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Held in
Annapolis, Maryland, USA
November 5-8, 1996

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ABSTRACT

This is a report on the CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements held at Annapolis, Maryland, USA November 5-8, 1996. This experts' meeting consisted of 140 participants from 21 countries; 65 invited papers were presented. The meeting was divided into five areas: (1) current and prospective plans of thermal hydraulic codes development; (2) current and anticipated uses of thermal-hydraulic codes; (3) advances in modeling of thermal-hydraulic phenomena and associated additional experimental needs; (4) numerical methods in multi-phase flows; and (5) programming language, code architectures and user interfaces. The workshop consensus identified the following important action items to be addressed by the international community in order to maintain and improve the calculational capability:

- preserve current code expertise and institutional memory,
- preserve the ability to use the existing investment in plant transient analysis codes,
- maintain essential experimental capabilities,
- develop advanced measurement capabilities to support future code validation work,
- integrate existing analytical capabilities so as to improve performance and reduce operating costs,
- exploit the proven advances in code architecture, numerics, graphical user interfaces, and modularization in order to improve code performance and scrutibility, and
- more effectively utilize user experience in modifying and improving the codes.

Following the workshop session summaries, 65 papers are provided.

KEY WORDS ARE:

CSNI
thermal-hydraulics
neutronics
thermal-hydraulic phenomena
numerical methods
multi-phase flows
programming language
code architectures
user interfaces

**PROCEEDINGS OF THE OECD / CSNI WORKSHOP ON TRANSIENT
THERMAL-HYDRAULIC AND NEUTRONIC CODES REQUIREMENTS
NOVEMBER 5-8, 1996**

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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- to achieve the highest sustainable economic growth and employment and a rising standard of living in Member countries, while maintaining financial stability, and thus to contribute to the development of the world economy;
- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

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The primary objective of NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

This is achieved by:

- *encouraging harmonization of national regulatory policies and practices, with particular reference to the safety of nuclear installations, protection of man against ionising radiation and preservation of the environment, radioactive waste management, and nuclear third party liability and insurance;*
- *assessing the contribution of nuclear power to the overall energy supply by keeping under review the technical and economic aspects of nuclear power growth and forecasting demand and supply for the different phases of the nuclear fuel cycle;*
- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

In these and related tasks, NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

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OECD/CSNI WORKSHOP ON TRANSIENT THERMAL-HYDRAULIC AND NEUTRONIC CODES REQUIREMENTS

MEETING SUMMARY

1.0 INTRODUCTION

A workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements was held in Annapolis, Maryland, United States, from 5 through 8 November 1996. The meeting was organized by the United States Nuclear Regulatory Commission (NRC) for the Organization for Economic Cooperation and Development's (OECD) Committee for the Safety of Nuclear Installations (CSNI). This workshop meeting was the fifth in a series sponsored by OECD/CSNI to review research related to transient two-phase flow. The first four meetings were held in Toronto, Canada (1976), Paris, France (1978), Pasadena, California, United States (1981), and Aix-en-Provence, France (1992). Each of these meetings consistently followed the theme initiated by the Thermal-Hydraulic Systems Behavior Task Group of the Principal Working Group No. 2, which was to discuss the achievements and define the needs of safety research in the critically important area of accident thermal-hydraulics.

The November 1996 workshop attracted some 140 participants from 21 countries. A total of 65 invited papers in important technical areas were selected for presentation. The meeting was designed to encourage the acquisition of all relevant information from the assembled group of experts. Through a process of discussion, debate, feedback, and validation, this information was used to identify a set of critical issues that must be solved. Consensus was sought on the degree of importance of each issue.

The meeting was structured in five sessions to explore the areas considered most critical to the successful definition of requirements for future codes: (1) current and prospective plans for thermal-hydraulic codes development; (2) current and anticipated uses of thermal-hydraulic codes; (3) advances in modeling of thermal-hydraulic phenomena and associated additional experimental needs; (4) numerical methods in multi-phase flows; and (5) programming language, code architecture, and user interfaces. In addition, three breakout sessions were held on the third day to address such important areas as advances and needs related to thermal-hydraulic modeling, numerical techniques and coupling interface requirements, and user needs and interfaces. During these breakout sessions, which lasted several hours, the meeting participants divided into approximately equal groups. Each breakout group discussion was facilitated by several internationally respected experts. The members of each group engaged in a "give-and-take" debate on the factors and needs required for success in the breakout subject area. On the final day of the meeting the facilitator for each breakout group presented the findings to the full assembly for further discussion, debate, and validation. Finally, after the end of the

essential to the successful modeling of phenomena in current and future computer codes. The need for such instrumentation will be the subject of the next CSNI meeting, which is the OECD/CSNI Specialists Meeting on Advanced Instrumentation and Measurement Techniques to be held from 17 through 20 March 1997, in Santa Barbara, California, United States.

Certain technical areas were identified as being of particular importance to code improvements. In the area of improved physical modeling, the addition of a transport equation for interfacial area was identified as a top priority item, as was improvement of models and correlations at low pressure/low flow conditions. In the area of improved numerical methods, the need for low diffusive schemes that can track steep gradients was identified. The highest ranked user needs include improved robustness and a graphical user interface (GUI).

3.0 DETAILED CONCLUSIONS AND RECOMMENDATIONS

3.1 Specific Areas for Improvement

1. Multi-field models, specifically separate liquid fields for film and drops

Codes with film and droplet fields already exist in the industry, so adding this type of model is possible within the present code structure and numerics. Multi-field models may be more physically based so that constitutive relations are simpler, even though a larger number are required. Additional experimental data are needed to validate such models.

2. Transport of interfacial area/dynamic flow regime definition

This area was identified as potentially having the greatest effect, since it may eliminate the use of flow regime maps based on steady-state and fully developed flows. Describing source terms is an area that may need additional work. Accurate modeling depends on getting properly scaled experimental data; there is a need for testing in three or four typical geometries such as small and large pipes, bundles, a direction change and an annulus.

3. Two- or three-dimensional hydrodynamics and their closure laws

The need to define flow regimes under three-dimensional conditions was identified. Multidimensional models have been added to existing codes because they were found to be needed, but the present models are not satisfactory. Validation of these models against experimental data is required. The need may be partly met by coupling a system code to an existing computational fluid dynamics (CFD) code. Two-phase CFD modeling is a long-term item that is unlikely to be developed within the horizon established for this work. Alternative approaches such as Large Eddy Simulation (LES) should be studied.

4. Turbulent diffusion models

The inclusion of turbulent diffusion models needs to be addressed in the code development effort.

5. Operation at low pressure/low flow

Correlations need to be validated for these conditions and the model implemented accordingly.

6. Operation in the presence of noncondensables

A mass transfer model will need to be implemented. For a new code, noncondensables should be included in the basic structure. There are very little data on condensation of bubbles with noncondensables, so there will be some requirements for experimental data in this area. A model will be needed for heat transfer to volumes of noncondensable gas, e.g., nitrogen from accumulator injection. For containment analysis, at least two noncondensables need to be modeled.

7. Three-dimensional neutronics, consistent with the level of detail of thermal hydraulics

Three-dimensional models are available and should be added to handle, for example, BWR void feedback during normal operation, power oscillations, and anticipated transient without scram (ATWS). Two issues to be considered are (1) homogenization and de-homogenization of characteristic variables, which needs to be addressed for transients, and (2) consistency in the level of noding detail. Implementation is required, as well as some theoretical research on homogenization/de-homogenization for transients. Also, uncertainties in neutronic calculations need to be quantified.

8. Modeling of containment phenomena and situations beyond the design basis for primary systems

Containment models are available and need to be implemented. This could be done in a modular fashion. For example, containment capability coupled to the system code is required to handle BWR ATWS where containment pressure strongly influences core voiding and power.

Some phenomena, such as countercurrent flow (CCF) in the hot leg, quenching of a degraded core, core flow blockage, and radiation heat transfer, are required for beyond design basis accident (DBA) events.

3.2 Numerical Methods and Features

1. The integration of different numerical schemes for use in different phases of the same problem solution, based on their effectiveness, would clearly be of calculational benefit to the thermal-hydraulics user community.
2. Improvement of the multidimensional capability of codes and exploratory numerical work should be carried out in parallel to the ongoing physics research supporting thermal hydraulics and neutronics code improvements.
3. In addition to physics, numerical methods are frequently a major cause of code deficiency. To improve these methods, low diffusive schemes must be developed.
4. The following are some required numerical computing features:
 - Cases run to completion without user intervention
 - Reliable results (accurate and repeatable)
 - Capable of handling a wide range of operating conditions and states

OECD published a book with such problems in the mid-1980s. It was agreed that a document could be published periodically with results from developers so that the benchmarks would remain current.

3. Numerical benchmark problems should be carefully designed to test only the numerical method and should either constitute very simple physics, such as the oscillating U-tube manometer, or have well-defined boundary conditions and source terms.
4. An automatic means of converting input decks (including the potential for an expert system for automatic input conversion) could speed up the process and reduce errors, although manual intervention will still be required.
5. A standard for building plant models should be established.
6. A database should be established to facilitate the conversion of plant input decks for different codes.
7. Deficiencies in code performance may be attributed not only to the models, but also to the user.
8. A new code should be fully implicit. Wall and interfacial shear, heat transfer, and other closure relationships will be treated implicitly to enhance stability.

3.5 User Needs

Table 3-2 presents the code features that are most needed, listed according to the order of their importance.

TABLE 3-2	
DESIRED CODE FEATURES WITH IMPORTANCE RANKING	
Ranking	Code Feature
1	Robustness (i.e., no code aborts due to properties errors or other problems)
2	Documentation (users and developers [programmers] manual)
3	Graphical user interface
4	Internal assessment of uncertainty (automatically performed by the code)
5	Investment conservation by maximizing the use of previous model development efforts and user experience
6	Identification of the range of validity of code models and correlations (warnings would be generated if validity range is exceeded)
7	Structure the code/input requirements to minimize the user effect (examples are time-step control and automatic nodalization)
8	Near-real-time code performance
9	Training guidelines (also user guidelines based on previous experience)
10	Portability (easy installation across a variety of computer platforms/compilers)
11	Modularity (allows substitution of different models for three-dimensional thermal hydraulics, turbulence, etc.)
12	Capability for coupling to other models (possible models to be coupled include kinetics, containment, and those used for severe accident analysis)

3.6 Data Needs

1. Developers must have access to data used for code validation and archival experimental data used in the code validation process.
2. Experimental data from unique tests such as LOFT may be lost. It is important to have the data stored with a stable organization in a retrievable manner.

Opening Plenary Session

CURRENT AND PROSPECTIVE PLANS OF THERMAL-HYDRAULIC CODES DEVELOPMENT

Co-chairs: G. Yadigaroglu (Switzerland) and L. Ybarrondo (United States)

Dr. Farouk Eltawila addressed the attendees at the workshop. This meeting was called to discuss current and future uses of thermal-hydraulic and neutronic codes, additional experimental needs, numerical methods, programming language, and code architectures and user interfaces for a future generation of safety analysis codes. The complete proceedings of this meeting will be published in a report. The excellent attendance, approximately 140 participants from 21 countries, shows that the international community realizes the importance of discussing and reaching consensus on these issues.

Dr. David Morrison, Director of the NRC Office of Nuclear Regulatory Research, also welcomed the attendees and introduced Dr. Shirley Jackson, the NRC Chairperson.

Dr. Jackson also welcomed the participants and discussed the purpose of the meeting, which was to reach a conclusion concerning the capabilities needed in thermal-hydraulic codes to accurately model reactor systems. She noted that this need is not new but goes back to the 1960s and early 1970s. The old codes developed during that era were very conservative. Testing in the 1970s and 1980s allowed more realistic modeling of phenomena and removal of these conservatisms. However, new demands have been placed on the best estimate codes as a result of advanced reactor development, severe accidents, and beyond design basis analysis. The NRC needs to develop a new set of coupled thermal hydraulic/neutronic codes for use in the 21st century. This meeting was designed to help determine the best way to do this, taking advantage of two-phase models and new computer capabilities, and to make them more user-friendly. Dr. Jackson noted that the NRC has preliminary answers, but wants the views of the CSNI member countries. The NRC is now working under severe budget constraints, and help is needed to focus and prioritize. The NRC needs to proceed in a framework of international cooperation. Dr. Jackson closed by stating that she will pursue this initiative through the next year.

Mr. Gianni M. Frescura, Head of the OECD/NEA Nuclear Safety Division, added his welcome. He thanked the NRC for arranging this meeting, which attracted the best qualified experts to discuss the issues, and pointed out that safety analysis has many roles, including design, audit, and event analysis. The CSNI has played a leading role in developing and validating safety analysis models, including periodic CSNI reviews of the bases and capabilities of the thermal-hydraulic models. While system computer codes have attained a high degree of maturity, these codes were developed some years ago and need to be more reliable and more accurate. The objective of this workshop, as stated by Mr. Frescura, was to

identify a set of requirements and attributes for new codes and to identify issues to be addressed by research. An international approach is desirable. Possible efforts include:

- Cooperation on code development and assessment
- Development and promotion of international QA program
- Development/comparison of specific models with specific codes

Summary by Prof. Yadigaroglu

Following this introduction, co-chair Professor Yadigaroglu (Switzerland) summarized the capabilities of current generation thermal-hydraulic codes as well as future plans, using material from the following papers:

- Methodology, Status, and Plans for Development and Assessment of the RELAP5 Code, (G. Johnsen, et al., Idaho National Engineering Laboratory [INEL], United States)
- Methodology, Status, and Plans for Development and Assessment of the TRAC Code, (B. Boyack, et al., Los Alamos National Laboratories [LANL], United States)
- Methodology, Status, and Plans for Development and Assessment of CATHARE Code, (D. Bestion, et al., CEA - Grenoble, France)
- Methodology, Status, and Plans for Development and Assessment of TUF and CATHENA Codes, (J. Luxat, et al., Ontario Hydro, Atomic Energy of Canada, Ltd., [AECL], Canada)
- Methodology, Status, and Plans for Development and Assessment of the Code ATHLET, (V. Teschendorff, et al., GRS, Germany)
- Methodology, Status, and Plans for Development and Assessment of HEXTRAN, TRAB and APROS, (T. Vanttola, et al., VTT Energy, Finland)

Dr. Yadigaroglu's summary and tables are included in the proceedings of this meeting in viewgraph form.

Paper Summaries

Thermal-Hydraulic Modeling Needs for Passive Reactors

(J. Kelly, NRC, United States)

Mr. Kelly reviewed RELAP5 code modifications and work-arounds that were adopted as a result of work performed by the NRC/RES and INEL. This work was performed for NRC-NRR to demonstrate the applicability of the RELAP5 code to passive designs such as the AP600. As the large-break LOCA performance of the AP600 is generally similar to that of operating reactors, it was decided to focus the assessment studies on small-break LOCA and transients.

Passive, natural circulation systems have relatively small driving pressures. In addition, the success of the transient mitigation depends on properly triggering the Automatic

Depressurization System (ADS). Therefore, after review of the Phenomena Identification and Ranking Table (PIRT), it was decided to look at phenomena from the SPES, OSU, and ROSA/AP600 facilities.

Events were judged according to a four-category criterion. The RELAP5 response was judged to be at least sufficient for all events. Results for most events were judged to be adequate or better.

Initially, RELAP5 was unable to perform the analysis due to code problems. These problems were fixed, and some improvements and work-arounds were found to improve predicted accuracy. These improvements are related to:

- Addition of Henry-Fauske critical flow model
- Elimination of nonphysical two-phase recirculating flows
- More physical interfacial heat transfer
- Core level improvements needed in the future

The end result was that RELAP5 Version 3.3 was judged to be applicable to the AP600. This version will contain all of the improvements mentioned above.

The Role of Uncertainty in Code Development

(F. Barre, CEA - Grenoble, France)

Dr. Barre's presentation on the above topic followed. The reader is referred to this paper and, in particular, to Section 8, page 13, "Conclusions," where the author summarizes, in addition to the topic of the paper, a methodology for code development.

The Role of the PIRT in Identifying Code Improvements and Executing Code Development

(G. Wilson, INEL; B. Boyack, LANL; United States)

The reader is referred to this paper and, in particular, to Section 4, page 4, where the PIRT process is summarized.

A discussion session followed the presentation of the above papers.

Technical Session 1

CURRENT AND ANTICIPATED USES OF THERMAL-HYDRAULIC CODES

Co-chairs: D. Grand (France) and R. Caruso (United States)

Paper Summaries

Current and Anticipated Uses of the Thermal-Hydraulics Codes at the NRC

(R. Caruso, NRC, United States)

This paper outlined the basis of the thermal-hydraulic codes developed to date by the NRC and the NRC's intended direction regarding future uses. These codes were originally developed for technical experts to help them provide information on the performance of nuclear power plants to regulators for the purpose of making licensing decisions. Thermal-hydraulic codes have been used to crosscheck vendor codes and calculations, to perform sensitivity calculations, for event analysis, and for plant simulations. A recent role has been to support PRA analysis for risk-informed decisions.

These uses of thermal-hydraulic codes have created three distinct user communities. The first group is composed of highly technical and specialized code users who are scientists and engineers with strong backgrounds in fluid flow, heat transfer, nuclear engineering, and computer science. They have detailed knowledge on code input, correlations, solution techniques, and output. The second community of users includes engineers who build simple models and have an overall knowledge of the code. However, this group typically does not have the time to learn the intricacies of running a thermal-hydraulic code. The third user community is composed of system analysts who have a basic knowledge of reactor fluid dynamics and system behavior, but run the codes to simulate plant performance. These users are primarily associated with PRA and operator training. Future thermal-hydraulic codes must be able to support all three user groups based on similar needs. Such needs include robustness, defensibility, linkability to other codes, computational speed, consistency, ease-of-use (GUIs), and proper documentation. Progress has been made thanks to growing cooperation between code developers and users and the application of lessons learned from current generation nuclear power plant (NPP) analysis.

Current and Anticipated Uses of the CATHARE Code at EDF and FRAMATOME

(J. Gandrille, Framatome; J. Vacher, F. Poizat, EDF; France)

This paper described the current and anticipated uses of the CATHARE code by EDF and FRAMATOME. The CATHARE code is used in safety studies and as a simulator. For safety studies, a realistic deterministic methodology (also called best-estimate) is applied for licensing calculations, realistic plant response analysis, and evaluation of advanced NPP

designs. A version of the CATHARE code (CATHARE-SIMU) forms the driver for an NPP simulator (SIPA). Current plans call for an upgrade of the simulator to use CATHARE 2 for improved system performance. Important requirements have been identified, such as the range of validity (overall plant operation modes), determination of code uncertainty, multidimensional capability, fast run times, good code documentation and user guidelines, and visualization tools.

Vacher continued with the uses of CATHARE, but concentrated on its use for simulators. The SIPA and SIPACT simulator versions were presented. A demonstration of SIPACT was available during the meeting. These simulators are used for training safety organization engineers and plant operators, and for studies of Emergency Operating Procedures. Future work will convert all simulators to CATHARE 2, so there will be only a single code available for safety, engineering, and training. This will require development of the capacity to analyze conditions at low pressure in real time, automatic generation of CATHARE modules, and extension of the simulation domain to all transients for all plant initial states.

Current and Anticipated Uses of the Thermal-Hydraulic Codes in Germany

(V. Teschendorff, GRS; F. Sommer, Preussenelektra; F. Depisch, Siemens; Germany)

This was a presentation on the uses of thermal-hydraulic codes in Germany. Thermal-hydraulic codes (e.g., ATHLET) are used by licensing organizations and utilities. Siemens uses S-RELAP5. Applications of the codes include operating plant performance, licensing calculations, evaluation of pressurized thermal shock (PTS), assessment of Accident Management plans, evaluation of plant upgrades, and verification of emergency core cooling system (ECCS) performance for advanced designs. There was emphasis on correctly modeling the secondary side in including control systems and validating the results. Future requirements will include low pressure models (including an interfacial area concentration model), boron mixing, multidimensionality, coupling to other codes, quality assurance, machine independence, and reduced user influence.

Summary of Papers by R. Caruso

These presentations were followed by a summary of papers from France, Germany, Italy, Korea, Japan, Spain, Switzerland, and the United States on current and anticipated uses of thermal-hydraulic codes presented by Mr. R. Caruso. A list of target code applications based on these papers and Mr. Caruso's summary is given in Table TS-1.

Information for each paper was extracted and placed into a common table format for current applications and future needs. For current applications, the table included the codes used, the problem application, and the application type (Licensing, Best-Estimate, and Research).

Under future needs, the application area and specific needs were listed for each country. There were common recommendations throughout all the papers. These included improved user interface, coupling to other codes, improved numerical methods (especially for low

pressure transients), assessment of uncertainties internal to the codes, minimization of the user effect, multiple fluids, modular code structure, and building on previous work.

TABLE TS-1
TARGET CODE APPLICATIONS

Number	Target Applications
1	Reactor safety analyses for both operating and planned reactors: <ul style="list-style-type: none"> • LOCAs (Loss of Coolant Accidents) and transients • RIAs (Reactivity-Initiated Accidents) • Containment analyses • Fuel behavior
2	Licensee calculations
3	Audits of licensee's calculations (including quantification of safety margins for EM (Evaluation Model) type calculations
4	Analysis of operating reactor events
5	Analyses of accident management strategies
6	Analysis of effectiveness of backfit measures
7	Analyses of emergency operating procedures
8	Generic issue resolution, e.g., BWR stability analysis
9	Support for test planning and interpretation, e.g., experimental facility behavior predictions
10	Support for PRAs
11	Design analyses: <ul style="list-style-type: none"> • Steady-state core analysis • Subchannel analysis
12	Nuclear power plant training and control simulators
13	Analysis of advanced reactor designs
14	Analysis of accidents beyond DBA (in domain where conventional thermal-hydraulics are still applicable)
15	Analysis of events for Eastern-type reactors

Summary of Papers by D. Grand

Next was a presentation by Dr. D. Grand of a summary of papers from the United States, France, Germany, the United Kingdom, Japan, and Canada on interface requirements for coupling thermal-hydraulic codes. The need for coupling comes from the need to solve complex problems in a multidisciplinary manner. Previous methods involved external iterations between codes or the creation of an integrated code. Either method was labor intensive for transferring the information between codes or for maintaining and improving the

integrated code. New methodologies involve merging separate processes or static linking. The coupling schemes for the core physics to the thermal-hydraulic can be made at the core boundaries or by overlapping in the core.

An important consideration when coupling the codes is time synchronization. This occurs because the two codes most likely will not have the same time-steps. Therefore, schemes must be developed so that one code does not overly slow down the complete calculation by using fully explicit, iterative, or simplified methods which require a small time-step size. Coupling with severe accident codes was also covered, and problems arising from tightly coupled phenomena (clad oxidation) were identified.

Coupling with containment codes was the third domain. Certain general requirements also drive this topic. These requirements include optimization (minimizing computer overhead and development and maintenance costs), physical relevance of coupling (conservation of mass, energy, and momentum), and the impact of new software technologies (parallelism, standards).

General Discussion of Technical Session 1

The final item on the agenda for this session was an open forum on the future development of thermal-hydraulic codes. Most of the discussion centered on how user requirements are developed and implemented. Some of the issues raised included: (1) what can be considered good enough; (2) how to define the success criteria and the relationship to improvement in the physics models; (3) the level of uncertainty needed in each code; and (4) the level of detail that adequately models the problem. It was understood that the rate of improvements in computer hardware makes the goal of reasonable run time a constantly changing requirement (a "running" target). Others emphasized the need to "get the physics right" as the first and foremost requirement. Still others, however, expressed the view that improvement in physics can proceed as a parallel process to shorter run times.

Technical Session 2

ADVANCES IN MODELING OF THERMAL-HYDRAULIC PHENOMENA, ADDITIONAL EXPERIMENTAL NEEDS

Co-chairs; Dr. Reocreux (France), Dr. Lillington (United Kingdom)

Dr. Reocreux opened the session by providing a brief description of the six papers to be presented and their relationship to the first day's proceedings.

Session 2 dealt with advances in modeling thermal-hydraulic phenomena and reactor physics. The session covered theoretical work, making only limited reference to experimental needs.

The first three papers dealt with thermal-hydraulic modeling. The first provided a broad overview of the remaining open issues, within the framework of the two-fluid model, and proposed recommendations for future developments. The next two papers dealt with specific issues related to variants of the six-equation model and on condensation modeling. Two additional papers described the status of reactor physics modeling and made recommendations regarding specific problems raised by coupling with thermal-hydraulic codes. The final paper of the session gave a view on possible extensions to multi-field description of the present two-fluid, two-field models.

Paper Summaries

Status of Thermal-Hydraulic Modeling and Assessment: Open Issues

(D. Bestion, F. Barre, CEA - Grenoble, France)

Dr. Bestion presented this paper, which focused on open issues regarding the ability of thermal-hydraulic system codes to predict the progression of nuclear power plant transients. It was first noted that more and more predictions were able to track the most important phenomena exhibited in integral effects tests (IETs). However, for some of these important phenomena, one is obliged to recognize that a severe misprediction or no prediction at all is obtained. These defects were analyzed and can be attributed to:

- Nodalization or schematization problems (user effect)
- Models used outside the range of validity
- Physical process not modeled
- Highly sensitive transients, e.g., loop seal clearing

The main limitations related to the basic assumptions used for the model were summarized. Averaging restricts the prediction to large-scale phenomena (space averaging) or filters fluctuations (time averaging). In space averaging, the limited number of fields generally used generates large limitations for the description of some complex phenomena. The closure relationships established for one-dimensional models were also discussed. Examples of limitations of these relationships were given, such as their general algebraic form; the use of relations established for steady-state in largely unsteady flows; the flow regime map dependence, where transition should be better described by additional transport equations; and

limitations in the validity ranges. For two- and three-dimensional models, extrapolation of the one-dimensional relationships is a large limitation, and the closure of multidimensional, two-phase flow appears to be still in its infancy. Treatment of complex geometries and the limitations related to the numerical scheme were also discussed.

Examples based on refill and reflood for a large-break LOCA were given in support of the preceding analysis. Finally, recommendations for future development were given, including:

- Multi-fluid models for some flow patterns
- Additional transport equations, e.g. interfacial area concentration
- Improved three-dimensional modeling, closure relations and turbulence modeling
- New experimental programs to provide data to qualify closure relations

During the discussion of the paper, questions were raised about problems that may result from the introduction of additional separate momentum equations when additional fields are introduced. In particular, it was stated that, in this case, it may be easier to use a formulation similar to drift-flux than to introduce additional momentum equations.

Dividing Phases in Two-Phase Flow and Modeling of Interfacial Drag

(T. Narumo, M. Rajamäki, VTT Energy, Finland)

Dr. Narumo described four models for one-dimensional, two-phase flow:

1. Six equation model
2. Six equation model with virtual mass term
3. Six equation model accounting for nonuniform transverse velocity distribution
4. Separation of two-phase Flow According to Velocity (SFAV)

Dr. Narumo discussed the characteristic velocities of each model. It was claimed that the SFAV model was giving propagation velocities of the same order of accuracy as the best virtual mass models. The friction model was tested in steady-state and sinusoidally varying inlet flux to a channel representing a section of a BWR bundle between spacer grids with no heating. At steady-state, the results agreed well with the drift flux model, but differences began to be seen at frequencies of 5 Hz.

This work showed the possibilities of SFAV modeling, particularly the following capabilities:

1. Equations are well posed, and derivation is based on physical reasoning.
2. One dynamic model covers the whole void fraction range and agrees with experimental data.
3. Progress has been made in modeling cocurrent vertical flow.
4. Horizontal stratified flow can be modeled.
5. Countercurrent flow limitation can be included in the model.
6. High velocity flows, critical flow, and approach to critical flow may be modeled.

Several questions were raised by the audience about the physical basis of such a model. As eigenvalues in two fluid models are well analyzed physically, what physical interpretation can be given to the new eigenvalues and eigenvectors obtained using SFAV? The answer was that the characteristic values are the two phase velocities: pressure wave propagation speed and void propagation speed.

A last series of questions concerned the physical basis for partitioning and how wall friction is divided between the two phases. In response, it was stated that the partitioning is done according to phase velocity, with different values of friction assigned to the slower and faster moving phases.

Advances in Modeling of Condensation Phenomena

(W.S. Liu, et al., Ontario Hydro, AECL, Canada)

Dr. B. Hanna presented this paper, which describes both analytical and experimental work related to the prediction of condensation in two situations: cold water injection and induced water hammer. Two experimental facilities were used to investigate these two condensation events: the Cold Water Injection Test (CWIT) facility and the Ontario Hydro Technologies (OHT) water hammer facility. These are both separate effects facilities. The CWIT facility is intended to provide data relevant to injection of cold water into a CANDU feeder channel. The OHT provides data to determine the threshold between the water hammer and no water hammer regimes. Two codes, CATHENA and TUF, that describe these phenomena use different approaches to model condensation. The TUF code tracks the motion of the injection front, while CATHENA identifies the location of the injection front from calculated liquid fraction gradients. The CATHENA results were compared with CWIT data, whereas TUF results were compared to OHT data. Overall trends were predicted and differences explained.

A member of the audience questioned how the increase in interfacial surface area due to increased entrainment was predicted. The response was that this was taken into account in the correlation used to predict interfacial area.

Another question was asked about the influence of dissolved noncondensable gases and how these effects were treated. The response was that no evidence has been found that dissolved gases have an effect in CANDU plants. However, this area is being investigated in conjunction with shutdown conditions.

At this point, Dr. Lillington summarized the papers to be presented in the remaining portion of the session, as well as the areas where multidimensional neutronics modeling is needed.

Multidimensional Reactor Kinetics Modeling

(D. Diamond, Brookhaven National Laboratory [BNL], United States)

This paper addressed three areas: (1) recommendations for the type of multidimensional reactor kinetics model that should be included in a coupled neutronics/thermal-hydraulics

code, (2) other important physical models needed for reactor dynamic capability, and (3) specific events for which coupled modeling is needed. The focus was on LWRs.

Recommendations were as follows:

1. Only three-dimensional capability should be considered (plus point kinetics and no kinetics), assuming isotropic flux, i.e., diffusion theory.
2. Two energy groups.
3. The solution space should be the fuel region or the entire reactor with reflector region.
4. Six delayed neutron groups.
5. Nodal methods or course mesh diffusion.
6. Time dependence by the direct method.
7. Modern matrix solution algorithms to minimize computation time.
8. Other important physical models include: cross section generator—data required for each mesh box includes exposure and spectral index (void and control rod history), reactivity feedback (control rods, boron), decay heat, initialization procedure (start from any operating state), ability to handle fixed source, equilibrium and transient samarium and xenon, flux reconstruction for critical heat flux (CHF), peak clad temperature (PCT) and pellet enthalpy, coupling to thermal-hydraulics subchannel analysis, in-core and ex-core instrumentation, calculation of temperature and boron concentration across core inlet, and fuel pellet temperature distribution.

Coupled model applications were listed separately for PWR/VVERs and BWRs and included return to power following steam line break, rod ejection boron dilution and ATWS for PWR/VVERs; and stability analysis, rod drop, ATWS, and overpressurization events for BWRs.

A member of the audience commented that in the United Kingdom, most of the features discussed have already been implemented, e.g., flux reconstruction pin by pin for pellet clad interaction (PCI) assessment, integrated core design and fuel studies, etc. In response to queries regarding qualification of the United Kingdom's methodology, it was stated that excellent results were obtained for the rod ejection benchmark.

Three-Dimensional Neutronic Codes Coupled with Thermal-Hydraulic System Codes for PWR, BWR, and VVER Reactors

(S. Langenbuch, K. Velkov, GRS; M. Rohde, FZR; Germany; and M. Lizorkin, Kurchatov Institute, Russia)

Dr. Langenbuch noted that thermal-hydraulics and neutronics codes have been separately developed. The need now is to couple the codes. Iterative schemes can be used, but these result in uncertainty related to feedback effects. Safety problems requiring coupled codes include boron dilution, cooldown with strongly negative moderator temperature coefficient (MTC), i.e. recriticality, ATWS, BWR instability, and new reactor concepts based on natural circulation.

Results of studies performed by coupling the BIPR-8 and DYN3D codes for VVERs and the QUABOX/CUBBOX code for LWRs with ATHLET were described. Two different approaches to coupling were used: (1) internal coupling, where the neutronics model is brought into the system code, and (2) external coupling, where the core region is modeled with the neutronics code, including the thermal-hydraulics. Both approaches were implemented using ATHLET and DYN3D. Internal coupling was implemented using BIPR-8 and QUABOX/CUBBOX with ATHLET. The author indicated a preference for internal coupling. In this case the thermal-hydraulics is fully consistent.

Events analyzed with the coupled codes were:

- Single pump coastdown in a VVER-1000 using ATHLET/BIRP-8
- Hypothetical control rod group ejection in a VVER-440 using ATHLET/DYN3D
- ATWS total loss of heat sink in a PWR using ATHLET/QUABOX/CUBBOX

Results were very promising for these first applications of the coupled codes.

A member of the audience stated that the situation for BWRs is much different than that for PWRs and VVERs in terms of the accuracy of results. In a recent benchmark, the results obtained using different codes were widely divergent. The basic problem is the inability to accurately predict void distribution.

Perspectives on Multi-Field Models

(S. Banerjee, University of California at Santa Barbara, United States)

Dr. Banerjee noted that a transition in our ability to model two-phase flows has been brought about by increased computational capability, including parallelization. He presented a tutorial on the multi-field approach (interpenetrating continua), noting its strengths and weaknesses. Structure resolving/subgrid modeling and particle methods were also discussed. The need for a three-field formulation to eliminate distribution effects was explained.

Multi-field formulations were shown to be acceptable for separated and dispersed flows (particularly when closure relations are less important), but they do poorly for oscillating or intermittent flows. The method has a real weakness when there is a nonlinearity in a constitutive relation. Reflux boiling in a PWR was used as an example to illustrate the point. In this case, using a flooding correlation is a preferred approach. The need for multi-field modeling in advanced passive PWRs was identified for the highest ranked (in the PIRT) phenomena for small-break and large-break LOCAs. Eight of the 12 phenomena for the large-break LOCA were identified as requiring multi-field models.

A representative of Siemens noted that the industry has been quite active in the area of multi-field modeling. They have demonstrated a capability to model three-dimensional flows in variable geometry. Dr. Banerjee noted that large utilities have also been quite active in this area because of the need to support plant operations. The licensing arena, using codes such as RELAP5, has not seen this same level of activity.

General Discussion of Technical Session 2

Adding transient capability to neutronics codes was stated to be straightforward. However, it was noted that a two energy group formulation may be poor in some circumstances and may not adequately capture spectral effects. It was noted that the recommended approach does not utilize the latest techniques, such as unstructured grids, transport theory, angular discretizations as a function of energy groups, etc. It was recognized that these techniques should be analyzed, and that there was a need for continued research and development of neutronics methods—even if, as stated, the present methods in many cases give satisfying results.

Besides these characteristics of the reactor physics codes themselves, the interface between the thermal-hydraulics and neutronics methods presents several problems, such as how to match the modules, (e.g., initial steady-state conditions) and how to match the level of detail (mesh sizes, time constants). Typically, neutronics models have orders of magnitude more detail than thermal-hydraulics models.

Concerning the multi-field related questions, an example was given that RELAP5 has added a phase separation model at TEE components and has successfully predicted reflux condensation in Semiscale and BETHSY experiments. The ensuing discussion revealed that the models used in RELAP5 are empirical correlations and not multi-field models. The potential shortcomings of using empirical models include potential scale effects. Concerning such shortcomings, the audience was reminded that the RELAP5 TEE model was validated against data at two different scales, and no scale effect was evident.

The discussion on the needs for future thermal-hydraulic physical models development focused on specific points of the multi-field approach, but concluded that the directions to be followed should be based on Dr. Bestion's very comprehensive presentation, which identified the following directions:

- Multi-field models
- Transport of interfacial area
- Multidimensional models including turbulence modeling
- Low-pressure, low-flow, and noncondensables

These topics were found to be key topics, and it was agreed that they would undoubtedly be the necessary starting points for discussion in the breakout session.

Technical Session 3

NUMERICAL METHODS IN MULTI-PHASE FLOWS

Co-chairs: V. Teschendorff (Germany) and J. Luxat (Canada)

The papers presented during Session 3 discussed approaches to improvements in numerical methods based on experience with versions of RELAP5, TRAC, and the CATHARE computer codes.

Paper Summaries

Problems with Numerical Techniques: Application to Mid-Loop Operation Transients

(J. N. Lillington, W. M. Bryce, AEA, United Kingdom)

Dr. J. Lillington presented this paper, which discussed problems with numerical techniques encountered when applying RELAP5 and SCDAP/RELAP5 to mid-loop operation transients. The focus of the paper was on generic lessons learned as opposed to proposed fixes to these computer programs. Calculations were performed using versions of RELAP5/MOD3 for the BETHSY 6.9 series of shutdown transients under experimental conditions at low temperature and pressure, both with and without the presence of noncondensables. Calculations were also performed using both SCDAP/RELAP5 and RELAP5 for the Sizewell B loss-of-residual heat removal (RHR) studies.

The types of problems encountered during these analyses were subdivided into six groups: (1) weaknesses in modeling noncondensables at low pressure, (2) poor time-step control, (3) problems with water packing, (4) non-stratified flow in sloping pipes, (5) numerical heat transfer instability, and (6) mass error. The problems were frequently found to be interdependent. In each case, alterations were made to the RELAP5 or SCDAP codes to correct the problem. Generally, single code modifications were used to fix problems with the existing models. Lessons learned included the need for:

- Careful initialization of properties before each property calculation iteration and consideration of side effects of altering any property such as noncondensable quality in the area of noncondensable modeling
- Better detection of time-step calculations that cause first-order property extrapolations to break down
- Careful checking of system mass and energy balances

Several questions were posed to Dr. Lillington, including the effect of nodalization on code behavior. It was suggested that some of the problems could be circumvented through judicious selection of node characteristics, as opposed to making code modifications. Volume differences were cited as being important. It was also noted that an important lesson learned is that the codes are being applied outside their range of intended application, requiring

development of new models or extending the capabilities of existing ones. Dr. Lillington believes that a combination of new models and model extensions is needed. He had no recommendation on how to handle steam and noncondensable flow without assuming that the two components are well mixed. In response to a question on mass error reduction, Dr. Lillington stated that convergence criteria were tightened in addition to other fixes.

Elimination of Numerical Diffusion in One-Phase and Two-Phase Flows

(Dr. M. Rajamäki, VTT Energy, Finland)

Dr. M. Rajamäki presented a paper that discussed the development of a new solution method called PLIM, or the Piecewise Linear Interpolation Method. This method was developed to avoid errors due to numerical diffusion and dispersion. The PLIM method is a shape-preserving characteristics method that is integrated into the hydraulics solver CFDPLIM. The CFDPLIM routines solve the system of N flow equations in an arbitrary hydraulic network consisting of nodes and one-dimensional flow paths. The CFDPLIM routines have been incorporated into a three-dimensional reactor dynamics code, HEXTRAN, resulting in a code called HEXTRAN-PLIM.

Boron dilution accidents under conditions close to natural circulation were analyzed using both HEXTRAN and HEXTRAN-PLIM to show the effects of numerical diffusion. Results based on the HEXTRAN analysis show clear indications of numerical diffusion, while the solutions from HEXTRAN-PLIM show little effect from numerical diffusion. The effect of numerical diffusion impacts predictions of the effect of boron dilution, since the reactivity worth of the boron slug, which is "smoothed" as a result of numerical diffusion, is decreased relative to the HEXTRAN-PLIM predictions. This decrease in predicted reactivity worth produces an underprediction of the fission rate and energy release to the vessel as a result of the event. Hence, numerical diffusion can mask erroneous results and have a significant impact on predicted plant behavior during a boron dilution event. The CFDPLIM package has also been applied to the SFAV two-fluid problem.

Advanced Numerical Methods for Three-Dimensional Two-Phase Flow Calculations

(I. Toumi, D. Caruge, CEA/IPSN, France)

This paper focused on new, fully implicit, finite volume methods that have been developed to analyze both one- and three-dimensional, two-phase flow problems. The one-dimensional solution scheme makes use of the Riemann solver approach to define backward and forward differencing to approximate spatial derivatives. The Riemann solver approach has been validated against various test problems, including the water faucet problem and the Edward's pipe problem. This method has been extended to a three-dimensional unstructured meshing, with improvements performed to obtain a fully implicit solution method. The method has been implemented in the FLICA-4 computer program, which is used to perform steady-state and transient calculations of rod bundles and PWR reactor cores and assemblies. The FLICA-4 program also has been used to analyze the effect of rod bow on hot channel coolant

flow and to perform PWR upper plenum flow calculations. The FLICA-4 program is planned to be coupled to the CATHARE code.

Recent Advances in Two-Phase Flow Numerics

(Dr. J. Mahaffy, R. Macian, Pennsylvania State University, United States)

In this paper Dr. J. Mahaffy presented a review of two-phase flow numerics. Topics covered included automatic differentiation, iterative solutions of sparse linear systems, interface tracking, higher order numerical methods, and quantification of numerical diffusion.

Automatic differentiation is seen as a tool useful to the code developer for developing analytic derivatives that are part of a new model or correlation for prototyping implicit numerical methods. Programs such as ADIFOR can be applied to generate the Fortran codes for the derivatives. However, it was noted that use of ADIFOR and similar codes requires improvements in efficient code production and in documentation. Iterative solutions of sparse linear systems have undergone a great deal of development in the past 20 years—to the point where there are many methods to choose from for a particular problem. Current methods include conjugate gradient methods and the Krylov subspace methods. The key to success with such methods is preconditioning of the matrix system for rapid convergence. A variety of iterative solution packages are available so that testing of a variety of options for a particular class of problems is not difficult. Interface tracking is of most use in following liquid levels in vertically stratified regions and plugs of liquid moving through pipes. Lagrangian methods have been used to track interfaces. The computer code OLGA, a major oil and gas pipeline analysis code, uses Lagrangian methods for tracking liquid slugs. In the area of higher order numerical methods, a wide range of methods have been refined for shock wave problems. Research using methods developed by Leonard and Smolarkiewicz has yielded promising results. Use of a well-posed equation set is a good idea with these methods. Quantification of numerical diffusion is important. However, an important first step is to quantify the degree of physical diffusion so that the relative importance of numerical diffusion may be ascertained.

Among the questions raised after Dr. Mahaffy's presentation were some related to the use of the method of characteristics on multi-processor parallel machines for the solution of hyperbolic systems. Dr. Mahaffy believes that finite element and finite volume methods are a better choice for solving these systems. Dr. Mahaffy also noted that most recent advances in two-phase flow numerics are adaptations of methods developed for single-phase flow. He notes that these adaptations frequently require far more effort than the original development for single-phase flow.

Current and Planned Numerical Development for Improving Computing Performance for Long Duration and/or Low Pressure Transients

(B. Faydide, CEA - Grenoble, France)

In his paper, Dr. Faydide presented current and planned development in the area of improved computing performance for long-duration or low-pressure transients. The CATHARE code

employs a fully implicit, six-equation, two-fluid model. A complete set of models for two-phase flow patterns, cocurrent and countercurrent flow, and heat transfer with wall structures and fuel rods is included. The CATHARE code has been benchmarked against experimental data. The CATHARE program has been simplified to allow real-time operation in plant simulators. This modified version, initially developed in 1986 and referred to as CATHARE-SIMU, utilized a two-fluid, six-equation model on the primary side and a three-equation model on the secondary side. Improvements in computational speed were achieved by optimizing the data management strategy in CATHARE-SIMU. CATHARE-SIMU is being improved by adding a drift flux model to the three-equation secondary side model and by developing a multi-processor version with a 100-millisecond CPU execution time per time-step.

A further stage of CATHARE development and application to simulators is the Simulator CATHARE Release (SCAR) project. The purpose of this project is to utilize standard CATHARE models without any simplifications in engineering and training simulators. Effort is being focused on improving calculation efficiency and code reliability and avoiding convergence failures. The version of CATHARE developed from the SCAR project will be benchmarked against a large variety of transient tests, including loss of RHR during mid-loop operation.

Questions on the availability of neutronic models in CATHARE were posed to Dr. Faydide, who stated that these are external modules provided by the user.

General Discussion of Technical Session 3

The desirability of using three-dimensional neutronics models in CATHARE was questioned, given that one-dimensional models are currently being used. Also, the impact of control system calculations on computation time in CATHARE was noted. In a simpler CATHARE model, control system calculation time is significant.

Answering questions regarding refinement of two-phase flow computational methods, Dr. John Mahaffy stated that higher order methods should be evaluated. He suggested a two-year program to evaluate and benchmark various approaches prior to selection of a method for installation in a computer code. Regarding a question on the connection between nodalization and numerics, Dr. Mahaffy also noted that the simple answer is that a fine mesh leads to a converged solution, and if this is not so, then there is a problem with the approach.

The possibility of using unstructured mesh was discussed. Dr. Mahaffy noted that unstructured mesh has been used in single-phase analysis. For two-phase analysis, use of unstructured mesh is complex and would require a significant development effort that would likely cost more than people are willing to pay. Actual engineering systems complicate the application of unstructured mesh. When the subject of adaptive methods was raised, Dr. Mahaffy noted that these methods have been applied to gas dynamics and that robust numerics are needed to extend these to two-phase flow problems.

Numerical diffusion was discussed. Dr. Mahaffy reiterated that the magnitude of physical diffusion needs to be estimated in any evaluation of numerical diffusion. It is acceptable if

physical diffusion dominates, and it is not necessary to totally eliminate numerical diffusion.

Further methods development was discussed by Dr. Mahaffy, who stated the best approach to improving numerical techniques is to identify and solve specific problems. He noted that benchmarks suggested by Dr. Vic Ransom and others could be used to focus the problem. Dr. Mahaffy also noted that in the area of single-phase turbulent modeling, analysts are just coming to the point where they believe that these models produce good results.

It was suggested that development of numerical methods is not independent of computer capability. With the move toward parallel computing architectures, model developers need to rethink the approach to numerical algorithms and how they can be developed to best take advantage of these platforms.

Technical Session 4

PROGRAMMING LANGUAGE, CODE ARCHITECTURE, AND USER INTERFACES

Co-chairs: T. Vanttola (Finland) and M. Naitoh (Japan)

During the past 10 years, rapid developments in computer hardware and software technology have considerably advanced the performance of detailed safety analysis calculations. However, this advance in nuclear safety calculational power has been due mainly to an increase in serial hardware architecture speed and memory capacity. This development trend may not continue; instead, future increases in speed may come mainly from the development of parallel hardware architecture (or single processors with inherent fine grain parallelism).

Attempts to parallelize safety analysis codes (e.g., TRAC, ATHLET, CATHARE, APROS, IMPACT) have produced fairly encouraging results. Parallel processing hardware and software have been available for some time, but the difficulty of thinking "parallel" and problems associated with architectural dependencies, correctness verification, and lack of reliable software tools have made this approach too difficult to apply. However, procedures are now available, such as languages supporting parallelization (F90, HPF, etc.) and message-passing protocols (MPI, PVM) that support the generation of portable codes.

Choices have to be made when starting a modern code development project. Three types of parallel hardware architecture are available: shared memory machines, distributed memory machines, and distributed networks. Portability is very important and should be kept in mind in all phases of code development. Distributed memory machines seem to be the most favorable for portability and for extensions of the number of processors.

As for programming style, loop-based parallelism, functional parallelism, data parallelism, or a combination of these may be chosen, of which data parallelism might be the most attractive (also applied in CATHARE and IMPACT). A high degree of rigor is necessary for object-oriented programming to successfully increase quality, maintainability, extendibility, and reusability of the code.

A graphical user interface (GUI) is a necessary and natural part of the development of a modern safety analysis code. GUIs are needed to increase productivity in such tasks as model development and display; run time control and display; and post-processor output, including playback and reporting. Backfitting a GUI to an existing code may require considerable effort, such as creation of the database and possible restructuring of the code. The database system is the core of the functionality of modern safety analysis software. It should contain all calculational level parameters, component definitions, documentation, etc.

In the conduct of a large software project, it is of great importance that well-structured procedures and standard tools are used, starting from the definition of requirements up to final release to the users. Feedback from various user groups is essential in the design, test, and validation phases. Feedback from end users is of particular importance for GUI development.

A large number of programming languages are available today, and no general recommendation for a preferred language can be given. Fortran still survives, at least in the calculational tasks through the F90 standard, or in new versions such as High Performance Fortran (HPF) in parallel architectures. They are also compatible with the existing F77 coding. Users of these extensions, however, need a lot of training, which is comparable to learning a real object-oriented language such as C++ (or JAVA). The object-oriented languages are more suitable for tasks like GUI development. C++ has been reported to produce as efficient coding as Fortran (Brun).

Paper Summaries

Current Implementation and Future Plans on New Code Architecture, Programming Language and User Interface

(B. Brun, CEA - Grenoble, France)

Dr. Brun pointed out that computer technology and tools develop more quickly than programming languages, whose typical renewal time constant is about 10 years, and safety analysis codes, which have a typical renewal time constant of 20 years. The rapid change of computer technology and the tightening of safety requirements, however, imply that safety codes such as CATHARE need to be updated more frequently.

Concerning parallel processing, the following observations were made: new languages (CRAFT, HPF) are inherently inefficient, but automatic tools (Preprocessors, Compilers) are very efficient for fine tuning. Message-passing (PVM/MPI) is more efficient and more portable. In the recent parallelization of CATHARE, data parallelism using a message-passing library (PVM) in shared memory computers has been applied successfully, with speed-up by a factor of 3 to 4 in a five-processor machine. In the conduct of a software project, Dr. Brun paid attention to a number of aspects such as the methods and requirements for object-oriented application development, life cycle, programming language, quality and metrics, documentation, portability, validation, and development team. In GUI development area, portability must be ensured by applying industrial standards. In the future, GUIs must also support user training and basic understanding of the physical models using all multimedia capabilities.

Parallelization and Automatic Data Distribution for Nuclear Reactor Simulations

(L. Liebrock, L-H Research, United States)

Dr. Liebrock described various options for parallelization from the point of view of hardware architectures and programming methods and gave some special recommendations for parallel reactor simulation. She also compared the advantages and disadvantages of several forms of parallel architectures.

Distributed Memory systems consist of separate computers, each handling separate mesh nodes. They are scalable and portable, but message-passing is a detailed bookkeeping process.

In the Distributed Network, the network is the bottleneck. It works well if portions of models are loosely coupled. It can use existing computers, but communication and support are complicated and expensive, and load balancing is difficult.

Loop-Based Parallelization has the advantages of fast and inexpensive use and extensive compiler support. Its disadvantages are that the approach targets shared-memory machines; it does not efficiently use all processors, and the parallelization overhead is high due to repeated creation and destruction of processes. Functional Parallelism means parallel execution of subroutines, where the advantage is the ability to do complex tasks in parallel, and the disadvantages are that separation of the subroutines and complicated control are required and difficulty occurs in the expression of loop or data parallelism. In Data Parallel Programming, the compiler language takes care of communications, which are slower but allow tool support. In the Combined Functional and Data Parallelism, data parallelism may be applied over a physical model, while functional parallelism may be used to link different codes—the advantage being flexibility, but with the disadvantage of complexity. A Data Parallel approach with automatic data distribution and program transformation is the most effective for two-phase flow problems, but will probably require rewriting existing solution algorithms.

Dr. Liebrock further stated that data organization in parallel applications should be organized by component, because this is the way the scientist thinks about the physical problem. Container arrays such as in RELAP may give better load balancing distribution information, but some optimization can be brought over. Pointers break optimization for parallelization. To improve optimization, Fortran statements GOTO, COMMON, and EQUIVALENCE should be replaced with more modern constructs. HPF and F90 modules allow reformulation of the component-based arrays. What is needed is to let the compilers do more of the work now instead of manually setting the pointers. This is a task which the optimizer does much better.

To avoid problems associated with the stability of the computing environment, standard languages, tools, libraries, and implementations that are generally supported around the world should be used. For a pilot development project, Dr. Liebrock recommended use of High Performance Fortran (HPF) and MPI protocol with explicit communication for implicit two-phase flow development.

In response to a question concerning Quality Assurance (QA) of compilers in parallelization, QA for compilers was cited as an issue in general, not only for parallelization. The data parallel approach must be checked by checking compilers as part of the QA process. This is one reason parallelization should be done by the compiler, not in the coding. For explicit communication, a full test suite for all configurations may have to be run. Dr. Liebrock further stated that data parallelization can be portable over the whole range of machine architectures being evaluated.

TOOKUIL: A Case Study in User Interface Development for Safety Code Application

(D. Gary, et. al., KAPL Inc., United States)

J. G. Hoole, KAPL, Inc., described TOOKUIL, a GUI for TRAC-P. The TOOKUIL development project started in late 1991, and the effort up to now has taken 12–13 staff years.

This GUI was developed to support the design and analysis process by providing features for creating TRAC models, running the code calculations, managing the resulting output files, and post-processing the data. TOOKUIL includes icon-based model generation, runtime control, on-line help, and output processing. Some functions, such as the three-dimensional vessel, control variables, and links to the database, are not yet implemented. In the development project several lessons were learned, such as: (1) runtime control is good for production shops; (2) model generation is the most difficult task; (3) access to manual through code is important; (4) completeness of GUI functional requirements are important; and (5) the team is important, requiring a good balance of engineers and computer scientists, as well as database experts. Finishing the GUI requires the addition of a database to automate sensitivity studies, to improve restart capability, to add XTV, and to improve the physical appearance and descriptiveness of the iconic display.

A question was asked about the current input capabilities of TOOKUIL. TOOKUIL is still at a fairly early stage in the area of input processing, so it does not untangle the nodalization diagram when it reads in an existing deck. The learning curve for TOOKUIL itself is only an hour or two, but it does not really help with the learning curve for TRAC, which is much longer.

It was suggested that (1) handling existing decks is very important; (2) it is also important to model the complete systems, not just thermodynamics, including controllers and balance of plant systems; (3) linking GUIs to expert systems will save a lot of time and be really valuable; and (4) there is a need to link the libraries of reference documents.

Requirements for a Multi-Functional Code Architecture

(O. Tiihonen, K. Juslin, VTT Energy, Finland)

Mr. Tiihonen presented requirements for a modern safety analysis code from a general point of view and gave special notes on user interface, code architecture, and programming languages and standards. There are two major aspects that should be taken into account: the user requirements and the continuous development of the code. The user requirements include an easy-to-use GUI; wide-range, robust code; and short time-to-solution. The code developers can benefit from highly structured, portable code based on standard compilers and tools that forms a maintainable, easily extendable analysis and simulation system. The code architecture should be layered, starting from separate program modules for different physical models, solvers, and a database with clearly defined interfaces. The database should be structured so that higher level objects such as process components, unit processes, and plant models can be made available to the actual users of the code. The GUI database should be included in the simulation database to preserve consistency of graphics and simulation data at all times.

As an example of a layered code architecture, Mr. Tiihonen described the APROS simulation software for NPP safety analysis (reactor, primary and secondary circuit thermal-hydraulics, containment—all interconnected), as well as automation and electrical systems. The object-oriented memory resident database allows the building of structures suitable for describing

process components and unit processes and provides a generalized standard interface for a GUI with on-line model building and data presentation capability.

Development of the Simulation System "IMPACT" for Analysis of Nuclear Power Plant Severe Accidents

(M. Naitoh, et al., NUPEC, Japan)

Mr. Naitoh presented a paper on the parallel processing software system, IMPACT. This system is designed and is being developed as a large-scale simulation system of interconnected hierarchical modules covering a wide spectrum of scenarios ranging from normal operation to severe accident conditions of LWR plants, as an example of future software systems. He indicated that IMPACT is a 10-year project that started in 1993, with financial sponsorship from the Ministry of International Trade and Industry (MITI). Six major requirements for the IMPACT software were explained: (1) minimum use of empirical correlations and constants, (2) maximum use of mechanistic models, (3) use of parallel computer, (4) user assistance from input generation to comprehension and retention of results, (5) modular structure, and (6) fast-running and detailed analysis. To avoid machine dependency and to keep scalability, IMPACT uses (1) Fortran-90 for analysis modules and C++ for control modules, (2) MPI as message-passing library, and (3) massively parallel machines or sequential vector machines.

The severe accident code structure also was shown. Mr. Naitoh indicated that the severe accident code would ultimately have about 30 modules and would be controlled by the simulation supervisory module with dynamic allocation of processor elements to optimize simulation elapsed time. Recent results were shown: (1) parallelization of an incompressible three-dimensional single-phase flow module with at least 30 times the normal speed-up ratio depending on the number of meshes; and (2) the pre-mixing sub-module for steam explosion analysis, which has good agreement with the MIXA experiments.

Asked about the number of engineers involved in software development, Mr. Naitoh said the project currently employs 8 inside NUPEC and about 20 as NUPEC contractors. Mr. Naitoh also stated that the parallelization method and results for single-phase flow analysis will be published in a journal in about six months.

Responding to an indication of difficulty in the development of the Human Interface during the Phase-1 period (by the end of 1997), Mr. Naitoh agreed and mentioned that it would be completed by the end of Phase-2 (2000), while temporarily using a commercial-based GUI.

Breakout Session 1

ADVANCES AND NEEDS ON THERMAL-HYDRAULIC MODELING

Co-chairs: J. Lillington (United Kingdom), M. Reocreux (France), and G. Yadigaroglu (Switzerland)

Discussion in this session was based on the characteristics of existing codes summarized in the Opening Plenary Session and the application needs identified in Session 1. Initially the discussion centered on the need for a new code and whether simply accepting the errors in present code predictions is a viable alternative. The consensus of the majority of participants was that improvements to the existing capability are absolutely essential. In particular, this capability is essential for the regulatory agencies that need to understand all situations taking place in operating reactors.

Proposals for Code/Model Improvements

It was agreed that the time horizon for code/model improvements is the next five to ten years. The following nine proposals were established and discussed:

1. Multi-field models
2. Transport of interfacial area/dynamic flow regime definition
3. Two- or three-dimensional hydrodynamics and their closure laws
 - a. system-wide global two-phase transports
 - b. single-phase detailed CFD capability
 - c. two-phase detailed CFD capability
4. Turbulent diffusion models
5. Operation at low pressure/low flow
6. Operation in the presence of noncondensables
7. Neutronics
8. Phenomena in Eastern reactors
9. Containment phenomena and situations beyond DBA in the primary system

For each code/model improvement, the following factors were considered:

- Why is the model or improvement needed? There should be identified uses of the code that make such improvements necessary.
- How should the proposed improvements be implemented and what is the feasibility of implementation; more specifically:
 - How mature are the approaches or the models?
 - How much more research is needed before implementation?
 - Do present code structures and numerical methods allow implementation?

In addition, the extent of any experimental support needed before implementation was considered. Finally, the various code and model improvements were prioritized.

Each of the nine proposed areas for code/model improvement was then discussed in detail within the pre-established framework. Results of these discussions are presented below.

1. Multi-Field Models

Needs: Multi-field models are essential for prediction of certain phenomena, such as BWR normal operation and transients, containment analysis, flow regime transition during large-break LOCA reflooding, entrainment and de-entrainment in the upper plenum and description of phenomena in the PWR downcomer. The need was clearly identified for codes with two fields for the liquid phase, namely film and droplets. Such multi-field descriptions already exist in industry codes. Adding this type of model is possible within the present code structures. Multi-field models are more physically based, so that closure relations are straightforward; however, a larger number are required. For example, it will be easier to treat drag on drops and films separately rather than develop a model for the average of the combined fields. Additional experimental data are needed to validate the models.

2. Transport of Interfacial Area/Dynamic Flow Regime Definition

Needs: All interfacial transfers are directly dependent upon the interfacial area. In the present generation of codes, the latter is determined using flow regime maps based on steady-state flow observations. In fact, to avoid unphysical flow descriptions it is necessary to describe the dynamic evolution of the interfacial area that governs flow regimes instead of using steady-state flow regime maps. For example, the evolution from bubbly to stratified flow after a bend cannot be properly described using a steady-state flow regime map.

It was agreed that in terms of present code weaknesses, this item potentially has the greatest effect. Ishii's paper outlines the manner in which interfacial area transport can be implemented. For multi-scale phenomena (e.g., a spectrum of droplets), more than one transport equation may be needed. Describing interfacial area source terms will require analytical and experimental work. Success will depend on getting properly scaled experimental data that are not now available. The need was identified for testing in geometries representative of small and large pipes, bundles, annuli, and direction changes.

3. Two- or Three-Dimensional Hydrodynamics and Their Closure Laws

Three different aspects of this general problem were identified:

- a. System-wide global two-phase transports
- b. Single-phase detailed CFD capability
- c. Two-phase detailed CFD capability

Needs: Regarding the first item, the need is to describe global mass movements, such as those occurring during vessel injection, multidimensional downcomer behavior, and

multidimensional core behavior driven by asymmetric loop operation. This capability has already been built into certain system codes, but these describe such situations with coarse meshing. The scale for such multidimensional treatments has yet to be established, but it was agreed that it would be between the present coarse meshing and that used in CFD codes.

The second item is related to the need to treat in detail certain single-phase, multidimensional phenomena such as thermal-mixing related to pressurized thermal shock (PTS), boron dilution, and mixing in containment volumes. This need may be met by coupling system codes to existing CFD codes.

The third item is the modeling of two-phase flows with CFD methods similar to the ones used today for single-phase flows. This is exploratory research that will hopefully result in multi-phase flow models that address the phenomena at a much more detailed, physical level. Alternative approaches such as Large Eddy Simulation (LES) should also be studied.

4. Turbulent Diffusion Models

Needs: Turbulence diffusion models are needed for the second and third cases described under area 3, above. Thus, additional separate discussion of this item was not necessary. It was noted, however, that inclusion of such models in two-phase flow codes requires implementation of low-diffusion, higher-order numerical techniques.

5. Operation at Low Pressure/Low Flow

This region of operation is characterized by rapid changes in flow regime and unstable flows due to the large density ratio. Such conditions appear at mid-loop operation, in passive ALWRs, in the containment, and during severe accidents.

Needs: Existing correlations need to be validated for these conditions and properly implemented.

6. Noncondensables

Needs: The needs are similar to the ones identified for low-pressure/low-flow operation: mid-loop operation, passive ALWRs, containment, and severe accidents. In addition, noncondensables are present during accumulator injection. For severe-accident and containment applications, several noncondensable gas fields may be needed.

One of the major problems with some existing codes is that the noncondensable models were added later and are not an integral part of the model and the solution scheme. For a new code, noncondensables should be included in the basic approach.

Data on heat and mass transfer in the presence of noncondensables exist for condensation in tubes and on walls, although some gaps may be present. There is little data on condensation of bubbles with noncondensables.

7. Neutronics

Needs: Multidimensional neutronics is needed to treat situations such as reactivity-induced accidents (RIA), ATWS, BWR stability, etc.

Three-dimensional neutronics models are available and should be used whenever necessary (rather than more limited one or two-dimensional models). Consistency in the spatial detail with the corresponding thermal-hydraulic models should be verified. The uncertainties of the neutronics need also to be quantified. Homogenization and flux reconstruction also need to be considered, particularly for the case of transients. Thus, three-dimensional neutronics is mostly a matter of implementing available techniques.

8. Eastern European Reactors

Differences in these reactor designs that must be modeled include horizontal steam generators and hexagonal fuel. There are ad hoc groups addressing these areas, and plant data exist. The fourth of a series of meetings on horizontal steam generator analysis will be held in Finland. Validation of models for Eastern-designed reactors is now underway [Ref. 1].

9. Containment Phenomena and Situations Beyond DBA in the Primary System

Needs: Models are needed for containment phenomena, including heat and mass transfer in the presence of noncondensables and pressure-suppression system response. A description of phenomena such as hot/cold steam countercurrent flow in the hot leg, quenching of overheated cores, core flow blockages and radiation heat transfer is required for beyond-DBA events. Water properties under extreme conditions need to be implemented.

Containment models are available and need to be implemented or coupled via special modules. This could be done in a modular fashion. Coupled code capability for severe accidents already exists; examples are RELAP/SCDAP and CATHARE/ICARE.

Priorities and Research Needs/Implementation

Priorities were established for each of the nine code/model improvement areas. The need for any additional experimental (E) and/or theoretical (T) research was identified. Areas where simple implementation will suffice were indicated (IMPL). The following table summarizes the results. Priorities have been characterized as Very High (HH), High (H), Medium High (MH) and Medium (M). Exploratory Long-Term research needs are shown as ELT.

<u>Code/Model Improvement</u>	<u>Priority</u>	<u>Further Research</u>
1. Multi-field models	MH	E
2. Transport of interfacial area	MH	E,T
3. 2D or 3D hydrodynamics and their closure laws		
a. system-wide global two-phase transports	MH	E,T*
b. single-phase detailed CFD capability	M	Comp.Sci**
c. two-phase detailed CFD capability	ELT	E,T
4. Inclusion of turbulent diffusion models	same as 3b,c	
5. Operation at low pressure/low-flow	HH	IMPL
6. Operation in the presence of noncondensables	HH	E, IMPL
7. 3D neutronics	H	T
8. Phenomena in Eastern reactors	underway by ad hoc groups	
9. Containment modeling and beyond DBA	H	IMPL

* *Need to consider numerical diffusion-higher order schemes.*

** *Computer Science effort needed.*

References

1. K. Liesch and M. Rocreux, "Concerted Actions on Safety Research for VVER-Reactors, Verification Matrix for Thermal-Hydraulic System Codes Applied for VVER Analysis, Common Report IPSN/GRS No. 25," July 1995 (limited distribution).

Breakout Session 2

NUMERICAL TECHNIQUES AND COUPLING INTERFACE REQUIREMENTS

Moderators: J. Luxat (Canada), J. Mahaffy (United States), V. Teschendorff (Germany)

The objective of this session was to establish the desirable characteristics of numerical techniques and coupling interfaces for system thermal-hydraulic and neutronics codes. During this process the general topics of numerical robustness, accuracy, models for coupling separate solution packages, objective evaluation of numerical methods, and some related programming issues were considered.

Robustness and Accuracy

A simple definition of robustness is the ability of a code to run a problem to completion without user intervention (time-step adjustment) or code failure. This is a practical definition, but there is a second aspect. The code must also give accurate, repeatable solutions. Both robustness and accuracy within a defined range of validity are required. A wider range of robust behavior is acceptable only if the code informs the user that it is beyond its verified range of validity. In general, the code must be able to handle any modeled fluid, from freezing to above the critical point (superheat). The pressure range must be from near zero to above maximum design system pressures for a PWR. This ability is also related to robustness but can be considered a "soft" limit (i.e., the code should have some ability to estimate an answer when going above or below the physical state limits).

The code should be expected to handle the full range of problem time scales associated with the physical processes. The current situation is that phenomena with high propagation velocities (pressure waves) force small time-steps to ensure accuracy. If these phenomena are always captured during a long-term transient, the complete calculation will take several days to weeks, even on the fastest workstations. It was suggested that an adaptive time-step controller be implemented in the code to give the user the small time-steps only when absolutely required and to change to the largest possible time-step (for a given accuracy) at all other times. Users could request detailed tracking of sound waves by requesting a rigorous Courant limit within the robust time-step controller.

Running time is a major issue when considering numerical methods. It clearly is a moving target, since it is dependent on the latest in computer technology and architecture. The general approach is to make a balance between run time and accuracy. Real time might be acceptable for many applications but unattainable for other cases. Real time is a good target, but it is a secondary requirement to robustness.

Discussion concerning the ability to accommodate situations involving "steep gradients" in process variables, as well as coupled feedback, identified that this is of great importance in

several key phenomena occurring in nuclear reactors. Therefore, the code must have the capability to track steep gradients, two-phase interfaces, and other similar situations.

Coupling of Models

It was considered desirable to maintain a high level of modularity within a code and, to the extent practical, maintain separation between disciplines, as reflected by the separation of programs that can be flexibly coupled according to the analysis needs.

The question of whether explicit or implicit coupling of modules is preferable was considered. There is no single solution, since this is truly process dependent. There is a risk of discontinuity between how one couples the code and sections of the plant (example: linking core and loop thermal-hydraulics). Thus, there are two levels of modularity: internal (core and loop thermal-hydraulic coupling) and external, with the linking of modules developed by different disciplines (RCS, neutronic and/or containment coupling). One must ensure that the interface is tightly controlled and that the physical condition of the fluid does not change when switching from one module to another. The general conclusion was that the interface should permit, but not require, implicit coupling.

Unified interface protocols should be established that allow modular coupling with clearly defined structures to control interactions and data transfer between coupled modules. Other disciplines have set standards for data transfer (example: reactor physics and their transport codes). This is important not only for data transfer but also for coordinating events between modules. The transfer must occur through one point to avoid the corruption of data from multiple transfer points within a module. However, careful thought should be given on how this would affect parallelization of the code. The QA and maintenance of the code would be simplified by having only one well-defined and controlled data transfer point. This transfer point must never involve intervention of one program into another program's database.

Objective Evaluation of Numerical Methods

The need to establish a set of numerical benchmark problems that provide an objective measure of numerical method abilities was identified. There can be no good measure of numerical effectiveness from one code to another unless there is some commonality in the testing. The problem is selecting the numerical benchmark and its boundary conditions in such a way as to separate out effects due to the physics versus those due to the numerics. Specific models must be provided for source terms such as phase change to test the response of methods to typical nonlinear terms. Solution of linearized equations should be tested, both in the context of flow problems and with specific matrix solution benchmarks.

In benchmarking to analytical solutions, one must be able to separate the physical and mathematical solutions. Based on mesh or spatial convergence and time-step convergence, one could produce a reference solution. It is also important to track the mass and energy error in an easily accessible form.

Test problems should cover:

- Robustness
- Accuracy
- Run time (e.g., floating point operations per second)

Within the context of :

- Basic two-phase flow solutions
- Solutions with specified source terms (mass and momentum sources, etc.)
- Basic matrix solutions

Measures of a methods quality would include:

- Ability to obtain solution convergence as mesh length or time-step are decreased
- Percent error in mass and energy
- L^2 norm of all results
- Variance of results when executed on a range of compilers and optimizations
- Run time at a specified level of accuracy

Other Factors

The discussion on which programming language to use was surprisingly civil. There are several related issues that are not controllable by the code developer. The programming language should have a standard definition (i.e., Fortran-90) and should be portable to other machines. However, as seen in the compilers currently available, there is no true standardization of language compilers. This can have an effect on the benchmark one may be using to assess code performance.

Parallel processing was also considered. It was agreed that allowance for parallelization of a code should be considered at the time of design. The important factor is that the computed results should not change, whether or not parallelization is employed.

Recommendations

The most important recommendation is the early establishment of benchmark problems. The second most important recommendation is establishment of protocols for a coupling interface. Finally, research into more accurate difference methods is recommended. These are important in the short term for following phenomena with sharp spatial gradients, and in the long term to permit implementation of turbulence models. Early development would include interface tracking techniques and research into promising higher order methods. All such methods must be tested early against typical two-phase benchmarks. The most promising high-order methods are those of Leonard and the generic group of high-order Riemann solvers. It is also noted that new methods will require reconsideration of the details of iterative linear systems solvers, particularly the choice of matrix preconditioning. It is recommended that code be structured to facilitate the testing of "computational engines" developed from the above research.

Breakout Session 3

USER NEEDS AND USER INTERFACES

Moderators: R. Caruso (United States), D. Grand (France), T. Vanttola (Finland), and M. Naitoh (Japan)

Breakout Session 3 addressed user needs and user interfaces to thermal hydraulic programs. The meeting was attended by about 25–30 people from the regulators, national laboratories, domestic utilities, vendors, and overseas institutes. The focus of the meeting was to obtain a consensus on the code capabilities desired by users, code features needed to assist users, characteristics of the user interface, and the mix of technical resources needed for code development. These points were previously posed as part of the call for papers prior to the CSNI meeting.

Discussion points for Breakout Session 3 are presented in Attachment 1. Modifications were made to these points based on discussion among meeting participants. The importance of code capabilities and features and the user interface characteristics were determined by ranking the attributes of each category by importance, based on discussion among the meeting participants. This ranking may be used by code developers throughout the OECD to guide their code development activities.

A summary of the discussion for each main discussion point is presented below.

What Capabilities Do All Users Want for the Next 10 Years?

Code capabilities required for the next 10 years were reviewed. The time window of 10 years was selected because it was judged to be the maximum time in which reasonable forecasting can be done, given the changes in computer technology. Much of the early discussion focused on defining the user. Generally, meeting participants felt that codes are developed to provide decision makers with information. These decision makers can be regulators, utility engineers, reactor vendors, and fuel engineers, among others. The needs of the users tend to vary and may be competitive, as well as diverse, thus complicating the code development process. As an example, the utility engineer interested in operating plant support may have different needs compared to an engineer working on the design of an advanced reactor. However, it was noted that six years of code development work for advanced reactors has proven valuable for current reactors for analyses involving mid-loop operation and PRA. In particular, the improvements made in handling noncondensable mixtures at low pressure for advanced reactors has been important for mid-loop operation analysis.

The level of code capability and features is directly linked to the needs of the users. The types of codes that were discussed included both thermal-hydraulic and neutronic codes. Mechanical engineering simulation capabilities (e.g., pipe stresses) were also mentioned. The question was raised as to whether a code that “does everything” is needed. Generally, it was agreed that

another hierarchy is needed to establish desired user capabilities, based on how the codes will be used. Although there may be a difference in perspective between the utility engineer and the regulator, the code capabilities needed are generally the same.

Meeting participants were asked to identify their code uses. Those mentioned included:

- Advanced reactor analyses, including small-break LOCA, large-break LOCA, and the spectrum of other design basis and beyond design basis events to evaluate reactor performance
- Heat sink strategy studies
- Licensing safety evaluations
- Appendix K break spectrum evaluations
- Time and frequency domain stability evaluations

Utility needs cited were analyses used to support power uprate and mid-loop operation, generally for a specific plant. In contrast, regulators must be able to analyze a spectrum of reactors and review models, including input provided by licensees. It was noted that a GUI would be invaluable in supporting input model evaluation. It was also noted that regulators approve codes (and code models) through a review of topical reports and audits of code capabilities.

As a result of this discussion, analysis types were requested and then ranked in importance, as presented in Table BOS-1.

TABLE BOS-1	
TYPES OF ANALYSIS TYPICALLY PERFORMED AND IMPORTANCE RANKING	
Ranking	Analysis Types
1	Design Basis Accidents
2	Operational Analysis (load runback and emergency operating procedure analysis cited. Plant transients would also be included.)
3	Simulator/Plant Analyzers
4	Accident Management
5	Mid-Loop Analysis
6	PRA Support Including Success Criteria and Event Timing
7	Component and System Design Analysis
8	Emergency Protection Analytical Support
9	Assessment of Other Codes (cross-code comparisons/assessments)
10	Fire Protection Support

What Code Features Should Be Provided To Assist Users?

Desired code features were identified by meeting participants. These are listed in Table BOS-2 along with their importance ranking.

TABLE BOS-2	
DESIRED CODE FEATURES AND IMPORTANCE RANKING	
Ranking	Code Feature
1	Robustness (i.e., no code aborts due to properties errors or other problems)
2	Documentation (users and developers [programmers] manual)
3	Graphical User Interface
4	Internal Assessment of Uncertainty (automatically performed by the code)
5	Investment Conservation (by maximizing the use of previous model development efforts and user experience)
6	Identification of the Range of Validity of Code Models and Correlations (warnings would be generated if validity range is exceeded)
7	Structure the Code/Input Requirements to Minimize the User Effect (examples are time-step control and automatic nodalization)
8	Near-Real-Time Code Performance
9	Training Guidelines (also user guidelines based on previous experience)
10	Portability (easy installation across a variety of computer platforms/compilers)
11	Modularity (allows substitution of different models for 3-D thermal hydraulics, turbulence, etc.)
12	Capability for coupling to Other Models (possible models to be coupled include kinetics, containment and those used for severe accident analysis)

Participants at the meeting identified several desired user interface features. Strong concerns were expressed about losing the investment in knowledge and experience in previous model development. This investment must be preserved, and it was proposed that knowledge base development be based on expert system techniques. The user interface features are listed in Table BOS-3, along with their importance ranking.

TABLE BOS-3

USER INTERFACE REQUIREMENTS AND IMPORTANCE RANKING

Ranking	User Interface Requirement
1	Post-Processing Plot Generation/Replay
2	Fluid System and Control System Logic Diagram Generation
3	On-line Component Library (allows user to select previously developed models for components such as steam generators)
4	Expert System Assistance (Input and Runtime; utilize animated graphics to show changes in important physical phenomena)
5	Error Resolution Assistance (Input and Runtime; clear diagnosis of problems when they occur)
6	User-Generated Input Documentation (allows notes and comments to be incorporated into the model for future reference and traceability)
7	Configuration Control of Input (previously developed models would be stored and users could access and modify these models to suit their needs. Changes could be highlighted using colors.)
8	Interactive Runtime Changes (changes in problem specifications during execution)
9	Runtime Display of User Selected Results
10	Input Translation Between Codes (e.g., TRAC, RELAP5, CATHARE, ATHLET)
11	Hardware-Based Input (example is to pick a Schedule 40 pipe of a given diameter and length and have the pipe automatically nodalized)
12	Common GUI for Multiple Codes
13	Assistance in Coupling Codes
14	Report Generation (input summary in tabular format)

One item noted was that nodalization for various components should be based on test data where applicable. This may not be practical in all cases, however, since nodalizations developed for topical report submittals by licensees for specific applications are not changed. It was also noted that on-line diagnostics during runtime could be done by utilizing color changes to highlight changes in a particular parameter (e.g., temperature limits, rate of temperature increase).

The role of the user in the code development process was extensively discussed. Generally, the code development process requires developing requirements that are translated to software

specifications. Software design specification (preliminary and final) are then developed, and the code development process proceeds. It was noted that knowledgeable users are needed to successfully implement this process. It was emphasized that feedback from the users is important and that user experience is an important component of this process. Conversely, developers should be involved in applications of their software periodically and probably visit some of the sites where application work is done to gain perspective on the use of the software.

The steps for integrating the user in the software development process were outlined by the meeting participants as follows:

- Use all available technical user (and software developer) resources in the international community.
- Involve the user in the code design and implementation process.
- Utilize useful information on software development (tools and techniques) from other engineering disciplines and from computer programming sources. Note that some of these were identified by Dr. John Mahaffy in his review of two-phase flow advances during Session 3.

Resources need to be considered in the software development process, and user requirements may have to be negotiated based on available resources. Software specifications should include manpower requirements.

Additional Recommendations

The meeting participants reiterated that it is necessary to have access to data used for code validation and archival experimental data used in the code validation process. It is recognized that companies may designate some of the data as proprietary, which would limit access to certain data. Also, information on how the data were measured (instrumentation details) and processed is needed and must be included. The need to have the data stored with a stable organization in a retrievable manner was strongly emphasized.

Finally, it was noted that the results of all computer analyses should be carefully scrutinized by a human analyst who understands the phenomena of interest and can identify anomalies in the results.

Attachment 1: Discussion Points

1. What capabilities do the users want for the next 10 years?
 - A. Operating reactors and advanced reactors—DBA and beyond DBA transients and accidents up to fuel damage
 - B. Operating reactors and advanced reactor events at low temperature/pressure
 - C. Simulators/Plant Analyzers—improve runtime, robustness, and user interface
 - D. More detailed core and system performance calculations and determination of available margins
 - E. Integrated Safety Assessments/PRA/PSA applications
 - F. Quantified code uncertainty

2. What code features should be provided to assist users?
 - A. Improved and expanded user guidelines and code documentation
 - B. Improved code robustness
 - C. Code identification of application outside limits of validity
 - D. Code internal determination and expression of result uncertainty
 - E. Establishment of user qualification and training guidelines
 - F. Structure code to minimize user effect
 - G. Users should be knowledgeable of the physical phenomena in the cases to be analyzed

3. What should the user interface be like, considering both the front end and back end of the analysis process?
 - A. Provide user interface that is visual and easy to use
 - ability to enter geometry information directly from engineering drawings (e.g., pipe sizes/schedules/endpoints, standard component input parameters)
 - “fill-in-the blanks” for component properties
 - B. Provide user interface that can read geometry from input deck and generate isometric drawings
 - C. Fully compatible with existing plant models
 - D. Design of interface should be sufficiently general as to accommodate other codes (e.g. containment, neutronics)

- E. Provide user tools at the back-end to help users visualize physical phenomena and results of calculations
4. What technical resources and what resource mix should be employed, considering the potential for contributions from international collaboration, academia, and industry?
- A. Use all available resources as appropriate
 - B. Involve users in code design and implementation process
 - C. Invite users to make specific recommendations for design features based on their past experience and anticipated needs
 - D. Look for useful information on software development (tools and techniques) from other engineering disciplines and from computer programming sources

Additional Recommendations:

- 1. Design code in a modular fashion so that new models or methods can be implemented early. Provide the capability to include detailed or simplified component models.
- 2. Design code so that it can easily be coupled to other codes (e.g., containment, neutronics, severe accidents).
- 3. Advanced T/H capability (e.g., model multiple fluids [gas, liquid], turbulence, 3-D).
- 4. Note that for all these recommendations, the physics in the codes must remain defensible and based on data.
- 5. Provide open access to data banks for code validation and experimental data used in the validation process.
- 6. Acknowledge that code development is a long-term continuous process.

Closing Plenary Session

CODE CAPABILITIES AND DESIRED ATTRIBUTES

(MINUTES FROM CLOSING PLENARY SESSION ON NOVEMBER 8, 1996)

Dr. Eltawila (NRC) made the opening remarks. He also moderated the discussion.

Dr. Eltawila asked if different numerical schemes could be used for different areas in the same problem based on their effectiveness. He said that the La Salle transient calculation would benefit from such a scheme. Dr. Mahaffy (PSU) replied with humor, asking, "How much would NRC pay for it?" He added that getting a higher order method in one region and first-order methods in other regions to talk to each other was very difficult. He also pointed out that, in a transient such as La Salle, driving forces and damping forces compete and eventually dictate the outcome, and such a scheme would be sometimes very dangerous.

Dr. Reocreux (France) said that the multidimensional capability in codes ought to be improved. He also asked the group to carry out the exploratory numerical work in parallel to ongoing physics research. He added that, as a group, they ought to be consistent in recommending both numerical methods and the physics.

According to Mr. Teschendorff (Germany), the numerical methods are a major cause of code deficiency besides the physics. To improve the methods, low diffusive methods must be developed. Referring to Dr. Ishii's presentation, he emphasized the importance of including the interfacial area transport in two-phase flow models. On the other hand, the numerical community was not ready to accomplish it today. In his view, it would be a mistake not to advance physical modeling and numerics at an equal speed. Therefore, he said, today's research should be directed by considering the needs of 10 years from today.

Mr. Kelly (NRC) stated that implementing new methods to the codes to test them was too expensive. He said he thought small pilot/test codes must be written to test a new method, e.g., low diffusive schemes.

Dr. Lillington (United Kingdom) reminded the group that there were already advanced two-phase methods in CFD codes and they were successfully applied in several areas, although interfacial transport had little or no significant importance in these applications. He said that these methods could be carefully tested with interfacial mass, energy, and momentum transport if it was desired to implement them in our codes.

A question from the audience about establishing common criteria for time-step selection noted that the time-step size was usually adjusted by ad hoc methods, but not criteria from first principles. It was also asked if there would ever be a single code to accomplish everything. Dr. Eltawila answered, "A single interface can be designed to call different modules from a library, and the user would not have any feeling that different codes are used in the background." Dr. Eltawila's answer opened up a discussion on the modularity of codes. On this matter, Dr. Grand (France) added that a level of modularity had been already achieved in

CATHARE with conventional programming techniques, and that it could be further facilitated by the object-oriented technologies. Mr. Teschendorff said he thought the subject of modularity should not be regarded as an easy way out from the problems, and a highly modular code would still have coupling problems. In his view, a general code must have certain specifications for transients, time scales, and flow regimes, etc. Dr. Reocreux reiterated that CFD codes and two-phase codes were fundamentally different. It is a fact that two-phase codes need careful assessment. In his view, breaking up the physics into individual modules must be carefully considered. When all models are brought together in a code, they usually compensate errors from each other. Therefore, the user will get radically different answers to a problem when he freely selects from a set of physical modules.

Dr. Lillington repeated that advanced numerical methods actually existed in today's CFD codes. Therefore, the research must concentrate on developing physical models. Dr. Reocreux reminded the group that everything developed for CFD codes must be tested with a comprehensive set of benchmark problems. As for getting hints from different fields, Dr. Grand added that the scientists in climate research have been developing new approaches to couple oceanic and atmospheric calculations with different time scales, and their methods could be a good example for coupling models with different time scales in nuclear safety.

Dr. Eltawila returned to the subject of implementing the interfacial area transport equation. He asked Dr. Mahaffy how one could put together the physical models and numerical methods for area transport. Dr. Mahaffy replied that both research areas could be advanced in parallel. He indicated that the interfacial area transport methods were in fact not new and that there were certain people with knowledge and experience in these methods. Adding to Dr. Mahaffy's reply, Dr. Luxat (Canada) said that the problem had to be defined clearly so that research on the numerical methods could be carried out in parallel to the work on the physical models. Another question on the subject came from Dr. Lillington, "Isn't it going to be straightforward implementing the method in one-dimensional flows?" Mr. Kelly answered him with an example from the industry: COBRA-TF has three fields and the interfacial area transport equation is already a part of the solution. This code employs a semi-implicit solver, and the time-step size is always limited by the Courant limit. Therefore, an extra equation for the interfacial area could be solved explicitly at the end of every time-step (very simple). On the other hand, Mr. Kelly and Dr. Mahaffy agreed that it would be a more difficult job to implement an extra equation for the area transport in an implicit solver.

It was noted by an audience member that advances in numerical linear algebra could be used to improve the codes referred to in Dr. Mahaffy's presentation of the previous day, adding that the physics can be incorporated into the pre-conditioners in some advanced linear solvers.

Another audience member complained that a set of challenging test problems did not exist. If a suite of problems were provided, the code developers could compare their methods against each other. Dr. Yadigaroglu (Switzerland) replied that OECD had already published a book with such problems in the mid-1980s. It was agreed that a journal could be published every six months to report results from developers so that the benchmark problems would not be forgotten.

On the same topic, Dr. Luxat raised another concern. He said that the numerical benchmark problems should be carefully designed to test only the numerical method and should either constitute very simple physics, such as the oscillating U-tube manometer, or have well-defined boundary conditions and source terms.

Dr. Eltawila asked if there was any work to do in automatic input deck conversion from one code to another. This question brought conflicting answers from the audience. Some members positively agreed to have an automatic means of converting the input decks, while others disagreed about spending any resources to develop an automatic converter. Dr. Luxat commented that an input deck for one code could not be converted to another without human intervention, and some work should be done manually unless the source plant design data were fully linked to the input data deck. Prof. D'Auria (Italy) said he thought time and other resources should not be spent to develop an expert system for automatic input conversion when it was possible to use dedicated man power, e.g., graduate students. Dr. Teschendorff added to the discussion that an input deck for a power plant was more than thermal-hydraulics and neutronics, but for the larger part of the balance-of-plant and control, no standard exists on how to model a plant. Therefore, he thought there are fundamental differences between the input decks for different codes. In his view, a standard for building plant models ought to be established before an automated input deck conversion between codes is achieved. Mr. Kelly and Mr. Caruso agreed that eventually a mega-database should exist from which plant decks for different codes could be converted. On the other hand, Mr. Johnsen (INEL-USA) disagreed on the subject and said the number of existing plant decks should be looked at before any consideration of an automatic deck converter, which, he thought, was finite. He also commented that deficiencies should be attributed not only to the models but also to the user. On the subject of automated deck conversion, it was concluded that an automatic converter could speed up the process and reduce errors, although human intervention was still required.

On the discussion of building an expert system into codes and user errors, Dr. Mahaffy said that, based on his background in numerical methods, even experienced users will accept results that could be regarded as nonsense. He said an expert system would provide the user with expertise from experts in different fields. Dr. Mahaffy elicited positive audience response from the code users when he commented that all developers should be forced to use codes on real problems. He also admitted that he was not a good TRAC user 11 years ago when he developed it, but that he was today.

An audience member said that the NRC was pursuing a graphical user interface that would incorporate an expert system.

Dr. Eltawila asked if there was any common definition for the concept of modularity. Dr. Grand explained that component-oriented technology, so-called objects, could be assembled together. It could be a particular physical model, numerical description of a plant, etc. Dr. Luxat suggested the definition that a module was an entity that had a defined function and attributes and was designed on "information-hiding" principles, so that it receives only the information it needs to perform its function and nothing else.

An audience member asked if the group should recommend that the developers of new models consider parallelization. Dr. Mahaffy replied, "Yes, we did." Another audience

member asked if time-step control should be built into a code rather than having to "baby-sit" the time-step. Dr. Mahaffy stated that the time-step control is an integral part of numerical method, and that it can induce stability problems unless carefully designed. Dr. Lillington commented that, in general, the time-step control fails to work in the current generation of safety codes. He gave an example: it is usually too late when a time-step controller discovers that the time-step size must be reduced and the code crashes. Mr. Teschendorff mentioned that many codes had different modules with different time scales. He continued by saying that when a time-step controller for thermal-hydraulics sets a time-step size, other modules must "get along" with it. He said he thought a master step controller must be set up.

A member of the audience asked for guidance from the group about the nodalization issues and added that it was currently a form of art. Mr. Wilson (INEL) complained, explaining he was a potential user of the new code, that developers were not advising the users about the ongoing work, and that they were simply told to "trust." He said he thought the developers must tell the users what their priorities are. Dr. Mahaffy stated that in his view, first-order numerics works and we can live with it. However, he thought developers often repeated themselves on the need for higher spatial differencing schemes. At this point, he was not sure which way they would go. On the other hand, he and Mr. Kelly agreed that a new code will be fully implicit. Wall and interfacial shear, heat transfer, and other closure relationships will be treated implicitly to enhance the stability.

Dr. Eltawila thanked the group and the audience and made the closing remarks.

Acknowledgements

This meeting involved the organization and challenges of coordinating the schedules and contributed papers of important and busy professionals from around the world. The meeting was very successful by any measure. Mr. Murlin Strand of SCIENTECH coordinated logistics and meeting arrangements. He was supported by Ms. Tracey Canty and other SCIENTECH staff. They did an extraordinary and thoroughly professional job.



UNITED STATES NUCLEAR REGULATORY COMMISSION

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OPENING REMARKS

BY

DR. SHIRLEY ANN JACKSON, CHAIRMAN
U.S. NUCLEAR REGULATORY COMMISSION

AT THE

OECD/CSNI WORKSHOP ON
TRANSIENT THERMAL-HYDRAULIC
AND NEUTRONIC CODES REQUIREMENTS
IN

ANNAPOLIS, MARYLAND
NOVEMBER 5, 1996

Good morning. I would like to welcome you to the OECD/NEA Committee on the Safety of Nuclear Installations Workshop on Transient Thermal-Hydraulic and Neutronic Computer Codes Requirements -- and to the beautiful city of Annapolis, Maryland. The purpose of this workshop is to reach some conclusions regarding computer code capabilities, and the need to ensure that thermal-hydraulic and neutronic codes are reliable, easy to learn, use, and modify. I am particularly interested in this subject because thermal-hydraulics and neutronics are fundamental to nuclear power technology, and understanding these disciplines is absolutely essential to ensuring reactor safety.

Of course, a detailed understanding of thermal-hydraulics and neutronics has been seen as important to reactor safety for a long time. One of the first safety studies in the United States involving these disciplines was published in 1956 as WASH-740, which helped to establish the concept of an engineered containment building. During the 1960s, when thermal-hydraulic code development was initiated, the U.S. Atomic Energy Commission emphasized the prevention of core melting, and the requirement for an emergency core cooling system (ECCS) to supply water to a reactor in the event of a large loss-of-coolant accident -- a LOCA.

The 1971 SEMISCALE experiment, which resulted in the large bypass of the emergency core cooling system, put a spotlight on thermal-hydraulics, and led to the protracted ECCS hearings conducted by the U.S. Atomic Energy Commission in 1972 and 1973. The result of the hearings was a set of very conservative regulations and assumptions for large-break LOCAs that were intended to cover the large uncertainties reflecting our rather poor state of knowledge at that time.

During the 1970s and 1980s, the NRC -- sometimes in cooperation with organizations like OECD and EPRI -- conducted many thermal-hydraulic tests in SEMISCALE, the loss-of-fluid test facility (LOFT), the multiloop integral system test facility (MIST), the full integral simulation test facility (FIST), and other facilities to confirm our understanding of large-break LOCAs. The NRC also engaged in aggressive computer code development to try to model the coupled neutronic and thermal-hydraulic phenomena mathematically. By 1988, we concluded that our knowledge and analytic capability had improved sufficiently to support modification of NRC regulations for large-break LOCAs to remove some of the earlier conservatisms.

Having concluded that our analytical capability was developed enough to support the then-current licensing reviews, including the new best-estimate analysis option, the NRC essentially went into a maintenance mode with these codes. However, several things occurred to change this posture. First, the new passive plant designs, that were submitted for certification in the U.S., pushed our computer codes into hydraulic regimes that required additional development and testing. Second, risk-informed regulation required a better understanding of event sequences beyond the design basis, resulting in a need for more robust and faster-running codes. Third, a computer revolution occurred, making our main-frame codes obsolete. Finally, budget constraints provided greater incentives to accelerate progress to a more efficient program.

Recently, we completed new experimental work on the low-flow regimes of the new passive plant designs, and we have developed improved models for the codes. We also have new state-of-the-art computing facilities. The challenge ahead of us is to develop a new set of coupled neutronic and thermal-hydraulic codes that will take us into the 21st century.

As we embark on this task, however, we need to address more specific questions. How can we be more efficient in the development and maintenance of our codes? How do we retain the value of our investment in existing codes and plant models? How do we best utilize modern computer technology? How do we take advantage of new developments in numerical methods and two-phase fluid dynamics? How do we identify features that can increase speed, accuracy, and reliability? How do we make the codes easier to use? Of course, we have our own preliminary answers to these questions, and these answers will be reflected in the presentations here. What we hope to accomplish in this workshop is to gain the perspective of the international community on these questions, and to factor your views into the decisions that we must yet make with respect to code development.

This workshop comes at a time of great change that is affecting the way we approach our research cooperation. One change is the

uneven pattern of growth in the use of nuclear power worldwide. In the Pacific Rim, ambitious nuclear programs are being implemented; while in other regions, the nuclear option has leveled-off or is in decline.

Also, as a result of economic constraints in many countries, all now must be more selective about our research programs. Each country must decide where to focus its own research efforts, and where to seek to join in efforts with others to save scarce resources, and to avoid duplication of effort. I believe that we can achieve more focussed and prioritized safety research on a global scale. This approach will require extra planning internationally, and will, of course, take a higher level of coordination than in the past.

International cooperation has a long history of success in the nuclear industry. The nuclear power industry has recognized the benefit of sharing information in the design, development, construction, and operation of nuclear power plants. Major vendors have exchanged manufacturing licenses. Recently, we have seen international mergers. Likewise, domestic and international operators' groups have banded together to share information and experience.

I believe that the world's nuclear regulators should follow suit and establish a better mechanism to exchange information, to identify common trends and approaches, and to provide better support for safety worldwide a mechanism which better reflects the needs and priorities of regulators. Therefore, I have initiated an effort to establish an international nuclear regulators forum, with a policy-oriented focus. At a meeting of senior regulators convened by the NEA near Paris in September, I discussed this proposal with some of my colleagues from other national nuclear regulatory organizations, and I found strong support for the forum idea. I will be pursuing this initiative more specifically early next year.

In closing, let me express the hope that this workshop will produce a useful exchange of views on thermal-hydraulics and neutronics code development.

Thank you.

**OPENING PLENARY SESSION: CURRENT AND PROSPECTIVE PLANS OF
THERMAL HYDRAULIC CODES DEVELOPMENT**

Co-Chair: Prof. Yadigaroglu (Switzerland), Dr. Ybarrondo (USA)

Capabilities of Current Generation of Thermal-Hydraulic Codes and Future Plans

Summary presentation of six papers on

**TRAC-P (Boyack & Jolly-Woodruff, LANL, USA)
CATHARE (Bestion et al., CEA, France)
RELAP5/MOD3 (Johnsen & Riemke, INEL, USA)
ATHLET (Teschendorff et al., GRS, Germany)
TUF and CATHENA (Luxat et al., Ontario Hydro/AECL, Canada)
HEXTRAN, TRAB, APROS (Vanttola et al., VTT Energy, Finland)**

by

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"Disclaimer of Responsibility"

- Presentation based on contents of papers (and additional summary information offered by authors) and reflects image given *in papers*
- Presenter responsible for misunderstandings/misrepresentations
- No clear distinction made between "official" code versions and near- or long-term plans/development efforts
- Authors' claims are reported "unfiltered"
- Difficulty in presenting information uniformly (based on material provided)
- Thanks to authors who provided summary information

Target Code Applications (based on TRAC and RELAP5/MOD3 papers)

- reactor safety analyses (transients) for both operating and planned reactors
- licensee calculations
- audits of licensee's calculations
- analysis of operating reactor events
- analyses of accident management strategies
- analyses of emergency operating procedures
- generic issue resolution
- support for test planning and interpretation
- support for PRAs
- design analyses
- nuclear power plant training and control simulators
- analysis of advanced reactor designs

Code Design Objectives (adapted from TRAC)

- Accurately model important accident phenomena in:
 - current generation
 - future generation plants
- deliver best-estimate predictions of accident progression
- have a practical running time
- be portable maintainable, extensible
- be adaptable to several reactor types

Codes/Plants/Transients

Codes considered	Organization(s)	Types of plants	Types of Transients
TRAC-P (→TRAC)	LANL, USNRC	PWR (→BWR etc.) and other (PIUS, AP600)	"all"
CATHARE	CEA, EdF, Framatome	PWR (EPR) (VVER, RBMK, adv. PWR, BWR?)	LOCA, non-LOCA containment t/h's (0D, 3D) mult. failures beyond DBA
RELAP5/MOD3	INEL, USNRC	PWR (BWR)	LOCA, non-LOCA ("all Chapter 15 events")
ATHLET	GRS	PWR, BWR (emphasis on combined injection), VVER, passive ALWRs	LOCA, non-LOCA beyond DBA
TUF, CATHENA	T: Ontario Hydro C: AECL	T: CANDU C: CANDU and small facilities	LOCA, non-LOCA
HEXTRAN, TRAB, ARPOS	VTT Energy	H: VVER T: BWR (RBMK) A: plant simuln. package, VVER, BWR	LOCA, non-LOCA plant transients (depndg on codes) see Table

Fluids/Fields/Numerical Method/Language

Codes considered	Fluids (beyond Steam and Water)	Fields/Equations	T/H Space Dimensions	Numerical Method	Coding Language
TRAC-P (→TRAC)	Solute in water n/c in steam	2C 2M 2E + solute concentration + n/c partial pressures	1D 3D (Cart, Cyl)	- SETS - higher-order for solute concentration	FORTRAN 77 (→ FORTRAN 90)
CATHARE	Boron in water Up to 4 n/c's gases in steam (radioactivity in gas/liquid)	2C 2M 2E + boron concentration + 4 n/c concentrations Multifield for 3D containment	0D, 1D, 2D, 3D modular	- fully implicit for 0D and 1D components - semi-impl. for 3D (Δp between phases present in mom. eqn guarantees hyperbolicity)	FORTRAN 77
RELAP5/ MOD3	Solute in water Mixture of up to 8 n/c's in steam	2C 2M 2E + gas/steam mixture + solute concentration	1D	two solution schemes: semi- implicit and two- step nearly-implicit (for slow transients)	FORTRAN 77 (FORTRAN 90 compileable)
ATHLET	Boron in water Up to 5 n/c's gases in steam	2C 1M 2E (drift flux) (2C 2M 2E used for reflood/downcomer)	1D 2D in downcomer	fully implicit	FORTRAN 77
TUF, CATHENA	Heavy water n/c gas in steam	T: 1C 1M 1E 1C 1M 2E (dr.flux) 2C 2M 2E C: 2C 2M 2E	1D	T: one-step and two-step semi-impl. C: one-step semi- impl.	FORTRAN
HEXTRAN, TRAB, ARPOS	H,A: n/c gas in steam A: solute in water	4,5,6 eqs See Table	1D	semi-implicit	FORTRAN 77 (and C)

Closure Laws, etc.

Codes considered	Flow regime map	Interfacial Exchanges	Wall Exchanges	Virtual Mass	Structures: conduction, etc.
TRAC-P (→TRAC)	yes, explicit for hydrodynamics	- area - mass transfer rate - friction - htc (int-liq, int-gas, liq-gas)	- friction to liquid - friction to gas - htc to liquid - htc to gas	included	- heat structures connecting two hydro cells - 1D and 2D
CATHARE	no, implicit ^a (smooth closure law transitions)	- friction (special case for reflooding) - htc (gas-int, liq-int) several regimes	- friction to liquid - friction to gas - wet and dry wall htc packages ^b	present in 1D 2-fluid eqs	- multi-layer - 2D conduction near QF - thermo-mechanical fuel rod model
RELAPS/ MOD3	yes, explicit for hydrodynamics (horizontal, vertical ^c and "high-mixing")	- area - friction ^c - int. h.t. in the bulk or near walls (from wall)	- wall friction apportioned to phases - htc selected by complex logic considering wall T, mass flux, void fraction, phase T's, CHF, TBHF and n/c fraction	included	- multi-layer (cyl., rect., spherical) - two-sided - 2D for reflooding with fine-mesh - fuel rod model with cladding deformation
ATHLET	various drift flux model options	- special condensation model - drift flux model recognizes CCFL	- friction - htc selection based on wall T and void fraction - QF's tracked by conduction-control	included in 2D parts only	- 1D - 3-layer - two sided

^a CATHARE: smooth evolutions of flow regime transitions are explicitly written for all closure laws (except for onset of droplet entrainment and stratification criteria)

^b CATHARE: special heat transfer package for the vicinity of a quench front

^c RELAPS/MOD3: using adaptation of EPRI drift flux model to obtain interfacial drag in bubbly and slug flow regimes; drag coeffs used otherwise. For post-CHF: inverted annular and slug are also considered

Component Models/Processes/Reactor Kinetics (only special/selected ones listed)

Codes considered	Components	Processes	Reactor kinetics
TRAC-P (→TRAC)	- pressurizer, tee, turbine - RPV volumes (downcomer, LP, UP)	- h.t. with 2D conduction and radiation - horizont. stratified flow (incl. CCFL) - vertical stratification in vessel and condensation	point
CATHARE	- phase separation at a tee - separators - entrainment and de-entrainment in UP - lower plenum voiding	- 2D conduction for quenching - k-ε turbulence model in 3D module (for containment t/h's) - condensation for ECCS injection	
RELAPS/ MOD3	- jet pump - simple steam separator, dryer - turbine - accumulator - ECC mixer - annulus	- rod-to-rod radiation h.t. - water packing mitigation - entrainment and water pull-through at take offs - mixture level tracking - boron front tracking - thermal stratification	point
ATHLET	- separator - jet pump - accumulator, pressurizer	- "dividing flow model" - tracking of mixture level - radiation among structures	point 1D (interface to 3D codes)
TUF, CATHENA	special CANDU components and control systems	see Summary Table	C: point (interface to neutronics codes)
HEXTRAN, TRAB, ARPOS	also hexagonal core geometry	see Table	1D, 3D (rect. and hex geometries)

Special I/O Features - GUI's - Unique Capabilities

Codes considered	Special Characteristics
TRAC-P (→TRAC)	Sophisticated input checking Consistent generation of st-st conditions Sophisticated GUI: TOOKUIL (by KAPL)
CATHARE	Simulators based on CATHARE have an advanced GUI
RELAP5/MOD3	Extensive input data checking Interactive with Nuclear Plant Analyzer (NPA) A GUI under development Implicit coupling to SCDAP severe accident models "Hooks" for explicit coupling to CONTAIN Renodalization "on the fly" Steady-state capability
ATHLET	Steady-state capability Interface with 3D neutronics
TUF, CATHENA	Modeling of CANDU's
HEXTRAN, TRAB, ARPOS	Modeling of VVER's

* GUI: Graphical User Interface

SUMMARY OF CANADIAN T/H CODE FEATURES

Legend: T = TUF C = CATHENA SOPHT = Ontario Hydro HEM code

FEATURE	DESCRIPTION
Purpose of Code (Applications)	<i>Safety Analysis (T,C) / Design Assist Analysis</i> including waterhammer & fluid structure interaction (T) / <i>Operational Support</i> - plant transients with commissioning test data feedback(T)
Number of fluids & treatment	Heavy water, light water, non-condensable gas (T,C) / <i>Modeling options</i> : EVET, EVUT, UVET, UVUT, drift flux - user selectable options (T) / UVUT, drift flux (C)
Flow regimes	<i>Vertical</i> : single phase liquid or steam, bubbly, annular, slug, churn-turbulent, mist, counter-current flow (T,C) <i>Horizontal</i> : single phase liquid or steam, bubbly, churn-turbulent, slug, mist, stratified (T,C)
Heat transfer	<i>Conduction, radiation (T,C) / Convective</i> : single phase, sub-cooled nucleate boiling, nucleate boiling, CHF, transition boiling, film boiling / <i>Metal-water reaction heat generation (T,C)</i>
Wall Closure	Wall friction at all solid surfaces (T,C) / Heat transfer explicit at all walls, temperature dependent metal thermal properties (T,C)
Interfacial Closure laws & virtual mass effects	Interfacial mass, energy & friction terms flow regime dependent; interfacial area and shear stress modeled (T,C) / Bulk fluid heat transfer rate includes pressure transient term (T) / Virtual mass effects explicitly accounted for (T,C)
Treatment of structures	1-D one and two region lumped parameter wall model for general piping; 1-D multiple element modeling for fuel channels (T) / 2-D modeling of multiple elements for fuel channel (C)
Numerical schemes	Staggered mesh flow rate equations; one and two-step semi-implicit methods. Matrix size = $L \times L$ sparse matrix inversion; separate steady-state and transient solutions, low numerical diffusion (T). / Staggered mesh separated fluid equations, one-step semi-implicit method. Matrix size = $(4N+2L) \times (4N+2L)$ sparse matrix inversion; transient solution only (C) <i>NOTE: L = no. of links; N = no. of nodes</i>
Special Processes	<i>Critical Flow</i> : Orifice and Henry-Fauske discharge options (T,C), Moody discharge and transient sonic options (T) / CCFL drift flux models (T,C) / CHF and post-dryout heat transfer degradation modeling based on full-scale water CHF & PDO experimental data (T)
Special component models	Special lumped parameter models for pressurizer and steam generators for void holdup (level swell) and entrainment processes. Explicit modeling of numerous valve types. Piping elasticity (T) / Four quadrant pump model (T,C) / Special component models for small reactor simulations (C)
Balance of plant	Complete balance of plant representation (T,C) / Interfacing process systems modeled (T) / Direct emulation of controllers through software modules (T) / Generalized controller routines - in one instance controllers from SOPHT were interfaced (C)
Input data conversion	Semi-automated software utility for conversion of SOPHT plant data files to TUF plant data files. (T)
Programming language	FORTRAN (T,C)

ANNEX

Summary of the properties of the HEXTRAN, TRAB and APROS codes in the form suggested by Prof. Yadigaroglu.

Feature	HEXTRAN	TRAB	APROS
Purpose of the code	3D reactor dynamics for hexagonal lattice cores combined with plant dynamics, from operational transients to ATWS scenarios. Safety analysis tool.	1D and 3D reactor dynamics for square lattice core combined with plant dynamics, from operational transients to ATWS scenarios. Safety analysis tool.	Full-scale modelling and simulation of different power plant processes, including the process automation and electrical systems. Design, safety analysis and training simulator applications.
Fluids and fields	1D water with solute, steam with non-condensable	1D water	1D water with solute, steam with non-condensable gas
Thermo-dyn. treatment	Simple thermodynamic treatment between steam and noncondensable gas	No thermodynamic treatment	Thermal dynamic treatment between gas components, no chemical reactions
Flow modelling	1D separated 4-eq., void fraction correlation for core TH. 1D separated 5-eq. drift flux model for the loop TH.	1D separated 4 eq., void fraction correlation	1D homogeneous 3-eq. / 5-eq. drift flux model with non-equilibrium / 6-eq. two-fluid model with separate phase momentum and non-equilibrium
Flow and heat transfer regime maps	No flow regime maps. In heat transfer a set of correlations with simple switching rules (e.g. DNB by correlation \Rightarrow post DNB heat transfer \Rightarrow oxidation). In loop full range drift flux model for vertical and horizontal flow. For HT wetted and non-wetted wall models.	No flow regime maps. In heat transfer a set of correlations with simple switching rules (e.g. DNB by correlation \Rightarrow post DNB heat transfer \Rightarrow oxidation))	3 Eq. model: no maps 5 Eq. model: full range drift flux model for vert.& horiz. flows. CCFL included in the drift-flux handling. 6 Eq. model: Flow regimes: bubbly, annular, droplet, stratified. Weighing factors for stratification and entrainment. Heat transfer: wetted wall, DNB, post DNB, quenching.

Wall closure laws	<p><u>Friction</u>: A set of correlations, e.g. McAdams, and two-phase multipliers with user defined parameters, e.g. Baroczy.</p> <p><u>Heat transfer</u>: A set of heat transfer and DNB correlations, particularly for VVER applications. Wetted and non-wetted wall models.</p>	<p><u>Friction</u>: A set of correlations and two-phase multipliers with user defined parameters.</p> <p><u>Heat transfer</u>: A set of standard heat transfer and DNB correlations. Particularly for BWR applications.</p>	<p><u>Friction</u>: 5 eq. A set of correlations, e.g. Blasius and two-phase multipliers with user defined parameters.</p> <p>6 eq. Blasius, distribution between phases on the basis of flow regime.</p> <p><u>Heat transfer</u>: A set of heat transfer and DNB correlations. CHF model.</p>
Interfacial closure laws	A non equilibrium boiling model in the core. In the loop full range drift flux model, flashing and condensation.	A non equilibrium boiling model.	<p>5 Eq. model full range drift flux model, flashing and condensation.</p> <p>6 Eq. model: interfacial friction and heat transfer with correlations depending on flow regimes</p>
Virtual mass	Not needed	Not needed	Not used
<p>Numerical scemes</p> <p><u>Neutronics</u>:</p> <p><u>Thermal-hydraulics / heat transfer</u>:</p>	<p>Fast two-level nodal method, Spectral matching method W_{11} in neutron kinetics.</p> <p><u>Core</u>: Implicit time discretization (flexible choice of time steps). The numerical method can be varied between the standard fully implicit theta method and the central-difference theta method.</p> <p><u>Loop</u>: Spatial discretization by donor cell method, time discretization by a non-iterative semi-implicit algorithm based on predictor-corrector -</p>	<p>Fast two-level nodal method, Spectral matching method W_{11} in neutron kinetics.</p> <p>Implicit time discretization (flexible choice of time steps). The numerical method can be varied between the standard fully implicit theta method and the central-difference theta method.</p>	<p>Nodal method, applicable to both square and hex lattices</p> <p>3 & 6 Eq. models: Implicit time discretization, with automatic time step adjustment.</p> <p>5 Eq. model: Spatial discretization by donor cell method, time discretization by a non-iterative semi-implicit algorithm based on predictor-corrector - method.</p>

	method. The sparse matrix methods make the code very fast.		
Structures	<u>Fuel</u> : 1D modelling of fuel and cladding. <u>Other structures</u> : 0 D heat slabs assuming cylindrical or slab geometry	<u>Fuel</u> : 1D modelling of fuel and cladding.	Fuel: 1D and 2D modelling of fuel and cladding. Other structures: 1D slabs with versatile interconnections
Special processes	CHF by correlations, Oxidation. In the loop CCFL included in the drift flux model. Critical flow.	CHF by correlations, Oxidation	CHF, CCFL, oxidation; cold startup, shutdown, critical flow
Special equipment models	Fuel follower control rods, PID-controllers, horizontal steam generators (with standard nodes), circulation pumps, jet pumps, safety valves, relief valves, injection pumps, simple automation for components	Partial length fuel elements, PID-controllers, pumps, valves, user defined algebraic of 1st-order differential dependences or delays between chosen variables	Fuel follower, partial length rods, automation and electrical systems, turbine, condenser horiz. & vert. steam generators, heat exchangers, etc.
Balance of plant components	Main components controlling steady state pressure, flow rate and core power included.	Main components controlling steady state pressure, flow rate and core power included.	Full automation system
Input deck generation	Standard editors	Standard editors	Through on-line graphical interface
Graphical user interfaces	No	No	Design-oriented interface for model definition and modification, analyser-type plant visualisation, CRT-based training simulator interface
Output	Normal files (listing, reports, events listing) online and post processor plotting	Normal files, online and post processor plotting	Structured data base dump, files, online and post processor plots, visualisation
Programming language	Fortran 77	Fortran 77	Fortran 77, C

Limitations/Improvements needed (as noted by authors)*

Codes considered	Coding/Numerics	Models
TRAC-P (→TRAC)	use of container array and pointers	blowdown rewet and reflood models
CATHARE	<i>See Table on Development activities</i>	
RELAP5/MOD3	numerical diffusion time-step control introduce FORTRAN 90 - eliminate old outdated coding nearly-implicit scheme not robust <i>see also Table on Development activities</i>	1D ^a interfacial area concentration st-st flow regime maps only one liquid field
ATHLET	<i>See Table on Development activities</i>	5-equation model

^a DOE version of RELAP5/MOD3 has 3D hydrodynamics and 1D, 2D, and 3D neutronics

RELAP5/MOD3 Code Improvements Needed

- 1D, 2D, or 3D hydro model
- Point- through 3D-kinetics model
- Semi- through fully-implicit solution schemes - automatic switching
- Improved interfacial area concentration models applicable to reactor geometries and non-fully developed flow
- More intelligent time-step control to improve code robustness
- Exploitation of FORTRAN 90 to eliminate outdated coding practices
- Parallellizable coding and data structure
- Powerful GUI that provides a front-end and back-end interface

ATHLET

Plans for Further Development and Improvement

- Fluid-Dynamics:**
- Dynamic flow regime evolution, interfacial area concentration model
 - Validity at full scale for condensation and interfacial friction model
 - 3D module based on non-staggered grid with flux-splitting method

Numerics:

- Non-diffusive schema for tracking of boron and subcooling gradients
- Speed-up for full-scope simulator application

Reactor types:

- Russian reactors VVER and RBMK, advanced type V-407
- Advanced western reactors EPR, BWR-1000, AP-600

Reducing the User Influence:

- Improved guidelines, enhanced input checking and run diagnostics
- Improved interactive user-interface with extended graphics

Assessment and Evaluation of Uncertainties:

- Complete assessment according to updated validation matrices (also for VVER and RBMK reactors)
- Application of GRS uncertainty method to generic reactor transients

CATHARE

Future Improvements Needed

Improvements of the code physical modelling

- Physical laws at low pressure
- Closure laws for the 3D model
- Improvements required by new reactor concepts

Numerical improvements

- Improvements of the reliability and robustness
- Reduction of CPU time (parallelism)
- Convergence of safety codes and plant simulators for operator training

Long term research

- Interfacial area transport equation
- Multifield approach
- 3D modelling with better turbulence modelling

Development Activities in Progress/Planned/Proposed - 1

TRAC-P

- Consolidation TRAC-P, TRAC-B and RAMONA 3D kinetics
- Adequacy assessment of closure and special models
- LB LOCA closure law packages for AP600 applications:
 "absolute/conditional pedigree", correlation kernel/coefficients
- Code modernization in 3 stages:
 - portability
 - improved computational efficiency
 - new code structure (FORTRAN 90)

TRAC modernization effort: [cited as example]

- apply modern software engineering principles
- achieve full portability to all single-processor Unix-based platforms
- significantly improve the maintainability of the code
- achieve a factor 10 improvement in run time on current single-processor platforms
- improve code operability and robustness
- position the code for parallelization
- separate the input/output and computational engine
- provide full functionality at all times during the modernization effort

Development Activities in Progress/Planned/Proposed - 2

CATHARE

- Apply the Discrete Adjoint Sensitivity Method (DASM) for uncertainty evaluation
- CIRCE: calculate the "basic uncertainties" of the closure laws
- SCAR - Simulator CATHARE Release project: insert standard CATHARE models in simulators
- Coupling capability with other codes: severe accidents, containment, neutronics
- Better physics:
 - low-p
 - 3D for core reflooding/de-entrainment in UP
 - advanced reactors
 - new physical models (e.g. interfacial area transport)
 - physics for VVER and RBMK
 - additional fields
- long-term: two-phase turbulence modeling

RELAP5/MOD3

- Code improvement for passive ALWRs
- Development of a GUI

Development Activities in Progress/Planned/Proposed -3

ATHLET

- Dynamic flow regime evolution
- Condensation and interfacial friction models
- 3D module for downcomer
- Non-diffusive scheme for boron tracking
- Speed up for full-scope simulation
- New reactor types
- Better interface with user
- Complete assessment (also for VVER and RBMK)
- Application of GRS uncertainty method to generic reactor transients

TUF and CATHENA

- Validation matrix for reactor physics
- Develop methods for uncertainty analysis
- Consolidation of two-fluid codes
- etc.

HEXTRAN, TRAB, APROS

- TRAB-3D with 3D neutronics under development (BWR)
- New numerical solution PLIM
- Improved formulation of conservation equations SFAV
- etc.

Needs of Passive ALWRs*

- Presence of n/c gases; their impact on:
 - condensation
 - flow circulation
 - heat transfer
- Small, gravity-driven pressure differences driving:
 - delivery of water at low pressure
 - circulation of coolant
- Sharp liquid/vapor interfaces
- Long transients (up to 3 days)

* from RELAP5/MOD3 and ATHLET papers

See also Table from RELAP5/MOD3 paper

Model Improvements Needed for ALWR Analysis (Johnsen and Riemke)

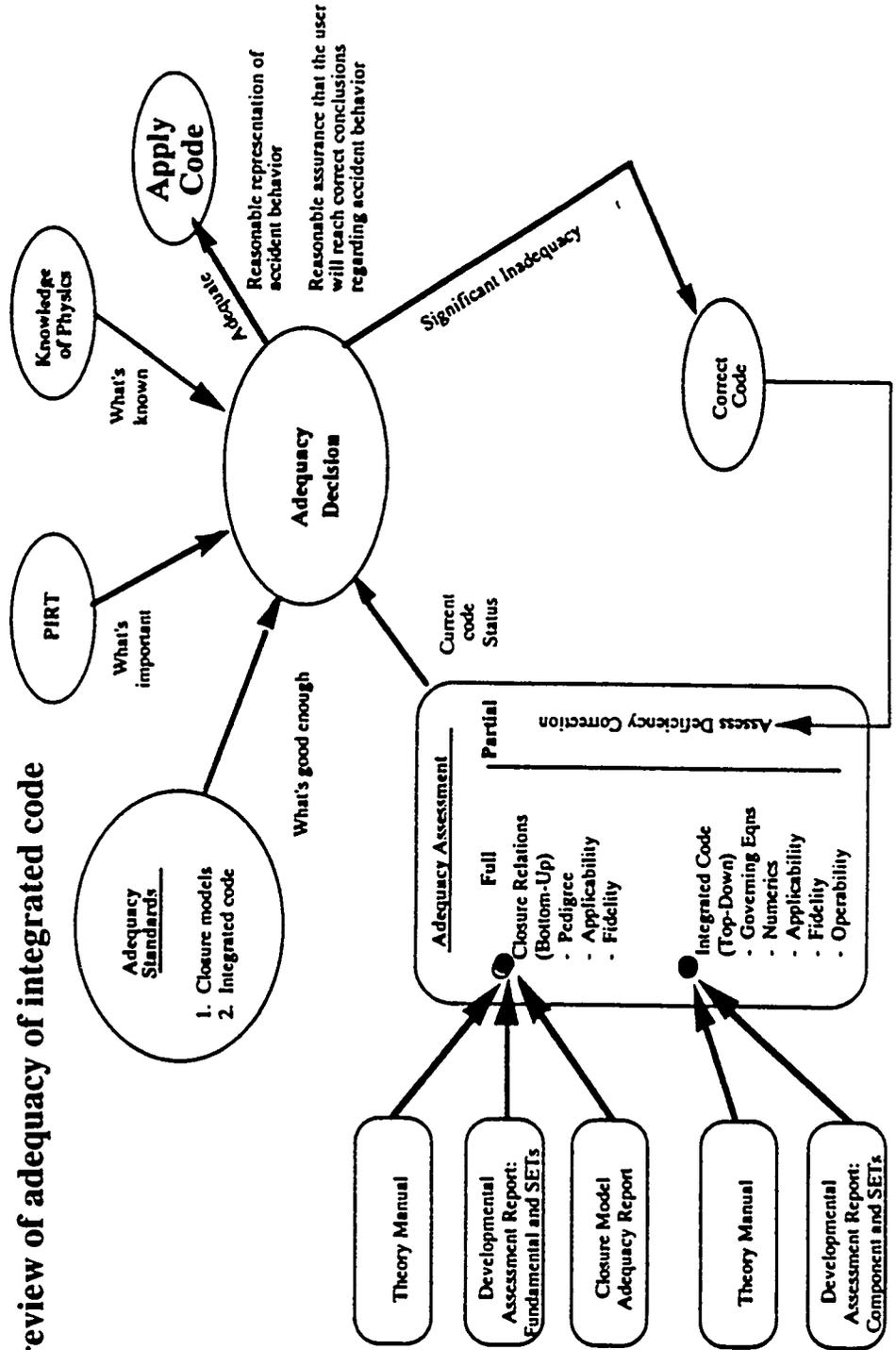
Phenomena/Characteristic	Code Modification
Sharp liquid/vapor and liquid/gas interfaces	Level tracking model
Steep temperature gradients in tanks, pools	Thermal stratification model
Critical flow through various geometry nozzles (experimental facilities)	Incorporate Henry-Fauske model
Sharp boron wave front in natural circulation SBWR (ATWS)	Apply Gudonov method to mitigate numerical diffusion
SBWR separator/dryer	Implement model from TRAC-B
AP600 spherical accumulator	Add spherical geometry capability
Low flow natural circulation	Incorporate Reynolds number dependence in form loss
Noncondensables prevalent	Improve code reliability in treating noncondensables
Horizontal tube bundle heat transfer	Incorporate suitable correlations
Filmwise condensation with and without noncondensables	New condensation model
Very long transients	Improve nearly-implicit solution scheme

Methods of Code Development/Validation/Assessment - TRAC Example

1. Bottom-up review of closure relationships:

“Pedigree”: physical basis of model, assumptions, limitations
 Applicability: consistent with “pedigree”
 Fidelity: validation effort, benchmarking,...

2. Top-down review of adequacy of integrated code



Methods of Code Development/Validation/Assessment - CATHARE Example

The constitutive relationships are developed and assessed following a **general methodology**:

- **Step A: Analytical experiments**, including separate effect tests and component tests, are performed and analyzed. Separate effect tests investigate a **physical process** such as the interfacial friction, the wall heat transfer. **Component tests** investigate physical processes which are specific to a reactor component, such as the phase separation in a Tee junction.
- **Step B: Development of a complete Revision of constitutive laws** from a large analytical experimental data base. Successive Revisions are implemented in successive code Versions. A new Revision contains a new physical modeling whereas a new Version may contain new numerical methods, new modules, new submodules, or a new code architecture, preprocessing or post-processing.
- **Step C: Qualification calculations of the analytical tests** in order to validate each closure relationship.
- **Step D: Verification calculations of system tests or integral tests** in order to validate the general consistency of the Revision.
- **Step E: Delivery of the code Version + Revision** fully assessed (qualified and verified) and documented (description documents and assessment reports).

When predictions are not correct or not accurate enough in step C, corrections will be made in steps A and B of the future Revision.

When predictions are not correct or not accurate enough in the verification calculations (step D), no correction of a closure law will be applied without coming back to analytical tests (step A). New analytical tests may be defined if a physical process was not treated before.

- A new Revision of constitutive laws is developed using some **general principles**:
- Data are first compared with **existing models**. If necessary, **original models** are developed. They can be either mechanistic (phenomenological), semi-empirical, or fully empirical, depending on the understanding of the physical processes which are involved. Each closure law is unique. No choice between several correlations is proposed to the user.
- When and where data are missing, **simple extrapolations of existing qualified models** are used. No mechanistic model is developed without the experimental evidence of its relevance. Some iterations may be necessary when experiments are sensitive to several constitutive laws.
- In a pre-qualification phase, some tests of each experiment of the qualification matrix are calculated. Corrections are sometimes necessary before finalizing the set of constitutive laws.
- A systematic qualification of the frozen Revision is then performed. All tests of the qualification matrix are calculated and qualification reports are written.

Items of Interest/Difficulties (from CATHARE)

Closure relationships for 2D and 3D t/h models

- today extrapolated from 1D models
(but, e.g., void fraction alone may not determine flow regime in 3D)
- lack of turbulent diffusion modeling
however, not restrictive when other effects dominate (e.g., in reactor core)

Differential terms in closure relationships

- they do affect character of set of system equations
in CATHARE: in added mass for dispersed flows, but also
in phase pressure difference/void fraction gradient for stratified flows

Effect of Singularities

- e.g.: CCFL at singularities needs special modeling
effect of ECCS water jet on condensation

Meshing vs convergence

METHODOLOGY, STATUS, AND PLANS FOR DEVELOPMENT AND ASSESSMENT OF THE RELAP5 CODE

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Abstract

RELAP5/MOD3 is a computer code used for the simulation of transients and accidents in light-water nuclear power plants. The objective of the program to develop and maintain RELAP5 was and is to provide the U. S. Nuclear Regulatory Commission with an independent tool for assessing reactor safety. This paper describes code requirements, models, solution scheme, language and structure, user interface, validation, and documentation. The paper also describes the current and near term development program and provides an assessment of the code's strengths and limitations.

Introduction

The mission of the RELAP5 development and maintenance project is to provide the U.S. Nuclear Regulatory Commission (NRC) with a best-estimate, fast-running, and user convenient transient analysis code for the simulation of accidents and transients in light-water nuclear power reactors. The NRC makes use of RELAP5 for a variety of regulatory tasks, including the evaluation of:

- transients in operating reactors
- generic issue resolution
- emergency operating procedures and accident management
- licensee analyses
- simulator fidelity
- advanced PWR and BWR designs.

The scope of applicability of RELAP5 encompasses a wide range of reactor designs and transient/accident conditions. Reactor designs include those of the U. S. pressurized water reactor vendors (B&W, Combustion Engineering, and Westinghouse) including design variations within a vendor (two-loop, three-loop, four-loop plants). In addition, RELAP5 must be applicable to experimental systems, so that its accuracy may be assessed.

Except for certain reactivity-initiated events, the code is applicable to all of the so-called Chapter 15 events. This includes loss-of-coolant accidents (LOCA), loss of feedwater, steam line break, steam generator tube rupture, and anticipated transients without scram (ATWS).

The approach taken in developing RELAP5 made use of the experience gained from its predecessor, RELAP4. The important principles underlying its development were:

- Best-estimate modeling - Utilize models without built-in conservatism and minimize modeling options.
- User friendly - Include free-format data input, random data order, extensive input data checking for consistency and permissible range.
- Fast running - Employ an efficient numerical solution scheme with a low grind time for faster execution.
- Feedback-based improvement - Promote wide usage of the code to provide user feedback on needed improvements.

The basic modeling concept of employing an Eulerian mesh to subdivide the coolant system into one-dimensional control volumes and interconnecting flow junctions was retained from RELAP4. So too were key models deemed satisfactory in their current form, including heat conduction, reactor kinetics, and the pump model. The basic hydrodynamic model, code structure, and input/output were completely rewritten.

The balance of this paper describes the code in each of its major constituent parts and developmental aspects, describes the current development program, and concludes with an assessment of the perceived strengths and limitations of the current code.

The constituent parts and major developmental aspects of the code are:

- Mathematical models
- Numerical solution scheme
- Code language and structure
- User interface
- Validation
- Documentation.

Hydrodynamic Model

A full two-fluid model is used in RELAP5 to simulate the transient one-dimensional flow of a two-phase fluid. The two-phase system consists of steam and water with the possibility of the vapor phase containing a noncondensable component and the liquid phase containing a nonvolatile solute. The phasic continuity, momentum, and energy equations are the basic field equations for the two-fluid model. The mass and momentum equations are used as sum and difference equations in the numerical scheme and are recorded here in that form.

The mass conservation relations are a sum mixture mass equation,

$$\frac{\partial}{\partial t} (\alpha_g \rho_g + \alpha_f \rho_f) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g v_g A + \alpha_f \rho_f v_f A) = 0 \quad (1)$$

a difference of the phasic mass equations,

$$\frac{\partial}{\partial t} (\alpha_g \rho_g - \alpha_f \rho_f) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g v_g A - \alpha_f \rho_f v_f A) = 2\Gamma_g \quad (2)$$

a noncondensable component mass fraction equation,

$$\frac{\partial}{\partial t} (\alpha_g \rho_g X_n) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g X_n v_g A) = 0 \quad (3)$$

and a nonvolatile solute mass equation,

$$\frac{\partial p_b}{\partial t} + \frac{1}{A} \frac{\partial (\alpha_f \rho_f C_b v_f A)}{\partial x} = 0 \quad (4)$$

The noncondensable component of the vapor phase is assumed to form a Gibbs-Dalton mixture with the steam so that the partial pressures sum to the mixture pressure. On the other hand, the nonvolatile component of the liquid phase is assumed to have no effect on the water properties. The noncondensable model is included to enable modeling the effect of nitrogen release from the accumulator, the presence of air in safety relief valve discharge piping, or air in containment components. The nonvolatile component is included to enable modeling and transport of dissolved boron salts and the associated reactivity effects in the core.

The phasic conservation of momentum equations are used in an expanded form and in terms of momenta per unit volume using the phasic primitive velocity variables. Two convenient independent momentum equations are obtained by a sum and difference of the phasic momentum equations (the difference is taken after division through by the product of the respective volume fraction and phasic density). The sum momentum equation is

$$\alpha_g \rho_g \frac{\partial v_g}{\partial t} + \alpha_f \rho_f \frac{\partial v_f}{\partial t} + \frac{1}{2} \alpha_g \rho_g \frac{\partial v_g^2}{\partial x} + \frac{1}{2} \alpha_f \rho_f \frac{\partial v_f^2}{\partial x} = -\frac{\partial P}{\partial x} + \rho_m B_x - \alpha_g \rho_g F W G v_g - \alpha_f \rho_f F W F v_f - \Gamma_g (v_g - v_f) \quad (5)$$

and the difference momentum equation is

$$\begin{aligned}
\frac{\partial v_g}{\partial t} - \frac{\partial v_f}{\partial t} + \frac{1}{2} \frac{\partial v_g^2}{\partial x} - \frac{1}{2} \frac{\partial v_f^2}{\partial x} &= - \left(\frac{1}{\rho_g} - \frac{1}{\rho_f} \right) \frac{\partial P}{\partial x} \\
&\quad - FWGv_g + FWFv_f \\
+ \frac{\Gamma_g [\rho_m v_l - (\alpha_f \rho_f v_g + \alpha_g \rho_g v_f)]}{\alpha_g \rho_g \alpha_f \rho_f} - \rho_m FI (v_g - v_f) & \\
- C \frac{[\rho_m^2]}{(\rho_g \rho_f)} \frac{\partial (v_g - v_f)}{\partial t} &
\end{aligned} \tag{6}$$

The sum momentum equation contains one interphase interaction term, the momentum transfer associated with mass transfer. The difference momentum equation contains interphase momentum exchange terms due to mass exchange, interphase friction, and virtual mass effects. The particular forms of the sum and difference momentum equations were chosen to provide smooth degeneration to the single phase case. Under single phase conditions, both equations remain determinant, and the constitutive model for the interphase drag is formulated such that interphase friction remains finite. Thus, in the single phase limit, the difference momentum equation reduces to a statement that the phasic velocities are equal.

The two phasic thermal energy equations are

$$\begin{aligned}
\frac{\partial}{\partial t} (\alpha_g \rho_g U_g) + \frac{1}{A} \left[\frac{\partial}{\partial x} (\alpha_g \rho_g U_g v_g A) + P \frac{\partial}{\partial x} (\alpha_g v_g A) \right] \\
= -P \frac{\partial \alpha_g}{\partial t} + Q_{ig} + \Gamma_{ig} h_g^* - Q_{gf} + \Gamma_w h'_g + Q_{wg} + DISS_g
\end{aligned} \tag{7}$$

and

$$\begin{aligned}
\frac{\partial}{\partial t} (\alpha_f \rho_f U_f) + \frac{1}{A} \left[\frac{\partial}{\partial x} (\alpha_f \rho_f U_f v_f A) + P \frac{\partial}{\partial x} (\alpha_f v_f A) \right] \\
= -P \frac{\partial \alpha_f}{\partial t} + Q_{if} - \Gamma_{if} h_f^* + Q_{gf} - \Gamma_w h'_f + Q_{wf} + DISS_f
\end{aligned} \tag{8}$$

The terms Q_{wg} and Q_{wf} are the wall heat transfer rates to the vapor and liquid phases, respectively. The terms Q_{ig} and Q_{if} are the interfacial heat transfer rates from the interface to the vapor and liquid, respectively. The terms $DISS_g$ and $DISS_f$ are the dissipation terms due to irreversible degradation of kinetic energy to internal energy. Only the dissipation effects due to wall friction and pump inefficiencies are included while minor effects due to interphase drag and mass transfer are neglected. The vapor generation rate is defined as

$$\Gamma_g = \Gamma_{ig} + \Gamma_w = - \frac{P}{\bar{P}} \frac{H_{ig} (T^s - T_g) + H_{if} (T^s - T_f)}{h_g^* - h_f^*} + \Gamma_w \tag{9}$$

The interphase energy transfer rates, Q_{ig} and Q_{if} , are formulated to account for flow regime and wall heat transfer effects on the interphase mass transfer rate. The sum of the phasic thermal energy equations, with the definition of the vapor generation rate, yields the correct mixture thermal energy equation.

The system of field equations is closed, insofar as relating differential quantities is concerned, by inclusion of the equations of state for the fluids. The constitutive models, necessary for evaluation of the nondifferential terms, are discussed later. The fluid state properties are obtained using a table lookup interpolation method. The liquid phase density is a function of the system total pressure and the liquid phase energy.

$$\rho_f = \hat{\rho}_f(P, U_f) \quad . \quad (10)$$

The vapor phase density is a function of the system total pressure, the vapor phase energy, and the mass fraction of noncondensable component

$$\rho_g = \hat{\rho}_g(P, U_g, X_n) \quad . \quad (11)$$

Numerical Methods

The two numerical methods for the hydrodynamic model use finite difference schemes having fixed, but staggered spatial noding. The scalar properties (pressure, energies, noncondensable quality, and void fraction) of the flow are defined at cell centers, and the vector quantities (velocities) are defined on the cell boundaries.

Semi-Implicit Scheme

To achieve fast execution speed, implicit evaluation is used only for those terms responsible for the sonic wave propagation time step limit and those phenomena known to have small time constants. Thus, implicit evaluation is used for the velocity in the mass and energy transport terms, the pressure gradient in the momentum equations, and the interface mass and momentum exchange terms. To further increase computing speed, time level evaluations are selected so the resulting implicit terms are linear in the new time variables. Where it is necessary to retain nonlinearities, Taylor series expansions about old time values are used to obtain a formulation linear in the new time variables. (Higher-order terms are neglected.) Linearity results in high computing speed by eliminating the need to iteratively solve systems of nonlinear equations.

The phasic density and phasic temperature equations are substituted into the five expanded density and energy difference equations. The equations are then ordered so that the noncondensable density equation is first, the vapor energy equation is second, the liquid energy equation is third, the difference density equation is fourth, and the sum density equation is fifth. A solver, which uses LU factorization without pivoting and factors the matrix into upper and lower triangular matrices using triangular decomposition, is used to obtain the bottom row of the inverse of the 5 X 5 matrix. This equation involves only the new time pressures and new time phasic velocities. Substituting the velocity equations into this equation results in a single equation involving pressures. This is done for each volume, giving rise to an N X N system of linear equations for the new time pressures in a system containing N volumes. Next, a sparse matrix solver is used to obtain the pressures for each volume. The pressure differences are then

substituted into the velocity equations to obtain the new time velocities. The new time velocities and LU factors are used to obtain the noncondensable qualities, energies, and void fractions.

Nearly-Implicit Scheme

For problems where the flow is expected to change very slowly with time, it is possible to obtain adequate information from an approximate solution based on very large time steps. The nearly-implicit scheme was developed for this purpose, and it consists of two steps.

The first step solves all seven conservation equations, treating all interface exchange processes, the pressure propagation process, and the momentum convection process implicitly. These finite difference equations are exactly the expanded ones solved in the semi-implicit scheme with one major change. The convective terms in the momentum equations are evaluated implicitly (in a linearized form) instead of in an explicit donored fashion as is done in the semi-implicit scheme. Because the momentum flux terms are implicit, the momentum equations cannot be locally solved for the new time velocities in terms of the new time pressures. In the nearly-implicit scheme, the equation involving new time pressures and new time phasic velocities is used to eliminate the new time pressure terms from the sum and difference momentum equations. A coupled pair of momentum equations involving only new time phasic velocities is obtained. This system of equations is next preconditioned in order to enhance the diagonal dominance of the matrix. This system of equations is then solved using a sparse matrix solution algorithm. Once the new time velocities are obtained, the new time pressures and provisional new time noncondensable qualities, energies, and void fractions are obtained through back substitution.

The second step is used to stabilize the convective terms in the mass and energy balance equations. This step uses the final new time level velocities from the first step along with the interface exchange terms resulting from the provisional variables of the first step. The phasic continuity and energy equations in this second step have the convected variables evaluated at the new time level. The three equations involving the gas phase have the same structural form for the convective terms, i.e., each equation convects with the vapor velocity. The coefficient matrix generated by one of the equations is inverted once, and then this inverse is used with different right hand sides to solve for the other two equations. In like manner, the two equations involving the liquid phase have the same structure and require only one inversion to be carried out to solve both equation sets.

Constitutive Models

The constitutive models are the real "glue" that holds the code together. While the basic two-fluid hydrodynamic model provides the conceptual framework for a two-phase fluids code, the constitutive models define the interaction of the phases with each other and the system boundaries. The constitutive models divide into four areas:

- interphase heat and mass transfer
- interphase drag
- wall heat transfer
- wall friction.

Unifying these four functional area are flow regime maps that define the interfacial area concentration and individual phase wall contact area. Three distinct maps are employed: vertical, horizontal, and high mixing (for pumps). **Figure 1** shows the map for horizontal components. The flow regimes possible are bubbly, slug, annular-mist, mist, and stratified. Transitions are included between stratified and non-stratified regimes and between slug and annular-mist. The determination of regime is based on the void fraction and the relative velocity between the phases. The transition void fractions are all empirically based. The critical velocity for transition from stratified to non-stratified flow is based on a Kelvin-Helmholtz instability analysis. For each of the flow regimes, an idealized topology, or geometrical arrangement of the two-phases, is assumed that leads to a calculation of the interfacial area concentration. For example, in bubbly flow, the interfacial area concentration is based on the assumption of spherical bubbles whose average diameter is predicated on a critical Weber number. Similarly, for slug flow, the composition of the vapor is assumed to be made up of large Taylor bubbles and much smaller bubbles in the bulk.

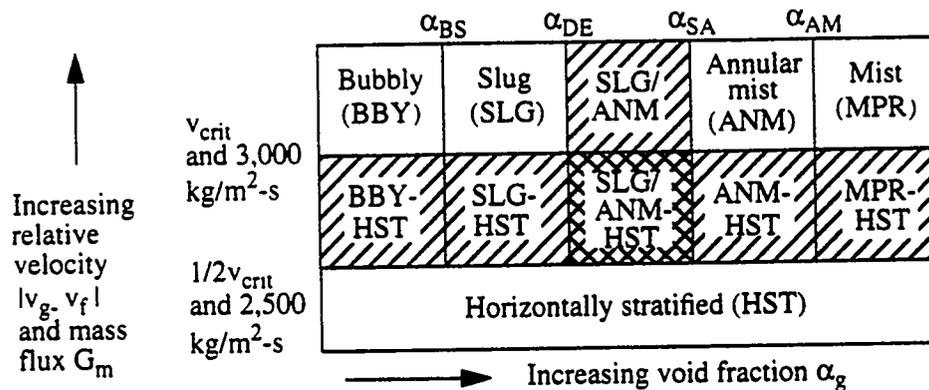


Figure 1. Schematic of horizontal flow-regime map with hatchings, indicating transition regions.

Interfacial Heat/Mass Transfer

Interfacial heat and mass transfer may occur in the bulk and/or in a thermal boundary layer near a wall. The former results from an energy exchange between the phases away from the wall while the latter is due to heat transfer at the wall. Mass transfer is assumed to occur at a saturated boundary, with the driving potential being the bulk to saturation temperature difference. In terms of vapor generation rate, the total vapor generation rate (Γ_g) per unit volume is given by

$$\Gamma_g = - \frac{\left(\frac{P_s}{P}\right) H_{ig} (T^s - T_g) + H_{if} (T^s - T_f)}{h_g^* - h_f^*} + \Gamma_w \quad (12)$$

where P_s and P are respectively the saturation pressure and total pressure, H_{ig} and H_{if} are respectively the vapor and liquid side product of the heat transfer coefficient and interfacial area concentration, T_g and T_f

are the bulk vapor and liquid temperatures, h_g and h_l are the vapor and liquid enthalpies defined such that the interface energy jump conditions at the liquid-vapor interface is satisfied, and Γ_w is the vapor generation rate per unit volume near the wall due to heat transfer. The vapor generation (or condensation) near the wall is determined by the wall heat transfer model.

Wall Heat Transfer Model

In RELAP5/MOD3.2 the total wall heat flux (q'') is the heat flux to the vapor plus the heat flux to the liquid:

$$q'' = h_g (T_w - T_{refg}) + h_l (T_w - T_{reff}) \quad (13)$$

where

h_g	=	heat transfer coefficient to gas
h_l	=	heat transfer coefficient to liquid
T_w	=	wall temperature
T_{refg}	=	gas reference temperature
T_{reff}	=	liquid reference temperature.

The reference temperatures can be the local gas or liquid temperature or the saturation temperature, depending on the heat transfer coefficient correlation being used.

A boiling curve is used in RELAP5 to govern the selection of the wall heat transfer correlations when the wall surface temperature is above the saturation temperature (superheated relative to the saturation temperature based on total pressure). When a hydraulic volume is voided and the adjacent surface temperature is subcooled, steam condensation on the surface is predicted. If noncondensable gases are present, the phenomena is more complex because while boiling is a function of the wall superheat based on the total pressure, condensation is based on the partial pressure of steam. When the wall temperature is less than the saturation temperature based on total pressure, but greater than the saturation temperature based on steam partial pressure, a convection condition exists. **Figure 2** illustrates these three regions.

RELAP5/MOD3 utilizes a complex logical algorithm to choose the appropriate heat transfer mode and correlation. The appropriate mode depends on a number of factors, including pressure, wall temperature relative to saturation, void fraction, phasic temperatures, mass flux, and noncondensable quality. There are a total of twelve heat transfer modes represented, including free convection, forced convection, subcooled boiling, saturated boiling, transition boiling, film boiling, and condensation.

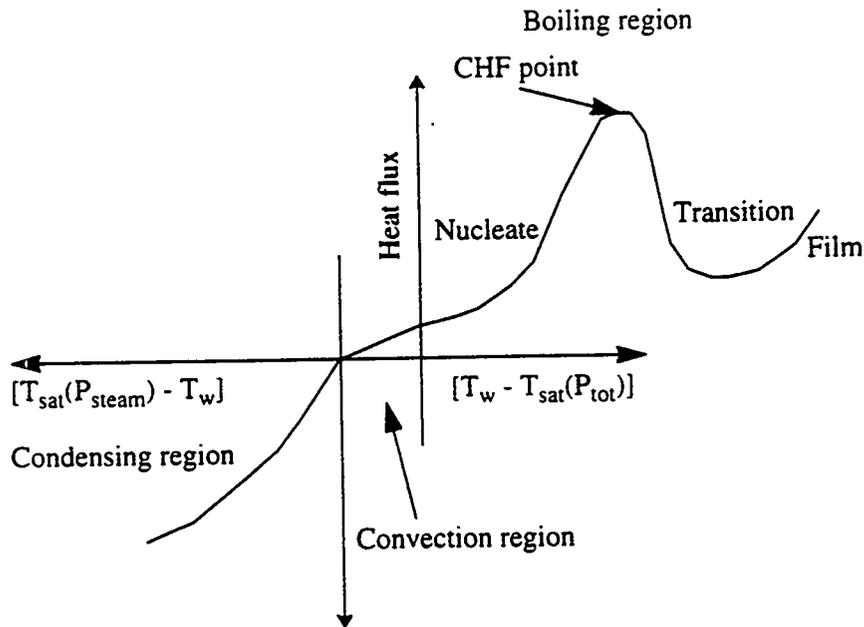


Figure 2. RELAP5 boiling and condensing curves.

Interfacial Drag Model

RELAP5/MOD3 uses two different models for the phasic interfacial friction force component, the drift flux method and the drag coefficient method. The drift flux method is used in the bubbly and slug flow regimes for vertical flow. The drift flux model specifies a distribution coefficient and vapor drift velocity. These are converted into a constitutive relation for the interfacial frictional force per unit volume. The drag coefficient method is used in all flow regimes except bubbly and slug flows in vertical components. The model uses correlations for the drag coefficient that depend on the flow regime. The general expression for the force on a body moving through a fluid is assumed:

$$F = \frac{1}{2} \rho v^2 C_d A \quad (14)$$

The interfacial friction per unit volume is given by

$$F_{ig} = \alpha_g \rho_g F_{IG} (v_g - v_f) \quad (15)$$

and

$$F_{if} = \alpha_f \rho_f F_{IF} (v_g - v_f) \quad (16)$$

where the terms FIG and FIF are determined by the drag coefficient or conversion of the drift flux parameters.

Wall Friction Model

The wall friction model, like the interfacial heat and mass transfer model, makes use of the flow regime map to determine the flow topology, and therefore the apportioning of the wall friction to the individual phases. The wall friction terms include only wall shear effects. Losses associated with abrupt area changes, elbows, or other complicated flow passage geometries are computed using a form loss model.

The wall friction model is based on a two-phase multiplier approach in which the two-phase multiplier is calculated from the HTFS-modified Baroczy correlation.¹ The individual phasic wall friction components are calculated by apportioning the two-phase friction between the phases using a technique derived by Chisholm² from the Lockhart-Martinelli model.³

The Lockhart-Martinelli model expresses the two-phase pressure drop gradient as dependent on the pressure drop gradient for one-phase flowing alone. For example, using the liquid phase, the two-phase pressure drop gradient is expressed as:

$$\left(\frac{dP}{dx}\right)_{2\phi} = \phi_f^2 \left(\frac{dP}{dx}\right)_f \quad (17)$$

where ϕ_f is the liquid-alone Darcy-Weisbach friction multiplier. A similar expression can be written based on the vapor flowing alone.

The HTFS correlation is used to calculate the two-phase friction multipliers. The correlation is expressed as:

$$\phi_f^2 = 1 + \frac{C}{\chi} + \frac{1}{\chi^2} \quad (18)$$

where χ^2 is the Lockhart-Martinelli parameter defined as:

$$\chi^2 = \frac{\left(\frac{dP}{dx}\right)_f}{\left(\frac{dP}{dx}\right)_g} = \frac{\phi_g^2}{\phi_f^2} \quad (19)$$

and C is the correlation coefficient, which is a function of the mass flux and the Baroczy dimensionless property index.

The partitioning of the wall friction between the two-phases is included through use of the rationale developed by Chisholm and employment of the quasi-static forms of the phasic momentum equations. The

method developed by Chisholm allows partitioning of the wall friction that is independent of the model for interphase friction, but depends on the fractional perimeter of the wall that is in contact with the liquid. The fractional contact of each phase with the wall is dependent on the flow regime.

Heat Conduction Model

In RELAP5, heat structures are coupled to fluid volumes for representing fuel pins, steam generator tubes, pipe walls, etc. The temperature distribution within the heat structures is calculated using a finite difference solution for the heat equation in one-dimensional rectangular, cylindrical, or spherical geometry. The temperature dependence of the material properties is specified by the user as a tabular function. The boundary conditions at the heat structure surface(s) are generally provided by the convective heat transfer model previously described. Alternatively, the user may specify other boundary conditions: adiabatic, specified temperature, and specified heat flux.

Process and Component Models

RELAP5 uses specialized models to simulate phenomena too complex to model mechanistically. These include both flow phenomena and the effects of components. Specialized flow phenomena include choking (Henry-Fauske model), countercurrent flow flooding, abrupt area change, form loss, two-phase mixture level, thermal stratification, and phase separation at tees. Component models include branch separator (simple or mechanistic), jet mixer, pump, turbine, valves (check, motor, servo, and relief), accumulator, ecc mixer, and annulus.

RELAP5 also has the capability of modeling trips to control events during a transient and an extensive array of control components. The control components include a constant, sum and difference, multiplier, division, exponentiation, table lookup, standard functions, delay, integration, differentiation, proportional-integral, lag, and lead-lag. Each component can access virtually any code parameter as well as other control components in a building block approach. This is a powerful feature not only for modeling control systems but also for manipulating code output. For example, analysts can integrate mass and energy flows to obtain a global perspective on system response.

Reactor Power Model

The reactor kinetics model is based on a generalized space independent (point) kinetic model. It models the feedback effects resulting from moderator density, fuel density, fuel temperature, and boron concentration in the moderator. The model computes both the immediate fission power and the power from the decay of fission products. The decay heat model is based on the ANS 1979 Standard.⁴ An actinide decay model is also included so that very long transients can be modeled.

The reactor kinetics model is integrated in time using a fifth-order Runge-Kutta like scheme modified to account for the reactor kinetics exponential reactor behavior with widely varying time constants. The reactor kinetics model has an automatic time step control and the attempted time step is taken equal to the hydrodynamic time step, but it may be reduced to maintain accuracy. After a reactor kinetics time advancement, an empirical error criterion is used to estimate the error. If the error is excessive, the time step is halved and the advancement calculation is repeated. This process is continued as needed until the error criterion is satisfied. The resulting reactor kinetics time step is an integral power of one-half times the hydrodynamic time step, which assures that a reactor kinetics calculation will be made at the same time level as the hydrodynamic time level.

Code Language and Structure

RELAP5/MOD3 is written in FORTRAN 77 for a variety of 64-bit and 32-bit computers. Here, a 64-bit computer is one in which floating point, integer, and logical quantities use 64-bit words; a 32-bit machine uses 32-bit words for those same quantities but also allows 64-bit floating point operations. Examples of 64-bit computers are Cray, Cyber-NOS-VE, and DEC/Alpha machines. Examples of 32-bit computers include IBM mainframes, such as a 3090, workstations, including those from DEC, HP, IBM, SGI, and Sun, and even personal computers.

A common source is maintained for all computer versions. The common source is conditioned for a particular computer and operating system through the use of two precompilers maintained as part of RELAP5. The first precompiler processes compile time options such as machine and operating system dependencies. Through the use of standard Fortran and a widely used standard for bit operations, there is very little hardware dependence. The primary hardware dependence is in matrix factoring routines where details of the floating point characteristics are needed to monitor roundoff error. The program has been compiled and executed using Fortran-90; a future full conversion to that standard should remove all hardware dependencies. RELAP5 is developed and maintained at INEL on computers using the UNIX operating system. Some user-convenient features have been incorporated into the code based on UNIX, but these are under compile time option, and the code does not depend on any particular operating system. The installation scripts distributed with the code are UNIX based, and control language to install and execute the code must be developed by the user for other operating systems.

RELAP5 is coded in a modular fashion using top-down structuring. The various models and procedures are isolated in separate subroutines. The top level structure is shown in **Figure 3** and consists of input (INPUT), transient/steady-state (TRNCTL), and stripping (STRIP) blocks. The input block (INPUT) processes input, checks input data, and prepares required data blocks for all program options. The transient/steady-state block (TRNCTL) handles both transient and the steady-state options. The steady-state option determines the steady-state conditions if a properly posed steady-state problem is presented. Steady-state is obtained by running an accelerated transient until the time derivatives approach zero. Thus, the steady-state option is very similar to the transient option but contains convergence testing algorithms to determine satisfactory steady-state, divergence from steady-state, or cyclic operation. The strip block (STRIP) extracts simulation data from a restart plot file for convenient passing of RELAP5 simulation results to other computer programs.

Figure 4 shows the functional modular structure for the transient calculations.

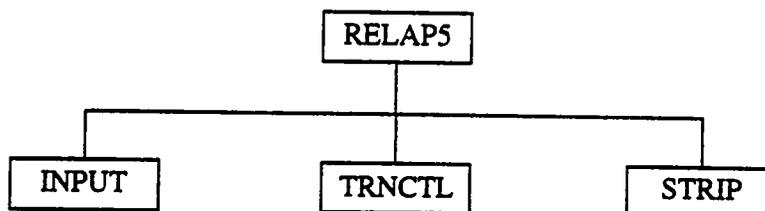


Figure 3. RELAP5 top level structure.

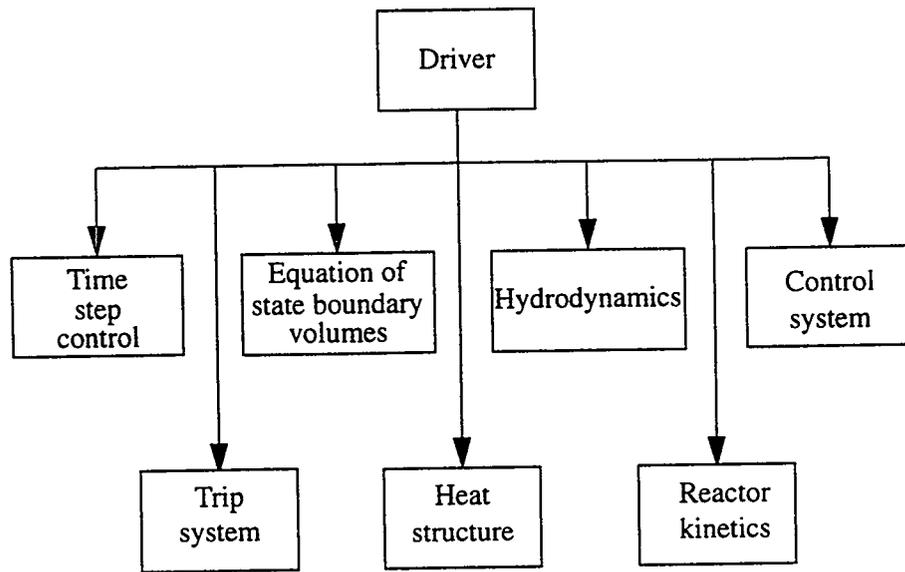


Figure 4. Modular structures of transient calculations in RELAP5.

User Interface

Data Input

Data input to RELAP5 is via 80-character records (or "cards"). Data is recognized by the leading card number on the record. Data consists of integers, floating point numbers, and alphanumerics. There is no rigid format (i.e., free format input) and random ordering of data records is permissible.

RELAP5 features sequential expansion format which enables users to save time in defining a series of items that have the same characteristics (e.g., pipe volumes).

RELAP5 provides detailed input checking for all system models using three input processing phases. The first phase reads all input data, checks for punctuation and typing errors (such as multiple decimal points and letters in numerical fields), and stores the data keyed by card number such that the data are easily retrieved. A list of the input data is provided, and punctuation errors are noted.

During the second phase, restart data from a previous simulation are read if the problem is a RESTART type, and all input data are processed. Extensive input checking is done, but at this level, checking is limited to new data from the cards being processed. Relationships with other data cannot be checked because the latter may not yet be processed. As an illustration of this level of checking, junction data are checked to determine if they are within the appropriate range (such as positive, nonzero, or between zero and one) and volume connection codes are checked for proper format. No attempt is made at this point to check whether or not referenced volumes exist in the problem until all input data are processed.

The third phase of processing begins after all input data have been processed. Since all data have been placed in common or dynamic data blocks during the second phase, complete checking of interrelationships can proceed. Examples of cross-checking are existence of hydrodynamic volumes

referenced in junctions and heat structure boundary conditions; entry or existence of material property data specified in heat structures; and validity of variables selected for minor edits, plotting, or used in trips and control systems. As the cross-checking proceeds, cross-linking of the data blocks is done so that it need not be repeated at every time step. The initialization required to prepare the model for the start of the transient advancement is done at this level.

Input editing and diagnostic messages can be generated during the second and/or third phases. Input processing for most models generates output and diagnostic messages during both phases. Thus, input editing for these models appears in two sections.

As errors are detected, various recovery procedures are used so that input processing can be continued and a maximum amount of diagnostic information can be furnished. Recovery procedures include supplying default or benign data, marking the data as erroneous so that other models do not attempt use of the data, or deleting the bad data. The recovery procedures sometimes generate additional diagnostic messages. Often after attempted correction of input, different diagnostic messages appear. These can be due to continued incorrect preparation of data, but the diagnostics may result from the more extensive testing permitted as previous errors are eliminated.

Output

RELAP5 output can be displayed in three formats: printed output, x-y graphs, and visually in conjunction with the Nuclear Plant Analyzer (NPA).

Printed output consists of major and minor edits. The user controls the frequency at which these edits are output, as well as the frequency at which restart files are written to the restart/plot files. Major edits contain most of the key quantities being advanced in time. The amount of output can be controlled by the user. Typical output includes a time step summary, trip information, reactor kinetics data, one to four sections of hydrodynamic volume data, one or two sections of hydrodynamic junction data, heat structure/heat transfer data, and control variable data.

Minor edits are generally used by analysts to print selected parameters more frequently than is practical with major edits. Users have available an extensive list of parameters from which to choose.

The most common method for analyzing code output is in graphical form. This can be accomplished by stripping selected data from the restart-plot file using the STRIP option to create ASCII data in a file called STRIPF. These data are then processed to put them in a format compatible with the user's plotting software. At the INEL, XMGR could be used to plot data from a STRIPF file. XMGR5 is an INEL extension to the XMGR computer code. XMGR5 adds features to conveniently plot information from restart-plot files or STRIPF files. Parameters available for plotting are the same as those available for minor edits.

The third method of analyzing code output makes use of the Nuclear Plant Analyzer (NPA), a separate computer code that can display transient results visually through a user-designed "mask" depicting the coolant system. RELAP5 output data "drives" this mask to show the state of the coolant system as the transient evolves. By using color gradients to represent the coolant condition around the system (e.g., dark blue for subcooled liquid, light blue for saturated liquid, white for saturated steam) the analyst can obtain an overall impression of the conduct of the transient. Other displays show the operating condition of pumps, valves, and safety systems.

The NPA can be used in either a playback mode or an interactive mode. In the playback mode, the analyst can view a completed calculation at virtually any speed s/he desires. The interactive mode makes use of a special feature in RELAP5 that allows the analyst to alter the boundary conditions of the calculation, much in the same way a reactor operator can interact with a power plant. This feature is especially useful for studying the efficacy of emergency procedures.

Code Validation

An essential part of the RELAP5 code package is the validation library that forms the basis for drawing qualitative and quantitative conclusions concerning the code's accuracy. Three types of validation cases are included in the library: conceptual problems, separate-effects experiments, and integral experiments.

Conceptual problems are "made-up" problems that have either a closed-form solution or an intuitive solution. These problems are useful for checking the basic soundness of the hydrodynamic model and numerical solution scheme. There are ten such problems currently in the library:

- Oscillating air-water manometer
- Water faucet
- 9-volume water over steam
- Horizontally stratified countercurrent flow
- Branch tee
- Crossflow tee
- Three-stage turbine
- Horizontal fill
- Primary and secondary loop
- Restart of primary and secondary loop.

Separate effects experiments usually focus on one or a few phenomena that can be isolated from "system effects". Examples include heat transfer experiments, blowdown experiments, and rod bundle boiloff experiments. In each case, the boundary conditions are carefully controlled and can be replicated in the code model.

Integral experiments are generally scaled-models of complete reactor coolant systems. Experiments in such facilities provide a simulation of the behavior of complete systems, including the interaction of components. These experiments are important parts of the library since they come close to replicating total system behavior.

Table 1 shows some of the key experiments contained in the RELAP5 validation library organized by the reactor component that is addressed by the experiment.

Table 1. RELAP5 assessment by component.

Component	Subset	Assessment case	Description
Reactor vessel	Core	THETIS ^a	Boildown and steady-state void profiles in rod bundles
		THTF ^a	
		FRIGG ^a	
		PERICLES ^a	
		ACHILLES ^a	
		ECN ^a	
		Flecht-Seaset ^a	
		Bennett's Tube	CHF and post-CHF heat transfer
		RIT Tube 262	
		Chen Post-CHF	
		THTF CHF	
		PBF LOC-11	Internal fuel rod heat transfer
		McMaster ^a	Subcooled boiling
		Shoukri ^a	
	Christensen ^a		
	Downcomer	Dukler Flooding ^a	Flooding (CCFL)
		Creare HI	
		Creare Mixing ^a	Thermal mixing
	Other	SRL Gd-Nitrate ^a	Boron transport
		LOFT L-6 ^a	

Table 1. RELAP5 assessment by component. (Continued)

Component	Subset	Assessment case	Description
Steam generator	Overall	MB-2	Various steady-state and transient tests in scaled facilities
		Semiscale ^a	
		Flecht-Seaset 23402	
	Inside tubes	MIT-Siddique ^a	Condensation inside tubes with and without noncondensables
		UCB-Kuhn ^a	
		Hein ^a	
		B&W ^a	
	Separator/dryer	TRAC-B test case ^a	G. E. data
	Plena	Thomas ^a	Subcooled jets entering saturated water from below (direct contact condensation)
		Sonin-Shimko-Chun ^a	
		Brown-Khou-Sonin ^a	
Brown-Helmick-Sonin ^a			
Pressurizer	Overall	G. E. 1 ft. ^a	Level swell during vessel blowdown
		G. E. 4 ft. ^a	
		MIT ^a	Insurge/outsurge
		Neptunus	Spray performance
Hot leg/cold leg	Main pipe	TPTF	Two-phase flow in large horizontal pipe
		Bankoff	Surface condensation in two-phase stratified flow
		Aoki	Condensation in dispersed flow
	Offtake	Smoglie	Tests were used to develop empirical model in RELAP5. Determines void fraction convected from main pipe
		Maciaszek et al.	
		Schrock	
		Anderson	

Table 1. RELAP5 assessment by component. (Continued)

Component	Subset	Assessment case	Description
Accumulator	Overall	LOFT L3-1	Accumulator discharge
		SRL Pressurizer	
Breaks/relief valves	Critical flow	ADS 1-3 ^a	AP600 valves
		Cumulus ^a	French relief valve
		Marviken ^a	Full-scale vessel blowdown
		LOFT-Wyle	Calibration of LOFT break nozzle
		Super Moby Dick ^a	S. S. critical flow through long L/D nozzle
		Sozzi & Sutherland ^a	S. S. data through various nozzles
		ROSA AP-CL-03 ^a	Used as a separate effects test
		Neussen ^a	Separate effects critical flow tests
		Carofano & McManus ^a	
		Fincke & Collins ^a	
Deich et al. ^a			
PRHR	Overall	<u>W</u> Tests ^a	
		ROSA Tests ^a	
CMT	Overall	<u>W</u> Tests ^a	

a. RELAP5/MOD3.2 or higher.

Documentation

RELAP5 is documented in a seven-volume users manual. The titles of the volumes are:

- Volume I: Code Structure, System Models, and Solution Methods
- Volume II: User Guidelines and Input Requirements
- Volume III: Developmental Assessment

- Volume IV: Models and Correlations
- Volume V: User's Guidelines
- Volume VI: Validation of Numerical Techniques
- Volume VII: Independent Assessment.

Volumes I, II, IV, and V were updated in July 1995 and are current with the latest release of the code, MOD3.2. Volume VI was released in 1994 but is considered valid for MOD3.2 since no changes to the solution scheme have been made since then. Volumes III and VII are currently out of date and are due to be replaced in early 1997.

Volumes I, II, IV, and V are available on the RELAP5 Home Page on the Internet at

http://www.inel.gov/capabilities/computing_resources/relap/RELAP5.html

Current Development Program

The current RELAP5 development program consists of a code improvement element focused on modeling the advanced reactor designs (Westinghouse AP600 and General Electric SBWR) and a maintenance element that includes user support, including support of the international members of the Code Application and Maintenance Program (CAMP).

The advanced reactor designs provide new challenges to the existing NRC-sponsored computer codes, including RELAP5. The new designs share some common characteristics, including:

- Intentional depressurization to allow gravity-driven injection of emergency coolant.
- Large, in-containment emergency coolant sources.
- Strong reactor coolant system/containment coupling for long-term decay heat removal.

These design features result in "new" phenomena during postulated accidents not encountered in current generation designs. Key among these phenomena are:

- Condensation in the presence of noncondensables.
- Small, gravity-driven pressure forces.
- Sharp liquid/vapor interfaces.
- Long transients (up to three days).

To address these and other requirements needed for the advanced reactor designs, an improvement program was initiated in 1993. **Table 2** presents a summary of the key code improvements and their relationship to the important phenomena or characteristics of these designs.

Table 2. ALWR model improvements.

Phenomena/Characteristic	Code Modification
Sharp liquid/vapor and liquid/gas interfaces	Level tracking model
Steep temperature gradients in tanks, pools	Thermal stratification model
Critical flow through various geometry nozzles (experimental facilities)	Incorporate Henry-Fauske model
Sharp boron wave front in natural circulation SBWR (ATWS)	Apply Gudonov method to mitigate numerical diffusion
SBWR separator/dryer	Implement model from TRAC-B
AP600 spherical accumulator	Add spherical geometry capability
Low flow natural circulation	Incorporate Reynolds number dependence in form loss
Noncondensables prevalent	Improve code reliability in treating noncondensables
Horizontal tube bundle heat transfer	Incorporate suitable correlations
Filmwise condensation with and without noncondensables	New condensation model
Very long transients	Improve nearly-implicit solution scheme

Code Strengths and Limitations

With development having begun in the late 1970's, RELAP5 by almost any measure must be considered a mature code. In considering the development of a successor code, or a refinement to the existing code, it is worthwhile to identify what are perceived to be the current strengths and limitations of RELAP5. Strengths and limitations can be cast in the following areas:

- Institutional
- Physics
- Numerics
- Programming
- User interface

From an institutional standpoint, RELAP5 is considered a strong code. It is the most widely-used code of its kind in the world, and this extensive user base has produced at least three important benefits: a

large volume of user feedback that leads to improved versions, international support for code maintenance, and extensive validation.

A second institutional strength is the inherent coupling to the severe core damage code SCDAP. The implicit coupling of RELAP5's thermal-hydraulic models to SCDAP's severe accident models results in a code that can analyze severe accidents from the very beginning of an accident.

The physics, or mathematical models, in RELAP5 are generally up-to-date and the code can be used to analyze a wide range of conditions. But there are definite limitations, some of which are inherent. RELAP5 is basically limited to one-dimensional flow situations with a provision to represent pseudo two-dimensional networks using the crossflow junction feature. Transients in which strong multi-dimensional flow patterns are important are beyond the scope of RELAP5. Similarly, RELAP5's reactor kinetics model is a point model, and therefore is limited in its applicability to reactivity excursion events where axial and radial power shifting is minimal.

Perhaps the most important limitation in RELAP5 is the use of flow regime maps. By and large these empirically-based maps were developed on the basis of steady-state fully developed flow. While there is evidence that the steady-state assumption is often applicable to transient situations, flows inside major portions of a reactor coolant system are never fully developed. Entrance effects on the distribution of steam and water are not accounted for when they are sometimes important.

Other limitations in the physics include the restriction of one liquid field (core reflood coolant behavior can have both films and droplets), and the lack of a dissolved gas model.

In the area of numerics, RELAP5's semi-implicit scheme is very efficient, leading to a very low grind time. However, with this scheme the time step is limited by the material Courant limit. The nearly-implicit solution scheme included with the code overcomes this limitation. Ideally, a fully implicit scheme should also be added, with logic to choose the most efficient scheme "on the fly".

Other limitations evident in the numerics are the occasional appearance of discontinuities in interfacial drag and interfacial heat and mass transfer terms. These can sometimes result in numerically-caused oscillations.

RELAP5's programming has both good and bad points. On the positive side, the code is very modular and very portable from one platform to another. But the data structure is outdated, the language level (FORTRAN 77) is also old, and the code's maintainability index is low. Adaptation of FORTRAN 90 would rectify both of these latter problems. The code's documentation also currently lacks a programmer's manual.

RELAP5's user interface has some strengths but is also out-of-date. The code is inherently very flexible from a user's standpoint, making it versatile in terms of modeling a wide variety of systems. The code also performs extensive input data checking, saving analysis time on preparing a problem. RELAP5's capability to be run interactively with the Nuclear Plant Analyzer, and to allow renodalization at restart are also code strengths. The code, however, currently lacks an integrated graphical user interface (GUI) that would significantly improve efficiency and accuracy in performing analyses. Ideally, a GUI should function as both a front-end and back-end interface. The development of a GUI is currently planned by the NRC.

Other areas where improvements could be made are improved user guidelines, and a formal training program, perhaps leading to certification of analysts.

References

1. K. T. Chaxton, J. G. Collier, and J. A. Ward, *H.T.F.S. Correlation for Two-Phase Pressure Drop and Void Fraction in Tubes*, AERE-R7162, 1972.
2. D. Chisholm. "A Theoretical Basis for the Lockhart-Martinelli Correlation for Two-Phase Flow," *Journal of Heat and Mass Transfer*, 10, 1967, pp. 1767-1778.
3. R. W. Lockhart and R. C. Martinelli, "Proposed Correlation of Data for Isothermal Two-Phase, Two-Component Flow in Pipes," *Chemical Engineering Progress*, 45, 1, 1949, pp. 39-48.
4. American National Standard for Decay Heat Power in Light Water Reactors, ANSI/ANS-5.1, 1979.

METHODOLOGY, STATUS, AND PLANS FOR DEVELOPMENT AND ASSESSMENT OF THE TRAC CODE*

by

B. E. Boyack** and S. Jolly-Woodruff†

Abstract

The Transient Reactor Analysis Code (TRAC) is a state-of-the-art, best-estimate, transient system analysis computer code for analyzing geometrically complex multidimensional thermal hydraulic systems, primarily nuclear reactor power plants. TRAC is used by government and industry for design and safety analysis, phenomenological studies, operational transient analysis, evaluating emergency operating procedures, simulator support and operator training, and for assessment of data involving basic experiments, separate-effects tests, and plant operations. TRAC will calculate one- and three-dimensional (rectilinear and cylindrical coordinates) fluid flow involving gas, liquid, and mixture states. Although TRAC has many capabilities, it also has limitations. Some limitations arise from its implementation, dating from the 1970s. Rapid advances in hardware and software engineering highlight TRAC's inefficiencies; however, other limitations relate to the level of scientific knowledge regarding two-phase flow physics. These limitations will continue until such time as the fundamental understanding of two-phase flows is extended. Presently, several development activities are either in progress or soon to begin that will fundamentally improve TRAC. Foremost among these are reimplementing of the current TRAC data structures in Fortran 90 and the integrated development of closure packages for large-break loss-of-coolant accident applications.

INTRODUCTION

The Transient Reactor Analysis Code (TRAC)¹⁻⁴ is an advanced, best-estimate computer program that calculates the transient reactor behavior of a pressurized water reactor (PWR). In the early 1980s, the Nuclear Regulatory Commission (NRC) branched the development of the boiling water reactor (BWR) version of TRAC off the main version of TRAC. All the BWR versions begin with the designation TRAC-B, and the PWR versions begin with the designation TRAC-P. The development of TRAC-B began at Los Alamos, but is currently being developed at the Pennsylvania State University. In September 1995, the NRC announced plans to consolidate the two TRAC versions along

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certain features from RAMONA. While acknowledging the consolidation objective, subsequent discussion of TRAC in this paper will focus on TRAC-P.

In the remainder of this paper, TRAC refers to the latest PWR version, which has the official NRC designation TRAC-P 5.4.15, that was released in January 1996. Before then TRAC-P was known as TRAC-PF1/MOD2 (MOD2). It is the latest in a series of TRAC codes including TRAC-PD2/ MOD1, TRAC-PF1, TRAC-PD2, TRAC-P1A, and TRAC-P1 (the earliest publicly released version).

Code development must be guided by a vision. For TRAC this vision is built on the foundation of specific code design objectives and targeted applications. The TRAC *design objectives* are as follows: TRAC should (1) accurately model important light water reactor (LWR) accident phenomena in current-generation and advanced-passive reactors, (2) deliver best-estimate predictions of accident progression, (3) have a practical running time, (4) be portable, maintainable, and extensible, and (5) be adaptable to other reactor types.

The *targeted applications* for TRAC are: (1) reactor safety analyses for both operating and planned reactors, (2) audits of licensee's calculations, (3) analyses of operating reactor events, (4) analyses of accident management strategies, (5) support for test planning and interpretation, (6) support for Probabilistic Risk Assessments (PRAs), (7) design analyses, and (8) nuclear plant training and instrument and control simulators.

Ultimately, the measure of TRAC or any computational tool is whether the tool fulfills its design objectives and can be used with confidence for its targeted applications. The determination of code adequacy is, of necessity, an ongoing process. However, it is important that there be, at appropriate intervals, a more searching consideration of code adequacy. The OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements* and associated activities is one such review.

In the remainder of this paper we will present TRAC-related information within the overall context of code adequacy. A code adequacy assessment is divided into two parts (Fig. 1). First, the adequacy of each closure model in the field equations is examined by considering its pedigree, applicability, and fidelity to appropriate fundamental or separate

* Held November 5-8, 1996, in Annapolis, Maryland, United States of America.

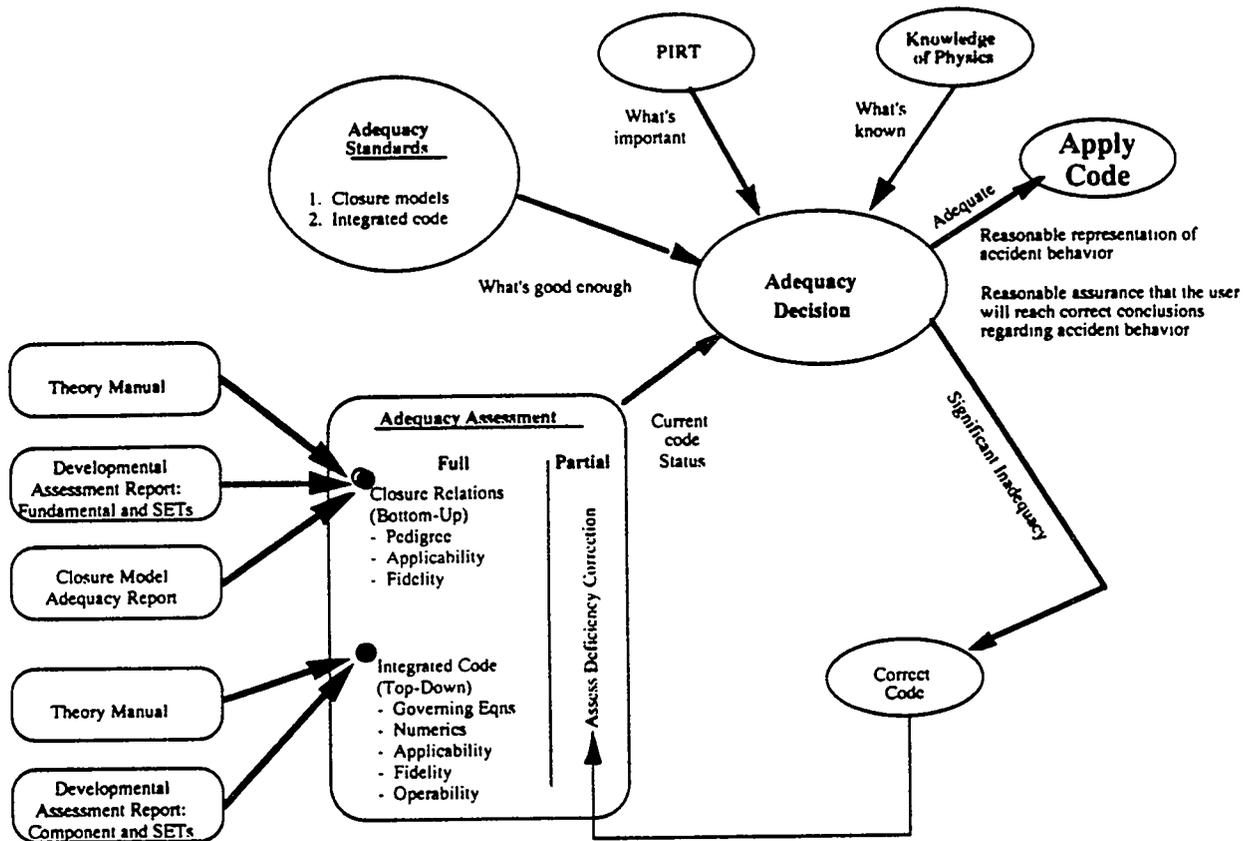


Fig. 1. Adequacy assessment overview.

effect test (SET) data. This part of the assessment effort is called the "bottom-up" review because it focuses on the fundamental building blocks of the code (e.g., closure relationships for interfacial heat and mass transfer). Adjunct features of the pedigree element of the adequacy standard are related to the physical basis of the closure model, assumptions and limitations attributed to the model, and details of the adequacy characterization at the time the model was developed. Adjunct features of the application element are related to whether the model, as implemented in the code, is consistent with the pedigree, or whether use over a broader range of conditions has been demonstrated. Adjunct features of the fidelity element are related to the existence and completeness of validation efforts (comparison to data), benchmarking efforts (comparison to other standards, e.g., a closed-form solution or results of another code), or some combination of the two.

Second, the adequacy of the integrated code is evaluated by examining the field equations, numerics, applicability, fidelity to the component or integral-effect test (IET)

data, and operability. This part of the assessment effort is called the "top-down" review because it focuses on the integrated code. An adjunct feature of the field equation element of the adequacy standard is that the equations are accepted by the scientific community. Adjunct features of the numeric solution element include convergence, stability, and property conservation. Adjunct features of the application element are related to whether the integrated code is capable of modeling the key plant systems and components. Model nodding issues also are addressed as an element of applicability. Adjunct features of the fidelity element are related to the existence and completeness of validation efforts using applicable IET data. Adjunct features of the operability element are related to code robustness and run time (e.g., does the code run successfully to completion for the required scenarios in an acceptable time interval?).

Several key perspectives must be considered during a code adequacy assessment effort. These perspectives provide insights regarding the relationship of the elements of code adequacy assessment to each other and to the whole of the assessment. These perspectives support the process of adequacy assessment of thermal-hydraulic (T/H) analysis codes by addressing the question "How good is good enough"? Three key perspectives relate to (1) knowledge of physical processes, (2) the relative importance of physical processes, and (3) adequacy standards. These concepts can only be covered briefly here, but they are discussed in more detail elsewhere.⁵

The current level of scientific knowledge regarding T/H processes that occur in nuclear power plants during accident sequences varies. The physics of some physical processes are well understood, whereas the physics of other physical processes are partially or poorly understood. The associated perspective is that a computer code cannot be expected to model precisely phenomena that are not yet fully understood by the scientific community.

Some processes and phenomena are more important than others and have a dominant influence on the course of an accident; therefore, it is important that the relative importance of systems, components, processes, and phenomena be assessed. Code models that are necessary to simulate highly ranked phenomena accurately must satisfy the appropriate adequacy standards fully; code models having less impact on the predicted course of the transient are held to a lesser standard. There are several recent examples of phenomena identification and ranking (PIRT) efforts.^{6,7}

Finally, standards for assessing adequacy must be identified. The standard for technical adequacy of the individual closure models is that (1) the model pedigree is known, documented, and acceptable; (2) the model is used appropriately (the application of the model is acceptable); and (3) the prediction of the phenomena being modeled is acceptable because the model predicts the appropriate data with acceptable fidelity or accuracy. The standard for technical adequacy of the total code is that (1) the field equations represent the key processes and phenomena, (2) the numeric solution approximates the equation set (field and closure) with acceptable accuracy, (3) the code is used appropriately (the application of the integrated code is acceptable), (4) the prediction of the performance of key systems, components, processes, and phenomena is acceptable because the model predicts the appropriate IET data with acceptable fidelity, and (5) the operability of the code is acceptable. The fidelity of code-calculated results to data is the best measure of "how good is good enough"? Judgments are based on the application of a standardized and consistent set of criteria that has been applied previously in the assessment of NRC-sponsored codes using data from fundamental tests, SETs, component tests, or IETs.⁸

METHODOLOGY

TRAC will calculate one-dimensional (1D) and three-dimensional (3D) (rectilinear and cylindrical coordinates) fluid flow involving gas, liquid, and mixture states. Two fluids are modeled with six equations to capture nonhomogeneous, nonequilibrium behavior. The field equations solved by TRAC are the combined-gas mass, liquid motion, combined-gas motion, total energy, combined-gas energy, noncondensable-gas mass, and liquid solute concentration equations.¹ The associated dependent variables are the liquid and gas velocities, liquid and gas temperatures, void fraction, pressure, noncondensable partial pressure, and solute concentration.

TRAC has a flow-regime-dependent constitutive equation package. Closure relationships are required for the interfacial area, interfacial mass transfer rate, interfacial drag coefficient, liquid wall-drag coefficient, combined-gas wall-drag coefficient, liquid interfacial heat-transfer coefficient, combined-gas interfacial heat-transfer coefficient, liquid-to-gas sensible heat-transfer coefficient, wall-to-liquid heat transfer, and wall-to-combined gas heat-transfer coefficient. A separate mass equation is added for a

noncondensable gas, and a separate equation is added for tracking solutes in the liquid phase.

A key modeling challenge of general purpose T/H systems analysis codes such as TRAC is illustrated in Fig. 2 for the liquid-mass and combined-gas-mass equations. Individual constitutive models must be provided at the two-fluid interface for closure of the two-fluid model for these equations. The interface-to-liquid heat-transfer coefficient for each flow regime that might be encountered (e.g., bubbly-slug, churn, annular-mist, stratified, plug, and reflood) must be provided. In a similar manner, constitutive models must be provided for the interface-to-gas heat-transfer coefficient and the interfacial area for the same flow regimes. Closure relationships must also be provided at the wall, as shown in Fig. 2.

The code sorts the problem of single-phase vs two-phase fluid at a very high level in determining the equation set to be solved. If the fluid is single-phase liquid or vapor, all of the interfacial processes are eliminated and the code considers only the interactions with the walls and the transport of a single-phase fluid. For the case of single-phase liquid, the code sets the vapor velocity to that of a bubble; for the case of single-phase vapor, the code sets the liquid velocity to that of a droplet. The code used this prescription to prevent accelerating the appearing (nascent) phase from zero velocity when the fluid first becomes two-phase.

TRAC is completely modular by physical component, such as the reactor core. The components in a calculation are specified through input data; available components allow the user to model virtually any PWR design or experimental configuration. Thus, TRAC has great versatility in its range of applications. This feature also allows component modules to be improved, modified, or added without disturbing the remainder of the code. TRAC component modules currently include Breaks and Fills, generalized Heat Structures, Pipes, Pressurizers, Pumps, Tees, Turbines, Valves, and Vessels with associated internals (downcomer, lower plenum, core, upper plenum, etc.). Accumulators and steam generators are constructed from more basic TRAC components such as Pipes and Tees.

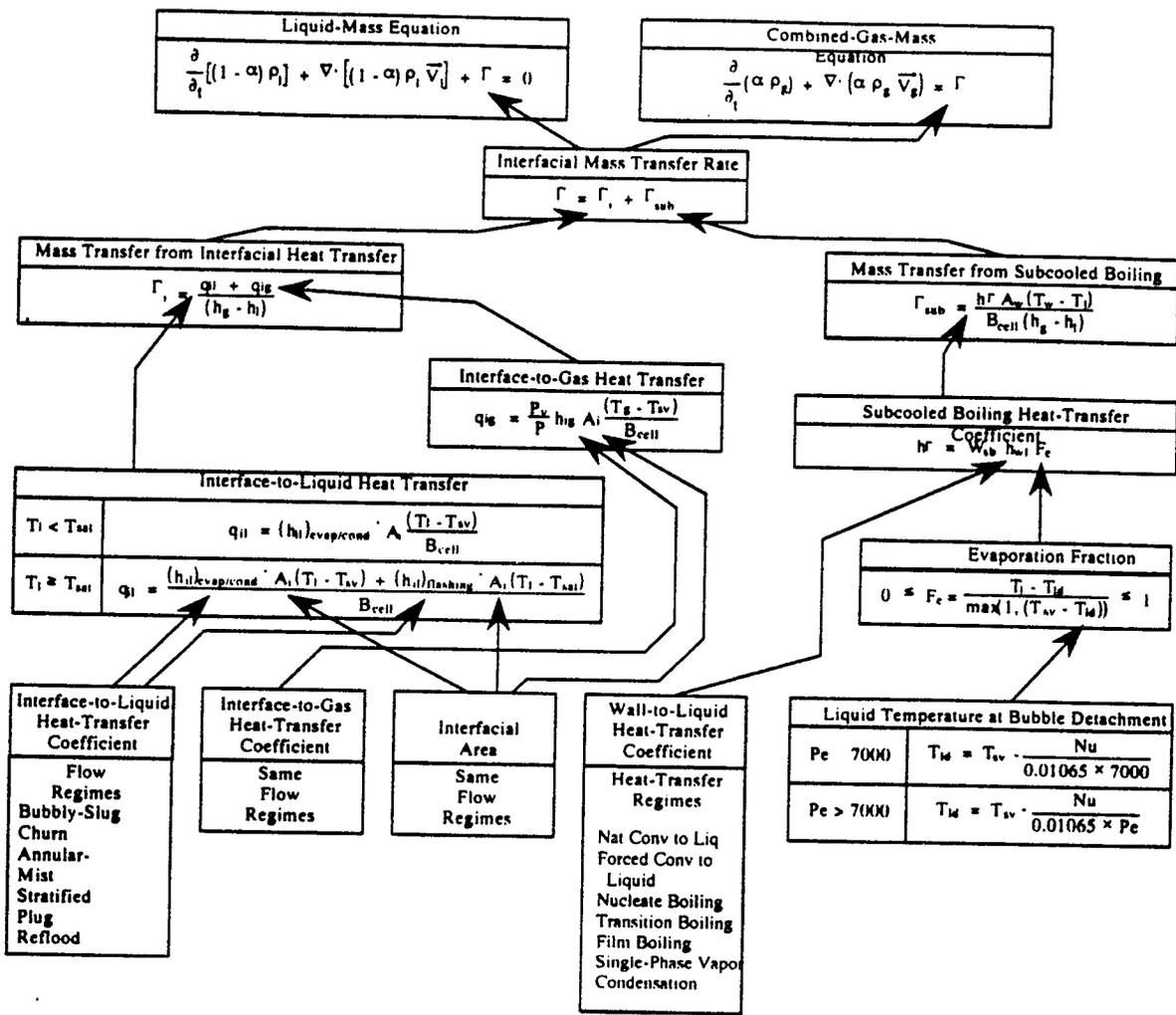


Fig. 2. Example relating flow-regime-dependent constitutive relations to field equations.

TRAC has additional models for nuclear reactor and other energy systems, including point-reactor or multidimensional kinetics with generalized reactivity feedback; general trip, control-system, and component-action models; and a comprehensive heat-transfer capability with 2-dimensional (2D) heat conduction and radiation. Each of these models adds to both the generality and the complexity of the overall code. For example, Los Alamos National Laboratory (LANL) has coupled the NESTLE and TRAC codes to produce a version of the code that can be applied to integrated multidimensional thermal-hydraulics and reactor kinetics problems. NESTLE, a code developed at North Carolina State University, solves the nonlinear form of the neutron diffusion equations. NESTLE has not been implemented in an NRC-sanctioned version of TRAC-P.

TRAC also is modular by function; that is, the major aspects of the calculations are performed in separate modules. For example, the basic 1D hydrodynamics solution algorithm, the wall temperature field solution algorithm, heat-transfer coefficient selection, and other functions are performed in separate sets of routines that are accessed by all component modules. This modularity allows the code to be upgraded readily as improved correlations and test information become available.

Various semi-implicit finite difference schemes have been used for solving problems in fluid flow. In many problems of interest, however, the stability limit on time-step size (less than the mesh size divided by the material velocity) associated with this class of method is far smaller than is necessary for reasonable accuracy. In such cases the standard approach for cutting computational costs is to eliminate this material Courant limit with a fully implicit difference method, or in multidimensional problems, employ an alternating direction implicit scheme. The SETs method^{1,9} was designed to propagate information needed for stability with minimal implicit coupling between spatial nodes. This method has been implemented in TRAC for both 1D and 3D calculations. Information about pressure wave propagation is provided with a basic step, which is simply a semi-implicit equation set. A stabilizing step is then added to provide the necessary flow of information about the density, energy, and momentum being transported across cell boundaries. The SETs method is especially valuable when applied to the full two-fluid model for two-phase flow. For this model, the stabilizer equations add less than 20% to the computational cost per cell per step of the basic equation set. A fully implicit method multiplies this cost by a factor of six. Adaptations of this method are now used in several other T/H codes.

Finally, a high-order method for solute tracking in two-phase thermal hydraulics was developed and tested.¹⁰ This algorithm uses a second-order, accurate, high-order Godunov method. Although the algorithm is available, it has not been implemented in an NRC-sanctioned code version.

MODELING CAPABILITIES

Most physical phenomena that are important in large-break (LB) and small-break (SB) loss-of-coolant accidents (LOCAs) and non-LOCA analyses can be treated by TRAC. The phenomena include the following: emergency core coolant (ECC) downcomer penetration and bypass, including the effects of countercurrent flow hot walls; lower-

plenum refill with entrainment and phase separation effects; bottom reflood and falling film quench fronts; multidimensional flow patterns in the core, downcomer, and plenum regions; pool formation and countercurrent flow at the upper-core support plate region; pool formation in the upper plenum; steam binding; average and hot rod cladding temperature histories; alternate ECC injection systems, including hot-leg and upper-head injection; and direct injection of subcooled ECC water, without the requirement for artificial mixing zones.

Models are provided for critical flow (choking) using an improved critical flow model; metal/water reaction; wall friction losses; natural circulation flows; horizontally stratified flows, including horizontal countercurrent flow driven by void fraction gradients down the pipe; vertical stratification modeling in the vessel component and in the interphase mass transfer (condensation) to better calculate pressurizer refill and the general refilling of any vertically oriented component; increased range in the water properties to permit the code to calculate fluid conditions beyond the critical point (pressures in excess of 22.12 MPa) and closer to the freezing point; noncondensable gas tracking, including the injection of the noncondensable gas from the accumulators and the effects of the noncondensable gas on the interfacial condensation; liquid solute (boron) tracking, which can be coupled to the reactivity feedback calculation; point reactor kinetics with a generalized representation of the reactivity feedback associated with the core average fuel temperature, the core average coolant temperature, the core average void fraction, and the core average boron concentration.

TRAC also has a balance of plant modeling capability; a Plenum component consisting of a single hydraulic cell with an essentially unlimited number of connections to simplify 1D connections; mixed 1D and 3D calculations or fully 1D calculations; fast computational speed for 1D and 3D problems when the transient is reasonably slow, as SBLOCA and some non-LOCA transients; very general trip, control system, and component action (such as feedwater pump flow characteristics) modeling capability; the ability to use trips and controls in the steady-state calculation; user convenience features, including free format input with capability to use comment cards or fields; forward and reverse additive friction factors for the hydraulics, the capability to choose to input Darcy K factors for the additive friction, the capability to choose to input cell centered elevations instead of the old gravity parameters at cell interfaces, and sophisticated input checking; consistent generation of steady-state conditions for initializing transients so that the same T/H models and numerics are used in both the steady state and the transient;

general orientation and magnitude of the VESSEL component for gravitational acceleration vector; and a generalized heat-structure component to allow the user to connect two hydro cells, resulting in increased accuracy for the modeling of steam generators, internal vessel structures, etc.

STATUS

TRAC will run on a Cray supercomputer or on Unix workstations (currently Sun SPARCstation, HP 9000, and IBM RISC 6000). TRAC requires a minimum of 32 MB RAM and 100 MB disk storage for practical applications on a workstation. A source code is provided, and Fortran 77 and ANSI standard C compilers are required for installation.

TRAC is configured with a main driver routine and 575 subroutines. The size of the source code is approximately 104,500 lines of which 70,000 are Fortran statements, 30,000 are comment lines, and 4,500 are precompile directives such as "include" statements and coding for platform dependencies.

At present, TRAC's grind effort is 10,000–20,000 floating point operations per fluid cell per cycle. This number includes the conduction solution for the heat structures. The range in the grind effort is associated with several factors, including the complexity of the closure models being exercised in a given calculation, the number of 3D nodes in the particular model, etc.

A graphical user interface (GUI) for TRAC has been developed at Knolls Atomic Power Laboratory (KAPL).¹¹ This X Window base GUI, named TOOKUIL, supports the design and analysis process, acting as a preprocessor, runtime editor, help system, and postprocessor to TRAC. The preprocessor is an icon-based interface that allows the user to create a TRAC model. When the model is complete, the run-time editor provides the capability to execute and monitor TRAC runs on the workstation or supercomputer. After runs are made, the output processor allows the user to extract and format data from the TRAC graphics file. Users may become functional in creating, running, and interpreting results from TRAC without having to know Unix commands and the detailed format of any of the data files. This reduces model development, debug time, and increases quality control.

At stages in its development, the various TRAC releases have been assessed against a broad spectrum of fundamental, separate-effect-test, integral-effect-test, and plant data. It is not possible to provide a complete list of the assessments in this paper; however, a sampling of the facilities for which TRAC assessments have been performed is provided without citation in Table I. These assessments are not repeated for each code version. In fact, we have conducted relatively few assessment efforts with recent code versions. Therefore, we offer the cautionary note that the previous assessment history will not fully apply to the present code versions. We do acknowledge that too few fundamental assessments have been performed throughout the TRAC development effort. Early in TRAC's development history, this was due primarily to the lack of the needed fundamental data. In later years (1989–1995), the code was placed in a maintenance mode and little fundamental closure model development or assessment was pursued. Even today, however, we are concerned that there are serious deficiencies in the fundamental data base, especially data related modeling processes at the liquid-vapor interface in our two-fluid models. We note that a significant development and assessment effort for the TRAC constitutive package as it applies to the AP600 LBLOCA is currently underway. This development and assessment effort is discussed in a subsequent section of this paper.

TRAC has been used to develop insights regarding nuclear power plant performance for a number of scenarios, including operational events or accidents initiated by reactor trips, loss-of-offsite power, LBLOCAs, SBLOCA, and steam-generator tube ruptures. It has been used in studies of unresolved safety issues including pressurized thermal shock and decay heat removal options. TRAC's adaptability for nonstandard reactor applications was recently demonstrated when it was used to support the preapplication review of the PIUS reactor.¹² Using a fully 1D model, a spectrum of initiating events was evaluated for both design basis accidents and severe off-normal conditions having a very low probability of occurrence. TRAC is currently being used for AP600 safety analyses. The primary focus is LBLOCA analysis, but it is also being used for SBLOCA analyses.

LIMITATIONS

Although TRAC has these many capabilities and features, it also has limitations. In fact, it is the very limitations in TRAC and other T/H codes of its generation that are the focus of present OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Code

TABLE I
LIST OF FACILITIES/PLANTS/DATA THAT HAVE BEEN USED FOR TRAC
ASSESSMENT

Fundamental	Separate Effect	Integral
Analytical Solution for Steady-State Conduction	19-Tube Once-Through Steam Generator Test	Davis-Besse Loss-of-Feedwater Event
Analytical Solution for U-Tube	ATLE tests	Ginna Steam Generator Tube Rupture event
Analytical Solutions for Stratified Flow	Babcock & Willcox (B&W) Annular Flow Distribution (AFD) Experiments	Jose Cabrera Plant Inadvertant Pressurizer Spray Event
Bennett Tube Experiments	B&W Mark 22 Assembly Facility	Loop Blowdown Investigation Test Facility (LOBI)
Berkeley Reflood Test	CISE Pressurizer Flooding Facility	Loss-of-Fluid Test Facility (LOFT)
Condensation Test Facility	Cylindrical Core Test Facility (CTCF)	Multi-Loop Integral System Test (MIST)
CREARE Countercurrent Flow Experiments	Edwards Blowdown Experiment	Primarkreislaufe facility (PKL)
Dartmouth College Air-Water Countercurrent Flow Tests	FLECHT Forced-Flooding Experiments	Rig of Safety Assessment (ROSA)
Direct Contact Condensation Experiments	Marviken Tests	Ringhals 2 Inadvertant Steam Line Isolation Valve Closure Event
Northwestern University Perforated Countercurrent Flow Limitation Tests	NEPTUNUS Pressurizer Test Facility	Ringhals 4 Loss of Grid Event
Safety Valve ATWS Separate-Effect Experiment	Savannah River Laboratory A-Tank Single-Assembly Flow Tests	Savannah River Plant 1985 L-Area Process Flow Test Series
Whatley Bladder Valve Experiments	Savannah River SPRITE and FA Rig Experiments	Savannah River Plant L-Area DC Tests
	Slab Core Test Facility (SCTF)	Semiscale Facility
	Upper Plenum Test Facility (UPTF)	Vandellos II Plant Load Rejection Transient

Requirements. As described in the background and purpose statement of the workshop notice: "The T/H codes that are currently being used were developed to study LOCAs in the 1970's. Over time, improvements have been made to the codes in a somewhat ad hoc

basis to include new capabilities and to analyze technical issues that some of these codes were not specifically designed to handle. Although these codes are being used to assess reactor safety issues and we are confident of the results obtained using them, these codes no longer provide the best estimate to T/H phenomena." The background and purpose statement continues: "In addition, the computer technology is changing at an ever accelerating rate and it is necessary to almost continually modify the codes in order to keep up with the advances. Past efforts to convert the existing codes to new computer environments did not make the codes more robust or reliable because of outdated coding and numerical methods inherent in the fundamental structure of some codes. Also, PRA requirements and the need to analyze beyond design basis accident (DBA) events impose new requirements on the codes compared with those that were used previously for DBA and would require code validation in new regimes and much faster codes."

We acknowledge that each of these statements applies, in some measure, to the present TRAC code. Development of the TRAC code series began in the 1970s. The architecture of the code was designed to efficiently utilize the best computational platforms of the time, but that same architecture is the root cause of some of the present deficiencies of the code. Among the most important is the use of a container array and "pointers." The container array was important in the original construct of the code because it facilitated the general modeling capability of the code, e.g., a small experimental facility for one application and a current-generation nuclear power plant for the next application. This innovative structure, so important for the early computational platforms with small-capacity, high-speed central processing units, now acts as a barrier to efficient computation on current computational platforms.

TRAC executes at approximately 6 million floating point operations per second (MFLOPs) on a Cray Y-MP. Typical rates are 70 MFLOPS for other complex scientific application codes. We have found that the container array approach obstructs compiler optimization and is one factor in the code running slower than needed for some applications, e.g., PRA analyses and simulators. Maintainability is also affected as the container array and pointers make the code difficult to learn and understand. Plans for addressing the container array deficiency are well advanced, as discussed in the next section.

Other important limitations are associated with the evolution of programming languages, the long-term development of the code, and the involvement of ~20 developers over the

years. The present code utilizes Fortran 77, which has led to overly complex protocols because of Fortran 77 limitations. Some of the coding is old and illogical, and there are multiple maintenance points. Extensive effort is required to implement changes. Plans for addressing issues related to the programming language, old and illogical coding, and multiple maintenance points are well advanced, as discussed in the next section.

As shown in Fig. 1, a full adequacy assessment consists of conducting reviews of both the code closure relations (bottom-up review) and the integrated code (top-down review). The code limitations previously discussed in this section, namely issues related to the container array, pointers, programming language, and old code, are not explicitly shown in Fig. 1. However, the code architecture and programming language form the fundamental code structure in which the T/H models are implemented. To the extent that these issues relate to the adequacy assessment envisioned in Fig. 1, they do so in the area of operability. We mentioned previously the impact of the container array on run time. Similarly, the use of nonstandard programming practices to compensate for the limitations of Fortran 77 also results in computational overhead that increases run time.

There are other limitations that directly affect code adequacy, as shown in Fig. 1. TRAC is currently being used to support the NRC's LBLOCA certification review for the AP600 reactor. Although the initial peak cladding temperature responses predicted by WCOBRA/TRAC and TRAC were similar, submittals by the vendor based upon more recent WCOBRA/TRAC calculations are markedly different.⁵ This has called the adequacy of the TRAC blowdown rewet and reflood models into question. As discussed in the next section, a development activity is now under way to address this issue.

With the rapid advancement of computer platforms, the analyst-machine interface is rapidly becoming an important limiting factor. The TOOKUIL GUI⁹ previously discussed is one element of the TRAC-related effort to address this limitation in the important areas of model creation, run-time management, and output extraction and formatting. However, we are still limited in our ability to process the voluminous data generated by TRAC. As discussed in the next section, a development activity is presently under way to address this issue.

DEVELOPMENT ACTIVITIES AND PLANS

The limitations discussed in the previous section have resulted in the NRC sponsoring several development activities. In addition, plans are well advanced for a significant TRAC modernization effort jointly sponsored by the NRC and the U. S. Department of Energy (DOE). Finally, at the request of the NRC, plans have been developed for consolidation of TRAC-P, TRAC-B, and the multidimensional kinetics modeling capabilities of the RAMONA code. Initiation of the consolidation effort is currently delayed, but it will be reported for completeness.

We first report on a recently completed activity, a developmental assessment plan for TRAC focused on the AP600 LBLOCA application.¹³ This effort has defined a developmental assessment plan for TRAC to support its application to the AP600 LBLOCA transient. As a part of this effort, we reviewed (1) the AP600 and its safety systems, (2) testing done in support of the design certification, and (3) a calculation of an AP600 LBLOCA transient. We used the AP600 LBLOCA PIRT,⁷ which rates the importance of processes and phenomena to the LBLOCA transient. We identified the code models corresponding to the processes and phenomena in the PIRT, and we combined the PIRT priorities with the adequacy of the code models to generate the developmental assessment priorities. Based on these assessment priorities and on the fluid conditions existing during the various phases of the transient, we identified separate-effects tests that can be used for developmental assessment. The nature of the PIRT leads to a concentration on separate-effects tests, and these tests seldom lead to comprehensive testing of the overall code performance. Therefore, we also identified integral tests for inclusion in the developmental assessment plan to check the overall quality of the code and to support enhancements to the robust nature of the code (the ability of the code to perform calculations without code failures). The resultant developmental assessment matrix is summarized in Table II.

We next report on three development activities currently in progress. The first is an adequacy assessment of TRAC closure and special models.⁵ In effect, we are nearing completion of the bottom-up review described in Fig. 1. As previously described, the pedigree (physical basis, assumptions and limitations, and original adequacy characterization), applicability (consistency with pedigree or other demonstrations of applicability), and fidelity (validation or comparison to data) and benchmarking (comparisons to other correlations) are evaluated. An example of the detailed

TABLE II
TRAC DEVELOPMENTAL ASSESSMENT MATRIX FOR THE AP600 LBLOCA

LBLOCA Phase	Separate-Effects Tests	Integral Tests
Blowdown	General Electric (GE) Level Swell 1004-3 5801-15 Idago National Engineering Laboratory (INEL) post-critical heat flux (CHF) data T-Junction Test Facility THETIS Boildown test T2L095 Winfrith steady-state post-CHF data	LOFT LP-02-6 LOFT L2-3 Semiscale S-06-3
Refill	GE Level Swell 1004-3 5801-15 INEL post-CHF data THETIS Boildown test T2L095 UPTF 5B, 6, 21A, 21B, 25B, 21D, and 27A Winfrith steady-state post-CHF data	LOFT LP-02-6 LOFT L2-3 Semiscale S-06-3
Reflow	CCTF Runs 14, 54, ... FLECHT-SEASET 31504 31701 33436 INEL post-CHF data Lehigh SCTF (total of 8 tests between CCTF and SCTF) Winfrith steady-state post-CHF data	LOFT LP-02-6 LOFT L2-3 Semiscale S-06-3

information tabulated for each closure model is provided in Fig. 3 for the bubbly flow interfacial area model in TRAC. Summary findings are tabulated for each closure model, e.g., interfacial area. Information from the adequacy assessment effort, when coupled with the conclusions of the AP600 LBLOCA PIRT,⁷ laid the foundation for decisions regarding the needed model development and developmental assessment.

ADEQUACY ASSESSMENT — BUBBLY SLUG FLOW INTERFACIAL AREA	
Pedigree	<p><u>Physical basis:</u> Ishii and Mishima (Ref. 5.88) assumed an idealized flow pattern in bubbly slug flow and developed an equation for the interfacial area concentration based on the geometrically idealized shapes. Over repeated lengths L, the following two distinct regions are assumed to exist within L.</p> <ol style="list-style-type: none"> 1) A region occupied by a liquid-bubble mixture. 2) A region occupied by a vapor slug and surrounding liquid. The slugs convert to cap bubbles if the channel diameter exceeds a critical diameter. From geometrical arguments, the area of cap bubbles is greater than slugs. <p><u>Assumptions and limitations:</u> Interfacial area models are mostly based on steady-state and fully developed flow data. In addition, almost all data are obtained from adiabatic air-water experiments, at or near atmospheric pressure.</p> <ol style="list-style-type: none"> 1) The bubble portion of bubbly slug flow can be represented as a population of spherical bubbles that are characterized by the Sauter mean diameter, D_b. D_b is evaluated using a simple expression by Ishii (Ref. 5.31). Bubble size and shape probability distributions are not considered. The upper and lower limits for bubble diameter are given by $0.1 \text{ mm} \leq D_b \leq 0.9D_H$. 2) Slugs or cap bubbles form depending on the diameter of the flow channel. Slugs form when the channel diameter is less than a critical diameter. Slugs form if $a > 0.3$ and the mass flux is $< 2700 \text{ kg/m}^2\text{-s}$ (see flow map review). Cap bubbles form if the $D > 50L_0$ where L_0 is the Laplace coefficient (MOD2/Eq. 4-13). The idealized cap bubble of Ishii and Mishima (Ref. 5.88) assumes a wake angle $\approx 55^\circ$. <p><u>Original adequacy characterization:</u></p> <ol style="list-style-type: none"> 1) Ishii's expression for the Sauter mean diameter, D_b, was stated to be an approximate arithmetic average of minimum and maximum bubble diameters observed experimentally. 2) Kataoka and Ishii (Ref. 5.12) state that slug bubbles cannot be sustained for channels with a diameter much larger than $40L_0$. The TRAC specification that cap bubbles form for $D > 50L_0$ is similar. Ishii and Mishima (Ref. 5.88) state that the observed wake angles range from 46 to 55°. Specification for slug to cap bubble transition is consistent with the data of Grace et al. (Ref. 5.13).
Applicability	<p><u>Consistent with pedigree:</u> Yes, except when quasi-steady and local equilibrium assumptions are violated.</p> <p><u>Otherwise demonstrated:</u> A mathematical treatment of the interfacial area for bubbly flow (spherical bubbles, no vapor slugs) is shown to be equivalent to the code's model for like conditions.</p>
Fidelity	<p><u>Validation:</u></p> <ol style="list-style-type: none"> 1) Model assessment studies were conducted using the data of Shilimkan and Stepanek (Ref. 5.14), Kasturi and Stepanek (Ref. 5.15), and DeJesus and Kawaji (Ref. 5.16). Each experiment was for upflow in a long vertical tube. Tube internal diameters varied from 0.6 to 2.54-cm i.d. With respect to the data of DeJesus and Kawaji, TRAC-PF1/MOD2 overpredicts the interfacial area concentration in the bubbly slug regime (MOD2/Sec. 4.1.11, Fig. 4-30). After back-calculating the Sauter mean diameter from the data, it was concluded that the available interfacial area data are not directly applicable for reactor safety analysis because the experimental setup does not allow a breakup mechanism into dispersed bubbles at the measured flow rates. The comparison with the data of Kasturi and Stepanek and Shilimkan and Stepanek is reported to have exhibited similar patterns during assessment. 2) None explicitly cited in MOD2 Theory Manual. <p><u>Benchmarking:</u> None explicitly cited in MOD2 Theory Manual.</p>

Fig. 3. Example of TRAC closure model adequacy assessment detailed information.

The adequacy standards for pedigree are that the model pedigree is known, documented, and acceptable. The adequacy standard for applicability is that the model application is acceptable. The adequacy standard for fidelity is that the model predicts the appropriate data with acceptable accuracy. The term "acceptable" is invoked repeatedly, and this implies judgment based upon documented information. The most concrete measure is fidelity. For fidelity assessments we use standardized fidelity criteria that characterize the agreement as excellent, reasonable, minimal, or insufficient. Reasonable agreement is the minimum standard for adequacy.

The second activity is the integrated TRAC development of LBLOCA closure packages for AP600 applications. Some background is provided for this effort. In the late 1980s, the NRC undertook to have its contractors improve the documented basis for the T/H systems analysis codes. The TRAC-PF1/MOD1 (MOD1) Correlations and Models Document¹⁴ was prepared to provide detailed descriptions of the various constitutive models used for closure of the field equations. This documentation was reviewed by several groups, specifically the Advisory Committee on Reactor Safeguards (ACRS) and the Technical Program Group (TPG) engaged in developing the Code Scaling, Applicability, and Uncertainty¹⁵ evaluation methodology. The following summarizes the key issues at that time.

The major criticism of TRAC based on [ACRS] review of the Q/A [TRAC-PF1/MOD1 Correlations and Models Document] document, was that many of its basic physical models were not based on a sufficient set of basic data. Since TRAC appears to achieve a reasonable representation of experimental data, LANL must have accomplished this by 'tuning' these basic models to integral system test data, rather than using basic data to obtain the necessary two-fluid constitutive relations. Therefore, use of the code beyond its integral system data base could lead to large uncertainties in the results.¹⁶

Although not stated in the above,¹⁶ a related concern of the reviewers was that a significant number of the closure relationships in MOD1 were of an *ad hoc* nature. These concerns were verified by LANL which, for example, reported " . . . the vertical flow map was basically invented to fulfill a need, no original reference exists for this map. . . This map was originally based on physical intuition . . ." ¹⁴

ACRS, TPG, and NRC criticisms played a significant role in the development of the next major code version, MOD2. The TRAC code-development team adopted an approach that will henceforth be identified as the "absolute" pedigree approach; this approach required that only closure models with an acceptable pedigree could be entered into the code. Further, these models could only be incorporated in their pedigreed or unmodified form.* Where it was deemed necessary, models affecting the blowdown and refill phases of a LBLOCA transient were implemented in MOD2, which satisfied this constraint.

MOD2 also included a new reflood model that used a modification of the "absolute" pedigree approach.¹⁷⁻¹⁹ The logic behind the generation of this modified approach is summarized as follows:

Whenever possible, correlations known to apply to a given regime for a particular closure quantity were used. Frequently, however, the original correlation could not be applied directly but had to be modified. For those cases, we tried to use the 'kernel' or 'functional' dependence of the original correlation and modify only its magnitude by use of a multiplier. When no correlations were available for given regimes, we tried to define known bounding regimes and use a weighting function between the known regimes to represent the unknown quantities.¹⁷

This approach will henceforth be identified as the "conditional" pedigree approach. The approach was built primarily upon the use of **basic** data from simple tube experiments. We know that limits exist on the current MOD2 reflood model, i.e., the coefficients were modified based primarily on only single-tube data. Extension of the work to fuel rod bundles was terminated when MOD2 was placed into a maintenance mode.

The NRC is currently sponsoring work at LANL to provide a code of demonstrated adequacy for AP600 LBLOCA confirmatory analyses. Of the various approaches possible for closure package development, we wish to discuss only the two approaches previously identified: the absolute pedigree and conditional pedigree approaches. Selection of these two approaches for further examination arises from a consideration of the interconnected inputs related to modeling concepts, constitutive equations sets, and data sets (Fig. 4).

* Even the "absolute pedigree" approach must be adapted somewhat because of discontinuities that will sometimes exist from correlation to correlation. The technique more frequently used in this case is interpolation from one correlation to the other over some region.

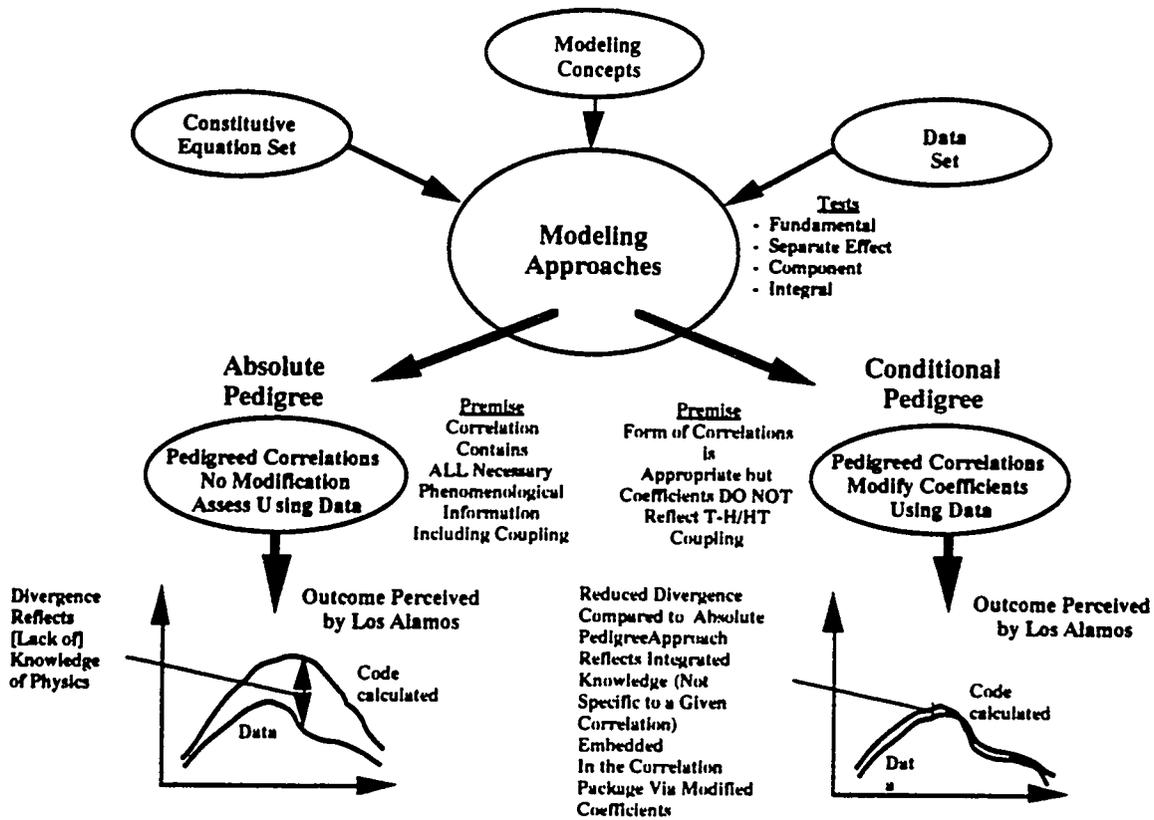


Fig. 4. Approaches to integrated closure package and accident phase modeling.

For the absolute pedigree approach, constitutive equations are selected on the basis of pedigree, applicability, and fidelity to basic data. The pedigreed constitutive equations are introduced into the code in their absolute (pure) form; no modifications are permitted. A basic premise underlies the absolute pedigree approach, namely, that the selected constitutive equations contain all the necessary phenomenological information for the modeled phenomena. This includes the various phenomenological couplings that may not have been measured in the experiments that produced the data sets used for creating the constitutive equation. For example, it is assumed that within the absolute pedigree that the wall and interfacial heat transfer and wall and interfacial drag have been properly coupled in the development of the constitutive equation. When this assumption is valid, and given correct implementation of each constitutive equation in the code, a positive outcome of this approach is that divergence between the code-calculated results and data provides a direct indication of the degree to which the physics are understood and captured in the constitutive relationships.

LANL has concluded that the absolute pedigree approach (Fig. 4) will have an undesirable outcome, namely that the difference between the code-calculated results and data for key parameters will be unacceptably large. As TRAC-PF1/MOD2 evolved from TRAC-PF1/MOD1, the absolute pedigree approach was followed. In the process, extensive information embedded in TRAC-PF1/MOD1 constitutive packages was lost as the code was broadly assessed against multiple integral test programs over many years.

The results obtained during a LANL-conducted investigation of various state-of-the-art models lead us to the conclusion that the conditional pedigree approach is the correct approach. For the conditional pedigree approach, constitutive equations are selected in the same manner as for the absolute pedigree approach. It is likely, in fact, that the same constitutive relationships would be used for either approach. The pedigreed constitutive equations are introduced into the code, but with a single, important difference. Modifications are permitted to a single part of the constitutive relationships, namely the coefficients.* These are adjusted so that reasonable code-data comparisons are obtained for a selected set of basic data and data from scaled integral experiments (Fig. 4). Thus, additional phenomenological information becomes embedded in the constitutive set as the relationship coefficients are adjusted to improve the code-data comparisons. A basic premise underlies the conditional pedigree approach, namely, that the form or kernel of the constitutive equation is appropriate, but that all necessary phenomenological couplings have not been included in the constitutive equations for the previously stated reasons. As additional fundamental data having ranges of applicability covering the spectrum of LWR operation become available, the conditional pedigree approach will merge with the absolute pedigree approach. This development activity, as presently planned, will provide results for both the absolute and conditional pedigree approaches.

The integrated development of closure packages will utilize nonlinear optimization techniques to "recorrelate" the model coefficients. Nonlinear optimization techniques are well established and have been used as part of complex system design for a number of years. The effort with integrated closure models will use the computer itself to accomplish the coupling and recorelation within the closure packages.

A visualization and plotting tool for TRAC, X-TRAC-View (XTV), uses the platform-independent X Windowing System to create its GUI. XTV was originally designed to aid

* This might be thought of as a recorelation of the model within the framework of the code.

in visualizing complex phenomena that result from LOCAs or other similar incidents, where line plots of critical variables do not easily indicate all of the interactions within a component and between components. XTV has been expanded to include line plot capabilities and is scheduled to eventually replace EXCON and TRAP, the current TRAC plotting features.

XTV allows the user to view up to 18 2D representations of components simultaneously. These visuals can be either static at a given time interval, or animated throughout time. Three dimensional components can be viewed in either Cartesian or cylindrical coordinates with any one of the three axes fixed at a particular value. For the multidimensional Vessel component, the additional capability exists to optionally plot either liquid or vapor flow vectors, as well as wall temperatures, in addition to any other scalar value at each cell. By placing adjoining components in neighboring viewpanes, one can visualize how the two components interact with respect to a certain variable; conversely, two different variables can be examined for the same component.

XTV is currently being expanded to improve its online plot capabilities as well as being able to perform calculations on any of the variable arrays. Additionally, capabilities to visualize any and all of the data generated in TRAC are being added. Its inherently modular data structure allows calculated values to be added as if they were produced in TRAC, which should also help XTV to function as an interactive controller for TRAC, allowing visualization as the results become available (a feature planned for implementation in late 1996).

We next report on the TRAC modernization effort. Both the NRC and DOE are sponsoring elements of this activity. Our overall objective is to provide a computationally efficient, portable, standard code in Fortran 90. We also seek significant improvements in extensibility by providing data structures required for new methods, models, and maintainability. The specific goals of the TRAC modernization effort are as follows:

- apply modern software engineering principles,
- achieve full portability to all single-processor Unix-based platforms,
- significantly improve the maintainability of the code,
- achieve a factor of 10 improvement in run time on current single-processor platforms,
- improve code operability and robustness

- position the code for parallelization,
- separate the input/output and computational engine, and
- provide full functionality at all times during the modernization effort.

The modernization plan consists of three stages. The first stage will reimplement the current data structures in Fortran 90 for portability without impacting the computational routines. We will also enhance information hiding between different data structures. We will take advantage of the current modular code design and object-oriented data structures and will transform the code rather than begin anew. Throughout the reimplementation effort, we will maintain an operational code relative to an appropriate test matrix. At the completion of the first modernization step, the following success metrics will apply. The run-time improvement will be quantified, special coding associated with multiple computational platforms will be eliminated with a concomitant improvement in portability, the container array will be eliminated, and the modularity of the code will be increased. A brief synopsis of each of the tasks within the first stage effort is provided in Table III. We anticipate initiation of this effort about September 1, 1996.

The second stage of the modernization plan is to develop new data structures to support improved computational efficiency, maintainability, and extensibility without impacting the computational routines. The third stage of the modernization plan reorganizes the computational flow and reimplements the computational routines to take advantage of the new data and new features of Fortran 90, such as array syntax. At the present time, there is no commitment from either the NRC or DOE to continue with the second and third stages of the modernization plan.

Finally, we report on the TRAC consolidation effort. As previously discussed, we are not presently pursuing this task at the direction of the NRC. However, we have been informed that the NRC may pursue this effort at a later time; therefore, a brief summary of the effort is provided here.

The NRC has developed several system transient codes, each for a slightly different mission. TRAC-P was developed at LANL to analyze LBLOCAs and system transients in PWRs. A version of this code was used to develop TRAC-B for analysis of

TABLE III

FIRST STEP TRAC MODERNIZATION ACTIVITIES

ID	Subtask Title and Task Description
20	<i>Dynamic system arrays:</i> Use Fortran 90 (F90) built-in dynamic memory management facility to dynamically allocate system-level arrays.
21	<i>Convert comdecks:</i> Convert existing common blocks, to F90 MODULES as appropriate to support dynamic memory allocation and ease code modification.
22	<i>Test object concepts:</i> Use the Heat Structure (HS) component to design the concept for implementing TRAC's component data structure in F90.
23	<i>Vessel data structure:</i> Modify the current inverted/equivalenced Vessel array data structure.
24	<i>Upgrade FIND:</i> Provide a universal, flexible, abstract, and efficient interface among TRAC's various data structures.
25	<i>Replace 1D hydro data base:</i> Replace 1D hydro component and boundary condition data bases and interfaces to driver routines.
26	<i>Replace plenum data base:</i> Replace the zero-dimension hydro Plenum component data base and interfaces in a manner that minimizes changes to lower-level core routines.
27	<i>Complete HS data structure:</i> Complete the modernization of the HS data structure and its interfaces with other modernized components to achieve full functionality.
28	<i>Control system/1D hydro communication:</i> Remove hard-wired knowledge of 1D component data structure from control system.
29	<i>Control system/HS communication:</i> Remove hard-wired knowledge of heat slab component data structure from control system.
30	<i>Object-oriented control system:</i> Replace current control system coding that is dispersed throughout all the various components with modular coding. Reimplement control-system data structure in a standard and portable fashion.
31	<i>PIPROD with FIND capability:</i> Replace current hard-wired communication between 1D hydro components and Heat Structures in PIPROD with use of FIND.
32	<i>Closure relations data structure:</i> Develop and implement any changes to closure relationships required to accommodate the new data structures.
33	<i>Neutronics and power:</i> Reimplement reactor power and neutronics capabilities with the new F90 data structures.
34	<i>Remaining non-standard/port constructs:</i> Automate the detection of any remaining nonstandard and/or nonportable constructs in TRAC.
35	<i>Steady-state initialization:</i> Implement the new hydraulic path steady-state initialization capabilities to be consistent with the new F90 data structures.
36	<i>Constrained steady state:</i> Implement constrained steady state capabilities to be consistent with the new F90 data structures.
38	<i>Radiation heat transfer:</i> Replace data base and interface (driver routines) associated with radiation heat transfer.
39	<i>Generalize output:</i> Provide generalized output interface using F90. Implement an array management methodology such that information that characterizes each array is embedded in the code using standard F 90 features.
40	<i>English units:</i> Standardize units processing within the code.
41	<i>Integrated testing 1D code</i>
43	<i>Special models :</i> Replace data base and interface (driver routines) associated with special models, e.g., TURB.
44	<i>Vessel full capabilities:</i> Complete modernization of Vessel coding.
46	<i>Integrated testing 3D code</i>

LOCAs and system transients in BWRs. The RAMONA code, with 3D neutronics capability for BWRs, was purchased by the NRC from Scandpower and modified by adding capabilities to perform calculations for BWR stability and anticipated transients without scram. TRAC-P is being maintained at LANL, TRAC-B at Pennsylvania State University, and RAMONA at Brookhaven National Laboratory. Maintenance of these three codes cost the NRC a considerable amount of funding each year. Consolidation of TRAC-P and TRAC-B, including the capabilities of RAMONA, will be cost beneficial.

We have proposed the following major tasks for combining the codes.

1. Modify software development procedures to meet the intent of American National Standards Institute, Inc., standards and NRC requirements using a cost-effective graded approach.
2. Write a Software Requirements Description (SRD) document that forms the overall basis for the consolidated code and associated GUIs.
3. Identify models that need improving, or identify where new models must be developed, considering various PIRTs for BWRs and PWRs and code adequacy requirements. Recommend a developmental assessment matrix based on the PIRTs and code adequacy requirements.
4. Examine current models and recommend those that should be included in the consolidated code. Select specific existing models from both TRAC-P and TRAC-B for the consolidated code. The intent of this phase of consolidation is to retain TRAC-P models that are judged adequate for both PWR and BWR applications and to add TRAC-B models as necessary for BWR applications. Modify the SRD to include discussions of specific models.
5. Modernize the software architecture of TRAC-P for improved portability, maintainability, and extensibility. Verify the modified architecture, including data structures and interfaces, with no changes in functional TRAC-P models. Note: this effort is precisely the stage 1 modernization effort previously discussed.
6. Modify the modernized TRAC-P to include selected existing BWR models, correlations, and functions from TRAC-B. This forms the consolidated code TRAC.

Verify the operation of the individual BWR models in TRAC. Some of this work can be done in parallel with modernization of TRAC-P, e.g., models not affecting data structures.

7. Examine the available 3D neutronics models suitable for TRAC, and select the best model and implementation details. Integrate these into TRAC, combining the best features from each. Modify the model to capture RAMONA features, and verify the results.
8. Extend GUIs—TOOKUIL from KAPL and XTV from LANL—for BWR models in TRAC. Integrate XTV with TOOKUIL. Add an input deck converter for TRAC-B to TOOKUIL.
9. Combine the standard verification and validation test matrices for both TRAC-B and TRAC-P into a single master test matrix for TRAC. Modify the matrix as necessary to meet testing requirements that are based on PIRT and code adequacy.
10. Verify TRAC, after full integration of all BWR models against the master test matrix, and resolve differences in test results between TRAC and either TRAC-B or TRAC-P.
11. Integrate the code documentation for TRAC-B and TRAC-P into a master set for TRAC, contemporaneously with programming, in electronic and paper editions.

CONCLUDING REMARKS

The TRAC code is presently applicable to many facilities and transients. Through its many versions, it has been broadly assessed against a broad set of separate-effect and integral-effect data. Its closure models have a documented pedigree; however, the applicability of numerous closure models is more limited. This is because the data from which the closure models were developed frequently cover only a fraction of the conditions encountered during calculated accident scenarios in nuclear power plants. Some of the strengths of TRAC are its generalized modeling capabilities, multi-dimensional Vessel component, point and multidimensional kinetics models, and the two-fluid model. TRAC approaches fulfillment of its design objectives in that it accurately models most important LWR accident phenomena in current-generation and advanced-

passive reactors, delivers best-estimate predictions of accident progression, and has proven adaptable to some other reactor types.

With the passage of time and the advancement in computational platforms and languages, the deficiencies in TRAC are becoming more serious. These limitations are most directly associated with the data structure and code architecture. The TRAC data structure and architecture date from the 1970s. Although they were advanced for their time, they now stand as liabilities when measured against current data structures and architectures. These limitations most adversely impact run time, portability, maintainability, and extensibility. Fortunately, the start of TRAC modernization efforts is imminent. We believe that these activities, when completed, will result in improved run time, portability, maintainability, and extensibility. TRAC will then have an improved capability for its targeted applications, namely, reactor safety analyses for both operating and planned reactors, audits of licensee's calculations, analyses of operating reactor events, analyses of accident management strategies, support for test planning and interpretation, support for PRAs, design analyses, and nuclear plant training simulators.

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REFERENCES

1. J. W. Spore, S. J. Jolly-Woodruff, T. K. Knight, J-C. Lin, R. A. Nelson, K. O. Pasamehmetoglu, R. G. Steinke, and C. Unal, *TRAC-PF1/MOD2 Code Manual, Volume 1, Theory Manual*, LA-12031-M (draft document), NUREG/CR-5673 (July 21, 1993).
2. N. M. Schnurr, R. G. Steinke, V. Martinez, and J. W. Spore, *TRAC-PF1/MOD2 Code Manual, Volume 2, User's Guide*, Los Alamos National Laboratory document LA-12031-M, NUREG/CR-5673 (July 1992).
3. L. A. Guffee, R. G. Steinke, and J. W. Spore, *TRAC-PF1/MOD2 Code Manual, Volume 3, Programmer's Guide*, LA-12031-M (draft document), NUREG/CR-5673 (November 1990).
4. J. C. Lin, V. Martinez, and J. W. Spore, *TRAC-PF1/MOD2 Code Manual, Volume 4 Developmental Assessment Manual*, LA-12031-M (draft document) NUREG/CR-5673 (August 1993).
5. B. E. Boyack, "TRAC-PF1/MOD2 Adequacy Assessment: Closure and Special Models," Los Alamos National Laboratory Draft document (December 5, 1995).
6. C. D. Fletcher, G. E. Wilson, C. B. Davis, and T. J. Boucher, "Interim Phenomena Identification and Ranking Tables for Westinghouse AP600 Small Break Loss-of-Coolant Accident, Main Steam Line Break, and Steam Generator Tube Rupture Scenarios," Idaho National Engineering Laboratory document INEL-94/0061, Rev. 1 (July 1995).
7. B. E. Boyack, "AP600 Large-Break Loss-of-Coolant Accident Phenomena Identification and Ranking Tabulation," Los Alamos National Laboratory document LA-UR-95-2718 (1995).
8. P. S. Damerell and J. W. Simons, Eds., "2D/3D Program Work Summary Report," prepared jointly by Japan Atomic Energy Research Institute, Gesellschaft fuer Reaktorsicherheit, Siemens AG, UB KWU, US Nuclear Commission, Los Alamos

National Laboratory, and MPR Associates, Inc., US Nuclear Regulatory Commission document NUREG/IA-0126, GRS document GRS-100, MPR Associates, Inc., document MPR-1345 (June 1993).

9. J. H. Mahaffy, "A Stability-Enhancing Two-Step Method for Fluid Flow Calculations," *Journal of Computational Physics* **46**, 329–341 (1982).
10. W. J. Rider and S. Jolly-Woodruff, "High-Order Solute Tracking in Two-Phase Thermal Hydraulics," Los Alamos National Laboratory document LA-UR-91-2263 (1991).
11. A. E. Kelly, C. K. Harkins, and R. J. Smith, "Development of a Graphical User Interface for the TRAC Plant/Safety Analysis Code," Proceedings of the 7th International Meeting on Nuclear Reactor Thermal-Hydraulics, NURETH-7, NUREG/CP-0142, Vol. 3 (1995) pp. 2003–2010.
12. B. E. Boyack, J. L. Steiner, S. C. Harmony, H. J. Stumpf, and J. F. Lime, "Transient Analysis of the PIUS Advanced Reactor Design with the TRAC-PF1/MOD2 Code," *Nuclear Safety*, Vol. 36, No. 2, (July–December 1995) p. 249–277.
13. T. D. Knight, "AP600 Large-Break Loss-of-Coolant Accident Developmental Assessment Plan for TRAC-PF1/MOD2," Los Alamos National Laboratory draft document (May 23, 1996).
14. D. R. Liles, et al., "TRAC-PF1/MOD2 Correlations and Models," Los Alamos National Laboratory report LA-11208-MS, NUREG/CR-5069 (December 1988).
15. Technical Program Group, "Quantifying Reactor Safety Margins: Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large-Break Loss-of-Coolant Accident," EG&G Idaho, Inc. report EGG-2552, NUREG/CR-5249 (October 1989).
16. L. M. Shotkin, "ACRS Meeting at LANL on TRAC-PWR," US NRC Reactor and Plant Systems Branch memorandum to B. W. Sheron, February 4, 1988.

17. R. Nelson and C. Unal, "A Phenomenological Model of the Thermal Hydraulics of Convective Boiling During the Quenching of Hot Rod Bundles, Part I: Thermal Hydraulic Model," *Nuclear Engineering and Design* 136, 277–298 (1992).
18. C. Unal and R. Nelson, "A Phenomenological Model of the Thermal Hydraulics of Convective Boiling During the Quenching of Hot Rod Bundles, Part II: Assessment of the Model with Steady-State and Transient Post-CHF Data," *Nuclear Engineering and Design* 136, 299–318 (1992).
19. C. Unal, E. Haytcher, and R. Nelson, "A Phenomenological Model of the Thermal Hydraulics of Convective Boiling During the Quenching of Hot Rod Bundles, Part III: Model Assessment Using Winfrith Steady-State, Post-CHF, Void-Fraction and Heat-Transfer Measurements and Berkeley Transient-Reflood Test Data," *Nuclear Engineering and Design* 140, 211–227 (1993).

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Methodology, status and plans for development and assessment of
CATHARE code

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ABSTRACT

This paper presents the methodology , status and plans for the development, assessment and uncertainty evaluation of the Cathare code. Cathare is a thermalhydraulic code developed by CEA (DRN), IPSN , EDF and FRAMATOME for PWR safety analysis. First, the status of the code development and assessment is presented. The general strategy used for the development and the assessment of the code is presented. Analytical experiments with separate effect tests, and component tests are used for the development and the validation of closure laws. Successive Revisions of constitutive laws are implemented in successive Versions of the code and assessed. System tests or integral tests are used to validate the general consistency of the Revision. Each delivery of a code Version + Revision is fully assessed and documented. A methodology is being developed to determine the uncertainty on all constitutive laws of the code

using calculations of many analytical tests and applying the Discrete Adjoint Sensitivity Method (DASM) At last, the plans for the future developments of the code are presented. They concern the optimization of the code performance through parallel computing - the code will be used for real time full scope plant simulators- the coupling with many other codes (neutronic codes, severe accident codes), the application of the code for containment thermalhydraulics. Also, physical improvements are required in the field of low pressure transients and in the modeling for the 3-D model.

1 INTRODUCTION

This paper presents the methodology , status and plans for the development, assessment and uncertainty evaluation of the Cathare code. Cathare is a thermalhydraulic code developed by CEA (DRN), IPSN, EDF and FRAMATOME for PWR safety analysis. First, the status of the code development and assessment is presented. The main characteristics of the code will be shortly described. A general strategy has been applied for the development and the assessment of the code. Analytical experiments with separate effect tests, and component tests are performed and analyzed. They are used for the development and the validation of the constitutive relationships. Calculation of many system tests or integral tests are used to validate the general consistency of the code models for each version. Conclusions are drawn from this extensive assessment work which is fully documented. Shortcomings are identified and listed in a synthetic document. User Guidelines are produced. The remaining problems are addressed by performing appropriate analytical tests. Further model improvements are then derived for future versions.

Investigations are in progress to apply the Discrete Adjoint Sensitivity Method (DASM) to determine the uncertainty on all constitutive laws of the code using the calculations of all analytical tests. This information may help the code developer to identify systematic biases and areas of higher uncertainty. It will also be used as part of a more general uncertainty evaluation method in view of determining the final uncertainty of the code response for a transient calculation.

At last, the plans for the future developments of the code are presented. They concern the optimization of the code performance through parallel computing - the code will be used for real time full scope plant simulators- the coupling with many other codes (neutronic codes, severe accident codes), the application of the code for containment thermalhydraulics. Also, physical improvements are required in the field of low pressure transients and in the modeling for the 3-D model.

2 THE CATHARE CODE STATUS

2.1 Main characteristics of the code

The code has a *modular structure*. Several modules can be assembled to represent the primary and secondary circuits of any PWR or of any analytical test or system test facility. There are 0-D, 1-D, 2-D, and 3-D modules available. All modules can be connected to walls, or heat exchangers with a 1-D conduction calculation. A 2-D conduction calculation is also available to calculate the quenching of a hot core during a reflooding process. Many submodules are available to calculate the neutronics, the fuel thermomechanics, pump characteristics, accumulators, sources, sinks...

All modules use the *2-Fluid model* to describe steam-water flows and four noncondensable gases may be transported. The thermal and mechanical nonequilibrium are described. All kinds of two-phase flow patterns - bubbly flow, slug flow, churn flow, annular flow, annular-mist flow, stratified flow - are modeled. Co-current and counter-current flow are modeled with prediction of the counter-current flow limitation (CCFL). Heat transfers with wall structures and with fuel rods are calculated taking into account all heat transfer processes, such as natural and forced convection with liquid, subcooled and saturated nucleate boiling, critical heat flux, film boiling, natural and forced convection with gas, film condensation,...The interfacial heat and mass transfers describe not only the vaporization due to superheated steam and the direct contact condensation due to subcooled liquid, but also the steam condensation or liquid flashing due to metastable subcooled steam or superheated liquid. The effects of noncondensable gases, such as nitrogen, air, hydrogen, are described.

The *range of parameters* is rather large: pressure from 0.1 to 16 MPa, liquid temperature from 20°C to 350°C, gas temperature from 20°C to 1800°C, fluid velocities up to supersonic conditions, duct hydraulic diameters from 0.01 to 0.75 meter.

Mass, momentum, and energy balance equations are written for each phase. Balance equations are also written for the radioactivity and for the mass of each noncondensable gas and of boron.

An important experimental program was carried out as a support for the development and validation of the code.

2.2 Status of the Cathare code

As will be explained later in section 3, the code development distinguishes code Versions and code Revisions. A code Version is a set of modules able to represent reactor components, with a numerical scheme and a solution procedure. A new Version may extend the code capabilities, may add new modules, may change the code architecture or optimize the solution procedure. A Revision is a package of physical closure relationships.

At present, the Version C2 V1.3U contains the revision 5 which is fully assessed. The Version C2 V1.3L contains the revision 5 with some improvements about the Reflood Modeling. The Version C2 V1.4 is delivered only to French users and contains the Revision 5. It has a completely new code architecture, a 3-D module which may be used for the pressure vessel or for the containment. It has also the Discrete Adjoint Sensitivity method, implemented for uncertainty evaluation. The Version V1.4E will be available to other users in autumn 96. The Revision 6 is now defined and will be implemented in the V1.5 Version.

3 METHODOLOGY OF DEVELOPMENT AND ASSESSMENT

3.1 General principles of the methodology

As a first step of the development, mass, momentum and energy equations are established for any module. They are derived from local instantaneous equations, using some simplifying assumptions and averaging procedures. Many closure relationships, or constitutive relationships, must be developed to express the mass, momentum and energy transfers between each phase and the walls, and at the interface.

The constitutive relationships are developed and assessed following a general methodology [1]:

Step A: Analytical experiments, including separate effect tests and component tests, are performed and analyzed. Separate effect tests investigate a physical process such as the interfacial friction, the wall heat transfer,...Component tests investigate physical processes which are specific to a reactor component, such as the phase separation in a Tee junction.

Step B: Development of a complete *Revision* of constitutive laws from a large analytical experimental data base. Successive Revisions are implemented in successive code Versions. A new Revision contains a new physical modeling whereas a new Version may contain new numerical methods, new modules, new submodules, or a new code architecture, preprocessing or post-processing.

Step C: *Qualification* calculations of the analytical tests in order to validate each closure relationship.

Step D: *Verification* calculations of system tests or integral tests in order to validate the general consistency of the Revision.

Step E: Delivery of the code Version + Revision fully assessed (qualified and verified) and documented (description documents and assessment reports).

When predictions are not correct or not accurate enough in the qualification (step C), it will be corrected in steps A and B of the future Revision.

When predictions are not correct or not accurate enough in the verification calculations (step D), no correction of a closure law will be applied without coming back to analytical tests (step A). New analytical tests may be defined if a physical process was not treated before.

A new Revision of constitutive laws is developed using some general principles:

- Data are first compared with existing models. If necessary, original models are developed. They can be either mechanistic (phenomenological) , semi-empirical, or fully empirical, depending on the understanding of the physical processes which are involved. Each closure law is unique. *No choice between several correlations is proposed to the user.*

- When and where data are missing, simple extrapolations of existing qualified models are used. No mechanistic model is developed without the experimental evidence of its relevance. Some iterations may be necessary when experiments are sensitive to several constitutive laws.

- In a pre-qualification phase, some tests of each experiment of the qualification matrix are calculated. Corrections are sometimes necessary before finalizing the set of constitutive laws.

- A systematic qualification of the frozen Revision is then performed. All tests of the qualification matrix are calculated and qualification reports are written.

3.2 Method for the code development

3.2.1 Derivation of the set of equations

Advanced thermalhydraulic codes use the two-fluid model where mass momentum and energy balance equations are written for each phase. These equations can be derived from exact local instantaneous equations . As described in [2], the process includes several steps: space and time averaging , simplifications through physical assumptions , derivation of closure relationships. Models are restricted to zero order closure so that no more partial differential equations are derived.

3.2.2 The averaging procedure

The averaging process which restricts predictions to large scale phenomena is necessary to allow reasonably coarse meshing and to make comparison with experiment easier. The time integration or averaging suppresses from calculated quantities fluctuations due to the turbulent nature of the flows. The space averaging is also very helpful in two phase flows as it allows to forget the complex structure of phase repartition and interface movements. The effects of small scale processes on macroscopic evolution can be taken into account by appropriate closure relationships.

3.2.3 Simplifying assumptions

Some simplifying assumptions are necessary for writing the final system of equations. They must be kept in mind when interpreting assessment calculations as they can be source of mispredictions.

The current simplifying assumptions are:

- In 1-D models, the axial diffusion of heat and momentum by molecular diffusivity or by turbulence is neglected. Moreover, all the correlation coefficients due to space averaging are taken equal to 1 by simple lack of knowledge. The loss of information associated with this simplification can be partly restored by an appropriate modeling of the transverse momentum and heat fluxes. This is possible when the transverse profiles follow a similar or affine solution. But in cases where the profiles are rapidly changing, the simplification cannot be justified. Then the best accuracy can be expected in the description of established flows in long pipes without singularities.

- In 2-D or 3-D models only diffusion towards walls or interfaces is correlated. The internal turbulent diffusion inside each phase is not modeled. A more complete diffusion modeling is possible with some limitations. The meshing must be fine and the numerical scheme must not be too diffusive. Moreover, considering the state of the art in turbulence modeling in two phase flows, the present knowledge is limited to dispersed flows. Thus a turbulence model (k.e) is available for the application of the 3-D module to containment thermalhydraulics and some research work is in progress to extend the modeling of turbulent diffusion to the full range of void fraction and to all flow patterns.

3.2.4 Closure relationships in a 1-D model

Closure relationships were extensively studied in the frame of the 1-D model [3]. Many separate effect experiments have been analyzed to determine constitutive relationships concerning mass momentum and energy transfers between phases or between fluid and walls. The difficulties come from the large variety of situations to deal with: variety of geometrical configurations, variety of flow patterns, variety of heat transfer modes, large range of thermalhydraulic parameters.

Constitutive relationships are essentially algebraic expressions of the principal variables. In the CATHARE 1-D model, only two differential terms are present in the interfacial momentum transfers : the added mass term associated with inertial effects has been derived for dispersed flows and another term proportional to the void fraction gradient plays an important role in stratified flows. Apart from these two terms, algebraic closure relationships are developed on the basis of steady and established flows (or quasi-steady and quasi-established flows). In unsteady or non established flows, it is implicitly assumed that this closure is still valid.

3.2.5 Flow pattern maps in Cathare code

Every flow regime has its internal structure and its transfer mechanisms. So it seems natural to use a flow pattern map in a code and to develop correlations for mass momentum and energy transfers which depend on the flow pattern. Unfortunately, at present, there is not a universal map valid in the whole domain of simulation . Experiments with steam water at high pressure and in large diameter pipes are very expensive and observations very difficult. So the available flow pattern maps are not validated in this domain. Moreover, it is not absolutely necessary to determine all the transitions and to use specific correlation for each flow regime. In the CATHARE code, only the onset of droplet entrainment and the stratification criterion are explicitly written. These two transitions are important because they limit a separated flow and a

more dispersed flow. Anyway, closure relationships can also be expressed directly as functions of the principal variables without reference to a particular flow pattern. So the absence of a unique and general flow pattern map in the codes is not a limitation by itself, but it reflects the limits of the physical knowledge in two phase flows.

3.2.6 Phenomenological and empirical correlations

A purely empirical correlation is a best fit of experimental data where the quantity to model is expressed as any function of the principal variables. It can be very accurate within the domain of experimental investigation but the extrapolation beyond it is very dangerous. On the other hand, this method does not take any benefit from the knowledge which may exist in certain subdomains where good correlations are available.

Dimensional analysis allows in principle to determine the dimensionless numbers to use in the expression of the quantity to correlate. But in 2-phase conditions, the number of independent parameters is very high so that simplifying assumptions are necessary. When the controlling physical processes are well identified, one can keep only the few dimensionless parameters which play a role. In this case, the extrapolation beyond the investigated domain is less hazardous. Nevertheless there is no guarantee since the controlling processes can be different in an other range of parameters. For example, slug flow does not exist any more in large diameter pipes.

The phenomenological or mechanistic approach consists in assuming a governing physical mechanism. The correlation is then derived theoretically without anything coming from experiments. An alternative is to keep some free parameters to adjust on experimental data. This semi-empirical approach was the most frequently used in the Cathare development. Even with this last precaution, the extrapolation beyond the qualified domain is not guaranteed. New effects, which are not present in the model, may become important in another range of parameters.

The experience shows that the 2-phase thermalhydraulics contains myriad of phenomena which make it difficult to generalize any theoretical breakthrough.

3.2.7 Closure relationships in 2-D or 3-D models

Closure relationships used in 3-D models are generally extrapolated from 1-D models [4,5]. This may lead to important shortcomings as quantities averaged over the cross section of a duct have not the same meaning as local values. For example, the void fraction is an important indication for the determination of the flow pattern in a 1-D model, whereas it is not so in a 3-D model.

The main problem is associated with the lack of turbulent diffusion modeling in present 2-D or 3-D models implemented in system codes. These models should be used only when the turbulent diffusion effects are dominated by other effects.

A first example is the core, a very porous medium where the diffusion towards rod walls or interfaces is much higher than the large scale turbulent diffusion. Moreover, in low velocity two phase conditions, gravity effects are likely to produce the most important large scale mixing effects. The lack of diffusion terms is not restrictive in this case.

The closure of multidimensional two phase flow models is still in its infancy. A tremendous lot of work is still required to reach the same quality as the 1-D models have, since there are much more physical processes to describe and more closure terms to correlate. So they must be used with caution only where and when 2-D or 3-D effects are important, and when the limitations of the multi-D model are not critical. As far as possible, the multi-D models must be validated with scale 1 data.

3.2.8 The problem of singularities

The presence of geometrical singularities in a circuit, such as bends, flow area contraction or enlargement, is a difficulty for the two-phase flow models. At these locations, the flow is perturbed and closure relationships obtained in quasi-established flows are not justified. As the flow structure is affected, perturbations may concern all the physical processes such as momentum exchanges, heat and mass transfers. The turbulence is generally increased, giving enhanced heat and mass transfers as well as irreversible pressure drops. Unfortunately, these local effects are dependent on many geometrical parameters and no general modeling can be proposed. Each case should be studied separately. For example, when the CCFL occurs in a geometrical singularity, specific local closure laws were found necessary in the same way as singular pressure losses are modeled. Also, the local effect of the ECCS water jet on condensation has been modeled to take into account the enhanced heat transfer due to increased turbulence.

3.2.9 Numerical modeling

The numerical method in the Cathare code uses a first order finite difference scheme with a staggered mesh and the donor cell principle. The time discretization varies from the fully implicit discretization used in the 0-D and 1-D modules to the nearly implicit multi-step scheme used in multi-D modules. These methods are known for their robustness and their stability but they are rather diffusive. The Cathare code takes care of the hyperbolicity of the system in order to warrant stability even for very small time steps and meshes. Theoretically, all calculations should be converged in space and time. In practice, convergence tests are easily performed for simple analytical tests, and some recommendations are deduced for system tests or reactor calculations.

The problem of convergence in meshing is somewhat different for multidimensional models. As long as there is no turbulent diffusion in these models, convergence tests cannot reach the exact solution. So closure laws must be validated for a given meshing (corresponding to a given numerical diffusion) and possibly with scale 1 experiments.

3.3 The qualification of constitutive laws

The qualification program aims at covering the whole range of flow patterns, physical processes and reactor components specific features. The tables 1 and 2 present the list of experiments used for the qualification of the Revision 5 of the constitutive laws. Each experiment is related to a principal phenomenon and some of them are also related to a reactor component. The constitutive laws which are validated by these experiments are classified into three groups:

- mechanical transfers
- interfacial heat and mass transfers
- wall heat transfers

Some experiments were devoted to the critical flows in nozzles of different sizes and shapes. They provided information on interfacial heat transfers in flashing flows, two phase wall friction, and interfacial friction in dispersed flows. All these processes control the break discharge flowrate.

Many experiments studied flow regimes and mechanical laws, particularly the interfacial friction. The duct geometries are:

- horizontal or vertical tubes ($0.01 < Dh < .135$)
- rod bundles (core geometry) or tube bundles (steam generators)
- annuli (downcomer geometry)
- geometry of the hot legs
- geometry of the U shaped intermediate leg

Five experiments have been necessary to cover the whole spectrum of phenomena occurring during the reflooding of a core. The reflooding consists in rewetting a high temperature dry core by Emergency Core Cooling System (ECCS) water :

- Wall heat fluxes were studied in tubes, rod bundle and tube bundle geometries.
- Direct contact condensation at ECCS injections were qualified with two test facilities at different scales.
- CCFL was studied for various geometries including scale 1 tests for the downcomer.

Experiments are also used to qualify:

- Phase separation phenomena at a T-junction
- Lower Plenum voiding
- Entrainment and deentrainment in an Upper Plenum
- Fuel behavior (clad ballooning, clad rupture, clad oxidation)
- Two-phase pump characteristics
- Multi-dimensional effects in a core and in a downcomer

Analytical tests were also performed in the BETHSY system loop. For such tests, additional measurements are generally required to better specify boundary conditions of the reactor component of interest. The BETHSY analytical tests investigated the pressurizer thermalhydraulic behavior, the core interfacial friction, and the two-phase pump characteristics.

At last, a few tests were specific to VVER type reactors.

All these separate effect tests are first used for the development or the improvement of the closure relationships. As the boundary conditions are well known this is the only way to determine the accuracy of each closure relationship. These qualification calculations are used also for:

- giving the range of validity of closure relationship
- estimating the uncertainty on each closure relationship
- defining the best schematization for each component in relation to the physical situation
- defining the node size and time step required for a converged calculation

3.4 The verification

The verification program aims at covering the whole range of accidental transients in pressurized water reactors. There are for example:

- Large Break Loss of coolant Accidents (LBLOCA)
 - Small Break Loss of coolant Accidents (SBLOCA)
 - Steam Generator Tube Ruptures (SGTR)
 - Loss of Feedwater (LOFW)
 - Steam Line Breaks
 - Loss of Residual Heat Removal (RHR) system
- The verification Program of Cathare V1.3 Revision 5 is presented. It can be divided into:

- System tests calculated by the Cathare team itself
- System tests calculated by the BETHSY analysis group

Some "independent assessment" calculations were also performed by:

- IPSN (French safety institute)
- Japan Atomic Energy Research Institute (JAERI)
- Pisa University (Italy)
- Joint Research Center ISPRA (EURATOM)
- Lappeenranta University (Finland)

All the existing system test facilities were used for the assessment of the successive Cathare versions and Revisions. These loops are presented in Table 3 with the main

characteristics about the scale ratios, maximum power, maximum pressure, number of primary loops and type of core. The system tests used for the verification of the Cathare Version V1.3 are presented in Tables 4 and 5.

3.5 The Cathare code documentation

The Cathare documentation comprises different types of documents:

- Code Use and Code Implementation
 - User's Manual
 - User Guidelines
 - Dictionary of operators and directives
 - Implementation manual
- Descriptive documents
 - Cathare general description
 - Description of each module & submodule
 - Description of constitutive laws
- Assessment reports
 - Qualification reports
 - Verification reports

All Cathare users participate to the Cathare Users Club (CUC) and report their work to CUC meetings. The minutes of these meetings are also parts of the Cathare documentation.

All the documents refer to a code Version and Revision. The User Guidelines contain many advises for writing an input deck and running calculations. It is the result of the experience of the code. These guidelines contain in particular :

- advises concerning the choice of Cathare modules for modeling reactor components
- advises concerning the choice of mesh size and maximum time step
- why, when and how to use the CCFL option model
- indication of physical processes which are not yet well modeled by any module
- warnings about most the frequent users errors.

3.6 The User's Effect

All system codes for nuclear thermalhydraulics are subject to the so called user's effect: different users may obtain different results for the same problem. This can be seen when the codes are used for blind "standard problems". The methodology to minimize this undesirable effect is:

- The code is fully portable on all machines, so that a unique code Version is released to all the users.
- No code options for physical models are proposed to the user. However, the CCFL in complex geometries requires the use of flooding correlations which are given by the user. Then, the User Guidelines should contain precise recommendation for using this option.

- Input decks should be qualified. It is recommended that an input deck should be checked by several users. For integral test facilities, preliminary calculations of characterizing tests - when they are available - are necessary to define pressure losses, heat losses, valve characteristics, pump characteristics....For reactor calculations, a few first transient calculations with a careful attention to bugs and inconsistent physical results are generally required.

- The Users Guidelines should be as precise as possible and take full benefit of the experience of the code.

- For each Version, successive sets of error corrections are released to the users. It is not recommended to calculate a sensitive transient with only a very new code version. The recently released Versions may contain more errors than the previous ones. A new version is first released to French users, who can test the new capabilities and participate to the debugging. After one year, the corrected version is considered as mature enough to be released to all users. A Cathare maintenance group is available for corrections and for preparing new releases.

4 PLANS FOR FUTURE DEVELOPMENTS

4.1 Qualification with evaluation of the closure law uncertainties

It is now clear that best-estimate codes such as Cathare have provided a pertinent insight into the complex thermohydraulic behavior of reactors during accidental transients and gave a more realistic view of flow phenomena than previous models based on a conservative approach. However, to be used in safety studies, the uncertainty of predictions should be estimated. As a first step, the Discrete Adjoint Sensitivity Method (DASM) is used for quantifying the uncertainty on each constitutive law of the Cathare code [6].

4.1.1 The future qualification program

The validation process, including both steps of qualification and verification, will be reconducted with the version V1.5 of the code which will include the Revision 6 of the closure relationships. In this program 1000 separate effect tests will be calculated for the qualification phase and 25 integral test will be used for the second phase. This represents an effort of work of 6 FTE during 5 years.

The objective of this validation process can be drawn as below:

-1- The qualification program of the version 1.3 will be reconducted in order to be sure that there is no-regression.

-2- Additional qualification will be performed to focus on the new aspects of the physical models. The main topics are:

* The reflooding because a large effort of development have been made in this field to prepare this new version

* The condensation problem because new correlation have been implements after fundamental studies performed by a PHD, especially in film condensation with non-condensable gases. In particular, the new French experiment CORTURNE will used.

* CCFL problem

* Three-dimensional problems, using devoted experiment as UPTF, PERICLES 2D, SEROPS, PIERO..

-3- The qualification includes a large effort for VVER reactors.

-4- One of the main objective of this qualification is to provide to the user the uncertainty on each closure relationships. The methodology is developed in a next section.

In addition to this validation program performed by the CATHARE developmental team, there is also:

* The qualification and verification performed by the French partners and by the international users.

* The qualification performed for the new possibility of CATHARE to describe containment thermalhydraulics with the Three-dimensional module: it includes film condensation along wall, turbulence models. Verification will also be made with large scale experiment as Battelle, HDR, Mistra, and Phebus FPT0.

4.1.2 The sensitivity analysis

The sensitivity analysis permits to answer to the following question: « how sensitive is the response of a code to any parameter? » The Discrete Adjoint Sensitivity Method (DASM) [6] has been developed in CATHARE to answer this question with a low CPU and manpower cost.

Let A^n be the algebraic discretized equations written at time n to calculate the vector X^n of principal variables.

$$A^n(X^n, X^{n-1}, \varepsilon) = 0$$

with: $\varepsilon = (\varepsilon_1, \varepsilon_2, \dots, \varepsilon_d)$

ε is a vector of parameters of the constitutive relationships. It contains many constants used in the relationships which were determined from experiments and which are known with some uncertainty.

The DASM gives the sensitivity of any code response R to some parameter ε_k :

$$\frac{dR}{d\varepsilon_k} = \frac{\partial R}{\partial \varepsilon_k} - \sum_{n=1}^N t(\phi^n) \frac{\partial A^n}{\partial \varepsilon_k}$$

N being the number of time steps

where ${}^t(\Phi^n)$ is the transposed adjoint vector at time n , which is solution of the following adjoint System of Equations (ASE) at time n :

$$\left[\frac{\partial A^n}{\partial X^n} \right] \Phi^n = - \left[\frac{\partial A^{n-1}}{\partial X^n} \right] \Phi^{n-1} + \left[\frac{\partial R^n}{\partial X^n} \right] \quad n = 1, N$$

This is a linear system which does not require a long CPU time to be solved. Two matrices are used at each time step, the direct jacobian matrix and the matrix of derivatives of equations A^{n+1} with respect to variables X^n at time n . The solution is independent on the parameter ϵ_k . Then, the calculation of all the sensitivities $dR/d\epsilon_k$ requires only one ASM solution.

The DASM has been developed in the code and is provided with the version. It runs as a post processing. It permits to systematically determine what are the most sensitive parameters in any calculations (separate effect tests, integral tests, reactor calculation) without performing a large number of calculation or without being based on expert judgment.

4.1.3 The uncertainties of the closure relationships: CIRCE

Circé is a tool which permits the calculation of the « basic » uncertainties of CATHARE 2, that is to say the uncertainties on the constitutive relationships [7]. It is based on the DASM method and takes into account the experimental uncertainties associated with the experiment used for the qualification. Its important feature is that it takes into account that several physical phenomena can take place in one experiment and also that one physical phenomenon can take place in several experiments. Thus it can provide a best estimate uncertainty .

This method will be systematically applied during the qualification process of the code. Several steps are planned in order to provide a first determination of the uncertainty at the end of year 1998 and to improve the determination of this uncertainties step by step in order to have the final one at the end of the qualification process.

4.2 Applications of Cathare to plant simulators

The use of Cathare based simulator software has been effective since the middle of the 80's. At this time a simplified version of Cathare, named Cathare-Simu, was developed and implemented as a kernel module of the SIPA simulator. This version was including :

- a 2-Fluid 6-equation model with some simplifications of the correlation set (qualified for SBLOCA or transients),
- the same numerical scheme with fully implicit time discretization,
- an improvement of the reliability by an enhancement of physical laws continuity,
- an improvement of the computation speed by an efficient coding on vector processors.

All these developments were verified against original Cathare calculations for all transients inside the simulation field.

A second stage of Cathare application to simulators is now under way ; it deals with the Simulator CATHARE Release (SCAR) project, whose purpose is to insert standard Cathare models inside engineering or training simulators without any simplification of the original model.

This project starts on the basis of the last version of Cathare (V1.4E) and is planned in three main directions:

- 1) implementation of standard Cathare models for several PWR inside SIPA simulator configurations and tests with simulator environment,
- 2) speed up of calculation process, using parallel processing, and improvement of reliability, in particular for low pressure transients,
- 3) development of some additional models needed to achieve an extensive description by Cathare of primary, secondary and auxiliary circuits.

All this work will be validated by a wide set (about 40) of actual NPP transient tests. will be made in close relationship with next CATHARE version (V1.5) development and will benefit consequently of the extensive validation program of CATHARE.

The final objective of the SCAR project is to allow an easy implementation of CATHARE models inside simulators and so, to ensure a maximum level of confidence and flexibility of the simulator software.

Therefore the convergence of safety codes used for safety analysis and for operator or safety staff training will be achieved. The result of the SCAR project will be a unique version of CATHARE inside and outside simulators.

4.3 Coupling of Cathare with other codes

The more recent Cathare Users Club meetings show clearly that the application field of Cathare has been considerably enlarged. For several applications, it is necessary to use the code not only in a standalone mode, but also in cooperation with other system codes (i.e. neutronic, fuel behavior, CSD, containment, ...).

This capability of coupling with other codes is particularly improved in the last version of Cathare (V1.4E) which allows an easy access to the main data structures. It has been demonstrated that a very small part of Cathare is modified to achieve the data exchanges with the others codes.

Most of the applications developed up to now use as coupling package the message passing library PVM. The major advantage of this tool is to be easily available on almost all workstations or multi-processor servers.

Coupling of CATHARE with the severe accident code TOLBIAC have been performed to calculate the external cooling of the pressure vessel when the corium is falling down to the lower plenum. Moreover, CATHARE is coupled to the ICARE2 code to analyze core degradation and fission product release.

Other coupling have been made with containment codes. Coupling of CATHARE with the three dimensional neutronics codes CRONOS and COCCINELLE are under development.

In the future it is planned to use some normalized and standard tools and methodology as CORBA for coupling purpose.

4.4 Future physical developments

Future physical developments are planned for the CATHARE code. The main topics are:

- * Low pressure physics
- * Three dimensional physics, in particular for the core reflooding and deentrainment in the upper plenum
- * Improvement of the physics for advanced reactors
- * Development of new physical models, such as the interfacial area transport
- * Improvements of the physics for the VVER and the RBMK reactors

Other subjects are under investigation such as implementing additional fields.

Long term developments deal with fine two phase turbulence modeling.

CONCLUSIONS

Best estimate thermal-hydraulic codes are irreplaceable tools for PWR safety analysis. They have already proven their capabilities to predict at least qualitatively and sometimes quantitatively many basic features of the accidental transients. But the knowledge of two-phase flow is still limited, and the balance equations written in numerical models suffer from a loss of information when applying the averaging procedure and when making simplifying assumptions. This loss of information can only be partly compensated by the development of models for the closure terms. In order to make the best use of such complex tools, a rigorous methodology must be followed for the code development and assessment in order to get a good knowledge of the code limitations.

The main aspects of the Cathare development and assessment methodology are the following:

- During the development, it is necessary to write a precise descriptive documentation with a list of all modeling assumptions. This will be useful during the assessment as mispredictions may be related to situations where some of the assumptions are not valid.

- Constitutive laws are validated using analytical tests with separate effect tests and component tests. The *qualification* calculation must precise also the range of validity of each model, the range of applicability of each module and the requirements for mesh size and time step. The uncertainty about each closure law must also be determined from these calculation.

- The second step of the assessment, called *verification*, validates the general consistency of the models. All mispredictions must be analyzed carefully. If they are attributed to models used out of the domain of qualification, or to physical processes which are not yet modeled, new analytical tests are necessary. Some users may be tempted to modify a constitutive law in order to improve a system test calculation. But, due to complex system effects and to a lower density of experimental information in such tests, one cannot justify a model change on system tests. A qualification of any model change on analytical tests is absolutely required.

- The code documentation must include precise *User Guidelines* in order to minimize the "user's effect".

References:

- [1] F. BARRE and M. BERNARD "The CATHARE code strategy and assessment" Nuclear Engineering and Design 124(1990) 257-284
- [2] J.M. DELHAYE , M. GIOT , M.L. RIETHMULLER "Thermohydraulics of two-phase Systems for Industrial design and Nuclear Engineering" ,McGraw-Hill Book Company, Hemisphere Publishing Corporation
- [3] D. BESTION " The physical closure laws in the CATHARE code " , Nuclear Engineering and Design 124(1990) 229-245
- [4] M.BERNARD, L.C.BERNARD, J.C.MICAELLI, P.VAN DEN HOVE, The new modules of Cathare and their specific assessment, NURETH 4, 1989, Karlsruhe, Germany, SETH/LEML-EM/89-164.
- [5] F. BARRE, I. DOR, C. SUN The multi-dimensional module of Cathare 2, 7th International Meeting On Nuclear Reactor Thermal-hydraulics, Saratoga Springs, NY USA - Sept 10-15, 1995
- [6] A. de CRECY, C. PERRET, F. BARRE, The sensitivity analysis by adjoint method for the uncertainty evaluation of the Cathare 2 code, 7th International Meeting On Nuclear Reactor Thermal-hydraulics, Saratoga Springs, NY USA - Sept 10-15, 1995
- [7] A. de CRECY, CIRCE: A tool for calculating the uncertainties of the constitutive relationships of CATHARE 2, to be published

Table 1: THE CATHARE QUALIFICATION MATRIX

Experiment	principal phenomenon	Mech. Transf.	Interf. Heat Flux	Wall Heat Flux	Component	
Moby Dick	Critical Flowrate	O	O		Break	
S M D TL		O	O		Break	
S M D TC		O	O		Break	
S M D TBet		O	O		Break	
Marviken		O	O		Break	
Rebeca		O	O		Break	
Dadine	Flow Regimes Interfacial Friction	O	O	O		
SMD Vert		O				
SMD Horiz		O				
CANON V Tube		O				
TAPIOCA		O				
CANON V rod		O			Core	
ECTHOR IL		O			Int. Leg	
ECTHOR HL		O			Hot leg	
G2		O		O	Core	
PERICLES Boil		O		O	Core	
PATRICIA SG1		O	O	O	SG Prim	
PATRICIA SG2		O		O	SG Sec	
ERSEC Tub		Reflooding	O	O	O	
ERSEC Rod			O	O	O	Core
ERSEC Osc	O		O	O	Core	
PERICLES Refl	O		O	O	Core	
ROSCO	O		O	O	Core	
OMEGA Tub	Wall Heat Flux	O	O	O		
OMEGA rod		O	O	O	Core	
TPTF		O	O	O	Core	
FLECHT SG		O	O	O	SG	

Table 2: THE CATHARE QUALIFICATION MATRIX (Cont'd)

Experiment	principal Phenomenon	Mech Transf	Interf. heat Flux	Wall Heat Flux	Component
EPIS	Condensation at ECCS		O		IS
COSI					IS & Accu
COSI Inc	Noncond. gas		O		IS
CREARE	CCFL	O	O		Downcomer
UPTF Do		O	O		Downcomer
MHYRESA		O			Hot Leg
SMD Tee	Phase	O			Break
INEL	Separation	O			Break
SEROPS	Déentr	O			Upper Plenum
PIERO	Voiding	O			Lower Plenum
EDGAR	Fuel			O	Fuel
REBEKA	Model			O	Fuel
EVA	Pump	O			Pump
PERICLES 2D	multi-D	O		O	Core
UPTF	Effets	O	O		Upper Plen.
<i>BETHSY ANALYTICAL TESTS</i>					
Pressu			O	O	Pressu
τ_i Core		O			Core
8.1a	Pump	O			Pump
<i>Experiments relative to VVER's</i>					
IVO Loop seal	Voiding	O			Int. Leg & Hot Leg
IVO CCFL	CCFL	O			Core
REWET II	Reflooding	O	O	O	Core
Guidropress	Horiz.SG	O		O	SG

Table 3: SYSTEM TEST FACILITIES USED FOR CATHARE VERIFICATION

LOOP	VERT. SCALE	VOLUME SCALE	POWER	PRESSURE	LOOP NB	CORE
LOFT	1/2	1/48	100%	16 MPa	2	Nucl
LSTF	1/1	1/48	14%	16 Mpa	2	Elect
BETHSY	1/1	1/100	10%	16 MPa	3	Elect
PKL	1/1	1/134	5%	4 MPa	3	Elect
LOBI	1/1	1/700	100%	16 Mpa	3	Elect
SPES	1/1	1/427	100%	16 MPa	3	Elect
PACTEL	1/1	1/305	?	8 Mpa	3	Elect
PMK	1/1	1/2070	100%	16 Mpa	1	Elect

Table 4: VERIFICATION MATRIX OF CATHARE 2 V1.3

LOOP & TEST	TEST TYPE
LOFT L2-5	LBLOCA
LOFT LP-LB 01	LBLOCA
BETHSY 6.7 a4	LBLOCA Reflooding
BETHSY 6.7 c	LBLOCA Reflooding
UPTF	LBLOCA Refill
BETHSY 6.2 TC	SBLOCA 6" CL break
BETHSY 4.1a TC	Natural Circulation
BETHSY 5.2 c	LOFW
BETHSY 4.3 b	SGTR 6 tubes
BETHSY 8.1a	2-phase Forced Circulation
LSTF SBCL 09	SBLOCA 10 % CL Break
LSTF SBCL 15	SBLOCA 0.5% CL break
BETHSY 9.1 b	SBLOCA 2" CL Break
BETHSY 6.1 a	SBLOCA 6" CL Brea
BETHSY 6.1 b	SBLOCA 3" CL Break
BETHSY 6.3	SBLOCA 10" CL Break
BETHSY 6.5	SBLOCA Break at Pressurizer
BETHSY 3.4b	SGTR 1 tube
BETHSY 4.1b	Natural Circulation

Table 5: VERIFICATION MATRIX OF CATHARE 2 V1.3
(independent assessment)

LOOP & TEST	TEST TYPE
LSTF SBCL 5	SBLOCA 5% CL Break
LSTF SBCL 21	SBLOCA 6" CL Break
LSTF TR-RH 02	Loss of RHR
LSTF TR-LF 03	Loss of electrical power
LOBI A2 81	SBLOCA 1% CL Break
LOBI BL 12	SBLOCA 1% CL Break
LOBI BL 34	SBLOCA 6% CL Break
LOBI BT 12	100% steam line break
LOBI BT 01	10% steam line break
SPES isp 22	LOFW
PMK spe 1	SBLOCA 7.4% break
PMK spe 2	SBLOCA 7.4% break
PACTEL	LOFW
PACTEL isp 33	Natural Circulation

METHODOLOGY, STATUS AND PLANS FOR DEVELOPMENT AND ASSESSMENT OF TUF AND CATHENA CODES

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ABSTRACT

An overview is presented of the Canadian two-fluid computer codes TUF and CATHENA with specific focus on the constraints imposed during development of these codes and the areas of application for which they are intended. Additionally a process for systematic assessment of these codes is described which is part of a broader, industry based initiative for validation of computer codes used in all major disciplines of safety analysis. This is intended to provide both the licensee and the regulator in Canada with an objective basis for assessing the adequacy of codes for use in specific applications. Although focused specifically on CANDU reactors, Canadian experience in developing advanced two-fluid codes to meet wide-ranging application needs while maintaining past investment in plant modelling provides a useful contribution to international efforts in this area.

1. INTRODUCTION

System thermal-hydraulics analysis codes are key computational tools in the nuclear industry and are usually designed for application in licensing safety analyses, in analysis to support process design of nuclear generating stations, and in reactor operational support. Each of these application areas impose specific requirements on the extent and detail of plant modelling and on functional capability in the code.

In the early years of safety analysis, conservative bounding analyses were used for plant licensing evaluations. With improved understanding of some of the underlying physics and thermal-hydraulic phenomena, and the desire to reflect this knowledge in advanced two-fluid thermal-hydraulics codes, has come a move toward best estimate safety analyses. This, in turn, has resulted in the need to more formally and rigorously validate these computer codes and assess the results obtained with formal uncertainty analyses. These are current topics of significant investigation in Canada, as well as internationally, as reflected in the work of the OECD/CSNI/NEA Principal Working Group 2.

In Canada two advanced two-fluid computer codes have been developed; the TUF code at Ontario Hydro (OHN) and the CATHENA code at Atomic Energy of Canada Limited (AECL). The objectives driving the development of these codes has differed, and to a large extent, have resulted in differing features and structure of these codes. This paper presents a brief overview of these codes, including the historical progression of thermal-hydraulic code development in Canada, together with discussion of areas of application, user needs and the methodology for assessing the adequacy of these codes for their intended applications.

2. OVERVIEW OF THE TUF AND CATHENA CODES

Several system thermalhydraulic codes have been developed in Canada, from the early 1970's to the present time, to provide analytical tools for the thermal-hydraulic analysis of CANDU reactors. AECL developed the FIREBIRD (Reference 1), RAMA (Reference 2) and CATHENA (Reference 3) codes for reactor safety analysis. In parallel, Ontario Hydro developed the SOPHT (Reference 4) and TUF (Reference 5) codes for both operational support and safety analyses of its 20 unit nuclear generation system. A one-fluid model was used in the FIREBIRD, RAMA and SOPHT codes, while a two-fluid model was implemented in the RAMA, CATHENA and TUF codes. The separated flow approach for two-fluid model was used in the RAMA and CATHENA codes, which is different from the mixture flow approach used in the TUF code. Currently, CATHENA and TUF are actively used in the safety analysis of CANDU reactors. Brief descriptions of the TUF and CATHENA codes are given below.

The TUF code, developed at Ontario Hydro, consists of two separate programs, one which provides a steady state solution and the other a transient solution that is initialized to the steady state solution. In the steady state program, the equations dealing with thermal-hydraulic variables, nodal heat flux, heat exchanger film resistance plant component state and control valve positions (or special link resistances) are solved. The set of simultaneous non-linear equations is solved by the Newton-Raphson iteration method. To match the steady state solutions with normal operating conditions, different control flags are used in the input data. These flags are used to define the degrees of freedom for the steady state simulation, particularly with respect to plant component and control systems states. TUF contains modules dealing with thermal-hydraulics (one-fluid, drift-flux and two-fluid), reactor physics (point kinetics or external coupling with other reactor physics codes), heat conduction (pipe wall, heat exchangers, pressure-calandria tubes and fuel pins), system components (pumps, valves, boilers, pressurizer, bleed condenser, turbine and accumulator), special models (discharge model, level swell, bundle movement, pressure tube strain model and metal-water reaction), and station controllers. A unique feature is the ability of the user to select one-fluid, drift-flux or two-fluid basic thermal-hydraulic models, thereby allowing the direct evaluation of the effect of the thermal-hydraulic modelling basis on transient behaviour. The control systems used in the code are station dependent and emulate plant control functions. The reactor controllers simulate the following control systems: overall unit control, reactor regulating system, steam generator pressure and level controls, heat transport (HT) system pressure and inventory controls, bleed condenser pressure and level controls and safety systems. An overview of the modules implemented in the TUF code and their role in the operational support and licensing safety analyses can be found in Reference 6.

The CATHENA code, developed at AECL Whiteshell Laboratories, is a transient two-fluid code designed primarily to analyze postulated loss of coolant accident scenarios for CANDU reactors and transients in small reactors and experimental facilities. CATHENA was developed from the RAMA two-fluid code with a different approach in the numerical scheme (a characteristic finite difference scheme with a non-staggered

grid is used in RAMA while CATHENA uses a non-conservative finite difference scheme with a staggered grid). CATHENA contains modules dealing with thermal-hydraulics (two-fluid model), reactor physics (point kinetics or external coupling with reactor physics codes), heat conduction model (a general package for piping wall, heat exchanger tubes, pressure-calandria tubes and fuel pins), system components (pump, valve, boiler and general tank model which is used in pressurizer, bleed condenser and accumulator), and special models (discharge model, pressure tube strain model, metal-water reaction and level swell). Conservation equations for mass, energy and momentum are solved for each phase (liquid, vapour and non-condensable gas). A detailed channel model which is similar to those used in other fuel channel codes has been implemented in the code. Radial and circumferential conduction are calculated for individual pins within a bundle. The effects of thermal radiation, pressure-tube deformation, zirconium and steam reaction, pressure and calandria tubes contact, and the presence of non-condensable gas can all be modelled. A simple controllers package has been set up for general applications, which requires user's interface to set up the specific station control logic. The reactivity changes due to mechanical control devices and shut-down systems are provided by the user's input data.

2.1 Numerical Techniques Used in TUF and CATHENA Codes

The thermal-hydraulics and heat transfer modules form the central core of systems analysis codes. Certain areas require special attention in these code modules: water packing and empty node treatment, symmetric behaviour of the solution, numerical instability, uncertainty in two-fluid parameters and wall heat transfer correlations. In this paper, only two particular areas are discussed: the symmetric behaviour of the solution and the numerical technique in thermal-hydraulics associated with pressure and density wave propagation.

Normally, the time-step size is controlled by the following modules: thermal-hydraulics, reactor physics, heat conduction and controllers. The code is usually designed so that the time-step size is controlled by the thermal-hydraulics module. In reactor physics, the stiff ratio of the differential equations is very large (many orders of magnitude) and the time-step size is much smaller than that for thermal-hydraulic equations. Therefore, the thermal-hydraulic time-step must be divided into smaller time steps for the point kinetics equations. The time-step size for heat conduction equations is normally larger than that for thermal-hydraulics if the number of finite elements in the fuel is not too large, as is the case in system codes. The sampling times used in the controllers are the final parameter in determining the overall time-step size.

Operational support analysis often requires that a code simulate certain types of pressure or density wave propagation problems. For example, there is a need in Ontario Hydro to use TUF for the simulation of condensation induced water hammer phenomena that can occur when cold water is injected into hot system piping which has led to the development of a unified version of the code that is capable of handling transients ranging in time scale from milliseconds (e.g. water hammer and fluid-structure interactions), though seconds and minutes (accident analysis), to hours (operational transients).

While the two-fluid model is generally considered to be a state-of-the-art method for modelling transient two-phase flows, it suffers from the fact that its time step size used is generally smaller than that used in the one-fluid model with the same numerical scheme. In applying the code to slow transients or cold water injection cases, the analyst may encounter an excessively long execution time due to stability limited time-step sizes in the finite difference equations. To reduce the computing cost, several stability enhancing methods, ranging from a simple two-step method to a fully implicit method, for two-fluid model have been

suggested in the literature (for example the two-step method implemented in the TRAC code, Reference 7) and are discussed later in this section.

TUF code: The two-fluid equations are reduced to a set of flow rate equations, which has a matrix size ($L \times L$) where L is the total number of links (excluding boundary links) and run-down pumps. In the steady state program, the thermal-hydraulic variables are pressure, specific enthalpies for mixture and vapour, quality, mixture flow rate and slip velocity. In the transient program, the variables are mixture mass, vapour mass, mixture internal energy, vapour internal energy, mixture flow rate and slip velocity. Currently, there are two numerical methods available in the code: the one-step semi-implicit method and the simple two-step implicit method. The simple two-step implicit method is a predictor-corrector type technique. In the first step, the mass and energy conservation equations are solved explicitly. These solutions are only used to update the link properties used in the transport terms, where the variables associated with pressure wave (pressure and mixture density) are not updated. In the second step, the implicit method is applied to obtain the final solutions. To verify the numerical method implemented in the code, the JUICE 1976 standard problems were simulated (Reference 8) and compared with the so-called exact numerical solutions obtained from the MECA code (Reference 9). Comparison of initial pressure oscillation in the problem of instantaneous heat addition (Standard Problem 1) of flowing sub-cooled water at high pressure in a vertical pipe indicates that the TUF solution displays a small amount of numerical damping in addition to the frictional damping associated with the problem. Nevertheless, numerical diffusion inherent in TUF is much less than in FIREBIRD, RAMA, and RELAP-UK codes as shown in Reference 10. Currently TUF has been used in operational support analysis (including safety system trip parameter assessment and water hammer simulation) and safety analysis at OHN. Abnormal plant operations have been simulated by TUF to provide estimates of system response for plant parameter not available in the plant data logs.

CATHENA code: The two-fluid equations are linearized and written in a set of matrix equations with a size $(4N+2L, 4N+2L)$, where N is the node size and L is the link size. The code uses a staggered-mesh, one-step semi-implicit, finite-difference scheme for the thermal-hydraulic equations. The one-step semi-implicit method is applied and the thermal-hydraulic variables used in the code are pressure, void fraction, phase specific enthalpies and phase velocities. These are arranged in the semi-implicit form and the resulting linear set is solved by a sparse matrix package. A stabilising corrector step based on mass conservation is applied. In the solution algorithm, the time step is not constrained by the material Courant limit (Reference 3). The introduction of the semi-implicit treatment of flux terms and the phase-to-interphase pressure difference does not allow the reduction of the equation set to a pressure field system of equations as done in RELAP5/MOD2. Comparisons between the solution speed of RELAP5 and CATHENA are given by Hanna et al. (Reference 11). The time-step control is based on conservation of the rate of change of variables. CATHENA has been used in safety analysis of MAPLE, CANDU-3 and CANDU-6 reactors and is being used in the preliminary safety analysis of the CANDU-9 reactor.

2.2 Numerical Techniques For Operational Analysis

Invariably most attention in two-fluid codes has been applied to modelling non-equilibrium effects that occur during accident transients. However, operational transients which can last over significant time periods require special consideration with regard to numerical techniques because of the sometimes conflicting demands of reasonable computing time, with a demand for longer time steps in the solution, and

the need to assure numerical stability and limit propagation of numerical errors. These considerations are discussed below.

Control of Round-off Error Propagation

In the development of reactor system analysis codes, there are three programming areas which require special attention: variations caused by the compiler, the accuracy of restart files and the round-off error inherent in the digital computers. Using the optimization option for the compiler, the results should be checked against those produced by other compiler options (for example the debug option). The round-off error has not received special attention in most system analysis codes. In reality, it may significantly affect the accuracy of transient solutions, depending on the order of matrix equations and the type of computing machine used. There are two particular concerns in the study of round-off error: accuracy of solutions and its propagation during the transient. The last concern has been resolved in TUF and CATHENA codes.

There are two fundamental sources of error in solving the initial value problem: truncation (or formula) error and round-off error. The round-off error depends on the type of computing machine used and the sequence in which the computations are carried out. Round-off errors stem from a finite number of digits in a computer word, while truncation errors are due mainly to finite approximations of limiting processes. When a decimal number which contains a fractional part is converted to its binary equivalent, a conversion error due to the finite word length of the computer may be introduced. Another source of round-off error may be introduced if the calculation requires more digits than available. The study of round-off errors and the control of their propagation is important in high-speed digital computations. In some cases, it may be needed to estimate the final round-off made in solving a given problem by a specific numerical method. The propagation of the round-off error may become a problem for a circuit with symmetric piping or branches since the error can be amplified as the transient progresses. The symmetric behaviour of the flow matrix equations will be destroyed. In the development version of TUF, two methods have been studied for the control of round-off error propagation: the iterative technique and the different precision levels approach.

Iterative Technique : In all thermal-hydraulic codes, the direct method for solving a system of linear equations has been employed. In this method, round-off errors at each time step of the calculations are usually carried to the next time step if they have not been controlled. If the equation number is quite large such as that for a reactor circuit simulated in safety analysis, these errors grow as the calculations progress, and considerable care must be exercised to prevent them from significantly influencing the transient solutions. In this case, the iterative techniques possess a certain advantage in that the round-off error of one iteration tends to be corrected in subsequent iteration. This technique with one iteration has been tested in the TUF and it has been concluded that the round-off error is generally less serious in the iterative technique than it is for direct methods. However, the computation time increased considerably (about 30%) and the propagation of the round-off error still exists as the transient progresses. As a result, the iterative technique for the matrix solver was abandoned for computational economics reasons.

Technique with Different Precision Levels : Rounding errors can often be eliminated by carrying one, two, or even more extra figures, known as guarding figures, in the intermediate steps of calculation. The causes for non-symmetric results in identical channels have been identified in the process of matrix inversion and solutions in steady state and transient programs. The number of extra figures theoretically needed, according to the analysis of von Neumann (Reference 12) gets to be almost prohibitive for the inversion of a matrix of the order of 100 or so. However, there is some indication that many of the matrices

encountered in practice are better behaved than those considered in the von Neumann analysis. A simple approach has been adopted in the TUF and CATHENA codes. A higher precision (for example, double precision) than that used for the rest (for example, single precision) of the calculations has been used in these two particular areas. Using this technique with different precision levels for the variables, the round-off error has been controlled. This error did not propagate to the subsequent time steps. Testing has confirmed that the technique implemented in these codes can indeed eliminate the propagation of round-off errors.

Further Enhancements for Long and Slow Transients

Currently, the numerical methods applied in the TUF and CATHENA codes do not satisfy the strong stability criterion. Further enhancements in numerical methods are desirable for long and slow plant transients. In thermal-hydraulic equations, the stiffness ratio of the largest to the smallest eigenvalue of the system is in the order of thousands. The region of stability for a method is defined as the domain on the time-eigenvalue complex plane. A method is called A-stable if the region of stability associated with that method contains the open left half-plane. In general, A-stable methods do not damp maximally as the product of time and eigenvalue approaches negative infinity. This undesirable asymptotic behaviour often results in oscillatory solutions for very stiff systems with a large time-step size. A method is called strong A-stable if it is A-stable and the absolute ratio of the results at preceding and current time steps approaches zero as the product of time step and eigenvalue approaches negative infinity. The fully implicit Rung-Kutta method is known to satisfy the condition of strong stability. However, this method requires solving a system of non-linear equations at each time step (i.e. requiring iteration in the matrix solver). For the strong A-stable technique, Rosenbrock (Reference 13) has developed a procedure requiring only the solution of a system of linear equations at each time step, a much simpler task compared to the fully implicit approach. In this procedure, the Jacobian matrix is directly inserted into the coefficients of the Rung-Kutta process, thereby yielding a strongly A-stable algorithm. This technique is under consideration as an enhanced solution method for TUF.

3. OVERVIEW OF CANDU CONTROL AND SAFETY SYSTEMS

The unique design features of the CANDU reactors and the intrinsic safety related features distinguish it from other types of reactors. A CANDU reactor is a pressure tube, heavy-water-moderated, high pressure heavy-water-cooled reactor consisting of two figure-of-eight loops. The fuel channels consist of two concentric tubes (pressure tube and calandria tube) with a space in between filled with an inert gas. The pressure tubes (390 in Pickering, 480 in Bruce and Darlington, 380 in CANDU-6 NGS) are horizontal and are connected to the end-fittings by rolled joints. The end-fittings are supported by the end shields. The calandria tubes, which are roll expanded at both ends into the calandria side tubesheets, separate the cold moderator in the calandria vessel from the hot pressure tubes.

The general features of CANDU plant controllers are briefly described to facilitate the discussion of code requirements for plant simulations. Although these are CANDU specific they serve to illustrate the need for adequate representation in thermal-hydraulic system codes of the many interfacing plant systems.

The following systems are to be included in a detailed plant representation of the CANDU reactor: primary heat transport system, secondary side steam supply and feedwater systems, feed and bleed system, D2O

purification system, emergency cooling injection (ECI) system, steam generator (or boiler) emergency cooling system and shut-down cooling system. Each nuclear power plant has unique control features. For example, the controllers for Pickering [540 MW(e)x8], Bruce [750 MW(e)x7], Darlington [850 MW(e)x4] and CANDU-6 [600 MW(e)], while possessing many similar general features, have differences in specific detail of the control algorithms. The CANDU control systems are designed to regulate the reactor power, the electrical power delivered by the generators and the conditions in process systems in an integrated and co-ordinated manner. All of the control systems, with the exception of HT pressure control which is an analog control function, are implemented in a system of two dedicated, redundant digital computers to perform the following major functions: reactor power control, plant load control, steam generator pressure control, steam generator level control, deaerator level control, moderator temperature control, control of miscellaneous systems, alarm annunciation and data logs. The three major areas which require constant monitoring and control under all operating conditions are: reactor, steam generator and turbine-generator. These areas are controlled in accordance with a pre-established overall plant control scheme.

Functions of CANDU Controllers

Automatic system control has been used in CANDU reactor design. The main functions of the control and safety system of a CANDU reactor are briefly described below. These controller functions have been implemented in TUF for all CANDU reactors at Ontario Hydro. The main purpose of this description is to point out the areas of interaction between the reactor controllers and the other modules in the code (thermal-hydraulics, reactor physics, heat conduction and system components).

Overall Unit Control: The function of this system is to match the reactor power and the turbine load while maintaining steam generator drum pressure at its setpoint value. It is executed by three control programs: the unit power regulator, the steam generator pressure control and the demand power routine of the reactor regulating system. There are two distinct modes of CANDU plant control: normal (auto, or reactor following turbine control) and alternate (manual, or turbine following reactor control) modes.

Reactor Regulating System: This system is an integrated system which directly controls the reactor power. It comprises the reactivity control mechanisms, the reactor power measurement (it is simulated by the point kinetics model in the codes), the demand power routine, and the reactor power stepback and setback programs. The stepback routine monitors the plant parameters and takes action to reduce the reactor power by dropping the mechanical control absorbers if any one of the parameters is met. The setback mode is automatically initiated when any of the setback parameters exceeds its setpoints.

In the power measurement, the point kinetics model with six-delayed neutron groups is normally used for neutronic power calculation in the system analysis codes. The reactivity changes in the point kinetics model consists of the following components: fuel temperature, coolant temperature and density, moderator temperature, refuel process, bundle movement, control mechanisms and shut-down systems. The reactivity changes due to control mechanisms include mechanical control absorber rods, liquid zone absorbers, adjuster or booster rods. The reactor power delivered by the fuel due to decaying fission products is modelled by three or more decay heating groups. The total power released in the fuel is the sum of the fission power and the power due to decaying fission products. Also the reactor power can be specified from the results simulated by reactor physics codes.

Since the point kinetics model does not yield the spatial distribution of the neutron flux, the normalized axial flux distribution is simulated either by the cosine curve or by the data obtained from a reactor physics code or plant design data. Axial and radial peaking factors, which describe the power density distribution in the core and also define the hot spots, are also input from the predictions of reactor physics codes. The following assumptions on the description of flux distribution are made by using the point kinetics model: (1) during an upset condition the power distribution is the same as that under normal steady state operating conditions, and (2) the effect on the power distribution of dropping control absorbers or shut-off rods can be expressed as a function of the reactor power.

Steam Generator Pressure Control System: This system manipulates either the reactor power setpoint (normal mode of operation) or the turbine-governor reference setpoint (alternate mode of operation) to maintain the steam generator pressure at its setpoint. It also controls the opening of the atmosphere steam discharge and condenser steam dump valves to trim the steam generator pressure. The calculation of steam generator pressure setpoint depends on the operating mode of steam generator pressure control: warm-up, cool-down, hold, pseudo poison prevent and poison prevent modes. When the unit control is in the normal mode, the steam generator pressure control program will calculate the required reactor power setpoint and send it to the demand power routine. When the unit control is in the alternate mode, the steam generator pressure control program will control the turbine load setpoint in response to the steam generator pressure error and the mismatch between the reactor power and turbine power. The turbine load setpoint demand rate is then processed to manipulate the turbine governor valves. The steam generator pressures are measured at each main steam line. The control program reads all steam generator pressures and checks the rationality and validity of the input before processing them to obtain the final measured steam generator pressure.

Steam Generator Level Control System: This system is designed to control the levels in all steam generators, by modulating the level control valves in the valve stations located in the feedwater lines. The control program runs in parallel in both digital control computers on a one second cycle time. The level in each steam generator is controlled individually using the same algorithm. The control algorithm consists of a single element, a three element and a default single element mode, depending on the valve lift required in the level control valves and the validation of the feedwater and steam flows. Whether the swelling level or collapse level should be used in the level control depends on the instrumentation location of the level measurement.

Heat Transport Pressure and Inventory Control System: This system comprises a pressurizer (Bruce, Darlington and CANDU-6 NGS), bleed condenser, bleed cooler, two feed pumps, pressurizer steam bleed valves, bleed condenser level control valves, reflux control valves, spray cooling valve, HT feed and bleed valves, D2O storage tank, HT liquid (or pressure) relief valves, isolation valves, bleed condenser over-pressure protection system and associated piping. The HT pressure controller maintains the reactor outlet header (ROH) pressure at its setpoint by modulating the pressurizer steam bleed valves and the pressurizer heaters. When the pressurizer is isolated from the HT circuit, the main circuit pressure is controlled by the wide range pressure controller via the feed and bleed valves. Under normal operating conditions, the HT inventory is controlled by the pressurizer level controller. When the pressurizer is isolated from the HT system under solid mode, the inventory control is done by the HT pressure controller. The bleed condenser pressure control is done by the operation of the reflux feed valve and spray valve controls. The liquid in the bleed condenser is controlled to a level below the reflux tubes, but above the outlet nozzle to maintain effective reflux cooling and to prevent steam escape to the bleed cooler. The bleed condenser level control

valves are controlled by the level controller and bleed cooler temperature controller. The HT liquid relief valves are used for heat transport system overpressure protection device to relief coolant to bleed condenser. Overpressure protection of the bleed condenser is provided by two spring loaded shell side relief valves.

CANDU Special Safety Systems

The special safety systems of CANDU reactors are totally independent of the control systems. They are automatically initiated when certain system parameters exceed pre-determined setpoint levels. The initiation of the safety systems are important for CANDU reactors: the shut-down systems (SDS1 and SDS2) ensure that fuel sheath and pressure tube integrity are maintained prior to the initiation of the emergency cooling injection (ECI) system; ECI system ensures that adequate cooling is maintained; steam generator controlled cool-down provides an additional heat sink for the secondary side system; and emergency cooling system for steam generators provides emergency cooling for the secondary side.

In an emergency situation, two fast-acting, independent shut-down systems are available to rapidly reduce reactor power to the shut-down level. These systems initiate a power reduction by dropping the shut-off rods into the core (SDS1), or by injecting a neutron absorbing solution (gadolinium) into the moderator (SDS2). The shut-down systems are automatically initiated when any of the parameters (for example ROH pressure, inlet feeder flow, neutron power and log rate, pressurizer level and boiler level) exceeds its pre-set setpoint values. In the primary side circuit the ECI system is initiated when process conditions in the heat transport system exceed setpoint values and specific conditioning parameters are registered. In the secondary side circuit, the injection valves for the steam generator emergency cooling system and the steam rejection (safety) valves of the steam generators are opened by separate initiation logic.

4. APPLICATION AREAS AND USER NEEDS

4.1 APPLICATION AREAS

The primary application of system thermalhydraulic codes are in a) safety analyses of accident and plant upset transients, b) operational support which includes simulating plant transients and assessing the behaviour of various systems, and c) design assist analysis for new designs and modifications to existing designs.

Safety Analysis

Safety analyses require a wide range of detailed phenomenological modelling and an ability to represent behaviour in events with widely varying time scales. For example, both short duration as well as long duration transient events associated with specific accident initiating failures have to be accommodated. In some accidents, such as large LOCA, many interacting phenomena occur, requiring interaction between all the major disciplines, including reactor physics, thermalhydraulics, fuel and fission product behaviour, fuel channel thermal-mechanical response, containment response and moderator system behaviour. Other accident events, such as small LOCA and secondary side failures can extend over relatively short to very long time periods. Additionally, accident events invariably involve physical phenomena whose modelling represents current state-of-the-art.

Operational Support Analysis

Operational support analysis places a very high demand on the ability to represent the plant systems and components with high fidelity. Since, by definition, operational support tends to be best estimate analysis of the plant behaviour, it very often requires detailed modelling of specific plant components, such as steam generators, pumps, pressurizer, bleed condenser and various valve types, as well as the various plant controls. This requirement has been a strong driver in the development of the SOPHT and TUF codes and is responsible for the control algorithms being simulated in dedicated software routines for each of the Ontario Hydro stations. Additionally, the requirement for upward compatibility in migrating from the SOPHT to the TUF code dictated that the investment in detailed modelling of the control algorithms be maintained by ensuring that the routines from SOPHT be directly transportable into TUF. These requirements were not applied in the initial CATHENA development, where the desire for flexibility led to a general purpose, input driven controller representation.

Design Assist Analysis

Design assist analysis is an important application for both new designs and modification to existing designs. As in the case of operational support analysis this application area requires attention to the detailed representation and modelling of interacting plant systems, major plant components and controllers.

Key features of these application areas are summarized in Table 1.

TABLE 1: KEY FEATURES OF APPLICATION AREAS

APPLICATION AREA	CHARACTERISTIC TIME SCALE	MODELLING NEEDS
Waterhammer Fluid-structure interactions	Milliseconds to hundreds of milliseconds	State of art two-fluid Detailed local phenomena (e.g. condensation front, pressure wave propagation)
<i>Accident Analysis</i> Large LOCA Small LOCA Loss of Flow Loss of Regulation Secondary side failures	Seconds to minutes	State of art two-fluid Interfaces to other accident analysis disciplines
Design Assist & Operational Support Analysis	Seconds, minutes, hours	High fidelity plant models of systems, components and controllers Stable numerical algorithms for large time steps

4.2 USER NEEDS

User Support

Both TUF and CATHENA have an established set of code documentation to assist users in the application of the codes; this usually being the initial means of transmitting detailed information about the codes to users. In addition, there are active user groups for the two codes which provide a vehicle for obtaining user feedback, identification of code deficiencies and communication of new user needs.

Investment in Plant Models and Data Sets

An important user requirement when migrating from one code to another is that they can protect their past investment in developing specific plant component models and plant data sets. These models and data sets usually represent both a considerable accumulated knowledge of plant behaviour and a major resource commitment by the user organization. This requirement was explicitly recognized at the outset of TUF development because of the investment that Ontario Hydro had made in developing and qualifying plant models and data sets for its five nuclear generating stations. As a consequence, TUF was designed to directly incorporate plant component models from the SOPHT code and a special conversion utility program was developed to allow the automated conversion of a SOPHT data set into a TUF data set. This has allowed rapid conversion of SOPHT data sets into TUF data sets for all five generating stations, as well as Hydro Quebec's Gentilly-II station, and the Pakistan KANUPP generating station.

Steady State Initialization

Many existing thermal-hydraulic system codes do not provide a steady state solution. Instead, pseudo-steady state conditions are calculated using pre-specified control system response (normally the controller responses are disabled) and the transient run is driven towards the specified initial conditions. In this case, there the possibility that even small imbalances in the initial conditions will override the transient solutions, especially for slow transients. Also, it cannot be assured that a subsequent induced transient is due solely to the transient event, and not due to improper initial conditions.

Currently the TUF code has both steady-state and transient solutions and the CATHENA code has a transient solution. In the TUF steady state program, the equations dealing with thermal-hydraulic variables, nodal heat flux for heat exchangers, film resistance for heat exchangers, and valve position (or special link resistance) for a CANDU reactor circuit are solved. This steady state program is used to calculate the normal operating conditions of the reactor heat transport system and balance of plant at a specific operating power levels and configurations of operating state.

Reactor Controller Responses

An accurate simulation of automatic controller actions and operator interventions is a governing requirement for the credibility of plant analysis and for gaining acceptance of the simulation results by operational staff. The interactions among the various control systems or components play the most important role in the operational support analysis. Experience at Ontario Hydro, including the small LOCA event that occurred in Pickering Unit 2 in December 1994, has confirmed that the interaction

among various control system must be properly described in order to have an accurate prediction of operational transients and accident events, especially if the code is to be used to assist further investigation of these events.

In the TUF code, although the control routines differ from one station to another, the code has been designed so that the control elements and the locations at which the input variables are measured are easily identified by means of location codes assigned in the input data for all CANDU reactors. Also, users can assign different control states for each major control function through the input data. For example, the overall unit control can be assigned either in normal or manual mode. The steam generator pressure control can be either in warm-up, cool-down or normal hold mode. In the CATHENA code controllers are specified to a generalized controller interface through input data. Recently a linkage procedure has been established to couple CATHENA and the simulated plant controllers of New Brunswick Power's Point Lepreau station which are based on controller modelling in the SOPHT code (Reference 14).

Incorporation of Commissioning Data

Commissioning is a vital part of reactor operation. The initial operation of a new nuclear plant must be carried out in carefully planned stages and each component tested separately to ensure maximum reliability and safety. The aim of a commissioning program is to obtain accurate information about the reactor core and its components prior to in-service full-power operation. The test results provide important design verification information about the characteristics of system components and control systems which can be used to improve the plant modelling in the system analysis codes. For example, the control rods characteristics (position indicators, withdrawal times and drop times), the characteristics of control and safety valves, and the swell curves of the pressurizer water level from the commissioning tests are usually incorporated in the input data set of plant simulations. To incorporate the commissioning data, modelling in these particular areas needs to be flexible in order for the user to adjust the specific characteristics of plant components to reflect as-built behaviour.

Availability of Special Auxiliary Components

The following system components must be modelled in CANDU plant simulations: pumps, valves, pressurizer, bleed condenser, steam generator, turbine and accumulator. The types of valves used in CANDU reactors include check valve, gate valve, global valve, ball valve, butterfly valve, pressure relief valve and safety valve. Modelling of these system components should be available for users to establish a high fidelity plant model.

Flexibility of Simulating Different Transients

The input structure of a code should allow users to specify different operational transients including the malfunctions of components and controllers, and the operator actions. In TUF, for example, the input data can indicate a control valve operating either in normal (or auto), failed open or failed close mode and a pump operating either in normal, run-down, brake, idle or restart mode. The input control vector data for each controller allows users to define various control functions including the malfunction of the controller. Also the operator actions can be simulated through the input time function, user input options or auxiliary vector data.

Accuracy of Restart Files

Restart capability is usually available in all reactor system codes. It allows user to manipulate different transient cases or to continue a long transient run. The restart files should include all necessary variables and common block data used in the program. The transient solutions should be independent of the time in the simulation at which the restart files are generated.

5. VALIDATION AND QUALIFICATION OF COMPUTER CODES

During the fifteen years leading up to 1990, there was an intense effort on code development and validation to support the CANDU reactors in operation and those under development. The task of code validation was supported by an R&D program, presently known as the Safety and Licensing R&D Program of the CANDU Owners Group (COG). The program was jointly funded and reflected the interests that were common to the three Canadian utilities operating CANDU power plants (Ontario Hydro (OH), Hydro Quebec (HQ), and New Brunswick Power (NBP)) and Atomic Energy of Canada Limited (AECL).

Since 1990, the R&D has become more focused on ensuring that code validation is carried out to satisfy both the needs of the industry, for its current design activities and plant operations, and the demands of the regulators. The R&D programs are reviewed both by COG Technical Committees and in-house by all the industry partners. In 1995 June, the industry formed a Code Validation Team, to coordinate code-validation activities in the four partner organizations (OH, HQ, NBP, and AECL). More recently, the Validation Team has been restructured into a Steering Group and several Working Groups. Building upon work initiated at Ontario Hydro, the Team's focus is the generic validation of the major codes used in safety analyses of CANDU reactors in operation and those under development. Generic validation refers to those activities that are code independent and provide the knowledge base necessary for the systematic validation of specific codes. One of the Team's first outputs was agreement on six main disciplines into which physical phenomena can be grouped conveniently for validation purposes (Reference 15). These disciplines are:

- i) System Thermalhydraulics,
- ii) Fuel and Fuel Channel Thermal-mechanical Behaviour,
- iii) Fission Product Release and Transport,
- iv) Containment Behaviour,
- v) Physics (comprising reactor physics, shielding, and atmospheric dispersion), and
- vi) Moderator and Related Thermalhydraulics.

Working Groups of specialists in each discipline carry out the work. Overviews of the current status of validation activities and planning to date in this multi-year validation program are given below.

5.1 FORMAL APPROACH TO VALIDATION

While the industry's traditional approach to code validation, as outlined above, has been in line with international practice, recent developments domestically and internationally have provided the stimulus for a re-examination. Increasingly, the CANDU industry and its regulators expect computer codes to be

formally validated within a systematic framework that can be readily audited. Such a framework exists, and its foundations are validation matrices. The Nuclear Energy Agency of the Organization for Economic Co-operation and Development (OECD/NEA) has developed and recently published (Reference 16,17) validation matrices for LWRs that represent an international consensus in the LWR community on (i) the major, hypothetical accidents, (ii) physical phenomena that might occur during these accidents, (iii) experimental facilities, and (iv) data from separate-effects experiments suitable for the validation of computer codes used in safety analyses and licensing submissions. These matrices address thermal-hydraulic phenomena in the primary heat-transport circuit, and for pressurized water reactors, also the secondary heat-transport circuit.

The CANDU industry has decided to adopt a validation-matrix based methodology for its validation activities, taking into account the state of the art internationally, available expertise, and cost/benefit considerations. Where no international precedents exist, the industry is proceeding with prudence. The steps are typically as follows:

- i) identification of accident scenarios to be analyzed,
- ii) identification and ranking of physical phenomena relevant to these accidents,
- iii) description of the phenomena,
- iv) identification of experiments that exhibit the phenomena,
- v) description of the source facilities/tests, and
- vi) generation of a cross-reference table of phenomena versus relevant experimental data.

The validation matrix comprises the tables in items (ii) and (vi) above.

The industry is examining its suite of safety-analysis codes, with a view to selecting the most appropriate ones for long-term development (if needed), application, and support. The validation matrices will provide the basis upon which to plan further code validation, if needed, to bring code development to closure. The above activities comprise a multi-year validation program, the front end, i.e. generic portion of which is described in the next sections.

5.2 VALIDATION MATRICES AND THEIR ROLE IN CODE VALIDATION

The validation-matrix methodology has five basic steps. In the first step, a Technical Basis Document is produced that provides a total overview of all postulated accidents in the design basis of the nuclear plant and the associated main physical phenomena governing the behaviour of plant systems and radionuclides. In the second step, validation matrices are produced for each discipline, relating all relevant physical phenomena to the relevant subset of accidents and to data from experiments, operating plants, mathematical solutions, and benchmark codes. Steps one and two provide the generic knowledge base which is code independent.

Steps three to five are code specific. In step three, a validation plan derived from the relevant validation matrices is produced for each code. The plan identifies validation work that is believed to be necessary to provide sufficient validation of the code for its intended applications. The execution of the plan demonstrates that the code version accurately represents the governing phenomena for each phase of the selected accident scenario, as identified in the validation matrices. In step four, validation exercises are performed to compare model predictions with selected data sets. Uncertainties in code predictions are

estimated. In step five, a validation manual is produced, summarizing code accuracy, sensitivities, and uncertainties for specific applications. The manual addresses the question whether the validation is adequate.

While the validation methodology shows a linear progression through five steps, actual work is being performed in parallel, on steps one and two, and in all six disciplines, to maximize progress on as many fronts as possible and to engage specialists in all disciplines. The Steering Group ensures that the activities are coordinated and that experience gained is shared among participants. The achievements to date and the near-term plans are summarized in the sections below.

5.2.1 Technical Basis Document

Draft sections of the Technical Basis Document are being produced by specialists in the six disciplines, with some sections being in an advanced state of preparation and undergoing peer review. The first document produced is the technical basis for analyses of large loss-of-coolant accidents (LOCA). The logic of that technical basis is such that it relates the safety concerns, behaviours of plant subsystems and radionuclides, and main physical phenomena. Similar descriptions are being produced for other accidents in the design basis.

5.2.2 System Thermalhydraulics

A validation matrix for system thermalhydraulics has been developed that is based on the physical phenomena that might occur during accidents which form the design basis of CANDU power plants. Seven accident categories have been identified and addressed. They are: (i) large LOCA, (ii) LOCA with loss of emergency coolant (EC) injection (LOECI), (iii) small LOCA, (iv) loss of flow, (v) loss of regulation, (vi) loss of feedwater, and (vii) steam-line break. For this ensemble of postulated accidents, 23 phenomena have been identified, assigned a unique identification number, and their relative importance during the different phases of the accidents has been estimated. That work has been summarized in a 23 x 7 matrix. For each of the seven accident scenarios, a table has been produced that divides the accident into two to four time periods and identifies primary and secondary phenomena in each period. Similar rankings have been produced for the other six postulated accidents.

In the next step, relevant available tests, both experimental and numerical, were identified and tabulated. Identification numbers were assigned to separate-effects tests, component tests, integrated tests, and numerical tests. At this point, the quality of the data was not judged; the data were simply identified as being potentially suitable and available for validation purposes. In the next step, the data were reviewed and assessed for suitability for code validation. One of three grades was assigned to each data set as it relates to each of the 23 thermalhydraulic phenomena: (i) not suitable, (ii) suitable for indirect validation, or (iii) suitable for direct validation.

To complete the generic part of the validation methodology, descriptions have been produced of the: (i) 23 phenomena, (ii) 37 experimental facilities, (iii) 25 separate effects tests, (iv) 5 component tests, (v) 17 integrated tests, and (vi) 10 numerical tests. The validation matrix comprises the two cross-reference tables: phenomena to postulated accident scenarios and phenomena to tests.

Staff from the Atomic Energy Control Board, the Canadian nuclear regulatory body, examined the validation-matrix document for system thermalhydraulics for CANDU power plants and discussed it informally with industry representatives. Their view was generally positive and they felt that the work done represents a significant advancement of generic validation. However, their final opinion is contingent upon specific issues being adequately addressed in future validation plans for individual codes.

The industry's future work will focus on specific computer codes and their interface with the validation matrix. The partner organizations may opt to retain their preferred codes and to identify potential gaps, if any, in the data base and the possible need for additional code development and validation against selected tests from the data base. The specific tests will be selected to ensure that all phenomena that are likely to be encountered during an accident are addressed. The selection of these tests will be done on the basis of a thorough understanding of the thermalhydraulic phenomena and their rank or relative importance during a postulated accident.

Although the focus of the above work was on CANDU safety analyses, the phenomena have broader applications to other thermalhydraulic systems such as research reactors and experimental loops.

5.2.3 Reactor Physics

Utilizing the same methodology employed in generating the system thermal-hydraulics validation matrix, together with specific guidelines developed at Ontario Hydro for applying the process - in particular for selecting phenomena to be included - a validation matrix has been drafted for reactor physics. This validation matrix covers both reactor statics and dynamics. An important observation from this exercise, as well as current exercises underway in other disciplines, is that achieving a common understanding of what constitutes a phenomenon and ensuring that there is consistency in application of the validation matrix methodology is a difficult task, requiring active discussion and interaction between disciplines. Achieving consistency of development is not possible if each discipline is expected to produce a matrix document in isolation.

5.3 Uncertainty Analysis

Accompanying the deployment of best estimate analysis approaches in safety analysis and the need for systematic formal validation of computer codes, is the need to apply uncertainty analysis to quantify the confidence in code predictions. Uncertainty analysis is a necessary component of answering the important issue of "how good is good enough?" when performing validation exercises. It is also a key component in establishing the confidence of code calculations performed in safety and licensing analyses to quantify the consequences of accident events.

An industry team has been formed in Canada to develop methods for uncertainty analysis of computer code calculations. Although there has been work in other countries in this area, the current concern is that the proposed methodologies are computationally prohibitive for application to large volume safety analysis work. A number of approaches are under investigation in an attempt to generate a methodology that is practical for large volume analysis and which also provides the acceptable level of confidence for those persons who have to make judgements on the acceptability of the safety analysis.

6. CONCLUDING REMARKS

The two-fluid codes that have been developed in Canada have evolved from different perspectives with significant differences in requirements imposed on these codes. Nevertheless, they both represent significant achievements resulting from well focused development groups operating with limited resources.

In light of the major industry involvement and co-operation in developing validation matrix based methods for systematic code validation, as well as in developing common uncertainty analysis methodology, an initiative is underway to consider consolidation of safety analysis computer codes into a Canadian industry standard toolset. One part of this initiative is to address the possibility of achieving consolidation of the two-fluid codes. This initiative parallels activities under consideration in other countries and it is believed that the experience within Canada in this area will be a valuable contribution to the international efforts.

REFERENCES

1. J.S.C. Tong and J.M. Bash, FIREBIRD-1 program description, TDAI-100, AECL Engineering, May 1976.
2. D. Bean et al., RAMA: A characteristic finite difference code for LOCA analysis, Simulation Symposium on Reactor Dynamics and Plant Control, Toronto, 1976.
3. D.J. Richards, B.N. Hanna, N. Hobson and K.H. Ardron, CATHENA: A two-fluid code for CANDU LOCA analysis, 3rd International Topical Meeting on Reactor Thermal-Hydraulics, Newport, RI, 1985.
4. C.Y.F. Chang and J. Skears, SOPHT - A computer model for CANDU-PHWR heat transport networks and their control, Nucl. Technology, 35, pp. 591-602, Oct. 1977.
5. W.S. Liu, W. Yousef, J. Pascoe, A. Tomasone, M. Williams and J.C. Luxat., TUF: A two-fluid code for thermal-hydraulics analysis, 10th Annual Conference of Canadian Nuclear Society, Ottawa, Ontario, Canada, June 4-7, 1989.
6. W.S. Liu, R.K. Leung and J.C. Luxat, Overview of TUF code for CANDU reactors, 5th International Conference on Numerical Methods in Nuclear Engineering, Montreal, Quebec, Sept., 1996.
7. J.H. Mahaffy, Numerics of codes: stability, diffusion, and convergence, Nucl. Eng. and Design, 145, pp. 131-145, 1993.
8. R.E. Nieman and M.R. Lin, Summary of JUICE standard problem submissions, presented at the JUICE meeting, Toronto, August 5, 1976.
9. W.T. Hancox, W.G. Mathers and D. Kawa, Analysis of transient flow boiling, application of the method of characteristics, Two-Phase Flow Symposium, 15th National Heat Transfer Conference, San Francisco, Aug. 1975; Also, AIChE Symposium Series No. 174, 74, 1978.
10. A. Tomasone, W.S. Liu and J.C. Luxat, Verification of the TUF code against the JUICE 1976 standard problems, 15th Annual CNS Nuclear Simulation Symposium, Mississauga, Ontario, May 1-2, 1989.

11. B.N. Hanna, N. Hobson and D.J. Richards, One step semi-implicit method for solving the transient two-fluid equations that is non-Courant limited, Computational Modelling of Thermal Fluid Systems, Denver, August, 1985.
12. J. von Neumann and H.H. Goldstine, Numerical inverting of matrixes of high order, Bull. Am. Math. Soc. 53, pp.1021, 1947.
13. H.H. Rosenbrock, Some general implicit processes for the numerical solution of differential equations, Computer Journal, Vol. 5, pp.329-330, 1963.
14. D.J. Richards and R. Girard, Integrating CATHENA with CANDU plant controllers, 13th Annual Canadian Nuclear Society Conference, Saint John, New Brunswick, Canada, June 7-10, 1992.
15. E.O. Moeck, J.C. Luxat, L.A. Simpson, M.A. Petrilli and P.D. Thompson, Validation of Computer Codes used in Safety Analysis of CANDU Power Plants, Proc. IAEA Technical Committee Meeting on Advances in Heavy Water Reactors, Bombay, India, Jan. 29-Feb. 1, 1996.
16. K. Wolfert and I. Brittain, CSNI Validation Matrix for PWR and BWR thermal-hydraulic system codes, Nuclear Engineering and Design, Vol. 108, 1988.
17. OECD/NEA, "Separate Effects Test Matrix for Thermal-Hydraulic Code Validation, Volume I, Phenomena Characterizations and Selection of Facilities and Tests; Volume II, Facility and Experiment Characteristics", Report OECD/GD(94)82, also NEA/CNSI/R(93)14/Part.1/Rev., Paris (1993).

Methodology, Status and Plans for Development and Assessment of the Code ATHLET

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Abstract

The thermal-hydraulic computer code ATHLET (Analysis of THERmal-hydraulics of LEaks and Transients) is being developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) for the analysis of anticipated and abnormal plant transients, small and intermediate leaks as well as large breaks in light water reactors.

The aim of the code development is to cover the whole spectrum of design basis and beyond design basis accidents (without core degradation) for PWRs and BWRs with only one code. The main code features are :

- advanced thermal-hydraulics
- modular code architecture
- separation between physical models and numerical methods
- pre- and post-processing tools
- portability

The code has features that are of special interest for applications to small leaks and transients with accident management, e.g. initialization by a steady-state calculation, full-range drift-flux model, dynamic mixture level tracking. The General Control Simulation Module of ATHLET is a flexible tool for the simulation of the balance-of-plant and control systems including the various operator actions in the course of accident sequences with AM measures.

The code development is accompanied by a systematic and comprehensive validation program. A large number of integral experiments and separate effect tests, including the major International

Standard Problems, have been calculated by GRS and by independent organizations. The ATHLET validation matrix is a well balanced set of integral and separate effects tests derived from the CSNI proposal emphasizing, however, the German combined ECC injection system which was investigated in the UPTF, PKL and LOBI test facilities.

ATHLET is being applied by numerous institutions in Germany and abroad.

Development and assessment of ATHLET will be continued with the aim to enlarge the range of validity and applicability of the physical models, to enhance calculational speed, to reduce the user influence on calculated results and to quantify the remaining code uncertainty.

Future fluid dynamics development will be focused on the following :

- The 6-equation two-fluid model will be completed as an option for low pressures ; the 5-equation model is maintained for most applications due to the advantages of the drift-flux model,
- Constitutive relations will be further developed and calibrated on data preferably from large scale experiments,
- For flow regime transition, a dynamic model is desired,
- For multidimensional flow simulation, the 2D downcomer model with non-staggered grid will be completed and extended to a 3D module.

Code speed-up is expected from improving the implicit time integration method with respect to selective updates of the Jacobian matrix. Non-diffusive space approximation schemes will be investigated in order to allow tracking of steep gradients. The capabilities of the plant analyzer ATLAS for interactive applications will be further increased.

Extended model adaptation and validation for Russian type reactors VVER and RBMK will continue in cooperation with foreign organizations.

For evolutionary PWR and BWR reactor concepts the following processes will receive special attention in future development :

- Flows under low pressure and low driving head,
- Presence of non-condensable gases.

The user influence will be reduced by :

- Improved user guidelines,

- Enhanced input checking and diagnostics.

The assessment task will be oriented on updated validation matrices. The needs for the advanced reactor projects EPR and BWR-1000 will receive special consideration.

The GRS method for determining the uncertainties of calculations will be applied to ATHLET plant calculations for typical transients and LOCAs.

1 Methodology and Status of Development

In the following, the main models and methods of the released version ATHLET Mod 1.1 Cycle C [1,2] are briefly described.

1.1 Code Structure

The ATHLET structure is highly modular, and allows an easy implementation of different physical models [3]. The code is composed of several basic modules for the calculation of the different phenomena involved in the operation of a light water reactor :

- Thermo-fluidynamics (TFD)
- Heat Transfer and Heat Conduction (HECU)
- Neutron Kinetics (NEUKIN)
- General Control Simulation Module (GCSM) ,

together with the numerical integration method FEBE.

Other independent modules (e.g. large models with own time advancement procedure) can be coupled without structural changes in ATHLET by means of a general interface. ATHLET provides a modular network approach for the representation of a thermal-hydraulic system. A given system configuration can be simulated by just connecting basic fluiddynamic elements, called objects. There are several object types, each of them applying for a certain fluiddynamic model. All object types are classified into three basic categories :

- pipe objects: apply for a one-dimensional TFD-Model with partial differential equations describing the transport of fluid. The nodalization (number of nodes or volumes) is defined by

input data. After nodalization, a pipe-object can be taken as a number of consecutive volumes (control volumes) connected by flow paths (junctions). The mass flow rates at the volume boundaries are calculated by the solution of momentum differential equations (local momentum balance) or by algebraic equations when the integrated momentum balance option is chosen. The calculation of the mass flows at the inlet and at the outlet of a pipe-object is included in the pipe-object model. A special application of a pipe-object, called single junction pipe, consists of only one junction, without any control volumes.

- branch objects: apply for any TFD-Model described by an arbitrary system of non-linear ordinary differential equations or even algebraic equations.
- special objects: used for components with complex geometry (e.g. the cross connection of pipes within a multi-channel representation).

Each fluiddynamic object supports a subset of the entire ordinary differential equation (ODE) system of the fluidynamics, which is integrated simultaneously (time advancement) by the ODE-solver FEBE. Within the pipe-objects, the ODEs are obtained from the partial differential equations by applying a spatial approximation method.

1.2 Fluidynamics

ATHLET offers the possibility of choosing between different models for the simulation of fluidynamics .

In the current released code version [1,2], the basic fluid-dynamic option is a five-equation model, with separate conservation equations for liquid and vapour mass and energy, and a mixture momentum equation, accounting for thermal and mechanical non-equilibrium, and including a mixture level tracking capability.

The spatial discretization is performed on the basis of a finite-volume approach. It means, the mass and energy equations are solved within control volumes, and the momentum equations are solved over flow paths – or junctions – connecting the centers of the control volumes. The solution variables are the pressure, vapor temperature, liquid temperature and mass quality within a control volume, as well as the mass flow rate at a junction.

Two types of control volumes are available. Within the so-called "ordinary" control volume a homogeneous mass and energy distribution is assumed. Within the "non-homogeneous" control volume a mixture level is modelled. Above the mixture level steam with water droplets, below the mixture

level liquid with vapor bubbles may exist. The combination of ordinary and non-homogeneous control volumes provides the option to simulate the motion of a mixture level through a vertical component.

A full-range drift-flux model is available for the calculation of the relative velocity between phases [4]. The model comprises all flow patterns from homogeneous to separated flow occurring in vertical and horizontal two-phase flow (Fig. 1). It also takes into account countercurrent flow limitations in different geometries.

Moreover, this fluid-dynamic option allows for the simulation of non-condensable gases, on the basis of the ideal gas formulation.

For pipe-objects, either on the basis of the 5-Equation or the still available older 4-Equation model, there is also the possibility to use the method of integrated mass and momentum balances (EIMMB - Method), an option for fast-running calculations, mainly in the frame of a nuclear plant analyzer. With the application of the EIMMB-Method, the solution variables are now the average object pressure, the mass flows at pipe inlet and outlet, and the local qualities and enthalpies (4-eq.-Model) or temperatures (5-eq.-Model). The local pressures and mass flow rates are obtained from algebraic equations as a function of the solution variables.

Furthermore, an additional mass conservation equation can be activated for the description of boron transport within a coolant system.

A two-fluid, 6-equation model, with completely separated equations for mass, energy and momentum for both phases is now under development.

1.3 Numerical Methods

The time integration of the set of local thermo-fluiddynamic equations is performed by the general purpose ODE-Solver FEBE (Forward-Euler, Backward-Euler). It provides the solution of a general non-linear system of first order differential equations by splitting it into two subsystems, the first being integrated explicitly, the second implicitly. Generally, the fully implicit option is used in ATHLET.

In its implicit option FEBE consists of four parts:

- A method which linearizes the nonlinear right-hand side of the ODE system. Within this context an algorithm is implemented for the efficient calculation of the Jacobian matrix by numerical differentiation.

- The linear-implicit Euler method, which calculates the sub-step or basic solutions of the ODE system at discrete points in time.
- By means of an extrapolation algorithm these basic solutions are used to calculate solutions of different levels of numerical accuracy with respect to their local time discretisation error. Comparison of these solutions among each other quantifies their local time discretisation error.
- A series of monitoring processes:
 - which checks by numerical tests whether the actual Jacobian matrix is still valid. In case it is not, the calculation of a new Jacobian is initialized.
 - which increases the error order of the solution or reduce the actual time step size, if convergence – the achieved accuracy in time is not sufficient – cannot be reached.
 - which determines a time step proposal for the next time step

By these means a rigorous control of the local time discretisation error is performed. According to the error bound specified by the user, the time step size and the order of the method are determined anew for every integration step.

In ATHLET applications the Jacobian matrix is a sparse matrix, i.e. most of its elements are equal to zero. The non-zero elements are collected to sub-matrices, the so-called blocks, introducing a block-structure. The ATHLET Jacobian is a predominantly block-pentadiagonal matrix with a limited number of additional – symmetrically positioned – blocks in off-diagonal positions. These off-diagonal blocks are generated by the interconnections between the network components.

To gain efficiency and high computational speed for the calculation of the Jacobian and the solution of the linear system the sparse matrix package FTRIX is applied in the ATHLET code.

The objectives of FTRIX package are :

- to generate the Jacobian block structure from the ATHLET input data
- to calculate the Jacobian numerically with a minimum of ODE right-hand side evaluations
- to store the sparse matrix economically (non-trivial blocks only)
- to calculate the sub-step (or basic) solutions by solving efficiently the equation system of the linear-implicit Euler method.

1.4 Heat Conduction and Heat Transfer

The simulation of the heat conduction in structures, fuel rod and electrical heaters is performed within the basic module HECU. It permits the user to assign heat conduction objects (HCO) to all thermal-fluiddynamic objects of a given network.

The one-dimensional heat conductor module HECU provides the simulation of the temperature profile and the energy transport in solid materials. The model has the following characteristics:

- The model can simulate the one-dimensional temperature profile and heat conduction in plates, hollow and full cylinders in the radial direction.
- In each heat conductor object (HCO) up to three material zones can be modeled. A material zone is simulated by a problem dependent number of layers. The material zones can be separated by a geometrical gap and a corresponding heat transfer coefficient.
- Heat generation can be considered in material zones. Within a material zone the specific heat generation rate per volume unit is assumed to be distributed uniformly.
- The subdivision of material zones into layers can be performed on the basis of equal layer thicknesses, or equal layer volumes, as well as with layer thicknesses specified by input data.
- The HCOs can be coupled on left and/or right side to TFD-objects by consideration of the energy transport between heat conductor surface and the surrounding fluid.

The heat transfer package covers a wide range of single phase and two-phase flow conditions. Correlations for critical heat flux and minimum film boiling temperature are included. A quench front model for bottom and top reflooding is also available.

1.5 Nuclear Heat Generation

The nuclear heat generation is generally modelled by means of the neutron kinetics module NEU-KIN. For the simulation of electrically heated rods or for a simplified, straight-forward representation of a reactor core the total generated power as a function of time can be optionally given.

The generated nuclear reactor power consists of two parts: the prompt power from fission and decay of short-lived fission products, and the decay heat power from the long-lived fission products. The steady state part of the decay heat and its time-dependent reduction after a reactor scram are provided in form of a GCSM signal. The time-dependent behavior of the prompt power generation is calculated either by a point-kinetics model or by an one-dimensional neutron dynam-

ics model. An input-specified fraction of the total power is assumed to be produced directly in the coolant. The remaining power determines the temperature distribution in the fuel rod, and the heat flux through the cladding surface.

The point-kinetics model is based on the application of the well-known kinetics equations for one group of prompt and for six groups of delayed neutrons. The reactivity changes due to control rod movement or reactor scram are given by a GCSM signal. The reactivity feedback effects for fuel temperature, moderator density and moderator temperature are calculated by means either from dependencies given by input tables or with reference reactivity coefficients. If the boron tracking model is switched on, the reactivity feedback due to changes in the boron concentration will be also taken into account.

The one-dimensional model solves the time-dependent neutron diffusion equations with two energy groups of prompt neutrons and six groups of delayed neutrons. The active core zone can be subdivided into zones with different materials. A reflector zone is also considered.

The model includes the coarse-mesh spatial approximation of the neutron flux by means of second order polynomials. It also accounts for moderator and Doppler reactivity feedback by temperature and density dependent cross sections. Control rod movement and reactor scram are simulated by means of local changes of group cross sections as a function of rod position. Libraries of effective cross sections for several types of light water reactors are also available.

1.6 Simulation of Components

In general, major plant components (e.g. pressurizer, steam generators) can be modelled by connecting thermo-fluiddynamic objects (TFO) and heat conduction objects (HCO) via input data. Simplified, compact models for those components are also available as special objects.

Additional models are provided for the simulation of valves, pumps, accumulators, steam separators, single ended breaks, double ended breaks, fills and leaks and boundary conditions for pressure and enthalpy. Except for the separator model, they are comparable to the corresponding model in other advanced codes. The steam separator model is an empirical approach for the calculation of carry-over and carry-under by means of input functions of the inlet mass flow rates, of the void fraction in the separator region, and of the mixture level outside the separator. Abnormal separator conditions, like flow reversal or flooding, can be simulated.

Critical discharge flow is calculated by an one-dimensional thermodynamic non-equilibrium model, with consideration of the actual geometry of the discharge flow path. A pre-processing tool, called CDR1D, generates automatically the input tables actually needed in ATHLET for interpolation of the critical mass flow rates. Optionally, an homogeneous-equilibrium model and the MOODY discharge model are available.

1.7 Simulation of Control and Balance of Plant (BOP)

The simulation of balance-of-plants systems within ATHLET is performed by the basic module GCSM (General Control Simulation Module). GCSM is a block-oriented simulation language for the description of control, protection and auxiliary systems.

The user can model control circuits or even simplified fluid systems just by connecting basic functional blocks (e.g. switch, adder, integrator). Most of the system variables calculated within the fluid dynamics, neutron kinetics or within other ATHLET modules (process variables) can be selected as input to these functional blocks. The output of such control blocks can be fed back to the thermo-fluid dynamics in form of hardware actions (e.g. valve cross sectional area, control rod position) or boundary conditions (e.g. temperature, heat and mass addition).

This simulation module allows for the representation of fluid dynamic systems (e.g. steam line, condensate system) in a very simplified way (quasi stationary approach) with the advantage of requiring very little computation time in comparison with the fluid dynamics module.

GCSM also provides a general interface to an external library of BOP models. This library contains detailed models with fixed structure and own input data for plant components (e.g. turbine, or even a containment model) or for control systems (e.g. power control, feedwater control or pressurizer pressure control for typical power plants).

2 Assessment

In 1987, the OECD/NEA/CSNI issued a report [5] compiled by the Task Group on the Status and Assessment of Codes for Transients and ECC. It contained proposed validation matrices for LOCA and transients, selected according to the dominating phenomena and the available test facilities. Meanwhile, the Task Group on Thermal Hydraulic System Behaviour is in the process of updating the integral test matrices [6] and extended their work also to separate effects tests [7].

The systematic validation of the ATHLET code is based on a well balanced set of integral and separate effects tests derived from the CSNI proposal emphasizing, however, the German combined ECC injection system which was investigated in the UPTF [8], PKL [9] and LOBI [10] facilities. The ATHLET validation matrices actually comprise 107 integral and 91 separate effects tests, including only a few VVER-specific tests until now. The ATHLET matrices consist of a matrix for large breaks in PWRs, small and intermediate breaks in PWRs, small and intermediate breaks in PWRs with once-through steam generators, AM for a non-degraded core in PWRs, transients in PWRs, transients in shutdown conditions in PWRs, LOCA in BWRs and transients in BWRs. Table 1 shows the validation matrix for integral experiments with the number of tests in each category. The specific selection of tests is based on the intention to cover each relevant thermal-hydraulic phenomenon and each test type in the matrices by at least three facilities of different scale, if available. A total of approximately 30 test types results in about 90 integral tests for code validation. Validation work is shared between GRS and independent organizations. By the middle of 1996, 58 integral tests and 71 separate tests were calculated.

An example from the ATHLET validation procedure was presented recently [11]. The specific needs for validation with respect to AM transients were outlined using a post-test calculation of PKL III Test B 2.1 as an example.

Facility or Plant	Scale	Pressurized Water Reactors *)				Boiling Water Reactors	
		Large Breaks	Small Leaks Intermediate Leaks	Transients	AM	LOCA's	Transients
UPTF/TRAM	1:1	4	2		3		
CCTF	1:25	2					
LOFT	1:50	1	4	1			
LSTF	1:50		2	2			
BETHSY	1:100		7	3	5		
PKL	1:134	3	6	5	5		
ROSA-III	1:424					5	1
FIST	1:642					2	1
LOBI	1:712	2	7	6	2		
GERDA	1:1686		1				
German Convoy				3			
Brokdorf				1			
Gundremmingen							3
Krümmel							2
Total		12	29	21	15	7	7

*) Experiments for VVER reactors not included

Table 1: ATHLET Assessment Matrix (No. of Integral Experiments)

3 Plans for Further Development and Assessment

The development and assessment of the ATHLET code will be continued with the aim to enlarge the range of applicability and validity of the physical models, to enhance calculational speed, to reduce the user influence on calculated results, and to quantify the remaining code uncertainty.

3.1 Fluidynamic Models

Further development is planned for both the basic equation system and the constitutive equations.

The six-equation two-fluid model, which is under development, will be completed. It is not intended to replace the existing five-equation model, but to supplement it as an option, e.g. for low pressure reflood situations. The advantages of the drift-flux model, i.e. direct relation of relative phase velocities to experimental data and easier mixture-level tracking, will be maintained.

The constitutive equations, namely for interfacial friction and contact condensation, will be further developed. This task is closely linked to the validation on the basis of separate effects tests. Predominantly large scale tests, e.g. the UPTF/TRAM tests, will be exploited as a data base. Fitting the closure relations to large scale test data is, however, not sufficient. The closure laws must be physically well-grounded, allowing to calculate the corresponding phenomena in scaled-down facilities as well, since integral experiments are the backbone of the overall code assessment.

Flow regimes are currently distinguished by a selection logic based on the actual values of void fraction and mass flow rate at each time step. It is intended to develop a procedure that allows to calculate the evolution of regimes over time, e.g. by means of a time-dependent interfacial area concentration model.

Multidimensional flow simulation is planned for the reactor pressure vessel. The current development for a two-dimensional downcomer representation is based on a flux-splitting method applied on a non-staggered grid with mesh sizes of a few tenths of a meter. For the planned extension to a three-dimensional module it is believed that mesh sizes of much less than a meter are necessary for accurate predictions of two-phase flow within the reactor vessel.

3.2 Numerics and Interactive Applications

Tracking of steep gradients, i.e. fronts of subcooled or unborated water, gives rise to investigate space discretization schemes with less numerical diffusion. The fully implicit time integration

method will be maintained including the accuracy-based time step control. A potential for speed-up is expected, however, from a selective update of elements of the Jacobian matrix based on physical considerations.

Speed-up is also a prerequisite for a wider use of interactive applications in a simulator environment. The present simulator ATLAS [12] is quite popular among users. Extension of the simulator capabilities is planned.

Among the extended modelling capabilities often requested by the users, the following will be treated with priority :

- larger variety of pre-fabricated BOP-models ,
- easier link of 3D neutron kinetics and its data base ,
- extended fuel rod model, with consideration of ballooning and cladding rupture.

3.3 Russian Reactor Types

The adaptation and extension of models for VVER and RBMK reactors will continue in cooperation with foreign partners. Development work will be focused on specific components like the horizontal steam generator in VVERs, and the steam separator drums and the graphite moderator in RBMKs. Advanced Russian reactor concepts, e.g. V-407 or a PWR pressurized by nitrogen in the vessel are considered.

3.4 New Reactor Types

The new evolutionary reactors, specifically the EPR and the BWR-1000, exhibit some flow phenomena that are not entirely new but gain more importance for the course of transients and accidents. Among them, the following will be primarily considered in future ATHLET development:

- Gravity-driven delivery of water at low pressures ,
- Circulation driven by small pressure differences ,
- Presence of non-condensable gases and their impact on flow circulation, condensation and heat transfer.

3.5 Reducing the User Influence

Measures from the developer's side to reduce the user's influence on calculated results are considered as an important task for future code development :

- improved guidelines for system mapping, nodalization and choice of model options ,
- enhanced input checking and run diagnostics ,
- improved user interface with modern graphics.

Experience and training remain indispensable, however, for a successful code application.

3.6 Assessment and Evaluation of Uncertainties

The ATHLET assessment will be systematically continued based on the validation matrices for integral and separate effects tests. These matrices will be updated as new experiments become available, especially for new reactor concepts. Since the ECCS concept presently considered for the EPR is based on cold leg injection, more emphasis will be given to this ECC mode in the ATHLET assessment. For VVER and RBMK reactors, specific tests will be selected based on the matrices that have just become available [13].

GRS has developed a method for determining the uncertainties associated with code calculated results [14]. This method was successfully used in applications other than thermal-hydraulics, too. For the ATHLET code, uncertainties were calculated for a separate effects test calculation (OMEGA) and for a small break integral test calculation (LSTF). Presently, the method is being applied to a PWR small break LOCA. Future plans foresee generic applications to typical transients and LOCAs.

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References

- [1] Lerchl, G. , Austregesilo, H.
ATHLET Mod 1.1 Cycle C , User's Manual
GRS-P-1 / Vol. 1 , Oct. 1995.
- [2] Austregesilo, H. , Deitenbeck, D.
ATHLET Mod 1.1 Cycle C , Programmer's Manual
GRS-P-1 / Vol. 2 , Oct. 1995.
- [3] Burwell, M.-J., Lerchl, G., Mirò, J., Teschendorff, V., Wolfert, K.
"The Thermalhydraulic Code ATHLET for Analysis of PWR and BWR Systems"
Proc. 4th Intern. Topical Meeting on Nuclear Reactor
Thermal-Hydraulics (NURETH-4), Karlsruhe,
Vol. 2, pp. 1234-1239, (1989).
- [4] Sonnenburg, H.-G., "Full-Range Drift-Flux Model Based on the Combination of
Drift-Flux Theory With Envelope Theory"
Proc. NURETH-4, Karlsruhe, Vol.2, pp. 1003-1009, (1989).
- [5] OECD/NEA/CSNI, "CSNI Code Validation Matrix of Thermo-Hydraulic Codes for
LWR LOCA and Transients", CSNI Report 132, (1987).
- [6] Annunziato, A., Glaeser, H., Lillington, J., Marsili, P. Renault, C., Sjöberg, A.:
"CSNI Integral Test Facility Validation Matrix For the Assessment of Thermal-Hy-
draulic codes for LWR LOCA and Transients; to be issued
- [7] Aksan, N., D'Auria, F., Glaeser, H., Pochard, R., Richards, C., Sjöberg, A.:
"OECD/NEA-CSNI Separate Effects Test Matrix for Thermal-Hydraulic Code Val-
idation", Volume I: Phenomena Characterisation and Selection of Facilities and
Tests, Volume II: Facility and Experiment Characteristics; NEA/CSNI/R(93)14 Part
1 and Part 2, Paris (1994).
- [8] Weiss, P.,
"UPTF Experiment, Principal Full-Scale Test Results for Enhanced Knowledge of
Large Break LOCA Scenarios in PWRs",
Proc. NURETH-4, Karlsruhe, Vol. 1, pp. 60-66, (1989).
- [9] Weber, P., Umminger, K.J.
"Accident Management Procedures on the Secondary and Primary Side for a PWR

– Experimental Investigations in the PKL Test Facility –“
Proc. NURETH-6, Grenoble, Vol. 2, pp. 1100–1108, (1993).

- [10] “LOBI Test Facility”
CSNI-SINDOC (83) 262 (1983).
- [11] Teschendorff, V. , Steinhoff, F. and Glaeser, H.
“ATHLET Validation Using Accident Management Experiments”,
7. Int. Conf. on Nucl. React. Thermal-Hydr. (NURETH-7), 10.-16.09.1995,
Saratoga Springs, N.Y., USA.
- [12] Beraha , D. , Voggenberger , T.
“Fundamentals and Main Features of the German NPA Project ATLAS”,
Proc. of the Simulators VI Conference (Tampa , FL, March 28-31, 1989)
SCS Simulation Series , Vol. 21 Nr. 3, 1989.
- [13] Liesch, K. , Reocreux M.
Concerted Actions on Safety Research for WWER-Reactors
Verification Matrix for Thermalhydraulic System Codes Applied for WWER
Analysis,
Common Report IPSN/GRS No. 25, July 1995 (limited distribution).
- [14] Glaeser , H. et al.
Contribution to the CSNI Workshop on Code Uncertainty Methods
Winfrith , U.K., 1995.

Abbreviations

AM	Accident Management
BWR	Boiling Water Reactor
CSNI	Council on the Safety of Nuclear Installations
ECC	Emergency Core Cooling
GCSM	General Control Simulation Module
LOBI	LWR Off-normal Behaviour Investigations
LOCA	Loss-of-Coolant Accident
NEA	Nuclear Energy Agency
PKL	Primärkreislauf (Test Facility)
PWR	Pressurized Water Reactor
RBMK	Water cooled graphite moderated Reactor (Russian type)
SG	Steam Generator
TRAM	Transient and Accident Management Programme
UPTF	Upper Plenum Test Facility
VVER	Water cooled water moderated Reactor (Russian type)

Drift-Flux Model in ATHLET

Component Geometry	Correlation for Drift-Flux j_{VL}	CCFL-Parameters V_{lim} , $V_{L,lim}$	Data Base Experiments
Rod Bundle	$j_{VL} = C_0 \alpha V_{L,lim}^* \left(-\frac{1}{2} + \sqrt{\frac{1}{4} + A} \right) / A^2$	Kröning	PERICLES THETIS
Downcomer		CREATE, Glaeser	UPTF
Tie Plate	$\text{mil } A = \frac{C_0 \alpha V_{L,lim}^*}{(1 - C_0 \alpha) V_{L,lim}}$	Bankoff, Glaeser	UPTF
Vertical Pipe	$V_{L,lim}^* = \frac{9}{16} V_{L,lim}$	Wallis, Kutateladze	Wilson, Ishii
Horizontal Pipe	$j_{VL} = \frac{C_0 \alpha (1 - C_0 \alpha)}{\frac{C_0 \alpha}{V_{L,lim}} + (1 - C_0 \alpha)}$	Bankoff/Lee	Richter, Ohnuki UPTF

α - Void Fraction

C_0 - Phase distribution Parameter

V_{lim} - Limit superficial vapour velocity

$V_{L,lim}$ - Limit superficial liquid velocity

Fig. 1 : Drift-Flux Model in ATHLET

Methodology, status and plans for development and assessment of HEXTRAN, TRAB and APROS

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Abstract

A number of transient and accident analysis codes have been developed in Finland during the past twenty years mainly for the needs of our own power plants, but some of the codes have also been utilized elsewhere. The continuous validation, simultaneous development and experiences obtained in commercial applications have considerably improved the performance and range of application of the codes. At present, the methods allow fairly covering accident analysis of the Finnish nuclear power plants.

1. Introduction

Code development in the fields of reactor physics and dynamics, as well as in thermal-hydraulics has been one of the key areas of reactor safety research in Finland since the middle of the seventies. An important motivator has been the need to analyse VVER plants against Western safety standards. This was problematic, because many of the VVER specific features could not be described properly with the Western codes. The effort has been remarkable compared to our limited resources. Major part of the code development has been performed by the Technical Research Centre of Finland, VTT.

A variety of calculation methods have been developed for the safety analysis needs, as well as for a wider range of application even in non-nuclear field. Two development lines have been followed: In one method extended versions for new applications have been constructed using most of the past experience and coding. In the other approach the development was started about ten years ago nearly from scratch, with a goal of a multipurpose simulation environment.

In addition to the code development, validation of the methods has been a very demanding task, when the relatively small resources are taken into account. On the other hand, particularly for reactor dynamics applications the validation data base is relatively limited. For thermohydraulic validation the available material is very large, including plenty of integral tests, separate effects tests and plant specific tests.

In reactor dynamics applications the combination of neutron-physical phenomena with thermal-hydraulics of the whole cooling circuit is of vital importance. It has therefore been a nearly built-in property of the Finnish reactor analysis codes, or in the combinations of core models with the circuit thermal-hydraulics models, from the first applications to the present day 3D models.

At present most of the licensing analyses of the Finnish NPP:s can be performed with our own codes, which have also been applied in the safety analysis of some foreign plants. The Finnish licensing policy differs from that of e.g. U.S., in the sense that the regulatory body does not license the calculation methods, but it inspects case by case the sufficiency of the used methods and the presented analyses. Conservative assumptions have to be applied even in such cases as ATWS, which is currently interpreted as a postulated accident.

The calculation system is not complete, and a number of deficiencies may be identified both in the basic models, validation, documentation and in the user interface. At the same time new requirements are set for the performance of the codes, such as the ability to reliably model inherent boron dilution, the mixing effects in large volumes or criticality during maintenance periods. Such factors as reliable simulation of detailed thermal-hydraulics of the core or time dependent pinwise power distribution could be of importance to reduce excessive conservatism in the analyses of the present day plants. Therefore, continuous code development still seems to be reasonable.

Another point of view in favour of continuous code development effort is that a trained group with deep understanding of the problems and the models is able to respond promptly to unpredictable new analysis needs, e.g. by modifying the methods.

Close cooperation with the customers has been very fruitful in code development. Our regulatory body STUK has strongly supported and funded the code development efforts and has been the main motivator for the strong position of reactor dynamics in Finland. The new fuel types introduced into the reactors of Teollisuuden Voima Ltd (TVO) has also emphasized the importance of own continuous development work. The Imatran Voima Ltd (IVO) has also participated in one of the major development projects.

The background and the current activities of the Finnish code development, validation and application is described in the following sections.

2. Past and present code development in Finland

Two types of nuclear power plants were ordered to Finland at the end of the sixties and in the beginning of the seventies, namely two units of the Soviet VVER-440 type and two BWR units of the Swedish Asea type. The plants started operation during the period 1977 - 1981. Hence, in order to raise analysis capability to meet the Western safety analysis requirements of that time, many U.S. safety analysis codes, such as RELAP, were taken into use in the middle of the seventies. However, also own code development was started in such special fields as reactor dynamics and fast simulation of thermal-hydraulics in small break accidents, as well as in the

generation of cross-section parameters and fuel burnup simulation in hexagonal reactor lattice. The own code development was particularly important for the VVER applications, because the available codes were not always directly applicable and no vendor support could be obtained.

In the field of reactor dynamics, which combines neutron kinetics, heat conduction, heat transfer and hydraulics of the cooling circuit, the first product was a LWR core model [1], which is basically one-dimensional two-group code, but includes a synthesis model for radially nonuniform dynamics. It also includes descriptions for the primary circuit components of a PWR, which were combined to a RELAP type node modelling of the secondary circuit. This combined code was during the first ten years applied for the transient calculation of the Loviisa VVER plant, e.g. in such cases as the analysis of a steam line break and ATWS.

Basically the same core model was also applied in the development of the BWR dynamics code TRAB [2,3], which is continuously used in the safety analysis of the TVO power plant. Typical applications are the pump trip and the steam line isolation. The code has also been used for the simulation of the RBMK reactor in accident conditions.

Another fast running simulation code, called SMABRE [4], was developed for such thermal-hydraulic accidents as small breaks, originally in order to facilitate parameter variations to support slow RELAP calculations. Its range of application was, however, soon extended to cover such types of accidents as small break LOCA, primary-secondary leak, steam line break and most parts of a large break LOCA in VVER plants. In addition to safety analysis, this code has been used as the thermal hydraulic model of various NPP full scope and compact simulators. It also serves as the cooling circuit model in the previous SMATRA (SMABRE circuit & TRAB 1D core) and in the present HEXTRAN (3D core) codes for VVER reactor dynamics analysis.

The HEXTRAN [5] core dynamics model is based on the combination of the stationary two-group diffusion code HEXBU-3D [6] for hexagonal geometries, with the fuel heat conduction and channel hydraulics description of the TRAB code. Currently it is the most widely used dynamics analysis tool for the VVER reactors with applications both in the Finnish Loviisa and Hungarian Paks VVER-440 safety analyses and in the analyses of the new Russian VVER-91 concept. A similar 3D reactor dynamics code called TRAB-3D is currently under development for rectangular lattice reactors, particularly aimed at the analysis of the TVO BWR plant.

While the standard 1D modelling of thermal-hydraulics seems to perform reasonably well in small and moderate disturbances, certain deficiencies are obvious in more demanding simulation conditions, such as numerical diffusion in the propagation of boron concentration and temperature gradients, when the numerical solution is searched in conditions far from the flow characteristics. On the other hand, the standard numerical modelling of two-phase flow is not either completely satisfactory, particularly in fast transients. Therefore, the development of a new numerical solution method for flow equations, PLIM [7], and an improved formulation of two-phase equations SFAV [8] has been under way already for a number of years. At present these methods are undergoing testing in reactor conditions and PLIM is being implemented in the TRAB dynamics code [9,10].

During the last ten years, parallel to the above code development, another approach has been taken to construct a multipurpose simulation environment APROS [11,12,13]. It has its origin in mid eighties, when it was foreseen that the future generations of nuclear safety analysts need new, interactive and more visual tools in their work. At the same time the automation department of the IVO power company had made a decision to search for a tool to be used in the plant automation design and testing. The basic needs were found to be parallel. No ready-made software (nor hardware) was found. The prospects were considered compelling thus justifying the start of such a relatively massive program development effort.

At present the APROS simulation software covers a broad range of applications in the nuclear safety analysis and in other industrial branches. APROS provides tools, solution algorithms and model libraries for full-scale modelling and simulation of power plant processes, including the process automation and electrical systems. The modular and hierarchical approach of APROS allows unique flexibility of process analysis. The different thermal-hydraulic two-phase flow models, 1D and 3D reactor models and the complete set of conventional power plant components such as heat exchangers and turbines facilitate full coverage in nuclear power plant modelling. The on-line features of APROS allow the user to make any parameter - or even model structure - changes on-line and immediately continue the simulation. The APROS simulation environment has been used in numerous projects covering plant design, system modifications, safety analysis and plant personnel training of different, mainly VVER type power plants.

3. Methodology of the HEXTRAN, TRAB and APROS codes

Currently the HEXTRAN reactor dynamics code for hexagonal fuel grid, the TRAB code for 1D cores and for 3D rectangular grid and the APROS code are under active use and/or development. In the following Table 1 the most important characteristics and the capabilities of the codes are presented.

3.1 Special features of the HEXTRAN code

In the development of the dynamics codes large emphasis has been put on the numerical methods used, their effectivity and stability.

The neutron kinetics model of HEXTRAN solves the two-group diffusion equations in homogenized fuel assembly geometry with a sophisticated, very fast two-level nodal method. In excess of full core calculations, calculations utilizing core symmetries of half-core, 1/3 or 1/6 core can be carried out. Advanced time integration methods are used. Time discretization is made by implicit methods which allow flexible choices of time steps. The numerical method can be varied between the standard fully implicit theta method and the central-difference theta method in fuel and cladding heat transfer and thermal hydraulics conservation equations. Spectral matching method W_{11} is used in neutron kinetics.

Table 1. Main properties of the codes.

Feature	HEXTRAN	TRAB	APROS
Core neutronics equations	two-group nodal eq.	two-group nodal eq.	two-group finite difference eq.
Core neutronics presentation	3D in hex. geometry	1D, 3D in rectang. geometry	1D, 3D in rect. and hex. geometries
Core heat transfer	1D radially	1D radially	1D radially + axial conduction
Hydraulics	1D 5-eq.	1D 4-eq. (6-eq.)	1D 3-, 5- and 6-eq.
Non-condensable gases	yes	no (easy to add)	yes
Mixing in large volumes	simplified/tuning	no	simplified/tuning
Heat structures	1D	1D	1D, 2D (cylindrical)
Material properties	tables, fluid with rational functions	tables, fluid with rational functions	fluid with tables, others tables, functions
Cooling circuit components	1D nodal	1D nodal	1D nodal
Turbine and generator	no	no	yes
Plant control/automation	simplified	PID controllers	60 different modules
Electrical system	no	no	yes
User interface	standard text editors, online and post processor plotting	standard text editors, online and post processor plotting	graphical model building, modification, on-line plots, visualisation
Input/output	normal files	normal files	data base dump, files

The process description of the circuit model SMABRE is based on generalized nodes, junctions connecting nodes and heat structures describing structure walls, fuel rods and steam generator tubes, similarly as in RELAP. The spatial discretization is based on donor cell method and for time discretization a non-iterative semi-implicit algorithm based on predictor-corrector -method is used. The flow equations are solved by applying sparse matrix methods. These methods make the code very fast.

The neutronics and thermal hydraulics are strongly coupled in the reactor core and mutual iterations are needed to achieve a stable solution. The solution method of SMABRE is non-iterative and there is a loose coupling between it and HEXTRAN, therefore no iterations are made with the circuit hydraulics.

The coupled code HEXTRAN/SMABRE has its own main program and some connecting subprograms, but as a rule the subprograms of HEXTRAN and SMABRE are used in the same way as in the separate codes. Both codes use their own input, output, restart and plotting capabilities. Thereby the versatility of the codes is not lost and all revisions made in the codes

separately can directly be included in the coupled code. The first applications with the coupled code were carried out as early as in 1991 - 1992.

With HEXTRAN it is possible to perform fully realistic time-dependent analyses starting from the actual core cycle conditions of the nuclear power plant. The same cross section data can be used as for burnup simulation. Methods for making conservative accident analyses with this best-estimate code have also been developed. Complicated transients and accidents in which there are strong interactions between neutron kinetics and thermal hydraulics can be reliably analyzed. Due to the effective methods the coupled code is so fast that even the longest accidents, e.g. ATWS cases, can practically be analyzed with it.

One reason for the speed of the current code is that the first versions of the reactor physics and dynamics codes have been used with very small and ineffective computers. Therefore effective mathematical methods and dynamic use of memory space must have been developed. Due to this work, the huge capacity of today's computers can be utilized for the completeness of the physical modelling of the reactors: three-dimensionality, detailed models of fuel, adequate number of nodes in hydraulic circuits, analyses of very long transients (e.g. ATWS).

3.2 Special features of the TRAB code

TRAB is a one-dimensional transient and accident analysis code for BWRs. It models the core and the main circulation system inside the reactor vessel, including the steam dome with related systems, steam lines, recirculation pumps, incoming and outgoing flows as well as control and protection systems. The core model includes a one-dimensional description of the geometry, neutronics, rod heat transfer, and thermal hydraulics. Radial power distribution effects can also be simulated by using the synthesis model of the code with parallel axial channels.

The neutronics model of TRAB has just been extended into a fully three-dimensional model with rectangular geometry. The solution methods applied in HEXTRAN have been utilized. The validation of TRAB-3D is being made during 1996.

3.3 Special features of the APROS code

APROS provides tools, solution algorithms and model libraries for full-scale modelling and simulation of different power plant processes, including the process automation and electrical systems. It has been developed for the design, analysis and training simulator applications. It has been built upon a real time database, which provides much of the flexibility of the modelling system based on graphical user interface and local area network connections. To facilitate plant model building, higher level objects, process components are used to automatically create calculational level model structures to describe real industrial components. They also provide ready-made connections to electrical and automation systems.

One of the visions emphasised throughout the APROS development process is the ability to use and extend the same plant model specification from the pre-design phase throughout the lifetime

of the plant. The model database can also store references to the sources of input data, modelling principles etc. and thus transfer design knowledge to the users of the plant.

The APROS 1-D and 3-D reactor models are based on two-group neutron diffusion equations. The models include calculation of iodine, xenon, promethium and samarium. Reactivity effects due to fuel temperature, coolant density, coolant void fraction, coolant boron content and control and scram rod groups are considered. The models are valid for both BWR and PWR cores with either square or hexagonal fuel lattice. The 3-D core can be divided a number of one-dimensional thermal-hydraulic channels extending from whole core being described with one thermal hydraulic channel into each fuel assembly being described with its own thermal hydraulic channel. The user can select either 3-, 5- or 6-equation thermal hydraulics for the channels.

More than 60 different elementary components are available in the APROS automation system library. They can be used to describe all the present day automation systems. The electrical system provides the subroutines to solve the electrical power consumption in the network.

4. Status, experiences and validation of the codes

All the codes are in every day use, except for the 3D version of TRAB, which is under validation. Currently the most urgent tasks are associated with the modernization of the Finnish NPPs, which projects include increase of power level.

An important feature in the use of these codes in Finland is that close communication with the code developers and the code users has been possible, which benefits both sides.

The main application field of the current codes during recent years appears in Table 2. Some important validation cases are given in Table 3.

A lot of measurement data is available for the validation of stationary reactor power distributions, that may be used as references for realistic initial states. Validation of core dynamics properties is more difficult, because interpretation of actual plant data is not very straightforward. Fortunately test reactor data is available for hexagonal geometry, which has been applied in the validation of the HEXTRAN code.

More accurate fuel property data for higher burnup also begins to be available, which improves accuracy in transient and accident simulation. Such effects have already been implemented and demonstrated in HEXTRAN.

Thermal hydraulic data seems to be abundant both for separate effects and for integral performance validation, but scaling of the test results to real power plants, particularly in two phase conditions remains to be uncertain. A difficulty in the thermal hydraulic validation, in addition to the vast volume of the material compared to our resources, is that many phenomena include 3D features that have to be modelled using basically 1D methods.

One good feature in gradual code development is, that with careful programming it has been possible to transfer the previously tested properties and validation results to the code extensions. As an example, the basic equations of HEXTRAN are written so that they reproduce the results of the stationary HEXBU-3D reactor analysis code, and the hydraulics solution of a core channel is equivalent to that of TRAB.

Table 2. Main applications of the codes.

Feature	HEXTRAN	TRAB	APROS
Nuclear plant types	VVER-440 VVER-1000	BWR (ABB) RBMK-1000 VVER-440	VVER-440 VVER-1000 BWR (ABB)
Licensing analyses	Loviisa: RIAs, ATWS, SBLOCA Paks (AGNES proj.): RIAs, ATWS, SBL	TVO transients and accidents	
Main accident types	Control rod withdr. Control rod ejection Boron dilution Steam line break SBLOCA Primary-secondary leak ATWS cases	Steam line isolation Pump trip BWR stability Boron dilution during maintenance Chernobyl scenarios ATWS cases	Steam line isolation Primary-second leak Boron dilution Steam line break Loss-of-feedwater SBLOCA LBLOCA ATWS cases
NPP simulator applications	Thermalhydraulics of Loviisa and Paks plant simulators and several PWR and BWR compact simulators		Kola VVER Chasnupp PWR Ringhals-1 BWR Forsmark-1 BWR TVO BWR Loviisa VVER
Non-nuclear applications			Gas turbine plant Paper mill Coal burning plant Diesel motor Distillation column
Plant performance studies			Control system design FW pump cavitation Condenser control Make-up tank design Plant power increase Control system analysis Predicting simulator

Table 3. Validation of the codes.

Feature	HEXTRAN	TRAB	APROS
Static power distributions	Loviisa VVER-440 stationary measurements	TVO and Loviisa stationary measurements	Loviisa stationary measurements
3D neutron kinetics measurements	LR-0 test reactor CR movements		
Power transients	Loviisa startup tests	TVO startup tests for pump stop and stabil. TVO stability incid. TVO over pressuriz.	Loviisa startup tests TVO over-pressurization
Other plant transients	Loviisa overcooling transient		Loviisa overcooling transient and feed water line break
3D benchmarks	3 AER dynamics benchmarks	NEA CRP benchm. Nordic benchmark	1 AER kinetics benchmark
Integral thermohydraulic tests	Several standard problems (LOFT, LOBI, ROSA-IV ...)		Standard problems (PACTEL, LOFT, BETHSY)
Separate thermohydraulic effects tests	e.g. phase separation, critical flow, dryout, heat transfer ...		e.g. reflooding, phase separation, critical flow, dryout, heat transfer ...

The parameter range in many of the current day analyses is much wider than was originally planned when developing the codes. This has led to continuous need to check correlations, material property presentations and numerical solutions. However, some uncertainty always remains, if all the essential phenomena have been modelled properly.

As a result of the diversity in the code development, it has been possible to calculate the same problematic scenarios using e.g. HEXTRAN, APROS and RELAP, and not very surprisingly, the results may have deviated considerably. One of the good side effects of this internal benchmarking has been, in addition to finding code errors and modelling weaknesses, that most calculation results are treated with reasonable scepticism.

5. Plans for development and assessment

In carrying out reactor dynamics calculations we need accurate data, suitable models, and good numerical solution methods. Continuous efforts are being made in all these sectors to improve the reliability and applicability of the reactor dynamics code system.

In order to remove problems that are associated with numerical diffusion and dispersion and some other problems of numerical origin, the PLIM method will be taken into use in the HEXTRAN and TRAB codes, first in the 1D version of TRAB.

The 3D version of TRAB for rectangular core dynamics applications is being developed. The first successful tests have already been made. The code will be benchmarked at least against TVO plant data and against the OECD/NEA PWR and BWR-benchmarks.

Some effort is put on more accurate estimation of the limiting fuel conditions in stationary state and during transients. Continuous evaluation and improvement of the modelling of several critical thermohydraulic phenomena are needed when making safety analyses (Table 4).

Table 4. Challenges in the simulation of plant transients and accidents

Event	Challenges of the simulation
Large break LOCA	Rapid depressurization, high mixture velocities, pressure wave propagation, liquid penetration in downcomer, multidimensional upper plenum flow with condensation, counter-current-flow in upper tie plate, rewetting of core, droplet carried by steam and core heat-up
Small break LOCA	Natural circulation modes including single-phase, two-phase, boiling-condensing modes, effect of noncondensable gases on natural circulation, phase separation in loop seals, horizontal stratification in pipes, level swell in core, core heat-up
Primary-secondary leak	Coupled pressure dynamics between primary and secondary side, isolation of broken steam generator, safety valve operation in the broken loop, primary loop isolation (VVER-440), overfilling of the broken loop secondary side
Loss-of-power and control rod withdrawal ATWS	Rapid primary repressurization possible to critical pressure, low condensation on water levels during repressurization, different natural circulation modes, hold-up of liquid in pressurizer, steam generator with reducing secondary liquid, boric acid dilution, core power with strong oscillations of pressure, inlet flow and void fraction, cross-section data validity over large variations of feedback parameters
Steam line break (PWR)	Pressure waves in steam lines after rupture, level swell in steam generator, heat transfer with reduced steam generator level, cold water channeling in the downcomer, automation on secondary side, core recriticality
Steam line isol. (BWR)	Pressure wave propagation in steam line, core power spiking, steam separator dynamics, effect of steam moisture on steam compressibility

VTT has committed itself to the development of safety analysis codes as a national support organisation. In addition, both IVO and VTT have committed themselves to continuous development of APROS as an analysis and design tool for different industrial processes, including

nuclear power plants. Training simulators are also obvious current applications. To increase the scope of nuclear training, a project to develop a set of severe reactor accident models has been started. In the future tools for real time assistance of plant operators will be developed. These require high power parallel solution algorithms, advanced process interfaces and a user interface capable of supporting these.

6. Conclusions

In Finland a number of transient and accident analysis codes have been developed during the past twenty years mainly for the needs of our own power plants, but some of the developed methods have also been utilized elsewhere. These applications are mainly associated with VVER safety analysis or with plant simulator models. As an example, the fast operation of the HEXTRAN code has enabled realistic analysis of 3D core combined to a full model of the cooling circuit even in such long reactivity scenarios as ATWS.

The methods allow fairly covering accident analysis of the Finnish nuclear power plants. The key persons in the code development group have been attached to the work since the beginning up to these days, which has guaranteed certain continuity and compactness.

The continuous validation, simultaneous development work and experiences achieved in commercial applications have considerably improved the performance and range of application of the dynamics codes.

As to the development of the APROS code, it has benefitted a lot from the references set by the TRAB and HEXTRAN codes, and on the other hand from the experience in the non-nuclear field.

Some modelling areas are still problematic for the codes, such as controlling of numerical diffusion, propagating fronts and separation of phases, but methods are being implemented to fix them. The treatment of 3D flow phenomena, such as upper plenum and downcomer mixing, probably needs considerable efforts in future.

References

- [1] Rajamäki, M. TRAWA, a transient analysis code for water reactors. Espoo 1980, Technical Research Centre of Finland, Nuclear Engineering Laboratory, Research Report 24. 150 p. + app.
- [2] Rajamäki, M. TRAB, a transient analysis program for BWR, Part 1, Principles. Espoo 1980. Technical Research Centre of Finland, Nuclear Engineering Laboratory, Research Report 45. 101 p. + app.

- [3] Rätty, H. Kyrki-Rajamäki, R. & Rajamäki, M. Validation of the reactor dynamics code TRAB. Espoo 1991. Technical Research Centre of Finland. Research Report 729. 31 p.
- [4] Miettinen, J., Development and assessment of the SBLOCA code SMABRE. Proceedings of the Specialist Meeting on Small Break LOCA Analyses in LWRs. Università di Pisa, Italy. 1985, Vol. 2, pp 481 - 495.
- [5] Kyrki-Rajamäki, R. Three-dimensional reactor dynamics code for VVER type nuclear reactors. Espoo 1995, Technical Research Centre of Finland, VTT Publications 246. 51 p. + app. 80 p. (Dr. Dissertation)
- [6] Kaloinen, E., Teräsvirta, R. & Siltanen, P. HEXBU-3D, a three-dimensional PWR-simulator program for hexagonal fuel assemblies. Espoo 1981, Technical Research Centre of Finland, Nuclear Engineering Laboratory. Research report 7. 148 p. + app. 5 p.
- [7] Rajamäki, M. & Saarinen, M. Accurate one-dimensional computation of frontal phenomena by PLIM. Journal of Computational Physics, 1994. Vol. 111, nro 1, pp. 62-73.
- [8] Rajamäki, M. and Narumo, T. Six-equation SFAV model for two-phase flow with correct propagating velocities of disturbances. Int. J. Numerical Heat Transfer, PartB, Vol 28, pp. 415 - 236, 1995.
- [9] Rajamäki, M. Elimination of numerical diffusion in one-phase and two-phase flows. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Md, U.S.A., November 5 - 8, 1996, Submitted.
- [10] Narumo, T. and Rajamäki, M. Dividing phases in two-phase flow and modelling of interfacial drag. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Md, U.S.A., November 5 - 8, 1996, Submitted.
- [11] Puska, E.K., Hänninen, M.J., Porkholm, K.J. and Kontio H.E., Assessment of APROS Against the Loviisa-2 Stuck-Open Turbine By-Pass Valve Transient, Proceedings of the 1994 ASME Power Plant Transient Symposium, November 6-11, 1994, Chicago, Illinois, American Society of Mechanical Engineers 1994, FED-Vol. 204, pp. 31-42.
- [12] Puska, E.K. and Kontio, H., Three-Dimensional Core in APROS Plant Analyzer, Proceedings of the International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses, April 30- May 4, 1995, Portland, Oregon, USA, ISBN 0-89448-198-3, American Nuclear Society Inc. 1995, Volume I, pp. 264-273.
- [13] Puska, E.K., Miettinen, J., Hänninen, M., Kontio, H. and Honkoila, K., APROS Simulation System for Nuclear Power Plant Analysis, Proceedings of ICONE-3, The 3rd JSME/ASME Joint International Conference on Nuclear Engineering, April 23-27, 1995, Kyoto, Japan, The Japan Society of Mechanical Engineers 1995, Volume 1, pp. 83-88.

ANNEX

Summary of the properties of the HEXTRAN, TRAB and APROS codes in the form suggested by Prof. Yadigaroglu.

Feature	HEXTRAN	TRAB	APROS
Purpose of the code	3D reactor dynamics for hexagonal lattice cores combined with plant dynamics, from operational transients to ATWS scenarios. Safety analysis tool.	1D and 3D reactor dynamics for square lattice core combined with plant dynamics, from operational transients to ATWS scenarios. Safety analysis tool.	Full-scale modelling and simulation of different power plant processes, including the process automation and electrical systems. Design, safety analysis and training simulator applications.
Fluids and fields	1D water with solute, steam with non-condensable	1D water	1D water with solute, steam with non-condensable gas
Thermo-dyn. treatment	Simple thermodynamic treatment between steam and noncondensable gas	No thermodynamic treatment	Thermal dynamic treatment between gas components, no chemical reactions
Flow modelling	1D separated 4-eq., void fraction correlation for core TH. 1D separated 5-eq. drift flux model for the loop TH.	1D separated 4 eq., void fraction correlation	1D homogeneous 3-eq. / 5-eq. drift flux model with non-equilibrium / 6-eq. two-fluid model with separate phase momentum and non-equilibrium
Flow and heat transfer regime maps	No flow regime maps. In heat transfer a set of correlations with simple switching rules (e.g. DNB by correlation \Rightarrow post DNB heat transfer \Rightarrow oxidation). In loop full range drift flux model for vertical and horizontal flow. For HT wetted and non-wetted wall models.	No flow regime maps. In heat transfer a set of correlations with simple switching rules (e.g. DNB by correlation \Rightarrow post DNB heat transfer \Rightarrow oxidation))	3 Eq. model: no maps 5 Eq. model: full range drift flux model for vert.& horiz. flows. CCFL included in the drift-flux handling. 6 Eq. model: Flow regimes: bubbly, annular, droplet, stratified. Weighing factors for stratification and entrainment. Heat transfer: wetted wall, DNB, post DNB, quenching.

Wall closure laws	<p><u>Friction</u>: A set of correlations, e.g. McAdams, and two-phase multipliers with user defined parameters, e.g. Baroczy.</p> <p><u>Heat transfer</u>: A set of heat transfer and DNB correlations, particularly for VVER applications. Wetted and non-wetted wall models.</p>	<p><u>Friction</u>: A set of correlations and two-phase multipliers with user defined parameters.</p> <p><u>Heat transfer</u>: A set of standard heat transfer and DNB correlations. Particularly for BWR applications.</p>	<p><u>Friction</u>: 5 eq. A set of correlations, e.g. Blasius and two-phase multipliers with user defined parameters.</p> <p>6 eq. Blasius, distribution between phases on the basis of flow regime.</p> <p><u>Heat transfer</u>: A set of heat transfer and DNB correlations. CHF model.</p>
Interfacial closure laws	A non equilibrium boiling model in the core. In the loop full range drift flux model, flashing and condensation.	A non equilibrium boiling model.	<p>5 Eq. model full range drift flux model, flashing and condensation.</p> <p>6 Eq. model: interfacial friction and heat transfer with correlations depending on flow regimes</p>
Virtual mass	Not needed	Not needed	Not used
<p>Numerical schemes</p> <p><u>Neutronics</u>:</p> <p><u>Thermal-hydraulics / heat transfer</u>:</p>	<p>Fast two-level nodal method, Spectral matching method W_{11} in neutron kinetics.</p> <p><u>Core</u>: Implicit time discretization (flexible choice of time steps). The numerical method can be varied between the standard fully implicit theta method and the central-difference theta method.</p> <p><u>Loop</u>: Spatial discretization by donor cell method, time discretization by a non-iterative semi-implicit algorithm based on predictor-corrector -</p>	<p>Fast two-level nodal method, Spectral matching method W_{11} in neutron kinetics.</p> <p>Implicit time discretization (flexible choice of time steps). The numerical method can be varied between the standard fully implicit theta method and the central-difference theta method.</p>	<p>Nodal method, applicable to both square and hex lattices</p> <p>3 & 6 Eq. models: Implicit time discretization, with automatic time step adjustment.</p> <p>5 Eq. model: Spatial discretization by donor cell method, time discretization by a non-iterative semi-implicit algorithm based on predictor-corrector - method.</p>

	method. The sparse matrix methods make the code very fast.		
Structures	<u>Fuel</u> : 1D modelling of fuel and cladding. <u>Other structures</u> : 0 D heat slabs assuming cylindrical or slab geometry	<u>Fuel</u> : 1D modelling of fuel and cladding.	Fuel: 1D and 2D modelling of fuel and cladding. Other structures: 1D slabs with versatile interconnections
Special processes	CHF by correlations, Oxidation. In the loop CCFL included in the drift flux model. Critical flow.	CHF by correlations, Oxidation	CHF, CCFL, oxidation; cold startup, shutdown, critical flow
Special equipment models	Fuel follower control rods, PID-controllers, horizontal steam generators (with standard nodes), circulation pumps, jet pumps, safety valves, relief valves, injection pumps, simple automation for components	Partial length fuel elements, PID-controllers, pumps, valves, user defined algebraic of 1st-order differential dependences or delays between chosen variables	Fuel follower, partial length rods, automation and electrical systems, turbine, condenser horiz. & vert. steam generators, heat exchangers, etc.
Balance of plant components	Main components controlling steady state pressure, flow rate and core power included.	Main components controlling steady state pressure, flow rate and core power included.	Full automation system
Input deck generation	Standard editors	Standard editors	Through on-line graphical interface
Graphical user interfaces	No	No	Design-oriented interface for model definition and modification, analyser-type plant visualisation, CRT-based training simulator interface
Output	Normal files (listing, reports, events listing) online and post processor plotting	Normal files, online and post processor plotting	Structured data base dump, files, online and post processor plots, visualisation
Programming language	Fortran 77	Fortran 77	Fortran 77, C

THERMAL-HYDRAULIC MODELING NEEDS FOR PASSIVE REACTORS

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ABSTRACT

The U.S. Nuclear Regulatory Commission has received an application for design certification from the Westinghouse Electric Corporation for an Advanced Light Water Reactor design known as the AP600. As part of the design certification process, the USNRC uses its thermal-hydraulic system analysis codes to independently audit the vendor calculations. The focus of this effort has been the small break LOCA transients that rely upon the passive safety features of the design to depressurize the primary system sufficiently so that gravity driven injection can provide a stable source for long term cooling. Of course, large break LOCAs have also been considered, but as the involved phenomena do not appear to be appreciably different from those of current plants, they were not discussed in this paper.

Although the SBLOCA scenario does not appear to threaten core coolability - indeed, heatup is not even expected to occur - there have been concerns as to the performance of the passive safety systems. For example, the passive systems drive flows with small heads, consequently requiring more precision in the analysis compared to active systems and raising the question as to whether the same confidence can be placed in the analysis methods for passive plants as compared to current plants with active systems. For the analysis of SBLOCAs and operating transients, the USNRC uses the RELAP5 thermal-hydraulic system analysis code. To assure the applicability of RELAP5 to the analysis of these transients for the AP600 design, a four year long program of code development and assessment has been undertaken.

The lessons learned during this effort were detailed in this paper by describing the relevant physical phenomena and the associated modeling challenges for each component.. Specific modeling challenges for our current generation of thermal-hydraulic codes include:

- Thermal Front Tracking: ability to resolve steep temperature gradients within the liquid in the flow direction and to use the temperature of a buffer layer in the interfacial heat transfer model.
- Mixture Level Tracking: ability to track the liquid/vapor interface, and correctly model the interfacial heat transfer phenomena for a stratified surface.

- **Thermal Stratification & Mixing:** provide for the accumulation of hot liquid in a buffer layer due either to convection or condensation, and provide for a mixing region that grows due to the addition of colder water either from wall heat transfer effects or convection.
- **Wall Conduction:** accurate solution of the transient conduction within thick walled vessels that is not sensitive to user specification of mesh spacing.
- **Cold Leg Thermal Stratification:** model thermally stratified single-phase flow (possibly flowing counter-currently) in large diameter horizontal pipes.
- **Critical Flow:** accurately calculate the critical flow for both valves (ADS) and thin orifice plates especially for low pressure and low quality conditions.
- **Phase Separation:** accurate prediction of entrained liquid fraction at ADS valves due to phase separation in the pressurizer and vertical off-take from the hot legs.
- **Low Pressure Boiling:** eliminate unphysical discontinuities in the interfacial heat transfer package and provide some form of subgrid resolution for the point of net vapor generation.
- **Low Pressure Void Fraction:** improve models for interfacial drag in rod bundles at low pressure, low flow, and low heat flux conditions.

In addition, a section on "numerical considerations" was included that discussed the need for further improvements in:

- **Computational Efficiency:** provide for a more implicit solution technique, minimize "numerical events" that reduce the time step, investigate parallel processing.
- **Code Robustness:** improve ability of code to run a transient to completion without requiring user intervention, this include improvements in the areas of phase appearance/disappearance, water packing, implicit treatment of wall heat transfer, time step control, and appearance of noncondensibles.
- **Code Accuracy (Numerical):** improve order of accuracy in differencing to minimize artificial diffusion, better conservation of mass in long term transients, reduce sensitivity to time step size, and reduce oscillations that are numerical in origin.

While the above list of challenges that can be encountered in the thermal-hydraulic analysis of passive reactor systems is imposing, it should not be taken to infer that the task is impossible. In the AP600 analysis program, extensive comparisons were made between RELAP5 (pre-release version of Mod3.3) and data from three integral test facilities all at different scales. Once the more serious problems were either corrected (or a workaround used) the overall transient behavior was well simulated and the key parameters judged to be in reasonable agreement with the measured quantities.

INTRODUCTION

The U.S. Nuclear Regulatory Commission has had two Advanced Light Water Reactor (ALWR) designs employing passive safety features submitted for design certification: Westinghouse's AP600 and General Electric's SBWR¹. As part of the design certification, the USNRC needed to have the capability of auditing the required vendor safety analysis calculations. For small break Loss-of-Coolant-Accidents (LOCAs) and operational transients, the RELAP5 system thermal-hydraulic analysis code is used by the USNRC. To assure the applicability of RELAP5 to the analysis of these transients for the passive reactor design, a four year long program of code development and assessment has been undertaken. The modeling challenges described below were uncovered during this process and have led both to the inclusion of new models (e.g., a subgrid resolution scheme for thermal stratification) and the fix-up of others.

The AP600 design was first-in-line for the design certification process and most of the USNRC effort to date has focused on it. In the process of applying the RELAP5 code to the AP600, much has been learned about the analysis of ALWR designs and their passive safety features. This paper will make the effort to summarize those findings. To do so, rather than discuss phenomena that need to be modeled in the abstract, each important phenomena will be discussed in the context of the component and phase of the transient for which it is important. In the following sections, the discussion will focus on a small break LOCA for the AP600 design. Of course, large break LOCAs have also been considered, but as the involved phenomena do not appear to be appreciably different from those of current plants, they are excluded from the discussion below.

First, a cursory description of the AP600 design and SBLOCA scenario is given in the section entitled "AP600 System & Transient Description". This is followed, in the section "AP600 Components & Phenomena", by a component-by-component description of the phenomena that are necessary to be well modeled in the analysis of a passive reactor design. In addition to the modeling of physical phenomena, there are a number of "numerical considerations" that must also be considered and they are treated next in a section of that title. A summary section concludes the paper.

AP600 SYSTEM & TRANSIENT DESCRIPTION

This section will give a brief description of the AP600 primary system and passive safety features followed by a summary of their behavior during a typical small break LOCA. A more detailed description of the individual key phenomena expected and the modeling considerations they give rise to is given below in the section entitled "AP600 Components & Phenomena".

¹ The SBWR design has since been withdrawn from the certification process.

AP600 System Description

The AP600, co-developed by Westinghouse Electric Corporation, the U.S. Department of Energy, and the Electric Power Research Institute, is an advanced light water reactor design that utilizes passive safety systems and modular design and construction techniques in an effort to reduce the capital costs, construction time, and operational and maintenance cost. The AP600 primary system has a four cold leg, two hot leg configuration (see Figure 1) and operates with a lower power density than standard PWRs to provide more margin. Also, injection flow is directly into the reactor vessel (Direct Vessel Injection) so that less cooling water would be lost through a cold leg break, making the passive safety systems more effective.

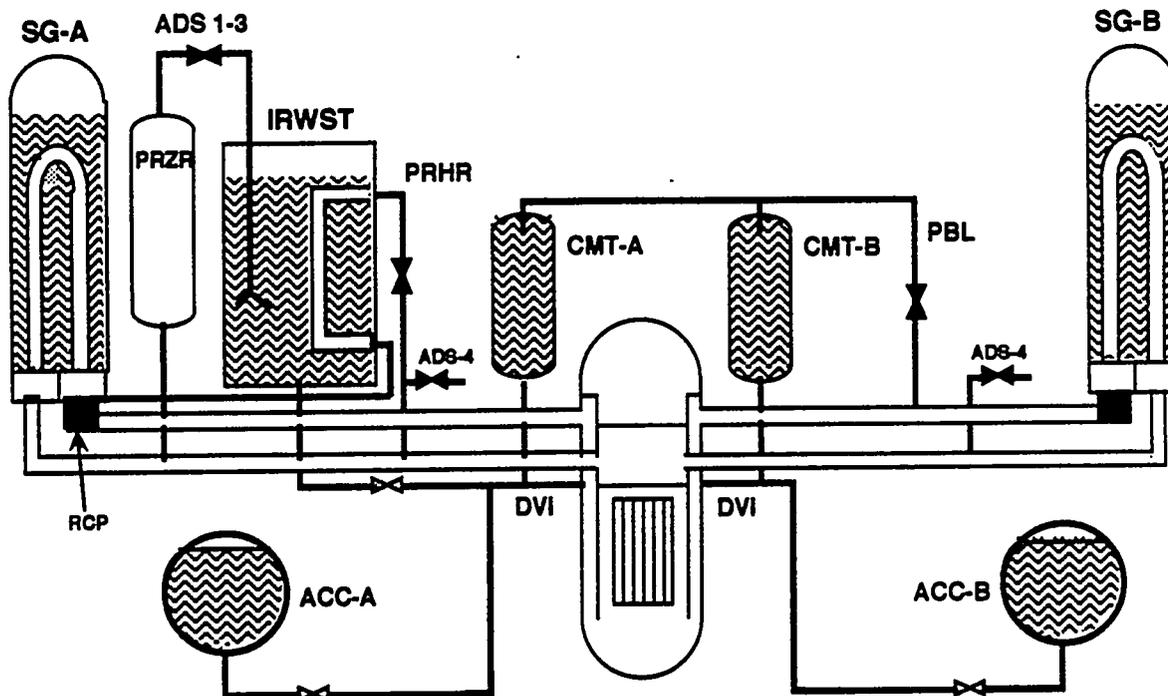


FIGURE 1: Schematic of AP600 primary system and passive safety features.

The unique features of the AP600 design are the use of a safety grade passive core cooling system and a passive containment cooling system. In the interests of allowing adequate depth of coverage of the subject area without excessive length, this paper will concentrate on the passive core cooling systems with only a cursory description of modeling needs for the containment cooling system. The passive core cooling systems are comprised of:

- Core Make-up Tanks (CMT): two full pressure tanks using gravitational potential to provide borated make-up water to the primary system in a loss of coolant transient (passive version of HPSIS).

- Accumulators: two gas pressurized accumulators discharging water at high flowrate in event of a large break LOCA (as in standard PWRs).
- Automatic Depressurization System (ADS): comprised of valves arranged in four stages, the first three stages connect from the vapor space in the pressurizer and blowdown through a sparger into the IRWST (see below), the fourth stage is connected to each of the two hot legs and discharges directly into the containment.
- In-Containment Refueling Water Storage Tank (IRWST): a very large tank situated high in the containment (relative to the core) to provide long term gravity fed cooling water to the core (passive version of LPSIS). In addition contains the ADS1-3 sparger and the PRHR (see below) heat exchanger.
- Passive Residual Heat Removal System (PRHR): a C-shaped heat exchanger submerged in the IRWST that removes decay heat during loss of steam generator inventory.

The above passive core cooling components are complemented by a passive containment cooling system that provides for the rejection of decay heat to the environment by transfer through the containment walls using in-vessel condensation and ex-vessel film evaporation and natural convection cooling.

Small Break LOCA Scenario

A typical small break LOCA scenario is described below to give the background necessary to better comprehend the discussion of component behavior and phenomena given in the subsequent section. A small break LOCA was chosen to illustrate the behavior of the new passive systems; it should be understood that the phenomenology for a large break LOCA is considered to remain substantially unchanged and that all of the associated modeling requirements are also required for the analysis of passive systems.

Figure 2, see below, illustrates the primary system pressure history expected to occur in a typical SBLOCA and illustrates the three distinct phases of the transient: the high pressure phase, ADS blowdown phase, and long term cooling phase. The long term cooling phase can be further subdivided into the IRWST injection and sump injection phases. Sump injection would occur many hours into the transient when the level in the sump has risen a meter or so above the cold legs.

In the initial part of the high pressure phase, the system pressure falls rapidly as the pressurizer drains; soon after a low pressure signal results in reactor scram, the steam generators are "bottled up", the CMT & PRHR isolation valves are opened, and the reactor coolant pumps are tripped. Upon equilibrating with the secondary pressure, the normal SBLOCA pressure plateau is not observed as the primary pressure continues to decrease as a result of the energy removal by the PRHR operation and CMT recirculation (cold water from the CMTs enters the primary system replacing hot water circulated to the top of the CMTs). When either the system pressure or inventory has decreased enough, the CMTs begin to drain, that is the circulation loop is broken and vapor displaces the CMT water. During this high pressure phase, little voidage occurs in the core, due largely to the efficacy of the PRHR, and the two-phase mixture level remains in the upper plenum.

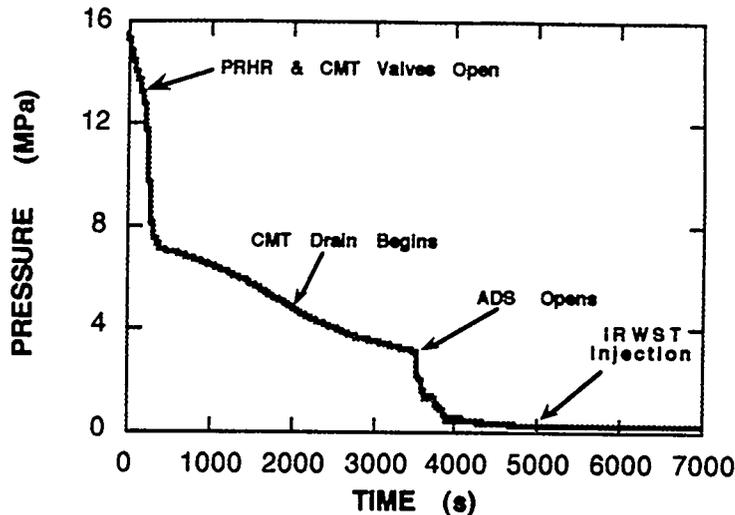


FIGURE 2: Pressure history during a small break LOCA.

When the CMT level reaches a setpoint, the actuation signal for ADS1-3 is given and a controlled blowdown commences. As the system pressure falls, vigorous accumulator injection occurs, and the core returns to a subcooled condition. As the accumulators empty, the CMT levels resume falling and the setpoint for ADS4 is reached. The ADS4 valves open at a relatively low system pressure (several atmospheres) and finish the depressurization of the primary system. After ADS4 opens, a combination of flashing and core boiling begins to decrease the core inventory.

The long term cooling phase is considered to start when the system pressure is low enough that gravity fed injection from the IRWST begins. The injection of subcooled water from the IRWST causes the vaporization to decrease, the core inventory to recover and return once again to a subcooled state. The minimum core collapsed liquid level occurs shortly about the time of the onset of sustained IRWST injection, however, the core remains covered (for all SBLOCA tests performed to date except for massive multiple failures of ADS4), and is in a subcooled condition for much of the transient. Eventually, sometime before sump injection begins, the core returns to a saturated condition and boiling recommences, exhausting a two-phase mixture out of ADS4 and recycling the effluent either to the IRWST (condensate from containment walls) or to the sump (liquid from ADS4 and break).

Although the above SBLOCA scenario does not appear to threaten core coolability - indeed, heatup is not even expected to occur - there have been concerns as to the performance of the passive safety systems, specifically:

- the potential for interaction either between the passive systems themselves or between non-safety active systems and the passive systems to decrease flows to the reactor vessel
- the possibility for non-limiting transients (steam generator tube rupture or main steam line break) to activate the ADS thereby precipitating a LOCA

- the passive systems drive flows with small heads, consequently requiring more precision in the analysis compared to active systems and raising the question as to whether the same confidence can be placed in the analysis methods for passive plants as compared to current plants with active systems.

To address these questions, separately, Westinghouse and the USNRC (in a confirmatory role) have conducted integral facility tests using the AP600 configuration in three different facilities. In concert with this experimental program, the USNRC together with its contractors is conducting a comprehensive code assessment program using the RELAP5 code to assure its applicability to perform auditing calculations of the licensee's submittal. This assessment effort is ongoing, however, in applying RELAP5 to the AP600 system, much has been learned about the analysis needs of passive systems. It is hoped that the following discourse can provide insight into these needs.

AP600 COMPONENTS & PHENOMENA

Rather than discuss phenomena that need to be modeled in the abstract, each important phenomena is discussed below in the context of the component and phase of the transient for which it is deemed important.

PRHR/IRWST: Heat Transfer & Thermal Stratification

The Passive Residual Heat Removal System (PRHR), as its name implies, provides for the rejection of decay heat from the reactor core via a natural circulation loop with the In-Containment Refueling Water Storage Tank (IRWST) serving as the heat sink. This system is of primary importance for transients where the steam generator heat sink is lost, such as station blackout, to provide for heat removal without A/C power. However, it can also play a significant role during an SBLOCA transient, helping to depressurize the plant by energy removal without inventory loss and to maintain core inlet subcooling.

During PRHR operation, the highest heat transfer rates occur near the heat exchanger inlet, where the primary fluid is the hottest, giving rise to nucleate boiling on the tube exterior and hence the limiting thermal resistance is due to the turbulent convection within the tube. As the primary fluid cools during its passage through the PRHR, the exterior cooling mode transitions from nucleate boiling to single-phase natural convection and the internal and external heat transfer resistances are then of the same magnitude. Within the IRWST, in the vicinity of the PRHR bundle, a buoyant plume is formed (see Figure 3), both enhancing the convective heat transfer coefficients on the tube exterior and entraining cold water from the tank into the PRHR bundle as heated water rises to the surface. The core inlet subcooling is directly affected by this recirculating flow within the IRWST as it both reduces the sink temperature and lowers the thermal resistance at the PRHR exit. If a simple 1-D axial stack of control volumes is used to model the IRWST, the effects of this recirculating flow are absent, and the PRHR outlet temperature will be over-predicted by 20-50° K.

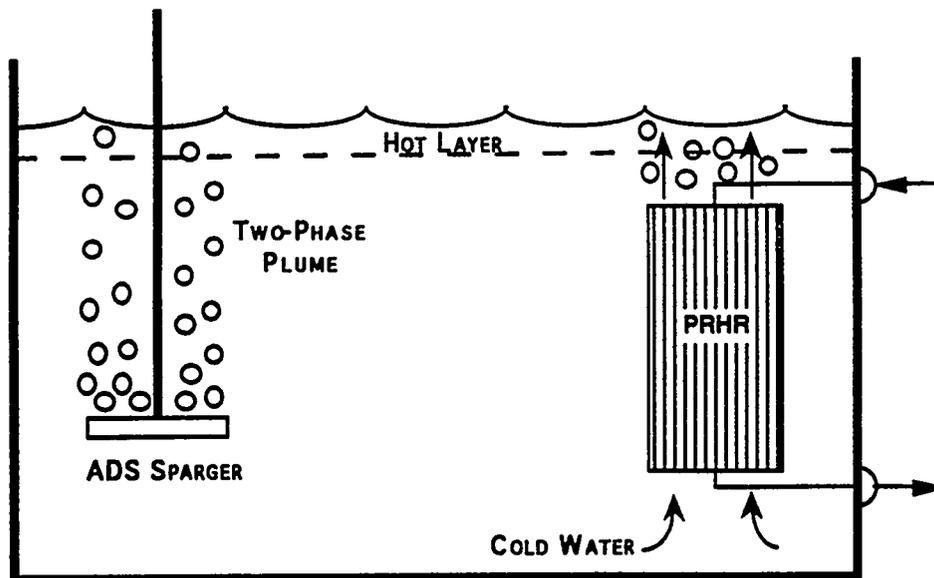


FIGURE 3: Schematic of the IRWST illustrating buoyant plumes caused by PRHR heat transfer and ADS sparging.

During actuation of the ADS system, a high quality two-phase mixture is injected into the IRWST through the ADS sparger. Rapid condensation ensues as the pool subcooled water is entrained into a rising two-phase plume, forming a hot layer at the pool surface that migrates downward as ADS continues. It is important to allow for this heated liquid to rise to the pool surface for three reasons. First, if a simple 1-D stack is used, then the control volume at the sparger elevation can saturate - especially for a transient such as inadvertent actuation of the ADS system - and the resulting expansion as the volume becomes two-phase can force large amounts of water to overflow the IRWST. Secondly, thermal stratification within the tank keeps the water at the lower levels cold so that when the IRWST injection phase begins, the water provided to the vessel is significantly subcooled. Finally, evaporation of the hot layer on the pool surface occurs adding a vapor source to the containment.

It is of primary importance to have a modeling capability for the IRWST that allows for convection of the heated liquid to the pool surface and the consequent thermal stratification. Whereas, predicting the exact structure of the plumes or the velocity profile within the PRHR bundle is relatively of less importance. It is clear, however, that a single lumped volume or a 1-D axial stack of mesh cells is unacceptable. Either some form of multi-D model or a special component model is needed. While a multi-D model is possible, it may be complicated by the need to implement a different flow regime and interfacial transfer package; for example, it is obvious that neither slug nor annular flow can exist in a volume located in the middle of a large tank. Also, for a reasonable number of computational volumes, the resulting cells can have aspect ratios orders of magnitude less than unity and negligible wall friction giving rise to numerical difficulties. An alternative would be to develop a special purpose component model, blending numerical and analytical models for the physical processes expected to occur in the tank.

Core Make-Up Tank: Mixing & Thermal Stratification

The proposed AP600 design contains two Core Make-Up Tanks (CMTs) to passively provide for inventory replenishment at high pressure and the injection of borated water into the primary coolant system. In addition, the CMT level serves as the actuation signal for the ADS system. Sensitivity studies have indicated that the minimum vessel inventory is somewhat insensitive to the CMT level (and hence time) at which ADS1-3 is triggered for a small break LOCA; a change in predicted inventory of only 10% for a change in ADS timing of 1000 seconds. Consequently, plant safety studies may not require highly accurate modeling of the processes which occur within the CMTs.

However, assessment of our computational models against test data from scaled AP600 integral facilities does require that the transient be reproduced with a high degree of fidelity so that important phenomena can be assessed over the appropriate parameter ranges. Also, many of the processes that occur within the CMT, e.g., the reduction of interfacial condensation due to the buildup of a buffer layer of saturated water, will be mirrored in the other systems. For these reasons, a fairly extensive discussion of CMT phenomena is given below.

Initially, the CMTs are filled with cold, relative to the reactor coolant operating temperature, borated water. Pressure balance lines from the cold legs are provided to keep the CMTs at the primary system pressure while isolation valves prevent injection of the CMT water. During a small break LOCA, these isolation valves are opened during the high pressure phase of the transient. At this time, the cold legs are still in a single-phase condition and a buoyancy driven flow, denoted as "CMT recirculation", convects hot water from the primary system to the top of the CMTs and injects cold CMT water into the primary system through the Direct Vessel Injection (DVI) nozzles, as illustrated in Figure 4, see below.

Within the CMTs, the superficial liquid velocity is on the order of a few millimeters per second, so that the addition of hot water on top of the initial cold inventory leads to the development of a thermal front. Figure 5 shows a comparison of the predicted and measured CMT axial liquid temperature profile at 2000 seconds during a small break LOCA in the ROSA test facility. In this RELAP5 calculation, the thermal front tracking model was turned off and the artificial diffusion resulting from the first order accurate upwind differencing scheme is readily apparent. Minimizing this artificial diffusion can be important for two reasons: first, the temperature in the cold layer at the bottom of the tank directly affects the core inlet subcooling, and second, the temperature in the hot layer can, as the system pressure continues to fall, lead to flashing and draining of the CMT. The phenomena occurring within the CMT are treated in more detail below, however, it is evident that some means to improve the prediction of a thermal front is needed, either a higher order differencing scheme for the liquid energy equation or a sub-grid resolution model (as is currently available in RELAP5) if a fixed Eulerian grid is used, or a special component model employing a Lagrangian scheme for fluid layers at different temperatures.

Having a numerical scheme that is capable of resolving (and not diffusing) a strong thermal gradient is one requirement for modeling the CMTs, but a number of other phenomena occur as well both during the recirculation phase (see Figure 6) and the draining phase (see Figure 8). As the hot fluid enters the CMT, there is a large temperature difference between the fluid (near initial operating temperature) and the walls (containment temperature). A convection current develops due to the wall heat transfer transporting the colder "near wall" fluid to a mixing region that develops

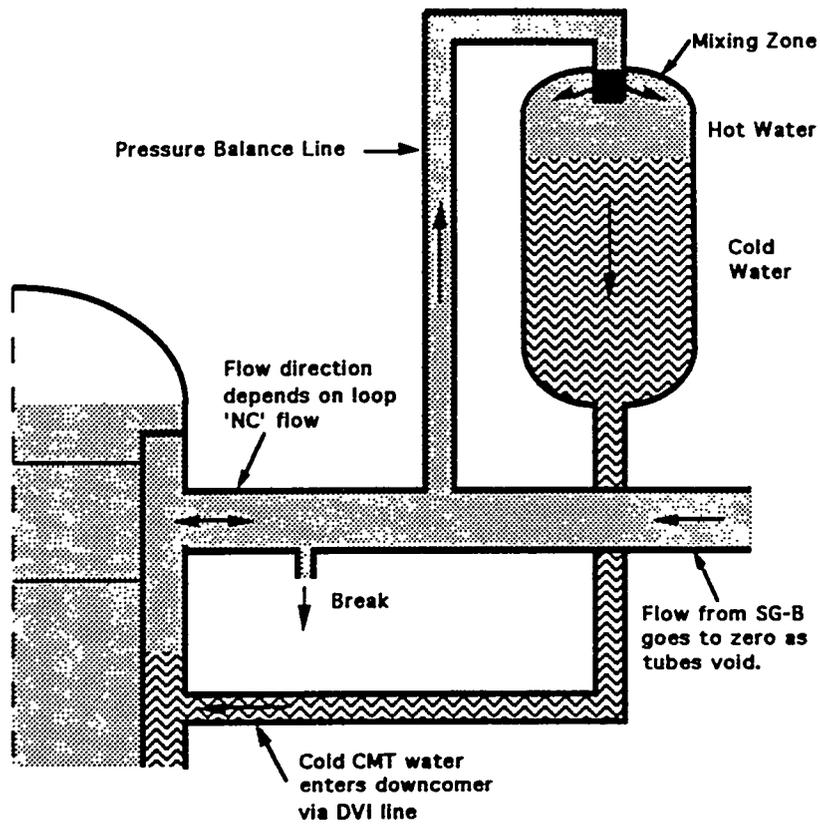


FIGURE 4: Schematic of reactor vessel and CMT during recirculation phase.

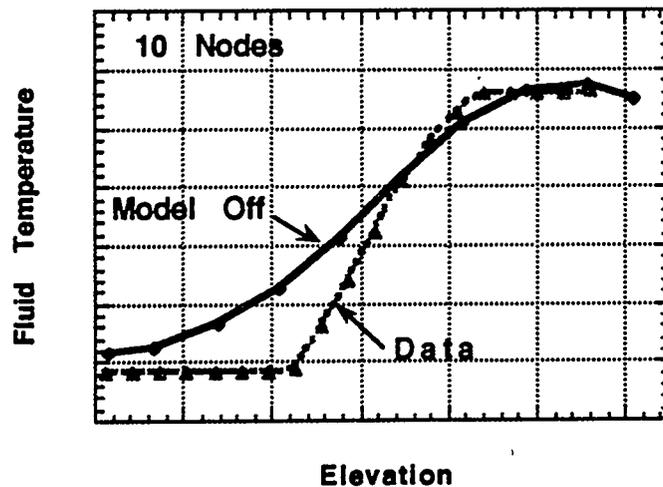


FIGURE 5: Example of artificial diffusion in the prediction of CMT axial liquid temperature profile for a SBLOCA in ROSA test facility.

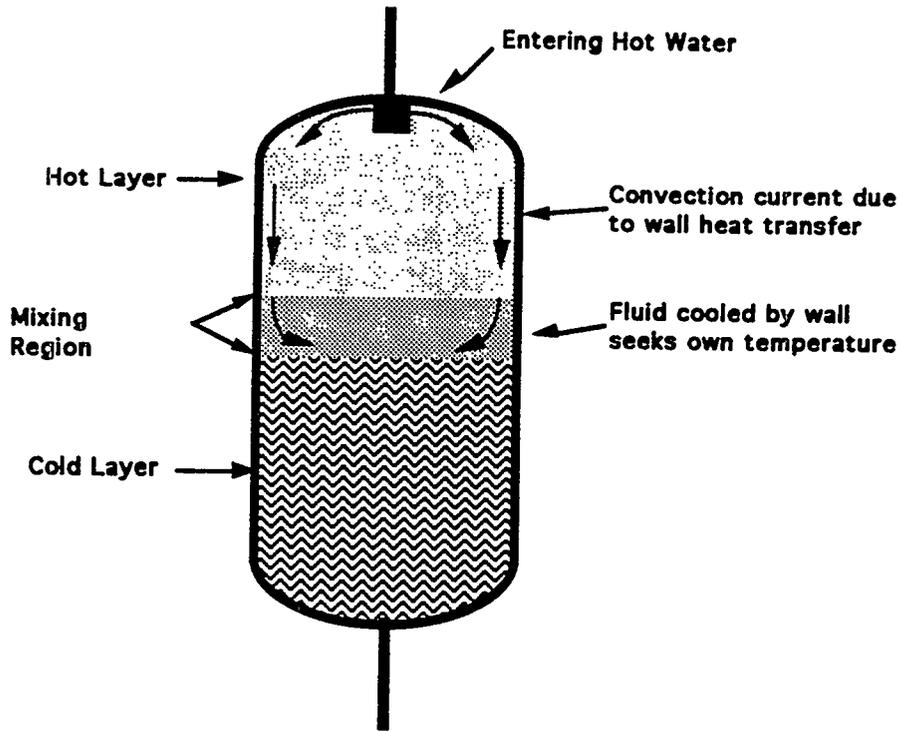


FIGURE 6: CMT phenomena during the recirculation phase.

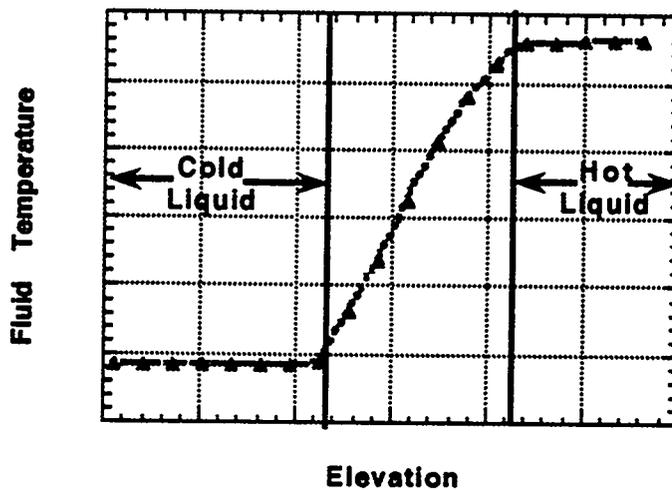


FIGURE 7: Example of measured CMT axial temperature profile depicting three distinct fluid regions.

between the "hot" and "cold" layers. An example of this behavior is given in Figure 7 which clearly shows the existence of three distinct fluid regions. Later in time, the temperature of the liquid in the primary system (and hence in the pressure balance line) will have decreased below that of the liquid at the top of the CMT, provision also needs to be made for this colder fluid falling through the hot layer and joining the fluid in the mixing region.

Eventually, the CMTs will begin to drain. The initiation and sustenance of CMT draining is governed by the availability of a vapor source to displace the liquid. Two mechanisms can provide this vapor source: the hot layer at the top of the CMT can flash as the primary pressure falls below saturation for its temperature (as depicted in Figure 8 below), or the primary system itself can begin to void, allowing vapor to travel from the cold leg up the pressure balance line to the CMT. In either case, the existence of the hot fluid layer now plays a key role as a buffer zone between the cold liquid and the vapor source inhibiting interfacial condensation.

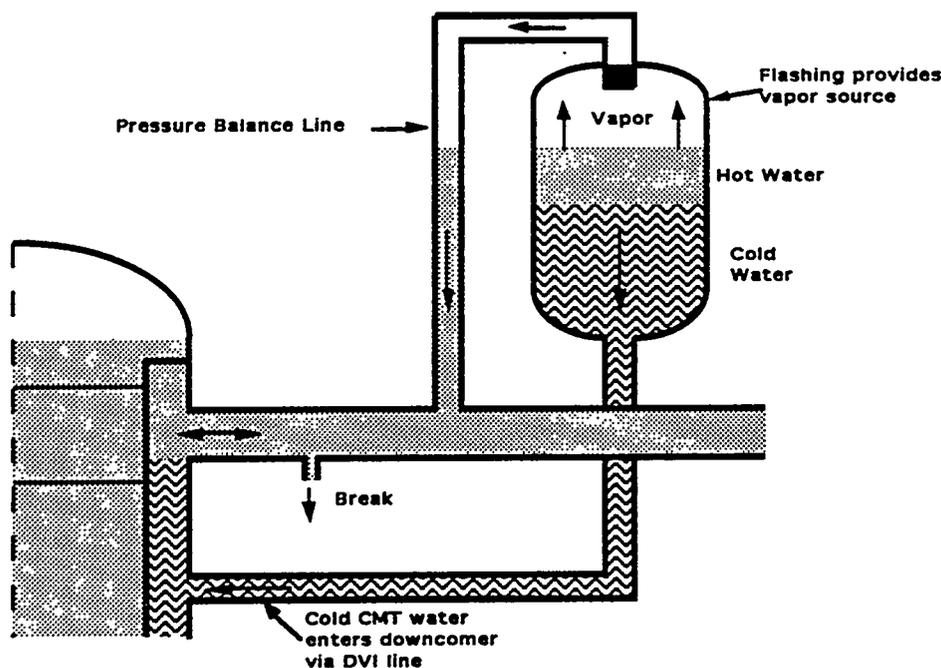


FIGURE 8: Schematic of reactor vessel and CMT during draining phase with internal CMT flashing providing the vapor source.

As the break size increases, the CMT recirculation phase shortens so that a CMT could drain in a cold state and interfacial condensation could be significant until a buffer layer of saturated water is built up by the condensate. Providing a reasonably accurate description of this condensation rate is necessary as condensation can hold up the CMT level and delay its reaching the setpoint for ADS actuation. Associated with the establishment of this buffer layer is the problem of tracking it as it passes through a fixed Eulerian mesh. If, as is usually done in two-fluid codes, the bulk liquid temperature in a cell is used as the driving potential for interfacial heat transfer, then

as the level passes a cell boundary, the bulk liquid temperature changes and interfacial condensation can follow a step-wise behavior. This can be minimized through the use of a large number of mesh cells for the CMT, however, it would be more efficient and physically correct to provide either a sub-grid resolution scheme or a Lagrangian mesh to track the buffer layer.

At the same time, as the CMT walls become progressively more uncovered there is a potential for wall condensation as, despite any warm-up due to convection from the hot liquid layer, the CMT walls are thermally thick and can remain a significant heat sink. It is not critical to predict the exact magnitude of the condensation heat transfer coefficient because the Biot no. would be much greater than unity and the heat transfer rate limited by conduction within the wall. However, it is necessary to specify what fraction of a mesh cell is uncovered and only compute condensation heat transfer on the appropriate surface area. So, once again, some form of sub-grid resolution or Lagrangian scheme is needed. Also, because the condensation heat transfer rate is governed by conduction within the CMT walls, the mesh spacing used for the wall conduction solution now becomes important and normal user guidelines for a pipe wall are inadequate. Leaving this specification to the user can contribute to the "user effect". It would be beneficial to provide either an advanced conduction solution (perhaps finite element or adaptive grid) or an automatic mesh selection to minimize the user effect.

In summary, to accurately model the processes occurring within the CMTs, a computational tool should have the following capabilities:

- **Thermal Front Tracking:** ability to resolve steep temperature gradients within the liquid in the flow direction and use the temperature of a buffer layer in the interfacial heat transfer model.
- **Mixture Level Tracking:** ability to track the liquid/vapor interface, correctly model the interfacial transfer phenomena for a stratified surface, and partition wall heat transfer appropriately.
- **Thermal Stratification & Mixing:** provide for the accumulation of hot liquid in a buffer layer due either to convection or condensation, and provide for a mixing region that grows due to the addition of colder water either from wall heat transfer effects or convection from the PBL.
- **Wall Conduction:** provide an accurate solution of the transient conduction within the CMT walls that is not sensitive to user specification of mesh spacing.

Cold Legs: Thermal Stratification

Due to the efficacy of the passive safety systems, there exists the potential for cold leg thermal stratification to occur as very cold water is returned to the primary system. As in the studies of Pressurized Thermal Shock (PTS), it was found that if natural circulation through the steam generators persists, then the cold fluid will be thoroughly mixed with the primary coolant preventing stratification. However, if the steam generator tubes void and the loop flow stagnates, then thermal stratification will occur.

In the ROSA SBLOCA tests, as much as a 180° K temperature difference between the top and bottom of the cold leg was observed for the loop containing PRHR injection. This large value is thought to be atypical of the AP600 design and rather be an artifact of a geometrical distortion in the ROSA facility due to the presence of a (reduced height) loop seal and the injection of the PRHR return flow into the loop seal rather than into the steam generator outlet plenum as in the AP600 design. For similar size scaled breaks in the OSU/APEX facility, the injection of the PRHR water into the steam generator outlet plenum prevented early stagnation of the loop flow and thermal stratification was not observed in the PRHR side cold legs.

However, on the other side of the plant, that is the side containing the CMT pressure balance lines, there is still the potential for the loop flow to stagnate and for thermal stratification to occur. During the ROSA small break LOCA tests, the situation depicted in Figure 9 was observed with a consequent level of thermal stratification of 100° K. Here, the lower plenum and downcomer have filled with colder water, from the PRHR return, that spills over into the CMT-side cold leg. For this test, the break was located on the bottom of the cold leg and became highly subcooled after thermal stratification developed whereas the pressure balance line continued to siphon off nearly saturated water from the top of the cold leg.

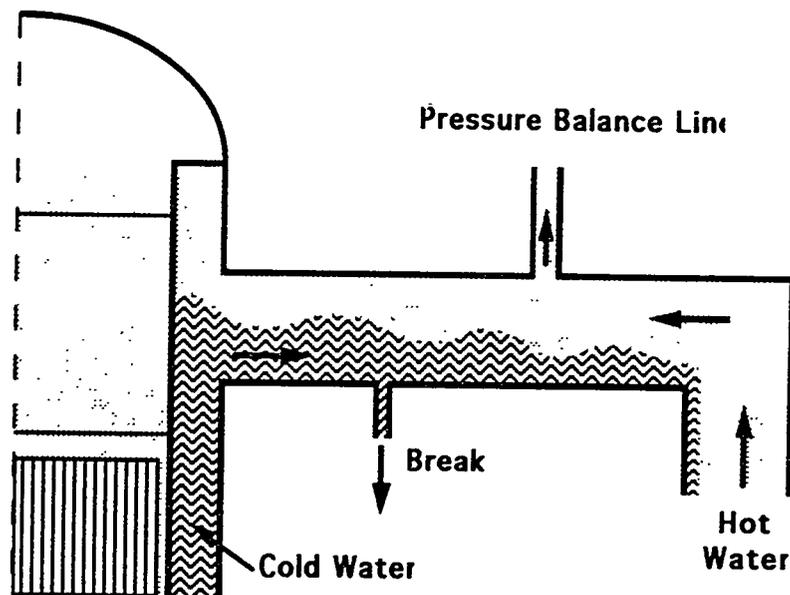


FIGURE 9: Schematic of reactor vessel and cold leg illustrating thermal stratification and its effects on the break and PBL temperatures as observed in ROSA small break LOCA tests.

Although the overall system thermal-hydraulic behavior was noticeably affected by the occurrence of cold leg thermal stratification in the ROSA facility, the effects were not overwhelming. That is, despite a 1-D representation of the cold legs, RELAP5 calculations of this test compared very well with the key performance parameters such as core collapsed level. However, for a realistic description of the local phenomena

occurring within the cold leg, some provision for thermally stratified fluid layers flowing either cocurrently or counter-currently would be necessary.

A simple approach to this problem might be to split the cold leg into two 1-D horizontal pipes, one over the other, that communicate via cross-flow junctions. While the two-pipe approach allows for some aspects of thermally stratified flows to be simulated, it clearly does not capture all of the physical phenomena correctly. This is especially the case if conditions within the pipe become two-phase. Although not a high priority item, it would be useful to have the capability for modeling pipes with either a 2-D (horizontal layers) or even 3-D mesh so that the effects of thermal stratification in passive systems could be examined in detail and PTS studies could be conducted using only one code as opposed to using RELAP5 results as boundary conditions to a mixing code. In addition to the numerical complications raised by such a capability, a model for turbulence within the liquid, and either the development of an interfacial package that would be applicable to discretized elements within a pipe or a scheme for collapsing the mesh back to a 1-D representation when two-phase conditions prevail would be needed.

ADS1-3 / Pressurizer: Critical Flow & Phase Separation

The first three stages of the Automatic Depressurization System are designed to provide for a controlled depressurization transient to a low enough system pressure that inventory can be replenished by the accumulators or ADS4 can be opened and IRWST injection begun. Additionally, it is desirable to maximize the energy loss while retaining as much mass in the system as possible. In the AP600 design, this is accomplished by taking the ADS1-3 off-take from the top of the pressurizer. Consequently, the mass and energy outflows during ADS1-3 actuation are governed by critical flow at the ADS valves and by phase separation in the pressurizer which affects the upstream quality.

The usual approach to describing critical flow in a two-fluid code is to evaluate the characteristic velocities directly from the two-fluid equations. This approach requires that the conditions at the "throat" be known, especially the degree of thermal non-equilibrium present. Describing the flow of a two-phase mixture in a geometry as complicated as the internals of a globe valve and trying to integrate the energy equations over a thermodynamic path to get the throat conditions would be extraordinarily difficult, if not impossible, as one cannot even define the shape of the interface much less the transport processes occurring there. This is particularly important for flow conditions very near the single-phase to two-phase transition, where thermal non-equilibrium effects can increase the critical flow rate by 100% to 500% above the equilibrium value. Instead, one could make a simplifying assumption, such as homogeneous equilibrium at the throat, and then conduct bounding calculations to account for the uncertainties. Alternatively, it would be desirable to have available as an option an empirically based critical flow model that would be flexible enough so that the results of valve characterization tests could be accounted for.

Of equal import to the correct calculation of the transient progression is the phase separation that occurs upstream of the ADS system, especially within the pressurizer. Upon ADS actuation, the pressurizer would normally be empty, so that the two-phase mixture entering from the surge line can separate primarily allowing single-phase vapor to be convected to the ADS valves. As the ADS blowdown phase continues, the pressurizer begins to fill and some liquid fraction is carried over to the ADS system, affecting not only the critical flow through the valves but also the inventory stored in

the pressurizer. Later in time, after the ADS4 valves have opened, this pressurizer inventory represents a large volume of water with a gravitational potential relative to the core, in effect becoming part of the passive ECCS system.

ADS4 / Hot Legs: Critical Flow & Off-Take

The ADS4 system is designed to take the primary system pressure low enough that gravity driven injection from the IRWST can provide for effective removal of the core decay heat. Once the system arrives at this state, the reactor vessel and containment act together as a two-phase natural circulation system with boiling occurring within the core, a two-phase mixture exhausted out of ADS4, condensation occurring on the inside surface of the containment vessel, and the condensate being returned to the IRWST. During this phase, the core flow rate is governed by the balance between the gravitational potential of the IRWST and the pressure losses associated with the venting of the two-phase mixture through the ADS4 valves.

For the ADS4 system then, it is important to be able to accurately predict not only the critical flow rate but also, later in time when the valves are unchoked, the two-phase pressure drop through the valves. The subject of critical flow in valves was discussed above and will not be re-iterated here except to note that the upstream pressure conditions for ADS4 can approach atmospheric and the critical flow model must be applicable at these low pressures². As for two-phase losses, the model present in the code must be flexible enough so that the losses in both valves and orifices (both abrupt and smooth entry are used in integral experiments to model ADS4) can be accurately calculated over a wide range of qualities at low pressure.

Finally, as was the case for ADS1-3, the quality of the flow convected to the ADS4 valves is important for determining the flow rate out of the primary system. Here, the quality is largely determined by the off-take from the top of the hot leg. For example, when the flow regime in the hot leg is predicted to be stratified, RELAP5 invokes a "horizontal-stratified-entrainment" model to determine what liquid fraction is convected out of a vertical off-take. Correct prediction of the conditions entering the ADS4 off-take then require: the correct prediction of the onset of stratified flow in the hot leg, and an off-take model that is applicable to both the range of pipe diameters in the experimental facilities and scalable to the AP600 design.

Downcomer: Mixing & Condensation

During PRHR operation the cold PRHR return flow is injected into the hot water of the downcomer via the cold legs. A negatively buoyant plume is formed, see Figure 10, and a recirculating flow pattern is induced where hot water rises counter-current to the plume. Local fluid velocities can be as much as ten times higher than the superficial liquid velocity, hot water is entrained in the falling plume spreading it, and the fluid is

² A flaw in the derivation of the choking criteria for the standard RELAP5 critical flow model can become evident at low pressure if the liquid and vapor phase velocities are not forced to be equal. This, and the need to include thermal non-equilibrium effects for the very thin orifice plates used in experiments, led to the implementation of the Henry-Fauske model as an option.

thoroughly mixed. So that by the time the falling plume reaches the bottom of the downcomer, the initially large azimuthal temperature differences have become only a few degrees K. This phenomena is of considerable importance in the analysis of the AP600 design as it reduces the propensity of the plant to operate in an asymmetric fashion. Note, that much of this and the subsequent discussion is also true for injection of cold water through the DVI nozzles.

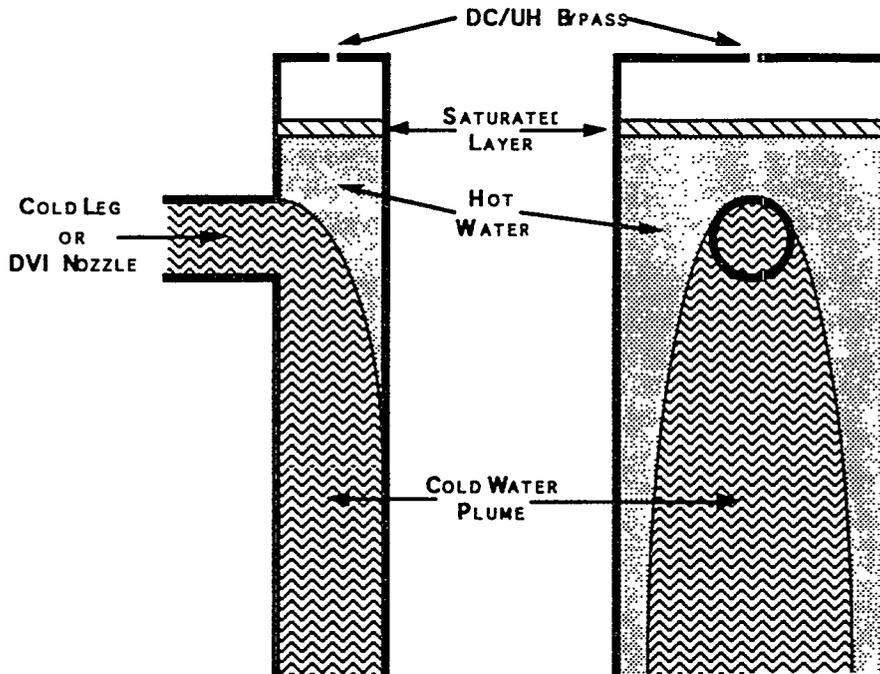


FIGURE 10: Schematic of downcomer showing negatively buoyant liquid plume and saturated buffer layer limiting interfacial condensation.

If the downcomer is well mixed, it would be reasonable to assume that it could be reasonably well modeled as a 1-D stack of mesh cells. However, this is not possible due to the "two-sidedness" of the AP600 design (the loops containing the PRHR on one side, and the loops containing the CMT pressure balance lines in the other). Consequently, a 2-D downcomer model is needed that allows buoyancy induced recirculation and mixing. Fortunately, both simulations of the CREARE downcomer mixing tests and comparisons to the results of CFD codes have shown that a very coarse description of the downcomer, about eight azimuthal sectors, is sufficient to capture most of the important flow features.

However, it is of equal importance to allow for the formation and maintenance of a saturated buffer layer between the incoming cold water and the vapor space in the upper downcomer that is connected via the upper head/downcomer bypass nozzles to the vapor source in the upper head. If the flow field solution artificially convects the injected cold water above its source, enhanced condensation can result. This bad situation can be made much worse if, due to the level crossing a cell boundary or some other perturbation, the flow regime in a cell at the top of the downcomer is predicted to transition from a stratified interface, where the interfacial heat transfer coefficient is small, to a two-

phase regime with a large interfacial heat transfer coefficient. The ensuing condensation spike can disrupt core flow and produce large oscillations in the core void fraction.

The above described "condensation event" can plague passive reactor calculations where the driving heads are due to gravitational potentials (and hence are small), and the system operates at low pressure where the liquid/vapor density ratio is huge. The prevention of such events must be a primary concern. However, the accurate prediction of the condensation rate at such an interface is relatively of negligible importance as - the physical situation being stably stratified - the real condensation rate is minuscule. This holds true as long as the liquid/vapor interface does not fall to the level of the injection point of the cold liquid where, of course, rapid condensation would be expected to occur.

Core: Boiling & Void Fraction at Low Pressure

In the AP600 design, the primary system pressure during the low pressure phase is on the order of 2 atmospheres. While in the OSU test facility, the combination of atmospheric backpressure (no containment) and 1/4 height scaling can lower this pressure to about 1.2 bar. At this pressure, the ratio of liquid to vapor phase density is more than 1300! Consequently, relatively small amounts of boiling can displace large amounts of water. In the discussion below, some of the mechanisms that were found to adversely affect the core vapor generation rate leading to void fraction oscillations are described. The ALWR code development effort identified and implemented improvements in RELAP5 to minimize these oscillations.

In early calculations of one of the SBLOCAs in the OSU facility, very large discrepancies between the calculated and measured core collapsed levels were observed. During this phase of the calculated transient, the net core flow rate was small (corresponding to a liquid velocity on the order of a few cm/s) and the liquid temperature was near saturation. The core heat input corresponded to about 1% of nominal power, so one would expect the core to resemble a large pot of water that is slowly boiling. Instead, the RELAP5 predicted flow pattern indicated a vigorous two-phase flow recirculation either within the core region or between the core and the lower plenum. Indeed, the magnitude of these recirculating flows was clearly unphysical with both liquid and vapor velocities on the order of 10 m/s directed upwards on the core periphery and flowing downwards in the central region of the core.

At that time, the RELAP5 input model for the OSU facility contained multiple parallel stacks, connected by cross-flow junctions, for both the core and upper plenum. It was demonstrated that some flaw in the formulation of the momentum flux terms in RELAP5, under certain circumstances, could lead to the growth of perturbations so that unphysical recirculating two-phase flows could develop. Basically, an unphysical momentum source may be present and can accelerate a nearly quiescent two-phase mixture until frictional forces are large enough to balance the momentum source. Consequently, until such time as this flaw can be eliminated from RELAP5, the core and upper plenum nodalizations of the AP600 plant and experimental facilities were changed to be one-dimensional axial stacks of computational volumes. After this nodalization change, the large discrepancy between measured and calculated core collapsed levels disappeared, however, some discrepancies remained as discussed below.

For an SBLOCA in the AP600 design, after the ADS-4 valves open, a short blowdown ensues followed by a relatively quiescent boil-off transient until IRWST injection is

sufficient to recover the vessel inventory. Figure 11 depicts the RELAP5³ calculated trajectory of the core collapsed liquid level during this period for an SBLOCA transient in the OSU test facility using the 1-D core nodalization. Significant events are indicated and the chronological sequence was much the same as observed in the experiment with the core remaining covered at all times and the minimum core collapsed level occurring at about the time of IRWST injection. However, relative to the measured core collapsed level (not shown), the predicted level was significantly under-predicted, that is, RELAP5 calculated too much voidage in the core. Also, another feature of interest in this figure is the "numerical noise" observed in the calculation: a variation of about 0.2-0.3 in the core collapsed level which is large enough to obscure potential physical oscillations. The cause of the remaining over-prediction of core void fraction and some of the driving forces behind this numerical noise are discussed below.

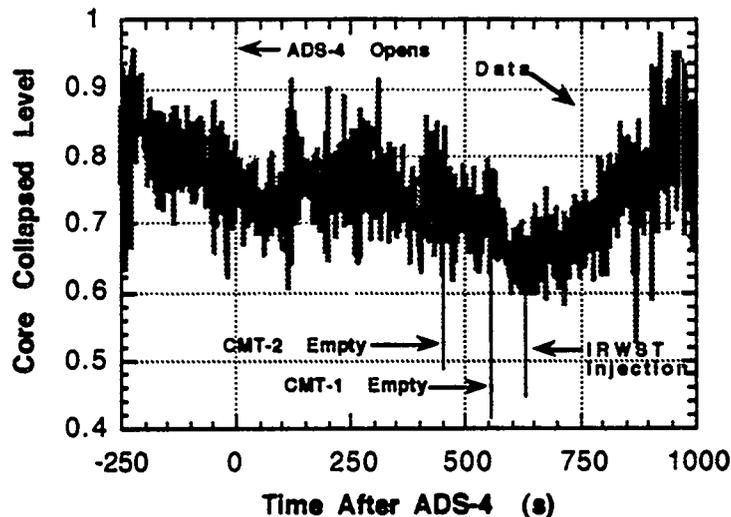


FIGURE 11: Early RELAP5 calculation of core collapsed level for an SBLOCA in the OSU facility illustrating "numerical noise".

Examining the over-prediction of core voidage first, it was determined that this was primarily due to an under-prediction of the core inlet subcooling. The RELAP5 calculated value was essentially saturated, whereas the experimental values exhibited a significant level of subcooling. In turn, this was traced to flow recirculation and oscillations in the downcomer that caused the subcooled water injected via the DVI ports to be convected upwards to the node containing the two-phase mixture level so that downcomer condensation was greatly enhanced. It was determined that a major source of the flow recirculation was due to the momentum flux problem discussed above for the core. However, as noted above in the discussion of downcomer mixing, a two-dimensional

³ These calculations were performed with a developmental version of RELAP5, one that does not have the improvements for low pressure boiling, and are presented here to illustrate potential code difficulties.

representation for the downcomer is needed, so the “fix” used for the core could not be applied here. Instead, the unphysical recirculations were eliminated by removing the momentum flux terms from the downcomer junctions. Subsequent calculations showed a greatly improved comparison for both the core inlet subcooling and the core collapsed liquid level.

However, the “numerical noise” illustrated in Figure 11 still remained, to investigate the driving forces behind this noise, let’s first examine the vapor generation rate in the core. The core was modeled using a 1-D axial stack of eight computational volumes. Figure 12 plots the RELAP5 calculated value for one computational volume for the time period after ADS-4 actuation using a sampling interval of one second. At this elevation, liquid subcooling has been lost and the heat input from the heater rods follows the exponential decay curve as is roughly indicated by Figure 12. However, large oscillations in the vapor generation rate, and hence the void fraction, are present in the calculation. What is the origin of these oscillations?

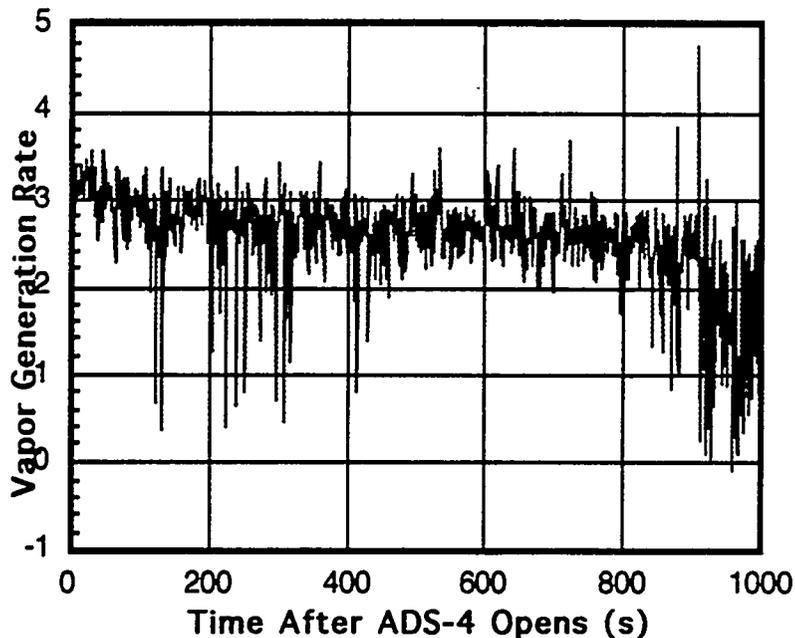


FIGURE 12: Early RELAP5 calculated value of vapor generation rate for one volume in the core during SBLOCA in OSU facility.

In a two-fluid code, such as RELAP5, the vapor generation rate is governed by the interfacial heat transfer using an equation of the form:

$$\Gamma = \frac{(h_{il} \cdot A_i) \cdot (T_l - T_{sat}) + (h_{ig} \cdot A_i) \cdot (T_g - T_{sat})}{(h_v - h_f)_{sat}}$$

For the fluid conditions of interest, the wall heat transfer serves to superheat the liquid phase and vapor is generated as a result of the interfacial heat from the liquid to the interface. In RELAP5, so-called “ad hoc” models were used for the superheated liquid

interfacial heat transfer coefficient for the slug and annular flow regimes. That is, from physical reasoning, it was supposed that these regimes could not maintain a significant level of liquid superheat and that it would be sufficient to use a large value for the liquid interfacial heat transfer coefficient in order to drive the liquid towards saturation. While making physical sense, this treatment of the liquid interfacial heat transfer coefficient does have pronounced numerical effects as follows.

In the definition of the vapor generation rate, the interface is taken to be at saturation corresponding to the bulk value of the vapor partial pressure for the computational volume. If the liquid interfacial heat transfer coefficient has a very large value, the calculated vapor generation rate is then very sensitive to the saturation temperature and consequently to small fluctuations in pressure (or in noncondensable quality). As small pressure perturbations abound in numerical calculations, the vapor generation rate and consequent void fraction cannot help but be extremely noisy. Furthermore, the introduction of very large values for the superheated liquid interfacial heat transfer coefficient in the annular and slug regimes results in a discontinuity across the saturation line as the subcooled value is about six orders of magnitude smaller. To "smooth" this discontinuity, a ramping function on the liquid superheat (or subcooling) is applied over the range ± 1 K. This, in turn, makes the interfacial heat transfer coefficient very sensitive to the superheat and hence to pressure fluctuations, etc. To reduce this sensitivity, the large "ad hoc" value of the super heated liquid interfacial heat transfer coefficient was removed and a physically based model implemented.

As the "numerical noise" level present in the calculation was reduced, other numerical driving mechanisms for oscillations were uncovered. One of these has to do with point of net vapor generation. For low heat flux conditions (on the order of 1 W/cm^2), the subcooled boiling model predicts negligible amounts of nucleate boiling until the bulk liquid temperature is very close to saturation. Indeed, for these conditions, the fraction of wall heat flux that produces vapor varies from essentially zero at a subcooling of about 0.5 K to unity as the liquid saturates, thereby acting as an "ON/OFF" switch. At low pressure with its attendant large vapor volumetric expansion, this switch can cause a computational volume (on the order of 0.5 meters in height) to rapidly transition from single-phase liquid to a void fraction in the slug flow regime, providing a numerical "geysering" effect. To avoid this problem, some method of tracking the point of net vapor generation within a computational volume is needed.

Yet another source of high frequency oscillations was uncovered when examining the results of low pressure and low power steady state boiling tests in rod bundles. For these conditions, the average liquid velocity was nearly stagnant (a few cm/s) with the vapor bubbles rising through it. In RELAP5, the bundle interfacial friction factor is derived from the EPRI drift flux model. As implemented in RELAP5, a discontinuity was present across the boundary between co-current upflow and counter-current flow. So, as the liquid velocity oscillated about zero, the interfacial friction factor varied by a factor of four, thereby causing void fraction oscillations. A ramping function was implemented between the two regimes to reduce this effect.

Finally, the question of accuracy in the calculation needs to be addressed. For SBLOCA analysis, the vessel inventory is used as a key parameter and this in turn is strongly influenced by the core interfacial friction. To examine the theoretical accuracy - without the effects of numerically induced oscillations - of the interfacial drag correlation used in RELAP5, the "predicted" void fraction for a steady state experiment can be calculated directly from the EPRI drift flux model (also known as the Chexall-Lellouche model) using input parameters determined directly from the experiment.

That is, input values such as liquid and vapor superficial velocities can be determined by performing a straightforward mass and energy balance. Figure 13 presents a comparison of predicted versus measured values for the core collapsed liquid level for a series of steady state low pressure and low flow boiling tests in a rod bundle at decay heat levels. For these conditions, which are similar to those expected in the AP600 during long term cooling, the EPRI void drift model would under-predict the core collapsed level by about 10%.

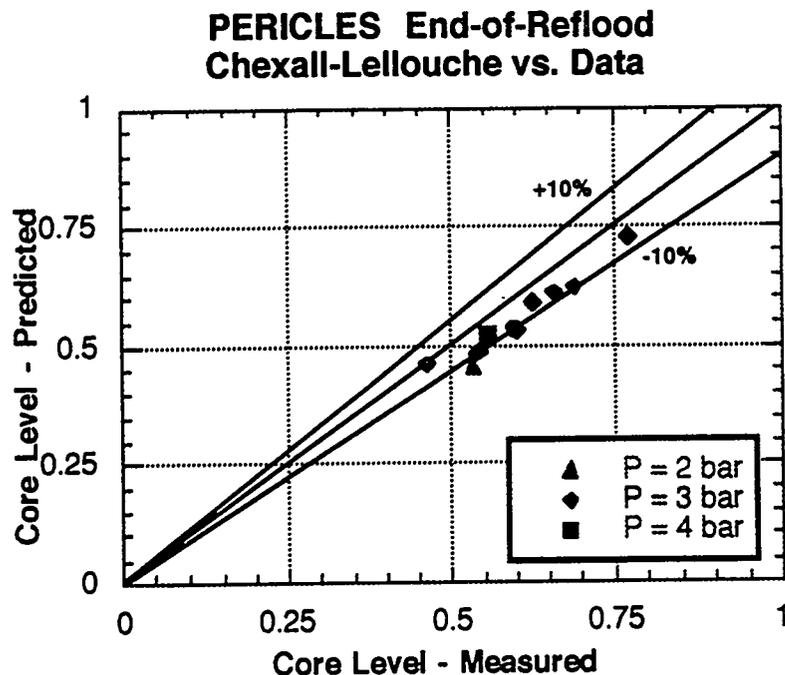


FIGURE 13: Comparison of predicted and measured collapsed liquid levels for the PERICLES end-of-reflood tests using the Chexall-Lellouche drift flux model.

Upper Plenum / Hot Legs: Phase Separation & Entrainment

During the long term cooling phase of an SBLOCA, that is, hours after IRWST injection would begin, the core can "return to saturation" and once again exhaust a two-phase mixture to the hot leg and ADS4. Experimentally, large amplitude oscillations of the IRWST injection flow rate (nearly $\pm 100\%$) have been observed to occur and to persist for more than an hour. Although these oscillations do not appear to have safety implications - they only occur when there is "too much" water in the system - it is worrisome that their amplitude is so large and that they continue for such a long time. Although predicting the amplitude, period, onset, and duration of these oscillations accurately would not be a high priority item, it would be very helpful to be able to calculate them. With reasonable calculations, one could investigate their underlying mechanism(s) and provide input on how to scale them to the AP600.

These oscillations appear to be associated with phase separation in the upper plenum and the relationship between the liquid level in the upper plenum and the hot leg elevation. At this time of the transient, the liquid in the upper plenum resembles a large nearly quiescent pool with vapor bubbling through it. As depicted below in Figure 14, the bubbles rise vertically through the liquid pool (the bubble rise velocity is much greater than the liquid velocity in the hot leg). If the liquid level is below the upper lip of the hot leg, then the flow in the hot leg is stratified and a clear vent path exists for the vapor to escape out of ADS4. If, however, the liquid level is above the hot leg, this vent path can be effectively sealed off. It appears to be this mechanism that causes the "return to saturation" oscillations.

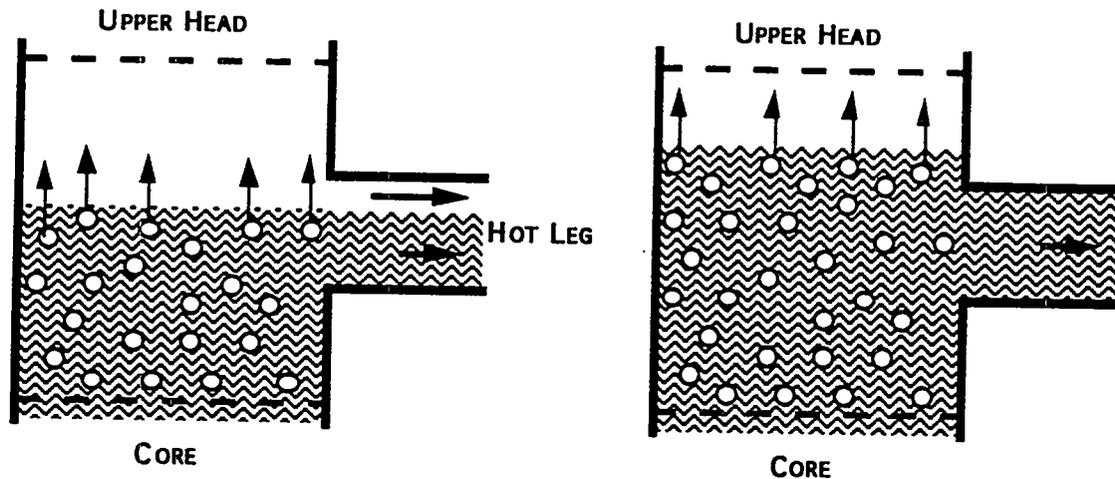


FIGURE 14: Schematic showing phase separation in the upper plenum and blocking of the hot leg / ADS4 vent path.

If the hot leg/ADS4 vent path is sealed off, then flow cannot escape out of ADS4 unless the primary system pressure is sufficient to raise a column of liquid up to the ADS4 elevation. Consequently, the vapor rising from the core, through the liquid in the upper plenum, into the upper head, serves to raise the primary pressure and begin to elevate a column of water in the ADS4 off-take line. The increase in system pressure, in turn, decreases the IRWST injection flow and causes the core vapor generation rate to increase as the portion of the core that is subcooled decreases. Eventually, the primary pressure is high enough to force water up and out of ADS4, at which point the vent path is cleared and the system pressure falls. The reduced system pressure leads to increased flow from the IRWST, more core subcooling, and less vapor generation. More liquid is now entering the core than is being carried out of ADS4, the liquid level in the upper plenum rises, and the cycle repeats.

To be able to calculate these oscillations, a code would then have to model the phase separation in the upper plenum and the interaction between the liquid level and the hot leg elevation appropriately.

NUMERICAL CONSIDERATIONS

The above discussion focused largely on the physical modeling needs for passive reactor analysis. Of equal, or perhaps more importance, are what I shall refer to as "numerical considerations". After all, if the code is simply unable to calculate the desired transient, that is, it crashes so often that an answer cannot be produced, then it matters not how good the physical models are. Numerical considerations involve not only the actual numerical technique applied but also the "gray area" between pure numerics and physical models, where interfacial coefficients are adjusted for special situations. The resulting issues are loosely organized into the categories of computational efficiency, code reliability (robustness), and code accuracy, however the distinctions are not always clear. In the following sections, a number of the issues that have emerged from the ALWR analysis effort are summarized.

Computational Efficiency

First, there is always the question of computational efficiency. Most of the SBLOCA transients have a duration measured in hours, and the long term cooling transients last for three days. Scientific workstations have eliminated the excessive costs associated with purchasing large blocks of time on a main frame computer, however, analysts cannot make efficient use of their time if they are forced to wait for days or weeks before a simulation is finished. Answers are needed in a timely fashion, this will become even more important as risk informed regulation increases the need for large numbers of calculations for PRA applications.

There have basically been four ways to increase computational efficiency:

- **Improve "grind time":** grind time is the CPU time necessary to advance a calculation one time step per computational volume. Making improvements here means more efficient coding, better matrix solution methods, or taking advantage of processes such as vectorization.
- **Use fewer nodes:** when possible without compromising the integrity of the answer, simplifying the noding can significantly reduce the CPU time because not only do the computations have to be performed for fewer nodes, but the grind time can decrease (smaller matrices), and the time step can increase (larger cells mean a larger Courant time step limit). For long term cooling transients, it would be helpful to have a utility to collapse noding so that a detailed nodalization could be used in the early more dramatic phases of the transient and a coarse nodalization used for the long term phase.
- **Use larger time steps:** to perform a simulation for a fixed transient time, larger time steps mean that less time steps are necessary. This has the potential for large improvements in CPU time as long as the selected numerical scheme does not require either the solution of much larger bandwidth matrices or large numbers of iterations thereby increasing the grind time so that it outweighs the gains achieved by computing fewer time steps. Successful efforts in this direction have been made by the development of the SETS method for the TRAC-P code and the fully implicit solution used for 1-D components in CATHARE.

- Buy a faster computer: although this sounds facetious, the advances in work station speed have been nothing less than revolutionary and have often made this option one of the most cost effective.

Future efforts should take advantage of all four of the above, but also allow for increased use of parallelization, that is running the same simulation on a large number of CPUs simultaneously. As multiple CPU work stations become increasingly available at modest prices, and the necessary software advances make writing parallel code machine independent, this option will become increasingly attractive.

Code Robustness

The above improvements in computational efficiency should be regarded only as potential speedups because the occurrence of "numerical events" can slow the calculation down far more than any of the above can speed it up. An extreme example, if a calculation is "in trouble" and reduces the time step to the order of 10^{-6} seconds, tens of thousands of time steps might be expended with little progression of the transient. Some of the more troublesome aspects of modeling two-phase flow, especially at low pressure, are treated below:

- **Phase Disappearance:** when one phase is disappearing, the terms on both sides of the conservation equations need to approach zero, small imbalances can lead to large fluctuations when little of a phase is present. For example, a mismatch in the liquid energy equation can lead to unacceptably large liquid superheats, and a mismatch in the liquid momentum equation can lead to unphysically large liquid velocities. While neither of these may materially affect the course of the transient (e.g., a large velocity that convects no mass), they can and do affect the code robustness and time step.
- **Water Packing:** this is the name given to the situation that arises from "over filling" a computational volume with liquid in a time step. Due to the incompressibility of the liquid, a large pressure spike is produced that can disrupt the flow field. This type of event is particularly troublesome because the code's normal first line of defense - that is, cutting the time step - only makes the situation worse as it gives less time for the liquid phase velocity to be accelerated in the opposite direction.
- **Implicit Heat Transfer:** more implicit coupling between the wall conduction and fluid energy equations can reduce potentially unstable oscillations that can lead to either "negative wall temperatures" or "water property errors".
- **Time Step Control:** more intelligent time step control algorithms should be developed to sense problems before they become catastrophic.
- **Non-Condensibles:** good techniques for handling the appearance of a non-condensable gas in a control volume are needed so that the appropriate derivatives will be available in the Jacobian. Problems with the vapor/gas temperature have also occurred for high non-condensable qualities with the temperature falling below 273.16° K and causing a code failure.

If these and other known problem areas are considered during the development phase of a code, as opposed to being retro-fit in a piece meal fashion, the resulting code robustness should be greatly improved.

Code Accuracy

Although accuracy is normally associated with the physical modeling aspects of a thermal-hydraulic code, there are numerous areas where the accuracy can be affected by "numerical considerations". A brief listing is given below:

- **Time & Space Differencing:** most two-fluid codes use first order accurate schemes for the temporal (forward time) and spatial (upwind) derivatives. The artificial diffusion caused by upwind differencing has been alluded to above in relation to the axial temperature profile within the CMTs. A similar problem occurs for the tracking of injected boron. More accurate differencing schemes should be investigated.
- **Mass Error:** long term calculations for a closed system need to have very good mass and energy conservation characteristics. Recent problems that have been improved in RELAP5 include mass error due to velocity "flip-flop" (phase velocity changes direction between momentum and mass/energy solutions) and truncation of a phase (very small volume fractions truncated to zero).
- **Liquid Films:** falling liquid films due to condensation have a film thickness on the order of $10^2 - 10^3 \mu\text{m}$, in a large vessel this corresponds to a minute liquid volume fraction (1×10^{-4}). Often, a fixed range of vapor volume fractions (e.g., 0.999 - 0.9999) is used to ramp between annular/mist and mist flow regimes. Thus, a falling liquid film can be incorrectly treated as mist flow.
- **Numerical Events & Oscillations:** whatever their origins - e.g., condensation events, sudden switch to saturated boiling, water packing, etc. - can lead to redistribution of liquid inventory and potentially different results. Even when such oscillations are benign, from a system thermal-hydraulic behavior viewpoint, they can raise questions as to the believability of the results.
- **Time Step Sensitivity:** the sensitivity to user selected parameters for time step control should be studied for any serious application. Further, to the greatest extent possible, "defensive" programming techniques should be used to reduce time step sensitivity and "intelligent" time step control algorithms should be implemented to minimize sensitivity and the user effect.

The above is not an exhaustive list of all the challenges that can be encountered in the thermal-hydraulic analysis of passive reactor systems, but does give an idea of the difficulties, especially in light of the longer transient times, lower system pressure, and smaller driving potentials. While not exhaustive, this list should also not be taken to infer that the task is impossible. In the AP600 analysis program, extensive comparisons were made between RELAP5 calculations and data from three integral test facilities at different scales. Once a couple of serious problems were corrected, the

overall transient behavior was well simulated and most key parameters were judged to be in reasonable agreement with the measured quantities.

During their development and application lifetimes, each systems thermal-hydraulic analysis code has faced some or all of these difficulties, in some cases truly innovative approaches have been taken to resolve the problem, while in others, "fixes" have been devised to ameliorate the worst symptoms. There is no doubt that if the total experience base were tapped (that is, the best from all of the codes), and these difficulties were considered from the beginning of the development process, a much more robust and accurate analysis tool would result.

SUMMARY

The U.S. Nuclear Regulatory Commission has received an application for design certification from the Westinghouse Electric Corporation for an Advanced Light Water Reactor design known as the AP600. As part of the design certification process, the USNRC uses its thermal-hydraulic system analysis codes to independently audit the vendor calculations. The focus of this effort has been the small break LOCA transients that rely upon the passive safety features of the design to depressurize the primary system sufficiently so that gravity driven injection can provide a stable source for long term cooling. Of course, large break LOCAs have also been considered, but as the involved phenomena do not appear to be appreciably different from those of current plants, they were not discussed in this paper.

Although the SBLOCA scenario does not appear to threaten core coolability - indeed, heatup is not even expected to occur - there have been concerns as to the performance of the passive safety systems. For example, the passive systems drive flows with small heads, consequently requiring more precision in the analysis compared to active systems and raising the question as to whether the same confidence can be placed in the analysis methods for passive plants as compared to current plants with active systems. For the analysis of SBLOCAs and operating transients, the USNRC uses the RELAP5 thermal-hydraulic system analysis code. To assure the applicability of RELAP5 to the analysis of these transients for the AP600 design, a four year long program of code development and assessment has been undertaken.

The lessons learned during this effort were detailed in this paper by describing the relevant physical phenomena and the associated modeling challenges for each component.. Specific modeling challenges for our current generation of thermal-hydraulic codes include:

- **Thermal Front Tracking:** ability to resolve steep temperature gradients within the liquid in the flow direction and to use the temperature of a buffer layer in the interfacial heat transfer model.
- **Mixture Level Tracking:** ability to track the liquid/vapor interface, and correctly model the interfacial heat transfer phenomena for a stratified surface.

- **Thermal Stratification & Mixing:** provide for the accumulation of hot liquid in a buffer layer due either to convection or condensation, and provide for a mixing region that grows due to the addition of colder water either from wall heat transfer effects or convection.
- **Wall Conduction:** accurate solution of the transient conduction within thick walled vessels that is not sensitive to user specification of mesh spacing.
- **Cold Leg Thermal Stratification:** model thermally stratified single-phase flow (possibly flowing counter-currently) in large diameter horizontal pipes.
- **Critical Flow:** accurately calculate the critical flow for both valves (ADS) and thin orifice plates especially for low pressure and low quality conditions.
- **Phase Separation:** accurate prediction of entrained liquid fraction at ADS valves due to phase separation in the pressurizer and vertical off-take from the hot legs.
- **Low Pressure Boiling:** eliminate unphysical discontinuities in the interfacial heat transfer package and provide some form of subgrid resolution for the point of net vapor generation.
- **Low Pressure Void Fraction:** improve models for interfacial drag in rod bundles at low pressure, low flow, and low heat flux conditions.

In addition, a section on "numerical considerations" was included that discussed the need for further improvements in:

- **Computational Efficiency:** provide for a more implicit solution technique, minimize "numerical events" that reduce the time step, investigate parallel processing.
- **Code Robustness:** improve ability of code to run a transient to completion without requiring user intervention, this include improvements in the areas of phase appearance/disappearance, water packing, implicit treatment of wall heat transfer, time step control, and appearance of noncondensibles.
- **Code Accuracy (Numerical):** improve order of accuracy in differencing to minimize artificial diffusion, better conservation of mass in long term transients, reduce sensitivity to time step size, and reduce oscillations that are numerical in origin.

While the above list of challenges that can be encountered in the thermal-hydraulic analysis of passive reactor systems is imposing, it should not be taken to infer that the task is impossible. In the AP600 analysis program, extensive comparisons were made between RELAP5 (pre-release version of Mod3.3) and data from three integral test facilities all at different scales. Once the more serious problems were either corrected (or a workaround used) the overall transient behavior was well simulated and the key parameters judged to be in reasonable agreement with the measured quantities.

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ON TRANSIENT THERMALHYDRAULIC
AND NEUTRONIC CODES REQUIREMENTS

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The role of the Uncertainty in Code Development

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-1- INTRODUCTION

From a general point of view, all the results of a calculation should be given with their uncertainty. It is of most importance in nuclear safety where sizing of the safety systems, therefore protection of the population and the environment essentially depends on the calculation results.

Until these last years, the safety analysis was performed with conservative tools. Two types of critics can be made. Firstly, conservative margins can be too large and it may be possible to reduce the cost of the plant or its operation with a best estimate approach. Secondly, some of the conservative hypotheses may not be really conservative in the full range of physical events which can occur during an accident. Simpson (1) gives an interesting example: in some cases, the majoration of the residual power during a small break LOCA can lead to an overprediction of the swell level and thus of an overprediction of the core cooling, which is opposite to a conservative prediction. A last question is: does the accumulation of conservative hypotheses for a problem always give a conservative result? The two phase flow physics, mainly dealing with situation of mechanical and thermal non-equilibrium, is too much complicated to answer these questions with a simple engineer judgement.

For a vendor or an utility, the alternative solution was to use best-estimate codes as RELAP-5, TRAC, ATHLET and CATHARE, solution admitted now by the safety authorities who have defined application rules for these codes. One of the rules is to prove the reliability of such codes, therefore to be able to quantify the uncertainty of the response obtained by the codes. In a safety analysis, the results of the calculations including the uncertainties must indicate that the

safety criteria are met with a high level of confidence. Already in France, EDF or FRAMATOME have admitted to conduct safety and licensing studies with CATHARE. Several methodologies have been proposed: the CSAU in the US, the EAE method in UK, the GRS method in Germany, the CEA-IPSN method in France, etc..... The purpose of all these methodologies is to propose tools to take into account the propagation of the uncertainties from the basic parameter uncertainties (physical models, numerical methods, plant data,..) to the relevant responses of the code. Thus, whatever methodology is used, the basic uncertainties due to the code have to be known. All the methods formerly listed include one step dealing with the determination of uncertainties, in most cases determination reduced to a simple evaluation. Therefore, at the end of this century, because of our knowledge, the strategy and methodology of development and validation of a new best-estimate code (or for a new version of a code), must take into account the ability of evaluating the uncertainties from the design phase.

The objective of this paper is to make a review of the quantification of the uncertainties which can be made during code development and validation. The origin of these uncertainties can be listed as below:

- * The uncertainties due to the choice of the basic models, namely the two fluid model.
- * The uncertainties due to the geometrical approximation: one-dimensional model, or three-dimensional model
- * The uncertainties due to the numerical method: spatial and time discretization
- * The uncertainties due to the closure relationships
- * The uncertainties due to the phenomena not taken into account in the models

Moreover, the user effect should be added to this list. This topic will be addressed also here because it is of major importance to think how to drastically limit it during the design phase of the code.

Other types of uncertainties can affect the results of a NPP calculation:

- * The uncertainties on the reactor data (geometry, core power, peak factor, boundary conditions...)
- * The uncertainties due to the scale effect (how to extrapolate to full scale most of the models derived from the analysis of small scale experiment); a method is proposed by D'Auria for this point.

They are not the subject of this paper.

-2- THE CHOICE OF THE MODEL

2.1 The two fluid model

In best estimate codes, the two fluid model was chosen in order to correctly describe the mechanical and thermal non - equilibria. The main option of the model is that two fields only are considered in all flow pattern situations: a liquid field for the water and a gas field to model the steam and the non condensable gases. At this stage of the modelling, the uncertainties are due to the lack of precision of this model in certain situations.

For example, in reflooding situations during a large break LOCA, it should be more accurate to model two liquid fields (a liquid film and a droplet field) in order to correctly predict the physical processes occurring in the upper plenum, as liquid entrainment and de-entrainment processes, which play a considerable role on the pressure repartition and thus influence the quench front pro-

gression. This problem is relevant and is addressed now in some code development. It is planned in the three-dimensional module of CATHARE to add a second liquid field to properly model entrainment and de-entrainment in the upper plenum. As only developing new numerical models is not sufficient, a basic 3-D experiment is planned to assess the code in such situations.

Nevertheless, the lack of modelling due to the choice of the two fluid model and the associated uncertainties can be taken into account in the constitutive relationships with a lumped approach.

2.2 The simplifications of the model

During the code development, simplifications are necessary to obtain a tractable problem to compute. Several examples can be given.

During the development of the models, the time averaging process makes disappear the fluctuation due to the turbulence. To restore pieces of missing information, several techniques exist:

- * adding turbulence model using additional equations as k-epsilon model for example,
- * adding diffusion terms with a lumped approach by introducing a coefficient of turbulent diffusion.
- * adjusting parameters in some constitutive relationships of the wall friction or the heat transfer, comparing with experimental data at large scale.

This last approach is generally chosen for best estimate codes.

The space averaging makes disappear the interface movements and the complex structure of the phase repartition. In fact as a consequence of this simplification, it is necessary to create flow pattern maps which are not accurate, and available only for a certain number of well defined geometries. In particular, stratification and droplet entrainment criteria have to be introduced. Different constitutive relationships have to be developed for all kinds of flow pattern.

In most of the code, only one average pressure is considered. It results in a lack of accuracy in particular for some situations where the fluid is stratified. The loss of information can be partially regenerated by adding algebraic relations in the equations in order to describe the pressure difference between the bulk pressure and the interface pressure. A typical example is the condensation in presence of non-condensable gases. It would need the calculation of the partial pressure at the interface to properly calculate the gas diffusion. This piece of information is restored in the condensation correlation by using an algebraic coefficient. This process is qualified by comparison with experiment where the global heat transfer is measured.

Another simplification appears in the choice of a one-dimensional or a three-dimensional model. It is clear that the choice of a one-dimensional model is reasonable to describe pipes as hot legs, cold legs, steam generator U-tubes, etc, namely in most situations. But, it prevents from modeling the temperature stratification occurring in horizontal legs in some situations, for example. therefore, it makes necessary to replace some of the information lost on the flow structure close to singularities as diaphragm. Singular pressure drop is one way to replace the information. Nevertheless, to chose a three-dimensional module for every situation does not resolve all the problems. This is due to a lack of very fine two phase flow three dimensional experiments able to provide suitable information for code assessment.

The conclusion of this section is that whenever simplifications are necessary in the models, pieces of information are regenerated in the constitutive relationships by means of a lumped approach. Therefore, the problem of uncertainties due to these choices can be implicitly affected to the model uncertainty. In next future, another approach will be to compare results of best estimate codes with the results of codes dealing with finer three dimensional physics. It is then necessary to develop appropriate experimental tools to assess these codes and to develop a methodology to be able to compare these codes.

-3- THE NUMERICAL METHODS

The uncertainties due to the numerical methods are connected to two problems: the choice of an appropriate method and the use of this method in its range of validity. It is well known that the problem discussed here is an ill-posed problem; in principle it can not be demonstrated that a consistent solution exists. Most of the best estimate codes are using finite volume or finite difference integration with staggered meshes with donor cell. Generally first order scheme in space or in time is used. The hyperbolic feature of the problem is obtained by properly writing the differential terms in particular the terms where the difference of pressure between bulk pressure and interface pressure is involved. Most of the codes have problem of numerical diffusion. But these problems are not so crucial; they only need to be quantified. A methodology has to be applied to evaluate those uncertainties.

The methodology used in the CATHARE code development can be proposed, as follows:

- * The numerical diffusion can be partially solved by performing systematic mesh convergence tests on validation calculations and then to recommend some mesh size criteria to the users.
- * To perform comparison of code results with analytical solutions of academic problems and to perform well known numerical benchmark.
- * To evaluate, with mathematical tools, the uncertainties due to the truncation of the problem. It can easily be done with the help of specialized university laboratories.
- * The code has to check the mass and the energy error systematically, for every time step. Then the error results have to be stored in a file in such a way that the user can plot it and therefore judge the accuracy of the code as well as the way he conducts his calculations.

The implicit feature of the code do not make necessary to compare the calculated time step with some Courant limitations. In addition it has no problem of stability.

Anyway some problems can remain. An example is how to predict, with a good accuracy, the propagation of boron plugs with a first order code. Advanced high order codes exist in fluid mechanics but not in two phase flow area. One possibility of coping with this problem could be to use high order single phase flow code and to define some systematic bias with expert judgement.

-4- THE USERS' EFFECT

The user effect is difficult to measure, but it can be easy to limit it. Five actions can be taken for this purpose:

- 1) **No code option:** in the code, even for physical model in order to prevent the user from choosing

or tuning the physics

2) **Full portability:** of the code in order to have **the same version for all the users**. During the benchmarking phase and the validation phase, the tests have to be performed on several computers and all difference have to be explained. Experience proves that programming ambiguite is the source of these differences

3) **Testing the new version:** The differences with other versions must be pointed out and explained in a report. Non-regression tests must cover the full range of use of the code for analytical tests, integral tests and NPP calculations (Large break LOCA, small and intermediate break LOCA, STGR, steam line rupture, etc)

4) **Users' guide lines** booklet has to be released with the version and updated with the users experiences. Advice on nodalization must be found into it. All this advice is the results of the qualification and verification phases of the code. Let us take an example: the meshing has to be advised. Therefore the meshing developed during the code validation phase must be used for the reactor calculation input deck. Typical examples can be given. In the CATHARE code, the break flow is calculated using the one-dimensional model and its eigen values are used to determine the sonic velocities. This approach needs a very fine meshing upstream to the break. During the assessment, converged meshing were found and therefore they are specified in the users guidelines. The same approach is followed for the bends of the legs (steam generator U-tubes, loop seal, etc) where converged meshing was determined during the assessment. Another example could be given with meshes of the wall and the rods.

5) **Active assistance and maintenance.** It can only be done by the development team.

-5- THE BASIC UNCERTAINTIES ON THE CLOSURE RELATIONSHIPS

In the second section, it has been shown that most of the uncertainties in the choice of the models and the associated hypotheses can be implicitly affected to the uncertainties of the constitutive relationships. Thus special attention must be paid to their evaluation.

5.1 The closure relationships

The closure relationships appear in the process of derivation of the systems of equations. By choosing at first a continuum model leads to the necessity of writing closure relationships to describe the state of the fluid. In order to obtain a solvable problem with reasonable means for industrial codes, the equations have to be averaged. This process makes disappear some information on the physical phenomena to describe. Therefore, additional closure relationships have to replace the information lost during the averaging process or because of simplifying assumptions.

The closure relationships are:

*Material properties, which include the equations of state for the phases as well as the models for the phasic transport properties

* Flow regime modeling, which closely depends on the geometry of the flow duct

* Interphase momentum interaction with three basic mechanisms: steady drag, dynamic drag, momentum transfer due to mass transfer

* Interphase mass and energy exchange

* Wall to fluid momentum and energy exchange

5.2 Methodologies to develop closure relationships

In general, to derive a closure relationships, two methods can be considered:

The first one, a purely empirical method, consists in using experimental results. It is based on the adjustment of a scalar law with parameters which seems to have some influence on the experiment. This relationship has a limited range of validity. It corresponds to the range of values of the experimental parameters and can not be extrapolated to another range of parameters. Within the range of validity of these relationships, the uncertainties are closely linked to the experimental uncertainties and the choice of the parameters used to the analysis.

The second method is a purely mechanistic method. It is based on the derivation of relationships or equations by using theoretical considerations. But the problem has often to be simplified in order to build a solvable model.

Generally an alternative approach is used, thus to start with a semi-empirical method where some theoretical considerations allow to link a limited number of parameters in a relationships. Then, these parameters are adjusted using experimental results. The source of uncertainties are:

- * The hypotheses used to simplify the problem and to obtain a theoretical model
- * The choice of the parameters to correlate
- * The experimental uncertainties

5.3 The choice of the experiments

The experiments never measure a closure relationship, for example the interfacial friction! It only measures pressures, temperatures, densities, flowrates, etc. Eventually, it can give additional information such as the flow structure.

It is difficult to design an experiment whose results are sensitive to only one closure relationship. Typically a critical flow rate experiment is sensitive to three parameters: the interfacial friction, the wall friction, the interfacial heat exchange in boiling conditions. In addition the relative sensitivity of these three parameters varies with the upstream conditions. The sensitivity of any parameter can change with physical conditions (pressure, void fraction, flow rate, etc)

In the same way several experiments can be used to develop a closure relationships in all the relevant range of physical parameters, flow patterns, geometries, etc...

A simple expert judgement is not really able to evaluate uncertainties in a such complicated situation. The solution is to put the maximum of uncertainties on each parameter, ... hoping that no important contribution has been forgotten. An alternative way is to have a strict development methodology associated with an uncertainty determination method, able to consider all together the experiment basis used for the qualification in order to take into account the correlation between the uncertainties.

To use this deterministic method, good experiments have to be chosen in order to get all the needed information: instrumentation, experimental procedure, bad runs, etc.

5.4 Strategy of development

The objective is to derive a consistent set of closure relationships with determination of

the uncertainties. They do not have to be separately developed. First all the thermodynamic and transport properties of the water, the mechanical closure laws, the interfacial heat exchange and then the wall to fluid heat exchange.

The method used to determine the uncertainty should be able at first to select the relevant parameters in an experiment, using a tool for sensitivity studies and then to determine the uncertainty of the selected parameters. In the following section an example of tools used for the CATHARE development is presented.

The problem to be solved is an engineering problem. It can be formulated in the following way. Let R be a response of the code; it can be, for instance, a physical quantity (as mass inventory, cladding temperature, break flow rate, heat flux, etc.) or the timing of an event, etc ... Let ϵ_k be any parameter of the code: physical quantity (pressure, temperature, etc.), steam-water physical properties, constitutive relationships (interfacial friction, wall friction, mass and energy transfer between phases, etc.), initial or boundary conditions, etc.

The first question to answer is: due to a modification $\delta\epsilon_k$ of the parameter ϵ_k , what will be the change δR of the response R ? Therefore it is necessary to be able to calculate the sensitivity profile:

$$\frac{\epsilon_k}{R} \cdot \frac{dR}{d\epsilon_k}$$

which is the percentage of change of the response R for one percent of change of the parameter ϵ_k . This can be done using the **DASM**.

The second question is how determine the uncertainty ΔR on R . This is the aim of the **CIRCE** methodology and software.

-6- THE SENSITIVITY ANALYSIS: example of a tool, the DASM method

The initial physical problem (i.e. the set of equations resolved in the **best-estimate system** code) is modelled by means of a partial differential system: $A(X_\epsilon, \epsilon)=0$, where X_ϵ is the solution of the equation, $\epsilon=(\epsilon_1, \epsilon_2, \dots, \epsilon_d)$ is the parameter vector and A is a **non-linear function** of both X and ϵ . In this paper, it is called the 'direct' problem. A response of the code is a real function R which can be considered as a function of the vector of parameters ϵ : $R(\epsilon)=F(X_\epsilon)$. The sensitivity evaluation consists of calculating the derivatives of R :

$$D_\epsilon \cdot R(\epsilon) = \left[\frac{dR}{d\epsilon_1}, \dots, \frac{dR}{d\epsilon_d} \right] \quad (1)$$

Several methods can be used to calculate this derivative vector.

6.1 . The brute force.

The most commonly used and easiest method is the one referred to as 'brute force'. To evaluate the sensitivity of R with respect to the parameter ϵ_k , one calculation is performed using the standard set

of parameters $\epsilon=(\epsilon_1, \epsilon_2, \dots, \epsilon_k, \dots, \epsilon_d)$, and one calculation with $\epsilon=(\epsilon_1, \dots, \epsilon_k + \Delta\epsilon_k, \dots, \epsilon_d)$. The derivatives are numerically evaluated:

$$\frac{dR}{d\epsilon_k} = \frac{R(X_{\epsilon + \Delta\epsilon_k}) - R(X_{\epsilon})}{\Delta\epsilon_k} \quad (2)$$

The advantage of this method is that the sensitivity of the code is obtained. The drawbacks are that one direct computation (with the best estimate code) is needed for each $\epsilon_1, \epsilon_2, \dots, \epsilon_d$ parameter. This results in a heavy computing cost for reactor computation dealing with a large range of parameters. Another drawback is the difficulty to choose appropriate $\Delta\epsilon_k$ increments.

This method will be used in this study to qualify the ASM.

6.2 . The direct sensitivity method.

Another method, oftently used, is the direct sensitivity method, which consists of resolving the derived equations of the initial system:

$$\frac{dA}{dX} \cdot \frac{dX}{d\epsilon_k} = \frac{dA}{d\epsilon_k} \quad (3)$$

The main drawback is that the computation time of each derivative is of the same order of magnitude as the computation time for the solution.

6.3 . The adjoint sensitivity method.

The proposed method is the Adjoint Sensitivity Method (ASM) [2] and [3].

If (X, ϵ) is a solution of the system, another solution around (X, ϵ) is $(X + \Delta X, \epsilon + \Delta\epsilon)$. At the first order,

$$D_X A(X, \epsilon) \Delta X + D_\epsilon A(X, \epsilon) \Delta\epsilon + O^2(I \Delta\epsilon) = 0 \quad (4)$$

where D_X and D_ϵ are differential operators. The change of the response R of the code, due to the change in ϵ parameter vector can be evaluated as follows:

$$\Delta R = \langle \nabla_X F(X) | \Delta X \rangle + O^2(I \Delta\epsilon) \quad (5)$$

The sensitivity profile vector can be written: $D_\epsilon R(\epsilon) = \langle \nabla_X F | D_\epsilon X \rangle \quad (6)$

As, $D_\epsilon X = -D_X^{-1}(X_\epsilon, \epsilon) \cdot D_\epsilon A(X, \epsilon) \quad (7)$, it can be written:

$$D_\epsilon R(\epsilon) = \langle {}^t(-D_X^{-1}(X_\epsilon, \epsilon)) \cdot \nabla_X F | D_\epsilon A(X, \epsilon) \rangle \quad (8)$$

$$D_\epsilon R(\epsilon) = \langle {}^t\Phi | D_\epsilon A(X, \epsilon) \rangle \quad (9)$$

where ${}^t\Phi$ is the adjoint vector, which is the solution of the adjoint equation:

$${}^t(-D_X A(X, \epsilon)) \cdot {}^t\Phi = \nabla_X F(X) \quad (10)$$

The advantage of this method is that only one linear adjoint equation for each response R is needed after calculation of one direct problem. In addition, it is very easy to introduce new parameters ϵ_k . There are two methods for applying the ASM.

The first one, the Continuous Adjoint Sensitivity Method (**CASM**), implies to write the adjoint system of the initial direct problem and then to discretize it. Therefore, two problems arise: the first one deals with the choice of the boundary conditions of the adjoint problem and the second one deals with the discretization of the adjoint problem: how to be sure that this discretization is consistent with the discretization of the direct problem. The sensitivity calculated using this method is not the sensitivity of the initial code.

The second method, the Discrete Adjoint Sensitivity Method (**DASM**), implies to derive the adjoint problem from the discretized direct problem. From a mathematical point of view, Ounsi and al. [4] have demonstrated that this approach is correct and that the calculated sensitivity is really the sensitivity of the initial code.

6.4. Implementation of the DASM in the Cathare 2 code.

The DASM has been chosen for the CATHARE 2 code as the standard tools to perform the sensitivity studies. The method of calculation is presented on table 1. At the n-th time step the adjoint equation can be written as:

$$\text{n-th time-step: } \left(\frac{\partial A^n}{\partial X^n} \right) \cdot \Phi^n = - \frac{\partial R}{\partial X^n} - \left(\left(\frac{\partial A^{n+1}}{\partial X^n} \right) \cdot \Phi^{n+1} \right) \quad (11)$$

It is apparent that in the adjoint system, derivatives with respect to explicit variables are necessary. As the CATHARE discretization is fully or nearly implicit, the number of additional calculations which will be needed to write the explicit Jacobian matrix is reduced. As the equation (11) is linear, it is very cheap in CPU cost. It is also cheap in manpower..

The sensitivity calculation is therefore performed in the code in three stages:

1) CATHARE computation: only one computation for the sensitivity study where the Jacobian

matrix and the main variables of the calculation have to be saved: $\frac{\partial A^n}{\partial X^n}(X_\epsilon^{n-1}, X_\epsilon^n, \epsilon), X_\epsilon^n$

2) Resolution of one LINEAR adjoint equation for a given response R :

* Computation of the derivatives of R : $\frac{\partial R}{\partial X^n}$

* Computation of the derivatives with respect to the explicit variables of the direct code: $\frac{\partial A^{n+1}}{\partial X^n}$

* Computation of the Equation (10), then storage of the adjoint flux vector Φ .

3) For each parameter ϵ_k , computation of the sensitivity profile: $\frac{dR}{d\epsilon_k} = \langle \Phi | \frac{\partial A}{\partial \epsilon_k} \rangle$ (12), which is only a simple vector product.

Thus, for each sensitivity study, one direct CATHARE calculation is needed, one CATHARE adjoint calculation is needed for every response R, and only one vector product per ϵ_k parameter is needed.

In the new version of CATHARE 2 (version 1.4), the adjoint calculation has been implemented. For hydraulic module (1-D, volume, Tee and boundary conditions), the heat conduction module and the fuel thermo-mechanical module, it is possible to perform an adjoint calculation. For the reflooding module and the 3D module development is still underway.

From a coding point of view, the adjoint modules use all the elementary subroutines of the CATHARE code. Then it ensures that exactly the same equations, the same discretization, the same physics are used for the adjoint calculation. Additional subroutines have been added to calculate the derivatives of the terms which are explicit in the direct code and the derivatives of the response.

When a CATHARE 2 calculation is performed, the sensitivity calculations are used as a **post-processing module**.

The method of qualification of the DASM is to compute a large number of analytical tests with CATHARE 2 and to compare the results of DASM with the brute force technique. This work has been under progress using the qualification matrix of CATHARE 2. It will be finished at the end of 1996. The first results indicate that for very simple sensitivity studies the results of both methods are exactly the same. To reach this quality of results, considerable attention has been paid to the debugging process. This was also of considerable value for the CATHARE code itself because some errors were found.

This method is applicable for non-linear problem and threshold phenomena. It has been demonstrated. It will be published at the NURETH 8 conference

6.5 . Advantage of this method.

The DASM is a convenient tool to perform systematical studies to point out the most sensitive parameters in a reactor calculation or integral test analysis. It avoids arbitrary choice to select the more relevant parameters or it avoids to perform a large number of sensitivity calculation by the 'brute force'. It can be very useful to develop new constitutive relationships: by being systematically used during the qualification process of the code, this tool can easily indicate what are the non regression test to compute after code modifications, for example.

For uncertainty studies, DASM also provides local derivatives, response surfaces can be easily drawn.

-7- THE DETERMINATION OF THE BASIC UNCERTAINTIES

7.1. The problem to be solved

In this section, the determination of closure relationships uncertainties (basic uncertainties) is con-

sidered, but not the evaluation of these uncertainties by an engineer judgement. The principle of a deterministic method is described: this method is used to predict the uncertainties with a good range of confidence, not a method of evaluation which can only give a result may be very far from the reality.

Establishing the range of parameters is very easy for parameters describing the conditions of the plant or for parameters describing thermophysical data (such as the conductivity of the UO₂). It is much more difficult for parameters relative to the constitutive relationships (such as the interfacial friction), because they cannot be directly measured in an experiment.

To this end, the results of the separate effect tests which are useful for establishing or assessing the constitutive relationships are used, as well as the associated experimental uncertainties. The corresponding results calculated by the code are also used and denoted R_j . The general idea is to calculate the uncertainties of the correlations from the code-experiment differences concerning the responses and from the experimental uncertainties.

7.2. The difficulty of the problem

Nevertheless, the relationships between correlations and separate effects tests is not always simple as we already mentioned it. To solve this problem, **all the correlations of the code and all the associated separate effect tests must be considered together**. There are roughly 30 correlations in the code, without taking into account, for instance, the submodels only used in some flow configurations. Thus the resolution of the problem requires a general and reliable method, which is the case of the methodology presented as follows.

7.3 Principle of a method of basic uncertainty determination.

All methods devoted to the determination of the basic uncertainty (closure relationships uncertainties) should follow the describing steps:

Step 1 Comparison between experimental results and code predictions: a wide range of experimental data has to be chosen: the experimental data selected for the constitutive relationships derivation and those used for the qualification process

Step 2 Experimental uncertainties It is of prime importance that the experimental data used for the constitutive relationship derivation and for their qualification are well known; in a first attempt, the uncertainties should be known to be sure that reliable data are used; in a second attempt, to allow a better determination of the basic uncertainties

Step 3 Sensitivity analysis To determine the basic uncertainties, it is clear that the most sensitive parameters or the most relevant parameters have to be known.

Step 4 Determination of the basic uncertainties. All the information determined in the first three steps has to be collected and analysed to provide the expected result.

The methodology presented here is a general one. Two methods can be applied:

***Using the brute force** A large number of sensitivity calculations can be performed by perturbing the closure relationships and by trying to give good results. The objective is to find the " envelope "

curves of the experimental results by determining the perturbation of the constitutive relationships which allows to fit the calculated results in the worst case. As one constitutive relationship can be influential in several experiments or as several correlations can be of influence for one experiment, this method needs a huge number of sensitivity calculation. This method may be impossible to practice.

* Using a statistical approach For the sensitivity step, a sensitivity tool can be used. To combine all the effect a statistical approach can be developed, in order to get a best estimate uncertainty at a cheap cost and low manpower. CIRCE is an example of this kind of tools. It has been developed in the framework of the CATHARE development.

7.4 Presentation of CIRCE.

This is an original work developed by A. De Crecy. [4,5]

Let us consider a closure relationships: CR . It can be written: $CR = e^\varepsilon \cdot CR_nominal$, where ε is a parameter which allows to performe sensitivity calculation when modifying it. In the standard version of the code $\varepsilon = 0$ and $CR = CR_nominal$.

Let us consider a set of constitutive relationships CR_k , $k=1,d$, associated with the vector of parameters $\varepsilon = [\varepsilon_1, \dots, \varepsilon_k, \dots, \varepsilon_d]$.

Let us consider n responses R_j , $j=1,n$. For one response R_j , it can be defined:

$$y_j = R_{j,exp} - R_{j,code}$$

where $R_{j,exp}$ is measured by the experience, and $R_{j,code}$ is the code response.

In fact, CIRCE tries to find the vector ε which allows to have $R_{j,exp} = R_{j,code}$. This value of the vector ε , ε^j , is called the j th realization of the d -vector ε : $\varepsilon^j = [\varepsilon_1^j, \dots, \varepsilon_k^j, \dots, \varepsilon_d^j]$. It is considered as a random variable, corresponding to the R_j response. ε is assumed to follow a statistical distribution.

Let us write now $y_j = R_{j,exp} - R_{j,true} + R_{j,true} - R_{j,code}$.

$R_{j,true}$ is the true value of the response R_j that the experiment tries to measure and that the code tries to calculate; it is unknown.

The first random variable, $e_j = R_{j,exp} - R_{j,true}$, is related to the experimental uncertainties. It can be assumed to obey a normal law, with or without biais. At the first order, the second random variable can be written:

$$R_{j,true} - R_{j,code} = \frac{dR_j}{d\varepsilon_1} \cdot \varepsilon_{1,true}^j + \dots + \frac{dR_j}{d\varepsilon_d} \cdot \varepsilon_{d,true}^j$$

The values $\varepsilon_{k,true}^j$ are the unknown quantities of the problem; they represent the values of the parameters to impose in order to have a prediction of the reponse R_j by the code, $R_{j,code}$, which is equal to the true value of R_j , $R_{j,true}$. The actual unknown quantity of the problem is a matrix con-

taining the variance of the parameters ϵ on the diagonals (the square of their standard deviation) and the covariance terms in the off-diagonals values: it is the covariance matrix, C . C^j is the covariance matrix of the j th realization of the d -vector.

The aim of **CIRCE** is to calculate the covariance matrix C . Using some statistic tools, the Bayes theorem and the principle of maximum likelihood, it is possible to have an estimation of the parameter (the vector ϵ) of the constitutive relationships from the n realization of the random variables. An iterative method, the E-M algorithm, is used.

7.5 Perspective of CIRCE.

CIRCE will be systematically used during the developmental assessment of the last version of CATHARE. This assessment will cover a wide range of parameters covering the physical phenomena occurring in a PWR or a VVER during normal operation, full spectrum of accidents, including accidents on the RHRs circuit during maintenance operation in an open reactor. More than 1000 analytical tests on 30 experiments will be calculated. DASM calculations will be performed to point out the relevant parameters. One of the main objectives of this qualification process is to provide an accurate determination of the uncertainties on all the closure relationships of the code. This will be done using CIRCE. It will be the first time in the thermal hydraulics that a deterministic methodology has been developed which permits to calculate the uncertainties of the constitutive relationships and then to provide pieces of information for any methods of error propagations.

-8- CONCLUSIONS

In this paper, an attempt to list the source of uncertainties and proposition to be able to evaluate them was made. As a conclusion, a methodology of code development is proposed. The author was engaged in the CATHARE development since ten years and it is clear that this proposition is completely influenced by the methodology followed by the French industrial partners for the CATHARE development. The cycle of development of a version could be as follows.

-1- During the development to use a development management software in order to keep memory of the modification made in this version.

-2- For the development of constitutive relationships, to choose analytical experiments whose all the characteristics are known. It is better to work in close relationships with the experimentalists. The code developers could well understand the experiment and its limits. The experimentalist can know what the code developer is waiting from his experiment.

-3- Before starting the validation, the version has to be **frozen**

-4- In order to avoid coding errors, **systematic control tests** including numerical benchmark, simple physical tests and reactor calculations have to be performed. Comparison has to be made with previous versions; all the differences have to be explained and written in a document. Comparison between several computers has to be performed: the following computers have to be tested cray, workstation, pc. Difference between solutions on different computers means coding error or coding ambiguity.

-5- After this systematic control of the version, the validation process can start. The first part is the **qualification** against separate effect tests and component tests. It allows to control the constitutive relationships in a larger range of parameters than used for their developments. It also allows to define the most adapted nodalization which is space-converged and to use tools, as DASM, to

point out relevant parameters and to determine the basic uncertainties on the constitutive relationships.

-6- The second part of the validation is the **verification** using results of integral test facilities. The same nodalization as qualified in the former step has to be used. The aim is to point out shortcomings on the constitutive relationships, not to fit them. DASM can be easily used to find the most relevant parameters. It is very useful to recompute the verification tests used at the last version validation for non regression test and to ensure continuity. Additional tests have to be chosen to extend the range of reliability of the code.

-7- It is very important to provide an adequate documentation with validation documents, systematic control tests results and **users guidelines**. validation by others users than the developmental team can be added.

-8- Then the safety authority should control that the safety calculations for NPP are using the same nodalization as for the verification tests as advised in the users guidelines. In such conditions, the uncertainties due to the users effect which can not be quantified will be limited.

REFERENCES

[1] H.C. SIMPSON

"Some thermohydraulics problems associated with the safety of water cooled nuclear reactors"
8th International Heat Transfer Conference, San Francisco,U.S., 1986

[2] A.OUNSY,F.DE CRECY, B.BRUN

"The adjoint sensitivity method; a contribution to the code uncertainty evaluation"
Nuclear Eng. Des. 149 (Sept. 1994)

[3] F.BARRE, A DE CRECY, C. PERRET

"The sensitivity analysis by the adjoint method for the uncertainty evaluation of the CATHARE 2 code"
NURETH 7 conference, Saratoga springs, U.S., 1995

[4] A.DE CRECY

"Determination of the uncertainties of the constitutive relationships in the CATHARE 2 code"
ASME-JSME, 4th International conference on nuclear engineering , ICONE 4,1996

[5] A. DE CRECY

"CIRCE: a tool for calculating the uncertainties of the constitutive relationships of CATHARE 2"
To be published in NURETH 8 conference,Kyoto Japan , 1997

The Role of the PIRT Process in Identifying Code Improvements and Executing Code Development

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1. Introduction

In September 1988, the USNRC issued a revised ECCS rule^[1] for light water reactors that allows, as an option, the use of best estimate (BE) plus uncertainty methods in safety analysis. The key feature of this licensing option relates to quantification of the uncertainty in BE safety analysis and inclusion of this uncertainty in the determination that an NPP has a "low" probability of violating the safety criteria specified in 10 CFR 50. To support the 1988 licensing revision, the USNRC and its contractors developed the CSAU evaluation methodology to demonstrate the feasibility of the BE plus uncertainty approach^[2,3]. The CSAU is described in detail in the references and the total methodology is not discussed further here. The PIRT process^[2,3,4], Step 3 in the CSAU methodology, was originally formulated to support the BE plus uncertainty licensing option as executed in the CSAU approach to safety analysis. Subsequent work has shown the PIRT process to be a much more powerful tool than conceived in its original form. Through further development and application, the PIRT process has shown itself to be a robust means to establish safety analysis computer code phenomenological requirements in their order of importance to such analyses. Used early in research directed toward these objectives, PIRT results also provide the technical basis and cost effective organization for new experimental programs needed to improve the safety analysis codes for new applications. This synergistic use of the PIRT process has been repeatedly demonstrated in applications to BE plus uncertainty analysis of a SBLOCA in a current generation NPP^[5], development of experimental programs and safety analysis requirements for two production nuclear reactors^[6,7], a proposed new research reactor^[8], two proposed advanced LWRs^[9,10,11,12] and support to resolution of a BWR licensing issue^[13]. Variations on the PIRT process have also been included in several international studies related to BE plus uncertainty analysis^[14,15,16].

The primary purpose of this paper is to describe the generic PIRT process, including typical and common illustrations from prior applications (Section 2). The secondary objective is to provide guidance to future applications of the process to help them focus, in a graded approach, on systems, components, processes and phenomena that have been common in several prior applications (Section 3). The paper is summarized and

concluded in Section 4. References providing further information are noted throughout the paper and identified in Section 5.

2. PIRT Process Description

The information obtained through the application of the PIRT process identifies the requirements that will be imposed on analytical tools used to simulate accident scenarios. In addition, those requirements are prioritized with respect to their contributions to the reactor phenomenological response to the accident scenario. Because it is not cost effective, nor required, to assess and examine all the parameters and models in a best estimate code in a uniform fashion^[2,3], the methodology focuses on those systems, components, processes and phenomena that dominate the transient behavior, although all plausible effects are considered. This screening of plausible phenomena, to determine those which dominate the plant response, insures a sufficient and efficient analysis. PIRTs are not computer code-specific, that is, PIRTs are applicable to the scenario and plant design regardless of which code may be chosen to perform the subsequent safety analysis. This also adds to the efficiency and generality of the process. A typical application of the PIRT process is conceptually illustrated in Figure 1 and described as follows.

2.1 Define problem

All PIRTs have a common basis in that they are developed to address plant behavior in the context of identifying the relative importance of systems, components, processes and phenomena in driving the plant response. However, details of PIRT development may vary depending on the specific problem to be resolved. In prior practice, PIRTs have been directed toward both: 1) research oriented more to code development associated with design confirmation^[2 - 12] and, 2) activities directed more to resolution of licensing issues^[13]. Accordingly, it is important to determine and define in some detail the specific problem for which resolution is desired. Further, it will eventually be necessary to develop an early match between the level of resources available and the level of effort to be expended in the PIRT development. It is foolhardy to set out to develop a broad based, highly detailed PIRT with insufficient funding, particularly if the chosen level of PIRT detail is not required for problem resolution. Thus, it is necessary to define the minimum achievement that has a high

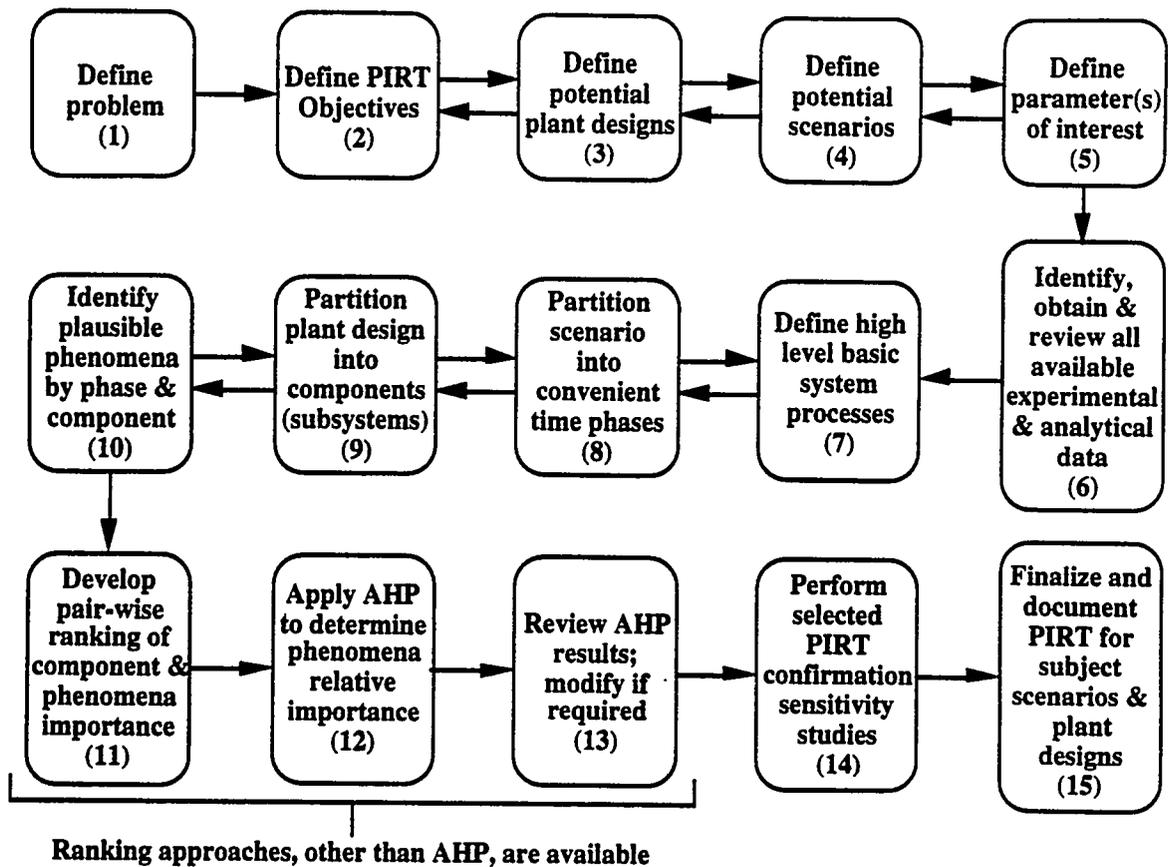


Figure 1. Illustration of typical application of PIRT process.

probability of effecting problem resolution. That is, specifically just what problem must be resolved and to what level. The references noted above can serve as guides based on prior experience.

2.2 Define PIRT objectives

The objective of a PIRT development is strongly oriented to the intended use of the PIRT. PIRTs have one primary and three adjunct functions depending on context and use (Figure 2). The primary function of a PIRT is to define plant behavior in the context of identifying the relative importance of systems, components, processes and phenomena in driving the plant response. This function is, therefore, the basis for the PIRT development, that is, to serve as plant performance indicators. Further, but subsequent to the primary purpose, a PIRT may serve one or more adjunct functions (Figure 2). That is, to provide guidance in establishing the requirements in:

- ① Separate and Integral Effects (SET, IET) experimental programs, where the objective is to help insure the experimental data fully reflect what may be expected in the plant,
- ② Code development and improvement, where the objective is to help insure the code is capable of modeling the plant behavior, and
- ③ Code uncertainty quantification, where the objective is to help insure the various contributors to uncertainty are identified and treated in a manner appropriate to their importance to plant behavior and, thus, to the overall uncertainty.

Implications of the above three items are further described in the ranking definition discussion in Section 2.11.

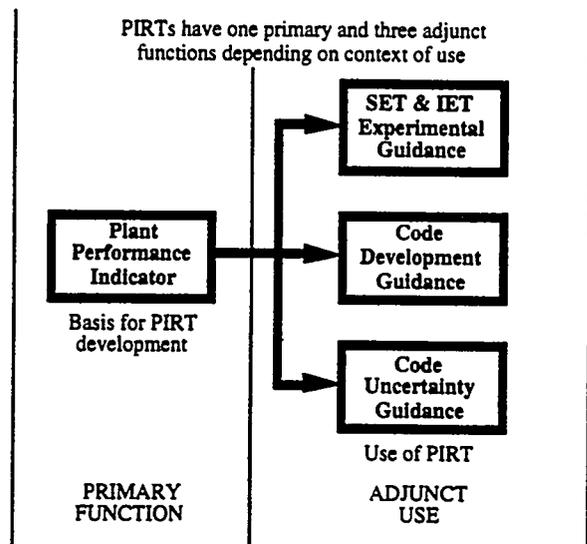


Figure 2. Conceptual use of PIRTs.

2.3 Define potential plant designs

The relative importance of phenomena/processes are plant design dependent to varying degrees. Thus, it is necessary to establish the NPP envelop to which the

PIRT(s) will apply. This step in the process must be coupled with the scenario(s) selection, discussed in the following section, to establish those plant systems/subsystems that will play a significant part in the plant behavior of interest. Further details in this regard have been documented in References [2]-[13]. That experience indicates two general findings:

- ① PIRTs addressing postulated accident transients (LBLOCA, SBLOCA, SGTR, etc.) in existing plant designs can often ignore the containment. The forced ECCS injection in these plants normally allows decoupling of the containment from the remaining plant systems. That is, the feedback from the containment to the primary, secondary and ECCS systems can be satisfactorily represented by boundary conditions.
- ② PIRTs addressing postulated accident transients in the new passive plant designs should consider the interactions between the containment and the remaining plant systems. Representation of the containment feedback as a set of boundary conditions should be demonstrated to be satisfactory before such decoupling is employed. This requirement arises because of the gravity driven ECCS condition that exists in many of the passive plant designs.

2.4 Define potential scenarios

The relative importance of phenomena/processes are scenario dependent. Although there are several systems/subsystems that are active in all plant designs in all scenarios, full understanding of the plant behavior also depends on other systems/subsystems that are specific to a particular accident scenario in a particular plant design. And as already noted, it is the combination of plant specific designs and scenario specific features that will dictate the system/subsystem envelop that must be considered in a PIRT development. More detailed guidance in this regard is available in References [2]-[13].

2.5 Define parameter(s) of interest

This step in the PIRT process deals with establishing the primary evaluation criteria that will be used to judge the relative importance of phenomena/processes in the plant behavior of interest. Primary evaluation criteria (or criterion) are normally based in regulatory safety requirements such as those related to restrictions in peak clad temperature, hydrogen generation, etc. The rank of a system, component, process or phenomena is a measure of its relative influence on the primary criteria (criterion). In US applications of the PIRT process, primary evaluation criteria are often derived from the regulatory requirements of 10 CFR 50^[1], as illustrated in Figure 3.

Peak clad temperature (PCT), clad oxidation, and hydrogen generation are specifically addressed in the regulatory requirements. Therefore, in accident transients were these parameters are likely (for example LBLOCA), they become prime candidates for selection as primary evaluation criteria. In practice, if it can be shown that the probability of PCTs above 982C (1800F) are low, then clad oxidation and hydrogen generation are insignificant and these parameters have reduced usefulness as primary evaluation criteria.

While PCT, clad oxidation and hydrogen generation regulatory limits remain in force for SBLOCA, analysis of

this class of transients are more normally directed toward insuring the fuel rods remain essentially covered by a two-phase mixture. Thus, it is common to use minimum core inventory, or a related parameter such as onset of significant voids, as the primary evaluation criterion.

PIRTs developed for containment analysis codes may use the regulatory requirements of Standard Review Plan (SRP) 6.2 as a basis for establishing the primary evaluation criteria.

2.6 Identify, obtain and review all available experimental and analytical data

Past experience shows that PIRT development is best accomplished using teams having broad base knowledge and expertise in relevant experiments, system analyses and plant operations. Further, because most PIRT process applications address state-of-the-art problems having finite resources, it is necessary the team exercise its collective engineering judgment (particularly in the initial development). Accordingly, the team must develop a collective knowledge base that represents the state-of-the-art understanding of all factors applicable to the problem of interest. Therefore, as early as possible in the PIRT process application, all relevant information should be identified, obtained and reviewed, individually and collectively, by the team. Sensitivity studies; however limited, to help better determine the relative influence of phenomenon performed early in the PIRT development have also proved worthwhile. Such information may come directly from experimental data analysis and/or code simulations of the experiments, and of the NPP/transient of interest. Often this type of analysis can eliminate phenomena by showing it does not exist, or is insignificant.

Experience has shown success in developing a PIRT, in a sufficient and cost effective manner, is strongly dependent on the composition of the team. Team attributes that promote success include:

- ① The collective expertise of the team should be extensive in depth. Team members should have extensive and current knowledge in their field of expertise, as may be reflected in individuals having well deserved international reputations.
- ② The collective expertise of the team should be broad based. The team make-up should have at least one member having expertise appropriate to the problem of interest in each of the following fields: Experimental programs, Code development, Code applications (safety analysis), Plant operations, and PIRT development methodology. There should be a clear team coordinator, preferably the team member having expertise in PIRT development methodology.
- ③ The team members should have a demonstrated capability to work in a team environment, particularly the ability to suppress individual agendas in the interest of the team objectives.

Level	Source	Criteria			Conservatism	Characteristic
1*	10CFR1.11	Protect public health & safety			Less limiting	Safety
2*	10CFR100	Limit fission product release				
3*	Appendix A	Limit fuel failure	Limit RCS breach	Limit containment breach		
4*	SRP 6.2 Containment	DNBR (PWR), MCPR (BWR), energy deposition, fuel temp., cladding strain	RCS & steam systems temp & pressure	Limit containment P & T, leakage, hydrogen, etc.		
	SRP 15.1.4 to 15.6.1 Non-LOCA					
	10CFR 50.46 & SRP 15.6.5 LOCA			PCT, oxidation, hydrogen generation, long term cooling, coolable geometry		
5	NUREG/CR-5818	Vessel inventory**				
6	Interim PIRT	Important parameters				
7	Interim PIRT	Dominant processes				
8	Interim PIRT	Ranked phenomena				

* Levels 1 - 4 are contained in NRC regulations or regulatory guidance
 ** Level 5 is key plant response criterion used for SBLOCA CSAU assessment

Figure 3. Illustration of the basis for development of primary evaluation criteria (SBLOCA example).

- ④ Experience has repeatedly shown that teams composed of more than six individuals become increasingly less effective as the number of members increases. However, the effectiveness of the team increases with the degree of technical support staff available to the team. Assignment of the team coordinator role to an individual having direct access to technical support staff is an effective technique. He/she then can call upon the technical support staff to execute the details of studies needed and defined by the team in the PIRT development and confirmation. The team coordinator should also have demonstrated skills in interpersonal relations in the context of effectively separating the wheat from the chaff in the various individual team member inputs, without suppressing the individual innovation of those members.
- ⑤ The customer for the PIRT of interest may be represented directly or indirectly on the team. Of more importance, the effectiveness of the team increases proportional to the degree of technical expertise, access to customer management, and program management skills possessed by the customer representative.

2.7 Define high level basic system processes

The initial development of the PIRT process, and the first several process applications, focused primarily on the relative importance of components and phenomena [2-10]. However, in more recent applications [11,13] the efficiency of introducing the identification and ranking of high level

system processes has been introduced. Specific identification of high level system processes has proven most valuable in efficiently organizing and focusing the subsequent identification of the components and phenomena that should be considered in the PIRT development. Further, perspectives of the relative importance of the high level system processes is a significant aid in ranking the components and phenomena. Often it can be shown a specific high level system process is of little consequence in a particular time phase (see Section 2.8), thus, further consideration of the associated components and phenomena is not necessary; a significant resource savings. High level system processes that have proved useful in prior PIRT process applications include:

- Depressurization
- Inventory reduction
- Inventory replacement
- Short-term dynamic core cooling
- Long-term evaporative core cooling
- Gas/vapor transport
- Suspended water transport
- Water depletion/accumulation/surface transport
- Debris transport
- Debris depletion

2.8 Partition scenario into convenient time phases

The relative importance of phenomena are time dependent as an accident progresses. Thus, it is convenient to partition accident scenarios into time phases in which the dominant phenomena/processes remain essentially constant. All, or nearly all prior applications of the PIRT process to LBLOCA have partitioned those transients into

blowdown, refill and reflood time periods. This partitioning has a basis in the regulatory requirements. Other time phase partitioning in prior PIRT process applications have included:

- SBLOCA in conventional PWRs: High pressure blowdown and long-term recovery
- Most transients in advanced PWRs: High pressure blowdown, ADS blowdown, short-term recovery and long-term recovery
- Most transients in advanced BWRs: Pre-isolation, isolation, depressurization (ADS), short-term recovery (refill) and long-term recovery

2.9 Partition plant design into components

From a modeling perspective, phenomena/processes important to a NPP response to an accident scenario can be grouped in two separate categories: 1) those local (within) to a component/subsystem, and 2) higher level system interactions (integral) between components/ subsystems. Thus, partitioning of the NPP into components/ subsystems is a significant aid in organizing and ranking phenomena/processes. Component partitioning common to prior PIRT process applications include:

- Accumulators
- Cold legs
- Downcomer
- Fuel rods
- Pressurizer
- Lower plenum
- Steam generator (PWR)
- Other unique systems
- Break
- Core
- ECCS
- Hot legs
- Pumps
- Separator (BWR)
- Upper plenum

For PIRTs directed toward analyses in which there are strong interactions between the primary systems and the containment, additional components may be needed such as:

- Containment interior
- Sump
- Vent (BWR)
- Drywell (BWR)
- Containment exterior
- Suppression pool
- Wetwell (BWR)

2.10 Identify plausible phenomena by phase and component

As noted in Section 2.6, PIRT development is best based on the collective expertise of broad based teams, and in the initial rounds tends to rely on the use of engineering judgment. The somewhat subjective nature of the process at these points in time introduces the question of completeness. That is, "how do the team members discover what they do not know" with respect to expanding state-of-the-art knowledge. The best technique discovered, to date, has been to formalize the process into two substeps:

- ① First, identify "plausible" phenomena/processes with strict adherence to not allowing ranking discussions during this substep. In effect this becomes a "brain storming" session(s). In this context, plausible phenomena/processes are those that have some significance to the plant behavior.
- ② Only after all team members are satisfied that the question of completeness can be defended, should the work proceed to phenomena/process ranking as subsequently described.

2.11 Rank components and phenomena importance

This step is the heart of the development of a PIRT. Figure 1 indicates a three step process specifically reflecting the use of a proven subjective decision making tool, the Analytical Hierarchy Process (AHP)[17]. The use of this tool is highly recommended to formalize subjective decision making into a product that is defensible, scrutinizable and complete. However, application of the AHP is not without resource penalties, and other less costly means are available. Accordingly, the following discussion is focused on the generic features of component and phenomena ranking regardless of whatever aids may be used to help in making subjective decisions.

The ranking process is dependent on the use of the resulting PIRT(s) as already discussed in Section 2.2 and Figure 2. In the context of that prior discussion, the most simple basis for ranking of a phenomenon/process regarding its relative importance to the primary evaluation criterion is to use a scale of low, medium or high. The low, medium and high ranks have definitions that correspond to the intended use. That is, with respect to the primary and adjunct uses summarized in Figure 2, the ranking definitions are:

- ① Primary use as plant performance indicators:
 - Low = Phenomenon has small influence on primary parameter of interest,
 - Medium = Phenomena has moderate influence ,
 - High = Phenomena has controlling influence.
- ② Adjunct use with experiments that may provide data for code development and validation:
 - Low = Phenomenon should be exhibited, but accurate measurements & prototypicality are of low importance.
 - Medium = Phenomenon should be exhibited; measurements may be derived; prototypicality may be somewhat compromised,
 - High = Phenomenon should be explicitly exhibited and well measured; phenomenon should be prototypical.
- ③ Adjunct use in the context of code modeling:
 - Low = Phenomena has small effect on the primary parameter of interest. Phenomena should be represented in the code, but almost any model will be sufficient,
 - Medium = Phenomena has moderate influence on the primary parameter of interest. Phenomena should be well modeled; accuracy maybe somewhat compromised,
 - High = Phenomena has dominant impact on the primary parameter of interest. Phenomena should be explicitly and accurately modeled.
- ④ Adjunct use in code uncertainty quantification:
 - Low = Combined uncertainty of phenomena may be determined in a bounding fashion, or may be eliminated when justified,
 - Medium = Phenomena should be evaluated to determine if uncertainty should be treated individually as are high ranks, or in a combined manner as are low ranks,
 - High = Phenomena uncertainty should be individually determined and then combined statistically with other uncertainty sources.

Ranking scales based on just low, medium and high are attractive in that they are the easiest to apply and have a simple numerical counterpart. That is, 1 = low, 2 = moderate and 3 = high. However, it is often helpful to differentiate between the lowest of the low, and highest of the high ranks. Prior experience suggests a numerical ranking scheme of 1 to 5 is a better scale, with the following meaning:

- 1 = Lowest of the low in importance
- 2 = Low importance
- 3 = Moderate importance
- 4 = High importance
- 5 = Highest of the high in importance

The final product of application of the PIRT process is a set of tables (PIRTs) documenting the ranks (relative importance) of phenomena and processes, by transient phase and system component.

2.1.2 Perform Selected PIRT Confirmation Sensitivity Studies

As reflected in Figure 1 and the preceding discussions, PIRT development is an iterative process with significant feedback between the various elements. At such time as may be deemed cost effective by the development team, key sensitivity studies should be performed by way of adding additional confirmation of the validity of the PIRT results. These studies may be a natural continuation of sensitivity studies performed early in the development (see Section 2.6). Continuing assessment of the moderately and highly ranked phenomena is of particular interest.

2.1.3 Finalize and Document PIRT for Subject Scenarios and Plant Designs

PIRT tables alone do not convey all the information that will be needed by the developers and users of the PIRTs. It is emphasized that excellent communication (documentation) of the PIRT process results is of paramount importance to the team members during PIRT development, to the team members and the customer during peer review of the PIRT process results, and to the customer, and/or other primary user of the PIRTs, following development. Experience strongly indicates success in developing useful PIRTs is a direct function of the degree to which supplemental products are well documented. Information typically important include descriptions of the plant(s), scenario(s), ranking scales, phenomena and processes definitions, evaluation criteria, and the technical rationale for each rank. References [9] and [11] are good examples of the level of documentation that has proven successful.

3. Typical Results from Prior PIRT Process Applications

The degree of phenomenological detail contained in a PIRT and, thereby, the direct applicability of the PIRT, is directly proportional to the specificity of the operating envelop considered in the PIRT. That is, PIRTs that convey the most phenomenological information tend to be very design and scenario dependent. Attempts to develop generic PIRTs by and large have proven to have limited usefulness. The move toward generic PIRTs by:

- ① "Lumping" several reactor designs together (for example all PWRs),

- ② "Lumping" several scenarios into a "class of scenarios" (for example all LOCAs),
- ③ Defining phenomena at higher levels (for example heat transfer rather than the specific modes of heat transfer),

has proven to be of limited value because the final results nearly always consist of everything being of high importance, or the phenomenological "classes" being too imprecise to be very useful to code development and/or improvement. Nevertheless, within "limited objectives", features common to all, or several prior PIRTs, can be derived. Two "limited objectives" have been selected for this paper:

- ① Identification of highly and moderately ranked phenomena that have been common in several of the prior PIRTs (Section 3.1),
- ② Identification of the relative importance of components in prior PIRTs by an arbitrary normalization scheme based on the frequency of occurrence of low, moderate and high phenomena ranks, and weighted by ranking importance (Section 3.2).

3.1 Phenomena Ranks Common to Prior PIRT Process Applications

Table 1 summarizes phenomena/processes that have typically been found to be of high importance during various general reactor response periods in the course of accident scenarios. Similarly, Table 2 summarizes phenomena/processes that are typically of moderate importance. The data reduction, in both tables, is considered to be appropriate to the objectives of this paper, but it is recognized the following data reduction procedures are somewhat arbitrary:

- Phenomena/processes and their ranks that are common to only one plant design or one scenario have been omitted from the tables.
- Cells that are shaded indicate that the time phase of interest does not exist in the subject transient/plant design, or is combined into another time phase shown in the table, or that a PIRT did not exist for the time phase of interest in the indicated transient/plant design.

Because of the above factors, the reader is cautioned that the tables should not be interpreted as indicating the only highly important phenomena/processes in NPP responses to accidents. The importance of phenomena/processes tends to be plant design specific. Thus, other phenomena/processes may also be highly important to specific designs. These tables only indicate the phenomena/processes that are highly important two or more plant designs/transients.

3.2 Relative Importance of Components in Prior PIRT Process Applications

Similar to the phenomena/processes importance shown in Tables 1 and 2, the relative importance of components in prior PIRT process applications can be derived through appropriate data collection and reduction techniques. Such information is provided in Table 3 based on the following data reduction procedures:

- The data focuses on components that are common to the majority of plant designs in the data base (for example core, fuel rods, downcomer, etc.).

Table 1. Phenomena/processes of typical high importance in prior PIRT applications.

General reactor behavior	Phenomenon	Frequency of high rank throughout the plant systems of interest										
		Total data base	WEC 4-loop LBLOCA	AP600 LBLOCA	B&W SBLOCA	AP600 SBLOCA	AP600 MSLB	SBWR MSLB	SBWR bottom drain line LOCA	SBWR GDCS line LOCA	AP600 SGTR	Production reactor DEGB
Rapid blowdown from high pressure through large breaks and/or ADS	Critical flow	17	1	1		1	1	2	5	5		1
	Flashing	15				1	1	4	4	4		1
	Subcritical flow	12				2		2	4	4		
	Voiding & distribution	10						3	4	3		
	Condensation	10						2	4	4		
	Entrainment/de-entrainment	10					1	1	4	4		
	Convective heat transfer	8	2				1	2	1	1		1
	Inventory/level	8				3	1		1	2		1
	Conduction heat transfer	6	2				1		1	1		1
	Decay heat	6				1	1	1	1	1		1
	Phase separation	5				2		1	1	1		
	Natural/intenal circulation	4						2	1	1		
	Evaporation	3						1	1	1		
	Stored energy	3	1					1				1
	Parallel channel flow	2					1					1
Energy transport by liquid	2				1	1						
Noncondensable effects	2							1	1			
Core inventory recovery, including refill and reflood	Decay heat	7	1	1			1	1	1	1	1	
	Convective heat transfer	7	3	1			1				2	
	Two-phase flow/delta-p	5	2					1	1	1		
	Inventory/level	4	2	2								
	Critical flow	4	1	1							2	
	Conduction heat transfer	4	1				1				2	
	Flow resistance/friction/form loss	3						1	1	1		
	Subcritical flow	2		1								1
Slow depressurization from high pressure through small breaks	Critical flow	2			1							1
	Decay heat	2			1							1
Long-term recovery	Subcritical flow	13		4	2	1		2	2	2		
	Noncondensable effects	9						3	3	3		
	Inventory/level	7				5		1	1			
	Convective heat transfer	5		1	1			1	1	1		
	Flow resistance/friction/form loss	4				1		1	1	1		
	Condensation	4		1				1	1	1		
	Conduction heat transfer	4			1			1	1	1		
	Decay heat	4				1		1	1	1		
	Natural/intenal circulation	3						1	1	1		

Table 2. Phenomena/processes of typical moderate importance in prior PIRT applications.

General reactor behavior	Phenomenon	Frequency of moderate rank throughout the plant systems of interest										
		Total data base	WEC 4-loop LBLOCA	AP600 LBLOCA	B&W SBLOCA	AP600 SBLOCA	AP600 MSLB	SBWR MSLB	SBWR bottom drain line LOCA	SBWR GDCCS line LOCA	AP600 SGTR	Production reactor DEGB
Rapid blowdown from high pressure through large breaks and/or ADS	Condensation	24				2	1	7	7	7		
	Flashing	23		4		4	4	2	4	4		1
	Voiding & distribution	19	1			1	6	2	4	4		1
	Stored energy	19				2		5	6	6		
	Subcritical flow	17		5		2		2	4	3		1
	Conduction heat transfer	16		1		2	2	3	3	3		2
	Convective heat transfer	15				2	2	2	3	3		3
	Noncondensable effects	11				2	2	3	2	2		
	Inventory/level	9		1		4	1	1	1	1		
	Entrainment/de-entrainment	7		1		2			2	2		
	Thermal stratification	6				3		1	1	1		
	Natural/intenal circulation	5						1	2	2		
	Critical flow	4				1			2	1		
	Flow resistance/friction/form loss	4				2			1	1		
	Two-phase flow/delta-p	3						1	1	1		
	Parallel channel flow	3						1	1	1		
	CHF/dryout	3				1	2					
	Phase separation	2		1				1				
	Boiling	2	1			1						
	Core inventory recovery, including refill and reflood	Subcritical flow	14	1	3			1	2	3	2	2
Convective heat transfer		9	3	3			1				2	
Voiding & distribution		8	2				5				1	
Conduction heat transfer		8	2	4			1				1	
Noncondensable effects		7		2			4				1	
Inventory/level		6		1			3		1	1		
Condensation		5	1	2			1				1	
Countercurrent flow/CCFL		4	1	3								
Natural/intenal circulation		3	1					1				1
Flashing		3	1				1					1
Flow resistance/friction/form loss		2					1					1
Entrainment/de-entrainment		2	1	1								
Stored energy		2		1				1				
Long-term recovery	Condensation	8				2		2	2	2		
	Subcritical flow	5		2		2			1			
	Noncondensable effects	5		1		1		1	1	1		
	Inventory/level	3		2		1						

$$(Component\ normalized\ rank)_i = 1 + \left[\frac{(Weighted\ rank\ sum)_i - (Weighted\ rank\ sum)_{min}}{(Weighted\ rank\ sum)_{max} - (Weighted\ rank\ sum)_{min}} \right] \times [9]$$

where:

$$(Weighted\ rank\ sum)_i = \sum_i Low\ ranks + 2 \times \sum_i Moderate\ ranks + 3 \times \sum_i High\ ranks$$

and $(Weighted\ rank\ sum)_{max/min}$ are for the total data base

- To help promote commonality in the PIRTs, certain component grouping has been used. For example several of the plant specific components in the AP600 and SBWR, such as the CMT, IRWST, suppression pool, etc. have been grouped into a single ECCS entry (see later comment).
- The data has been normalized to a scale of one to ten as shown above:

The relative component importance given in Table 3 is a measure of the relative importance of the indicated components in all the prior PIRTs identified. For example, based on the total data available, the downcomer, break and core components are shown to be of primary priority in the plant behaviors. Similarly, the hot legs, pressurizer, pump and containment exterior components are shown to be of lesser importance. Lesser importance should not be interpreted to mean of little importance. For certain scenarios and time phases these components may, and probably will, have associated phenomena of high rank. The lesser relative importance in Table 3 is better characterized as meaning these components have fewer high ranked phenomena for shorter periods of time. Thus, it should be recognized the normalized relative component importance shown in the table is only of an approximate nature. For example the effort to achieve more commonality in the data base by lumping a number of components in the listed ECCS component results in a large number of entries in each of the rank categories (low, moderate and high). This tends to inflate the normalized importance of the ECCS component. Similarly, because accumulators do not exist in all the designs listed, the relative importance of this component may be underestimated. Nevertheless the data in Table 3 can be used as general guidance in future PIRT development. In addition, there is sufficient data in Table 3 that a reader could refine the analysis, say to just PWR designs, if so inclined.

4. Summary

The PIRT process was originally formulated to support the BE plus uncertainty licensing option as executed in the CSAU approach to safety analysis. Subsequent work has shown the PIRT process to be a much more powerful tool than conceived in its original form. Through further development and application, the PIRT process has shown itself to be a robust means to establish safety analysis computer code phenomenological requirements in their

order of importance to such analyses. Because it is not cost effective, nor required, to assess and examine all the parameters and models in a best estimate code in a uniform fashion, the methodology focuses on those processes and phenomena which dominate the transient behavior, although all plausible effects are considered. This screening of plausible phenomena, to determine those which dominate the plant response, insures a sufficient and efficient basis for identifying needed code improvements and subsequent code development.

While the usefulness of PIRTs tend to increase with their specificity to each particular application and its objectives, there are certain commonalities in all such applications. The more important of these common features have been described in this paper in the context of typical results from prior applications of the PIRT process. This information may be expected to help future applications of the PIRT process, particularly in identifying typical:

- Primary evaluation criteria for judging the importance of phenomena/processes, including their licensing basis,
- Partitioning of accident scenarios into time phase,
- Partitioning of NPP designs into components/subsystems,
- Phenomena/processes ranking approaches, including the meaning of the ranks for guidance to experimental, code development and code uncertainty quantification work,
- Phenomena/processes commonly of moderate and high importance in prior applications of the PIRT process, and
- Desired elements in the organization and use of expert teams to develop PIRTs.

5. References

- [1] U. S. Federal Register, Acceptance Criteria for Emergency Core Cooling Systems for Light Water Reactors, 10 CFR 50 (1988).
- [2] TPG (Technical Program Group), *Quantifying Reactor Safety Margins: Application of CSAU to a LBLOCA*, NUREG/CR-5249, EG&G Idaho, Inc. (1989).
- [3] TPG (Technical Program Group), *Quantifying Reactor Safety Margins: Application of CSAU to a LBLOCA*, Nuclear Engineering and Design 119 (1990):
B. E. Boyack et al., Part 1: An overview of the CSAU Evaluation Methodology,
G. E. Wilson et al., Part 2: Characterization of Important Contributors to Uncertainty,
W. Wulff et al., Part 3: Assessment and Ranging of Parameters,
G. S. Lellouche et al., PART 4: Uncertainty Evaluation of LBLOCA Analysis Based on TRAC-PF1/MOD1,
N. Zuber et al., Part 5: Evaluation of Scale-Up Capabilities of Best Estimate Codes,
I. Catton et al., Part 6: A Physically Based Method of Estimating PWR LBLOCA PCT.
- [4] R. A. Shaw, T. K. Larson and R. K. Dimenna, *Development of a Phenomena Identification and Ranking Table (PIRT) for Thermal-Hydraulic Phenomena During a PWR LBLOCA*, NUREG/CR-5074, EG&G Idaho, Inc. (1988).
- [5] M. G. Ortiz and L. S. Ghan, *Uncertainty Analysis of Minimum Vessel Liquid Inventory During a SBLOCA in a Babcock and Wilcox Plant*, NUREG/CR-5818, EG&G Idaho, Inc. (1992).
- [6] R. G. Hanson et al., *Development of a PIRT for a Postulated Double-Ended Guillotine Break in a Production Reactor*, Nuclear Engineering and Design 136 335-346 (1992).
- [7] G. E. Wilson et al., *Phenomena-Based Thermal Hydraulic Modeling Requirements for Systems Analysis of a Modular High Temperature Gas-Cooled Reactor*, Nuclear Engineering and Design 136 (1992).
- [8] G. E. Wilson, *Statistically Based Uncertainty Analysis for Ranking of Component Importance in the Thermal Hydraulic Safety Analysis of the Advanced Neutron Source Reactor*, EGG-NE-10078, EG&G Idaho, Inc. (1992).
- [9] C. D. Fletcher, et al., *Final PIRTs for WEC AP600 SBLOCA, MSLB and SGTR Scenarios*, INEL-94/0061-Rev. 2, Lockheed Martin (1996) [Distribution at the discretion of the USNRC].
- [10] G. E. Wilson et al., *Use of PIRT Process in Research Related to Design Certification of the AP600 Advance Passive LWR*, International Conference on Nuclear Engineering, Vol. 2 ASME (1996).
- [11] B. E. Boyack, *AP600 LBLOCA Phenomena Identification and Ranking Tabulation*, LA-UR-95-2718, Los Alamos National Laboratory (1995) [Distribution at the discretion of the USNRC].
- [12] P. G. Kroeger et al., *Preliminary Phenomena Identification and Ranking Tables for SBWR LOCA Scenarios*, Technical Letter Report W-6092-5 6/95, Brookhaven National Laboratory (June 1995) [Distribution at the discretion of the USNRC].
- [13] G. E. Wilson et al., *BWR Drywell Debris Transport Phenomena Identification and Ranking Tables (PIRT)*, Letter Report, Idaho National Engineering Laboratory (Initial Issue June 28, 1996) [Distribution at the discretion of the USNRC].
- [14] H. Glaeser et al., *Uncertainty and Sensitivity Analysis of a Post-Experiment Calculation in Thermal Hydraulics*, SMIRT-12, Post Conference Seminar No. 15, Heidelberg, Germany (1993).
- [15] E. Hoffer, *The GRS Programme Package for Uncertainty and Sensitivity Analysis*, *Proceedings of the Seminar on Methods and Codes for Assessing the Off-Site Consequences of Nuclear Accidents*, EUR 13013, Commission of the European Communities (1990).
- [16] H. Holmstrom, et al., *Status of Code Uncertainty Evaluation Methodologies*, *Proceedings of the International Conference on New Trends in Nuclear System Thermohydraulics*, Pisa, Italy (1994).
- [17] T. Saaty, *Decision-Making For Leaders*, Belmont, CA, Lifetime Learning Publications, Wadsworth Inc. (1982).

**TECHNICAL SESSION 1: CURRENT AND ANTICIPATED USES
OF THERMAL-HYDRAULIC CODES**

Co-Chair: Prof. Yadigaroglu (Switzerland), Dr. Ybarrondo (USA)

Current and Anticipated Uses of the Thermal Hydraulics Codes at the NRC

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Abstract

The focus of Thermal-Hydraulic computer code usage in nuclear regulatory organizations has undergone a considerable shift since the codes were originally conceived. Less work is being done in the area of "Design Basis Accidents," and much more emphasis is being placed on analysis of operational events, probabilistic risk/safety assessment, and maintenance practices. All of these areas need support from Thermal-Hydraulic computer codes to model the behavior of plant fluid systems, and they all need the ability to perform large numbers of analyses quickly. It is therefore important for the T/H codes of the future to be able to support these needs, by providing robust, easy-to-use, tools that produce easy-to-understand results for a wider community of nuclear professionals.

These tools need to take advantage of the great advances that have occurred recently in computer software, by providing users with graphical user interfaces for both input and output. In addition, reduced costs of computer memory and other hardware have removed the need for excessively complex data structures and numerical schemes, which make the codes more difficult and expensive to modify, maintain, and debug, and which increase problem run-times. Future versions of the T/H codes should also be structured in a modular fashion, to allow for the easy incorporation of new correlations, models, or features, and to simplify maintenance and testing. Finally, it is important that future T/H code developers work closely with the code user community, to ensure that the codes meet the needs of those users.

Background

Thermal-Hydraulic (T/H) code development began 40 years ago, with the application of the first generation of computers to analyze the performance of the first generations of nuclear power plants. The codes and the computers of that age were both limited in their capabilities. The computers were not very fast. Their input and output systems were very cryptic, difficult to understand, and unforgiving. The size of the problems that they could handle was small, because computer memory was very expensive, and schemes to increase the size of the problem slowed down processing speed even more.

In addition, the physics of fluid flow, especially in the two-phase region, was not well understood. Relatively little test data existed, especially for the flow regimes that were of interest to nuclear applications. Computers were in their infancy, and numerical methods to make the best use of digital computers were just being developed. Some analysts were insisting that the best way to perform complex modeling of physical systems was with analog computers, not digital ones. Since then, as the power of the computers has increased, and as experimental data been developed, so has our need and desire to apply these codes to new problems.

Code Applications

Design Basis Analyses and Operating Event Analyses

In the early 1970s, T/H code development was driven by the need for tools to model "Design Basis Accidents (DBA)." These accidents are formally defined in regulatory documents, and were thought, at the time, to conservatively bound the limiting operating conditions of reactor systems and components during transient and accidents. The AEC (and later, the NRC) developed its own T/H codes in order to establish an analytical capability independent from the reactor vendors. The goal of the NRC program was to develop T/H codes that could be used to check the adequacy of the vendor codes for DBA calculations, and the agency created a large experimental program to develop actual test data for comparison with code predictions. With this data, and as computer power increased, it became possible to model reactor behavior in more detail, and it appeared that it might be possible to create "best estimate" calculations. The efforts of the NRC since then have been focused on the development of T/H codes that reproduce the phenomena associated with reactor transients and accidents, to the highest fidelity that is both possible, and necessary for making regulatory decisions. NRC codes have been used to benchmark licensee and applicant calculations, to understand the behavior of plants during actual transients and accidents, and to understand the consequences if the events had proceeded differently.

In addition to performing analyses of DBAs in support of licensing actions, T/H codes have been used to perform analyses of events after they have actually occurred, in order to better understand the sequence of events, as well as to examine other possible courses that an event might have followed.

These functions are expected to continue, as long as nuclear power plants are operating. Under pressure from other sources of electricity to reduce costs, nuclear utilities are continually looking for ways to improve fuel performance by extending the time between refueling outages, by reducing thermal margins, and by increasing reactor power levels. Some licensees are also using reactor cores that are designed to reduce neutron fluence at the reactor vessel wall, in order to reduce embrittlement, and such designs lead to higher power peaking factors. All of these improvements in performance need to be supported by technical calculations by licensees and/or fuel vendors, and nuclear regulators will therefore need to maintain the ability to perform independent verification calculations.

Probabalistic Risk/Safety Assessment

In the mid-1970s, the art of Probabilistic Risk Assessment (PRA) began to flourish, with the publication of WASH-1400, the "Reactor Safety Study". This study considered many different accident scenarios, not just the stylized DBAs, and determined that the majority of the risk from nuclear power production arose from scenarios that had originally been thought to be more benign than the DBAs. In addition, PRA analysis considered multiple failures of systems and components beyond the failure definitions of the DBAs.

The March 1979 accident at Three Mile Island, which was not a DBA, but instead was caused by a collection of equipment failures and operator errors, pointed out the need to be able to analyze the scenarios discussed in PRA studies. Close scrutiny of other reactor transients and events following TMI revealed the existence of "severe accident precursors", events which could have eventually led to severe accidents, had additional equipment failures or operator errors occurred. Unfortunately, PRA analysis considers very large numbers of slightly different scenarios, and it had not been practical to use the best T/H codes to simulate more than a handful of PRA scenarios with the best T/H codes, because of the large amount of time that is needed to set up and run each individual scenario.

In recent years, licensees have started to use fast-running codes, such as MAAP, to support PRA calculations. The fast-running codes can produce results for one PRA sequence in about one hour, and with a network of powerful workstations and some clever programming, it is relatively easy to run through rather some large sets of sensitivity calculations in a few weeks of computer time. Nuclear regulators need to be able to validate the ability of these simplified codes to accurately predict reactor behavior. Because PRAs are supposed to be "best estimate" tools, without the addition of conservatism, the thermal-hydraulic tools that model the individual sequences also need to be "best estimate". Regulators do not need to re-create the entire spectrum of PRA sequences that are generated by a licensee, but they do need the ability to check a selected set of sequences, and it should be possible for PRA practitioners to perform these checks.

Thermal-Hydraulic User Community

Traditional Users

Historically, T/H computer codes have been used by scientists and engineers with extremely specialized and focused backgrounds. First of all, these individuals have needed strong backgrounds in fluid flow, heat transfer, and general nuclear engineering, because an understanding of the physics of the systems is essential to the production of good analytical products. In addition, code users have also had to have a strong background in computer science, computer programming, and computer operating systems, along with a very tolerant mental attitude towards computers. Even then, good analysts take a long time to develop and mature.

The current generation of codes are deliberately designed to be general purpose tools, with many options and opportunities for customization. This allows them to be applied to the widest spectrum of analyses.

The best analysts know the code options thoroughly, and they also know how to use those options to make the codes produce results that are very close to experimental data. These analysts take drawings and descriptions of plant piping and control systems, and translate them into the input models of the facility under study for the T/H code. They know best how to nodalize the piping, where and how to attach the heat structures, and how to model the break flow characteristics. This level of expertise takes a considerable amount of time to develop, though, and is not a skill that every engineer can master. It also requires continuous exposure to both the codes and to challenging analytical problems to maintain. These people are very valuable to an organization, but they are rare. For the purposes of this paper, I characterize them as "Category 1" users. For future analytical work, two new categories of code user have emerged.

Knowledgeable Engineers

Category 2 users include the nuclear, mechanical, and reactor engineers who have a need to model reactor system performance, but may not have the time, or talents, to learn the intricacies of running a T/H code. They are the first people called upon to assess the implications of an event at an operating reactor, and are also the people who have to make the initial recommendation for the acceptance or rejection of a licensing modification request. Often, their experience with the behavior of other plants or systems is sufficient to allow them to make assessments without recourse to calculations. In other cases, they may have an initial impression about a technical issue, but may want to verify it with a calculation. Sometimes the calculation can be performed by hand, but many times, it would be more useful to have an easy-to-use computer tool to calculate the flow of water or steam in a simple network of piping, or a simple heat up.

The most common situation where this arises is for events that occur during reactor shutdown, when a maintenance worker opens the wrong valve, or a freeze-seal fails, and a large amount of water is drained out of a reactor coolant system. Alternatively, if RHR cooling is lost, a heat up can begin, and the question that is always raised is "How long would it take before the core starts to boil?" or "How long would it take to drain the reactor vessel and uncover the core?" With easy-to-use tools at their disposal, engineers with minimal specialized code training should be able to develop a model of a simple piping system, impose a break, and calculate simple flow rates and water levels as a function of time. The current generation of codes is much too cumbersome to solve these problems in any reasonable time, and they require highly trained people to use them.

Over the next few years, as maintenance practices receive higher levels of scrutiny, and as licensees and regulators need to determine the relative risk associated with various shutdown/maintenance evolutions, the need for quick, accurate calculations of "what-if?" scenarios will increase significantly. This class of user is already well served in the mechanical and

structural engineering profession, where several very sophisticated tools exist to model structures and components for mechanical stresses and strains. With these tools, which are currently used in engineering courses in universities, knowledgeable engineers can model a structure or component in three dimensions very quickly, using a drawing tool on a screen, and then subject it to the desired loads, and have the resulting stresses and strains plotted automatically. This is the sort of capability that needs to be made available to our reactor and systems engineers in the nuclear industry.

Simulator Users

The third category of T/H code users is the newest, and the fastest growing. It includes nuclear professionals who may have a basic knowledge of reactor fluid dynamics and system behavior, but who do not need to know anything about the detailed phenomena in the core or individual pipes or components. Their needs are for a code that functions like a simulator, at the overall plant level, and allows them to manipulate the operation of each individual valve and pump and component, to turn equipment on and off, and to create breaks and equipment failures in a wide variety of locations.

These individuals are primarily associated with PRA, but could also be involved in operator training, or operating procedure development. They need to be able to run many different scenarios, with many variations, and to be able to simulate the behavior of the operators as they react - correctly or incorrectly - as the scenario unfolds. They do not want to be involved in the development of the computer model itself. They do not want to have to know all of the error messages from the system. They want to be able to use the T/H code and plant model as a simulator, to understand how the reactor system will behave on a macro level. It should be noted that several organizations in the United States are considering the use of existing best-estimate T/H codes as the drivers for engineering workstation-based plant simulators, which would be used to train operators, perform engineering calculations, and verify operating procedures.

The NRC is taking great efforts to include risk-informed decision making in its regulatory processes, and it is difficult to make good risk-informed decisions if you do not have the tools to calculate the performance of the systems accurately. It is also not possible to train a sufficient number of expert users to support the PRA needs. The T/H codes that calculate these scenarios need, therefore, to be quite robust, quite user-friendly, and able to warn the user when their results venture into ranges for which they are not valid. The plant models that they use will likely be developed by the experienced code users, but the goal should be that once a model is complete, the experienced user will release it to the end-user and his future involvement in simulator-like calculations will be minimal.

Typical Analyses

At the NRC, several different organizations use the T/H codes to perform analyses. The Office of Research, which is responsible for T/H code development and maintenance, has been heavily involved in the use of the codes for studies of advanced reactor performance during DBA

conditions. The Office for the Analysis and Evaluation of Operational Data uses T/H codes to develop simulation scenarios for exercises in the incident response center, to evaluate actual reactor events, and to train NRC staff members at the Technical Training Center.

The Office of Nuclear Reactor Regulation is using the codes in support of the licensing of new advanced reactor designs, for the analyses of operating reactor events, and in support of reviews of vendor and licensee computer codes. Some of the tasks that have been performed include:

1. In support of an ALWR licensing review, NRR analysts used the RELAP5 code to perform check calculations of a series of PRA success-path sequences, to verify the performance of the applicant's T/H code. The sequences that were calculated included several loss of feedwater transients with various combinations of equipment operable, several small-break loss of coolant accidents, steam generator tube rupture accidents, and intermediate size loss of coolant accidents. In addition, a series of sensitivity calculations was performed for one particular sequence to determine the sensitivity of the calculation to variations in various input parameters and assumptions. One important conclusion that arose from this series of calculations was that the decay heat assumptions used by various analysts was not consistent. As a result, the analyst prepared an information notice to alert other analysts about the various factors that need to be considered in determining appropriate decay heat levels for reactor calculations.
2. In 1995, a boiling water reactor in the United States that had just been shutdown for maintenance experienced a loss of residual heat removal(RHR) cooling for a sustained period of time, and experienced an unplanned mode change. An NRR analyst used the TRAC-P code to model the internals of the reactor to determine the sensitivity of the reactor to variations in downcomer water level and RHR flow rate. He specifically modeled the event that occurred, and then considered several similar scenarios with different initial conditions. He determined that boiling did not occur in the reactor core during the transient.
3. NRR analysts have been called upon several times to perform check calculations of steam main steam line breaks, actual generator tube rupture events, or postulated steam generator tube rupture events, for licensing reviews. In one case, an analyst was asked to calculate the differential pressure across the tube support plate in a steam generator during a main steam line break, in order to determine the deflection of the support plate. The deflection was needed to determine whether the support plate would continue to restrain the tube, which had sustained a crack in the support plate region. If the support deflected sufficiently, then the crack would be exposed, and it would be possible that the tube would rupture. The licensee initially used a proprietary code that was not validated for this application, but after questioning by the staff, shifted to RELAP5. The staff reviewed the RELAP5 calculation, and then performed an independent TRAC-P calculation to verify that the magnitude of the loads calculated by the licensee was reasonable.
4. During a maintenance outage, a PWR in the US discovered that the performance of one of its ECCS pumps had been degraded for about one year, because of a damaged relief valve. An NRR analyst calculated the plant performance during several small-break LOCA scenarios assuming the degraded ECCS system as an input parameter. He also considered several scenarios

where the ECCS performance was degraded more than the as-found condition, and determined that, even with the degraded systems, the plant retained margin for limiting fuel temperatures.

5. As a result of allegations by plant staff, NRR investigated the behavior of spent fuel pools under degraded cooling conditions. One of the concerns that was raised related to the shielding effect of the water in the pool, and how radiation levels in the spent fuel pool building would be affected as the water above the fuel boiled away. An NRR analyst used the TRAC code to perform an analysis of the boiling phenomena in a spent fuel pool without external cooling, to determine the void profile in the water above the fuel.

6. In a PWR that was shutdown for maintenance, an operator who was conducting motor-operated valve testing misaligned the valves in one flow path, and drained approximately 9200 gallons of water from the reactor. At the request of AEOD, NRR performed an analysis of the consequences of such a leak that was not isolated, for various different combinations of decay heat and reactor coolant pump operational states. The analysis was used to determine the amount of time that an operator would have to react to the event, and how high fuel temperature would rise.

7. In support of ALWR licensing reviews, NRR analysts have performed ATWS and station blackout calculations, to compare against applicant calculations. For the ATWS case, the analyst considered the significance of the licensee's assumptions for moderator feedback at beginning of life, and determined that this was an important factor that needed to be addressed in more detail by the applicant.

8. In response to an allegation, NRR evaluated the significance of a return-to-power scenario in a PWR following a large break LOCA accident with a failure to scram. A detailed analysis of this scenario was performed by a contractor using a coupled three-dimensional T/H and three-dimensional neutron kinetics calculation. When the contractor report was submitted for approval, an NRR analyst who was not involved in the contract was asked to perform an independent calculation of the accident to verify the reasonableness of its results and the phenomena that it predicted. Several sensitivity cases were run to examine possible behavior changes due to void reactivity feedback effects, and the independent calculation verified the contractor's results

Probabilistic Risk/Safety Assessment

Resource Implications

Regulatory organizations are under continual pressure to do more with fewer resources. Future T/H codes should be easier to use than the current generation, so that less time is needed to generate plant models and evaluate their output. They must also be compatible, in some way, with the models that are the input to the old T/H codes. Every organization that uses the current generation of codes has invested a considerable resources in training staff members to use the codes, and has also invested considerable resources to develop plant models. New versions of T/H codes must include the capability to read old plant models and convert them into new input formats so that these investments are not lost.

Summary

We believe that in the future, the number of Category 2 and 3 users will grow at a rapid rate, in order to support risk informed regulation, and to support the need for better technical analyses of maintenance and shutdown events. Regulatory organizations do not have the resources to develop sufficient numbers of Category 1 users to support these needs, so the T/H codes need to be adapted to the user community. Future T/H codes should make use of user interface technologies that are already in existence in other technical disciplines, and they must include sufficient "intelligence" to warn unsophisticated users when they venture into operating regions or modeling situations that have not been well validated. They must be "robust". They must be consistent. They must be traceable. They must be transparent. And they must be correct.

Current and Anticipated Uses of the CATHARE Code at EDF and FRAMATOME

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ABSTRACT

This paper presents current industrial applications of the CATHARE code in the fields of Safety Studies and Simulators where the code is intensively used by FRAMATOME, EDF and CEA, the development partners of CATHARE. Future needs in these fields are also recapitulated.

Safety Studies :

In the context of CATHARE original development for Loss Of Coolant Accidents (LOCA), in order to demonstrate Emergency Core Cooling System (ECCS) adequacy and compliance with safety criteria, FRAMATOME currently uses CATHARE in so-called "Better Estimate" or "realistic deterministic" methodology relying upon use of Best-Estimate code, with conservative initial and boundary conditions; the limiting case is identified in a deterministic way cumulating elementary conservatisms, with the demonstration of code adequacy : proper accounting of code uncertainties, justification of nodalization and modeling scheme by sensitivity studies.

FRAMATOME has used CATHARE in this realistic deterministic approach for licensing calculations of small breaks LOCA for French 4-loop plants, Koeberg South African and Ringhals 3 Swedish plants. The same realistic deterministic approach is under development for large breaks LOCA. Such LOCA analyses justify new plant configurations : core peaking factor or power increase, SG replacement or tube plugging, fuel management or design (high burnup, mixed UO₂-PuO₂). The next step for CATHARE LOCA applications will consist in the development of Best Estimate methodology featuring the statistical combination of uncertainties.

CATHARE has been used for realistic plant response to support emergency recovery procedures, with assessment of :

- reactor vessel level instrumentation system, at degraded RCS mass inventory;
- time delay before core uncover in the case of total loss of high or medium head ECCS pumps (beyond design basis accident, BDBA);
- feed and bleed efficiency in the case of total loss of SG feedwater (BDBA);
- long term plant safe state in the case of coincident steam line break and multiple (100) SG tube ruptures (BDBA).

CATHARE has been used for new reactors and new system designs :

- automatic RCS water supply for loss of Residual Heat Removal system; all states (partial or full RCS opening, mid-loop operation) can be considered thanks to CATHARE noncondensable gas modeling;
- assessment of passive safety reactors, with gravity driven or stored gas energy (accumulators) components;
- severe accident passive systems: cooling system of core catcher sole plate.

CATHARE is also the basic tool for the new FRAMATOME-SIEMENS EPR reactor.

Since CATHARE modeling capabilities are not limited to UTSG PWRs, but have been extended to VVERs, mainly featuring horizontal SG, FRAMATOME extensively uses CATHARE for all kinds of VVER plants and transients, LOCA and non-LOCA design basis accidents, and also BDBA.

FRAMATOME also uses CATHARE as a reference code for simpler models, by benchmarking them against CATHARE, or by improving them with more detailed modelization of component response or specific physical phenomena, resulting from CATHARE in-depth analysis.

Simulators :

The training of Electricité de France NPP operators on simulators benefits from the wealth of the French PWR generating capacity and from nearly 20 years of experience. In the past few years, EDF has been leading wide-ranging changes in simulator design and operation and increasing its operator training effort, while rationalizing its range of simulation tools.

In this context, the Post-Accident Simulator SIPA has been developed, using CATHARE-SIMU, a speeded-up version of the CATHARE1 code (CATHARE1 is a former version of CATHARE2 using the standard 6 equation model for the primary circuit of a PWR and a 3 equation model for the secondary circuit).

From 1991, three of these simulators have been delivered with two configurations (900 MW and 1300 MW) of the French NPPs : one was installed at SEPTEN (Basic Design Department of the Engineering and Construction Division of EDF, Villeurbanne, next to Lyon), one at CEA/IPSN (Fontenay aux Roses, next to Paris) and more recently one at CEA/STR in Grenoble where a team is in charge of the maintenance of CATHARE-SIMU in a simulator environment.

At EDF, where this simulator is intensively used for the training of both Operators (Shift Safety Advisors, Operating Managers...) and for the members of the National Crisis Organization, the richness of information provided by the tool, its user-friendliness, the realism of the images of the Pedagogical System have been unanimously recognized. Moreover, in 1995, a new configuration was implemented to represent the new 1450 MW N4 French NPP, whose first application will be the validation of Emergency Operating Procedures.

In the very near future, three full-scale simulators using the SIPA principles will be installed on the BUGEY, FESSENHEIM (900 MW-CPO type) and CHOOZ (1450 MW-N4 type) sites. The EDF's Production and Transport Division has also decided to renovate all of the 9 current full-scale simulators (installed in the training centers) and to install, from 1996, SIPACT (Sipa comPACT) simulators on each of the 18 NPP sites (running on work stations).

In the longer term, EDF's ambition is to incorporate CATHARE2 in all of its simulators, in replacement of CATHARE-SIMU, so that there will be only a single code available to study, engineering and training. Adapting CATHARE 2 to real time simulators, and extending the validity domain of its simulators to all transients occurring from any state, including situations with open primary circuit are EDF's new perspectives. These objectives require developments in three directions : physics (especially for low pressure), real time capabilities, and automatic generation of the CATHARE modules. These developments are the subject of the SCAR (Simulator Cathare Release) project.

INTRODUCTION

This paper presents current industrial applications of the CATHARE code in the field of Safety Studies and Simulators where the code is intensively used by FRAMATOME, EDF and CEA, the development partners of CATHARE. It consists of two independent sections : Section I is dedicated to the use of CATHARE in the field of Safety Studies, Section II is dedicated to simulators.

Section III presents a summary of the needs relative to these utilizations.

SECTION I

USE OF CATHARE FOR SAFETY STUDIES

CATHARE uses can be characterized by three main features :

- i) methodologies,
 - ii) plants, components,
 - iii) transients and range of conditions,
- over which the code runs.

i) Methodologies

In principle, a Best Estimate code can be defined as a consistent set of models intending to describe most of physical phenomena that occur in a domain of accident transients, with accuracy in agreement with current knowledge and available experimental data base. Each of these models should be compared with experimental data and be able to provide a best fit of tests results.

CATHARE 2 is a Best Estimate advanced thermohydraulic code, according to the criteria and definitions of Regulatory Guide 1.157 (reference /USNRC, March 1989, "Best-Estimate Calculations of Emergency Core Cooling System Performance"), which describes the essential features of a Best Estimate code: mass, energy and momentum conservation equations for liquid and steam phases (possibly with multiple fields for each phase) and non condensable gases, accounting for non equilibrium effects between phases (thermal and mechanical), with acceptable accuracy, multidimensional capability for some phenomena (but 1D approximations are acceptable if justified).

Until recently, LOCA analyses were performed in compliance with the provisions of 10 CFR 50.46 "Acceptance Criteria for Emergency Core Cooling Systems for Light Water Nuclear Power Reactors", published by former USAEC in January 1974. This document describes the criteria to be met and also

the required and acceptable features of the evaluation models in Appendix K to this document (among those, ANS 71 + 20 % for fission products decay heat). Since 1974 and issue of 10 CFR 50.46 and Appendix K, international R&D programs, including experimental and analytical developments programs, have allowed to considerably enhance both understanding and predicting capabilities for physical phenomena that occur during the course of LOCA events. Appendix K models appeared to be utterly conservative. In addition to that demonstration, R&D programs have provided suitable data for reasonable estimate of uncertainties and quantification of this conservatism.

This development gave rise to an update of 50.46 regulations in September 1988 in the USA, which allow the use of Best-Estimate Evaluation Models based on realistic codes and assumptions. This new regulation requires the quantification of uncertainty on results and accounting for it in the comparison of results with safety criteria, in order to demonstrate that they are not exceeded with high confidence level. Regulatory Guide RG 1.157 describes an acceptable methodology that complies with prescriptions of "new" § 50.46. §4 "Estimation of Overall Calculational Uncertainty" is devoted to estimating the calculation uncertainty, the sources of which are identified as :

- code uncertainty (related to accuracy of models);
- experimental data uncertainty (against which code assessment is performed);
- uncertainty related to initial and boundary conditions;
- uncertainty resulting from simplifying assumptions.

The same kind of approach is proposed with use of the CATHARE code in so-called "Better Estimate" or "realistic deterministic" methodology, consistent with the USNRC method:

- objectives are to provide an estimate of the calculation uncertainty and to demonstrate compliance of results with safety criteria at a high confidence level ;
- penalizing mode is chosen so that no unrealistic results are predicted by the code. Very often, dominant parameters (models, boundary conditions) are not independent, therefore their conservative bounding may be difficult. Transient physical analysis and understanding, supported by sensitivity studies analyses, intend to demonstrate that conservative bounding of dominant parameters has been correctly selected to produce the limiting case and results.

Therefore, the following basic steps are applied for safety studies:

- transient analysis resulting in identification of key phenomena and judgement on code adequacy. Key parameters can be code models or simplifying assumptions or nodalization scheme or initial and boundary conditions. Such analysis relies upon physical understanding, experimental data base and code assessment examination. It can be supplemented by sensitivity studies.
- evaluation of calculation uncertainty with emphasis on dominant parameters (through sensitivity studies), or check of bounding conservative approach of key phenomena by the code; such analysis also relies upon the assessment status of the code;
- introduction, if necessary, of conservative biases as close as possible to uncertainty on key phenomena. Such conservative biases can be imposed in a code model or in a nodalization scheme or in a decoupled calculation (e. g. hot assembly calculation with boundary conditions coming from the global system calculation);
- deterministic determination of limiting case, cumulating elementary conservatism in initial and boundary conditions.

FRAMATOME has already used CATHARE in this realistic deterministic approach for licensing calculations of small breaks LOCA for French 4-loop plants, Koeberg South African and Ringhals 3 Swedish plants (at 108 % power level). The same realistic deterministic approach is under development for large breaks LOCA. Such LOCA safety analyses intend to justify new plant configurations: core peaking factor or power increase, SG replacement or tube plugging, fuel management or design (high burnup, mixed UO₂-PuO₂). The next step for CATHARE LOCA applications will consist in the development of Best Estimate methodology featuring the statistical combination of uncertainties.

II) Plants, Components

FRAMATOME intensively uses CATHARE for global safety assessment of NSSS during incident or accident conditions:

- pressurized water reactors (PWR) of current western design;
- PWRs of current Russian design, VVER 440-230, VVER 440-213, VVER 1000, since CATHARE modeling capabilities are not limited to UTSG PWRs, but have been extended to VVERs, mainly featuring horizontal SG for which modelization of primary and secondary sides has been validated by means of sensitivity studies and verification against relevant experiments (PMK, PACTEL integral test facilities); CATHARE qualification against IVO loop seal tests (1:1 scale) also made it possible to address VVER specific loop layout with loop seals in both hot and intermediate legs; lastly, the CATHARE possibility of simulating the top-down quenching of the core is useful for VVER hot side ECCS injection;
- new PWRs: design of FRAMATOME - SIEMENS EPR model, assessment of passive safety reactors, with gravity driven or stored energy (accumulators) components.

Due to its modular characteristics, CATHARE can model any complex fluid system where two-phase flow conditions could develop: it has already been used to assess the performance of a passive cooling system of core catcher sole plate with natural circulation driven flow.

As CATHARE features noncondensable gases and a 3D capability (V1.4), it can be used for containment response during accident conditions.

Another interesting application of CATHARE is the determination of two-phase degradation of reactor coolant pump thanks to its mechanistic 1D pump module. From the geometric description of the modeled pump, CATHARE represents the fluid behavior inside the different parts of the pump, therefore providing the pump hydraulic performance (head and torque), given the inlet fluid conditions and the rotation speed. Such capability was verified by predicting the performance of a petroleum pump, quite different in design from a nuclear reactor coolant pump, therefore providing good reliability for predicting the performance of any kind of pump. Generally, the single phase pump performance is known through measurements performed by the designer. However, the two-phase degradation of the pump characteristics rely upon costly test programs, such as the EVA program achieved in CEA-Cadarache within the frame of a joint R&D program between CEA, EDF, FRAMATOME and WESTINGHOUSE; this EVA program addressed a scale (0.382) model of a 93A reactor pump model and provided two-phase degradation in all operating conditions; the results were applied to similar design reactor coolant pumps, and also used to qualify the CATHARE 1D pump module. When such two-phase data do not exist for a quite different design reactor (or other fluid system) pump, the CATHARE 1D pump module is particularly useful in developing such two-phase data, in two possible ways : either by using it as a part of the modelization of the considered fluid system (NSSS, or other) in transient conditions, or in a stand alone approach where the hydraulic head and torque performance are calculated at successive various operating conditions, therefore making it possible to derive two-phase data in the form usable by simpler models, such as the CATHARE 0D pump module which relies upon a degradation factor as a function of void fraction only, and a "totally" degraded head (and torque) performance as a function of the operating conditions (homologous flow).

Some interest recently arose with respect to steam injectors, that can be considered as a passive pumping system only relying upon use of some steam which is available, for instance, in the SG secondary side, in order to perform the pumping function in a fluid system such as the SG emergency feedwater system; the CATHARE prediction of such component performance would be helpful for its design.

iii) Transients and Range of Conditions

Like most of advanced two-phase flow computer codes, CATHARE was originally intended to address the loss of coolant accidents (LOCA) resulting from RCS pipe break or rupture of any connected line. The short term transient calculation should verify the compliance with safety criteria in terms of peak clad temperature, local and total core oxidation. Appendix K methodology, deterministic Better Estimate or statistical Best Estimate methodologies have been or are being developed for this purpose. Middle and long term transient calculations are also performed in a realistic way to demonstrate long term core cooling, which may rely upon adequate emergency recovery guidelines based on a realistic assessment of plant behavior. Long term boron concentration in the core is a LOCA concern which needs proper recovery actions, as well as appropriate code modeling. According to break sizes, transient durations and emergency procedures, these LOCA scenarios extend between nominal pressure and a few bar, while the clad temperatures should remain below 1204 °C. Multi dimensional effects can occur at various RCS locations or transient stages: in large "open" volumes without flow channelling (reactor vessel lower and upper plena), in the core itself during the reflooding phase by steam and liquid flow redistributions between assemblies at different power, or during the long term core cooling with possible internal circulation flows; therefore, the 0D and 1D approaches should be properly justified according to the calculation objective (for instance, conservative modeling for demonstration of compliance with safety criteria); the 3D CATHARE capability of V1.4 version could be helpful in such justification.

FRAMATOME also employs CATHARE for safety assessment of any scenario resulting in similar decrease of reactor coolant system mass inventory: inadvertent opening of a primary relief or safety valve (pressurizer), or intentional opening of pressurizer discharge for bleed function when this operating feed (ECCS) and bleed (pressurizer) operating mode remains the only possibility for core decay heat removal in the case of total loss of SG feedwater flowrate (multiple failure beyond design basis accident, BDBA), which failure initiated the TMI 2 accident. In the TMI 2 aftermath, more emphasis was put on these concerns: multiple failure accidents (BDBA), RCS and pressurizer behavior in the case of leak at the pressurizer (stuck open valve), reactor coolant pump performance in two-phase conditions and consequences of delayed trip in the case of loss of coolant. Since that time, FRAMATOME currently performs safety analyses with CATHARE in order to develop adequate recovery guidelines for BDBA:

- total loss of high or medium head ECCS pumps in the case of small and intermediate breaks,

- total loss of SG feedwater flow,
- multiple steam generator tube rupture (up to 100 SGTR) coinciding with steam line break.

FRAMATOME also conducted CATHARE analyses to support the use of reactor vessel level instrumentation system at degraded RCS mass inventories in emergency procedures.

Experience feedback from operating reactors highlighted the need for analysis of transients occurring at shutdown conditions, in particular the loss of Residual Heat Removal System at mid-loop operation with partial (RCS vents) or full (pressurizer or/and SG man holes) RCS opening. Such transients are particularly challenging for computer codes due to low pressure (1 bar), low flowrates and long duration with potential emphasis of numerical problems, and presence of noncondensable gas. Thanks to this latter CATHARE capability, FRAMATOME has already performed analyses to design an automatic RCS water supply under such circumstances.

Also, some SGTR actually occurred on power plants: in order to develop adequate emergency procedures, to assess the performance of required instrumentation for accident management (radioactivity detection), and to evaluate the releases, the code should model radioactive product transport, which CATHARE does.

In addition to LOCA transients which normally comply with safety criteria, same kinds of LOCA transients that evolve into severe accidents due to loss of safety systems can be assessed by CATHARE, provided that core degradation has not yet begun, and materials and fluid temperatures remain low enough; CATHARE can accurately describe the severe accident first phase in comparison with other severe accidents integrated codes; V1.4 version extends the CATHARE capability toward this high temperatures range.

FRAMATOME also uses CATHARE as a reference code for simpler models generally devoted to non LOCA transients, by benchmarking them against CATHARE, or by improving them with more detailed modelization of component response or specific physical phenomenon, resulting from CATHARE in-depth analysis. An example is given by detailed CATHARE calculations of SG secondary side in the case of feedwater line break, which are used to develop a correlation of break flow quality versus residual SG mass inventory, supplied as a boundary condition to another code that does not model the SG in as much detail as CATHARE.

CATHARE is also used by itself, or as reference code, to assess non LOCA transients such as ATWS, resulting in high RCS pressure for which the code simulation range was extended; neutronics calculation is obviously required in such a case.

From the above listed current or future uses of CATHARE, some important requirements or needs can be pointed out:

- simulation and validity range: although it is difficult to foresee new initiating events and plant transients that would actually occur and need analytical capabilities, it seems easier to define this needed range in terms of potential plant states: RCS pressure from 1 bar (shutdown conditions with open RCS) up to design maximum pressure (around 230 bar) in the case of subcooled overpressurization; RCS fluid temperatures from a few tens of °C up to gas temperatures achieved during the course of severe accidents; RCS flows from near stagnating conditions to maximum flowrate resulting from large break LOCA; the presence of non-condensable gases both at low temperature (shutdown conditions, open RCS) and high temperatures (severe accidents); boron and radioactive product transport; neutronics calculation; clad thermomechanical response to differential pressure and temperature variations, with potential creep deformation and burst.
- determination of code uncertainty: this is a key element of any better or best estimate methodology; this determination should be systematically conducted during any qualification or verification process. Also, the experimental data base should adequately cover the simulation range of the code, which seems to be in the case for current reactor applications, but should be verified for new applications to other fluid systems or components (e.g. steam injectors).
- multidimensional capability: when such a possibility exists (large open volumes without strong flow channelling, reactor vessel lower and upper plena, reactor core, reactor containment), a simplified 0D or 1D approach should be properly justified, and 3D capability can support such justification, provided that it itself benefits from sufficient qualification.
- for industrial use, the code should not be excessively time-consuming; as computer performances increase rapidly, the structure of the code should be flexible enough to take advantage of any hardware advance (e.g. parallel processing); long duration transients at low pressure (1bar, shutdown conditions) are the most time-consuming.
- in addition to standard code documentation, accurate and exhaustive users guidelines should be available in order to minimize the user effect; this can be achieved by systematic sensitivity studies during the qualification and verification processes, demonstrating convergence of modelization,

numerical scheme and solution according to time and space, therefore making it possible to develop documented recommendations for code users. User training, user clubs for mutual exchange of experience and information about the code use, also help to achieve the same objective.

- as the amount of information delivered to users constantly increases (e.g. 3D modelization results), they should be provided with suitable visualization tools or computer aided analysis tools, in order to facilitate the analysis and interpretation of code results. Also, the preprocessing stage should facilitate the user's modifications of input data deck, for the purpose of sensitivity studies (e.g. modelling).

Provided that previous requirements are satisfied, which is the case for CATHARE either in its current status or in its development program within the next 2, 3 or 4 years, CATHARE will continuously and extensively be used for the following purposes:

- assess safety margins of existing plants, both western or eastern designs, for all kinds of Design Basis Accidents and Beyond Design Basis Accidents, but more particularly LOCA transients and initiating events that finally result in loss of primary coolant (e.g. feed and bleed); define technical specifications of maximum power level, peaking factor, hot channel enthalpy rise factor, number of SG plugged tubes; support new fuel management, with increased burnup, long fuel cycles, mixed fuel UO₂-PuO₂ or reprocessed Uranium; validate emergency recovery procedures and accident management strategies; all operating conditions will be covered, from full power to cold shutdown;

- design new reactors and cost effective safety systems, with optimized margins: emergency core cooling system with assessment of response of NSSS, primary circuit and core to ECCS performance, other active or passive safety fluid systems (e.g. natural circulation passive system to cool the core catcher in the case of severe accident);

- design new components that would rely on two-phase flow mechanisms (e.g. steam injectors);

- assess the thermohydraulic behavior of fluid components, such as the reactor main coolant pumps in two-phase conditions;

- more generally assess the thermohydraulic behavior of any complex fluid system, in multi-phase flow conditions, under large driving forces as well as low driving forces (natural circulation, gravity-driven phenomena).

SECTION II

USE OF CATHARE FOR SIMULATORS

II-1- THE CURRENT EDF SIMULATOR NETWORK

II-1.1. The French Operational NPP Capacity

It consists of :

- six CP0 3-loop 900MWe units
- twenty eight CPY 3-loop 900 MWe units
- twenty P4 and P'4 4-loop 1300 MWe units

This NPP capacity represents roughly 80% of the French power generation.

Moreover, four units of the new N4 design (4-loop 1450 MWe) will be connected to the grid by 2000.

The large standardization of the EDF nuclear program can be noticed, with three different main series (3-loop 900 MWe, 4-loop 1300 and 1450 MWe). This standardization also structures the simulators network and developments.

II-1.2. The different Types of Simulators

II-1.2.1. Definitions, Vocabulary

When talking about simulators specifications, construction or assessment, we need to consider three main features :

- *the physical domain* which is representative of the complexity of the physical phenomena taken into consideration. This domain determines the choice of individual codes (thermohydraulics, neutronics).

- *the geographical extent* which is representative of the parts of the process and the plant systems which have to be simulated. It includes a range of "initial" states to be covered. It characterizes a set of codes rather than any individual code.

- *the Human Machine Interface System (HMIS)*, more and more diversified with the arrival of work stations.

We prefer to consider complete replica simulators as "full-scale", by reference to the notion of one to one scale representation and use the "full-scope" term (incorrectly used to designate usual simulators) to refer to the physical domain and geographical extent.

The different types of EDF simulators in service on Dec. 31st, 1995, are briefly presented below.

II-1.2.2. First Generation Simulators

This category includes two types of simulator :

- the "*part-task*" simulators, which are dedicated to in-depth learning of basic functions such as Chemical and Volume Control System (CVCS) of the primary circuit, reactor control for the sub-criticality approach, or Turbo-Generator coupling.

- the usual "*full-scale*" simulators, which are used for collective training in normal, incidental and accidental situations, as well as for operating personnel licensing. Ten simulators of this type are currently operated. They are equipped with the DEF12 thermal-hydraulic code and are able to simulate minor accidents, such as LOCA with break sizes not exceeding 4 inches.

II-1.2.3. New Generation Simulators

In their principles, these simulators are close to the "part-task" simulators, except that, firstly they deal with one or some particular accidental sequences instead of a specific system or function and secondly their HMIS is composed of work stations. In the eighties, they have been installed on each of the EDF power plants.

Originally, they were developed for Steam Generator Tube Rupture (SGTR) simulation to train operators to SGTR detection and mitigation. They were supplemented by an expert system (SEPIA) so that the operator diagnosis and actions could be assessed and corrected. More recently, these simulators have been upgraded into "multi-part-task" simulators, named "MicroPWR", with an extension of the simulation domain to eight scenarios, ranging from the main normal transients to small accidents (rupture of 3 SG tubes, LOCA with break size lower than 1 inch).

II-1.2.4. The SIPA Simulators

The SIPA project marked a breakthrough in simulator technology in France. The first simulator of this type was installed in 1991 at SEPTEN (Basic Design Departement of the Engineering and Construction Division of EDF, in Villeurbanne, next to Lyon). It was duplicated at CEA/IPSN (Fontenay aux Roses, next to Paris) in 1992. It differs from the previous simulators mainly because of its capability to simulate and illustrate a wider range of accidental situations, and because of its generation methods.

In 1996, compact versions of the SIPA simulator, named "SIPACT" (SIPA comPACT), and running on work stations, are being installed on each of the eighteen French NPP sites.

The relevance of the simulations performed on SIPA mainly relies on the use of CATHARE-SIMU, a speeded-up version of the CATHARE code.

The main features of these simulators are presented in the following sections and an exhibition of SIPACT will be offered during the OECD-CSNI Annapolis meeting.

II-2. FEATURES OF THE SIPA SIMULATORS

II-2.1. The Thermohydraulic Code (CATHARE-SIMU)

SIPA is using CATHARE-SIMU, a speeded-up version of the CATHARE code. For the representation of the primary circuit, the physical model is the standard 2-phase (liquid/steam), 6-equation model : separate mass, energy and momentum balances are carried out in each phase, allowing stratification, counter-current flows, core uncovering and reflood. The numerical scheme is based on a fully implicit Newton's iterative method. The nodalization scheme for the 4-loop 1300 MWe configuration is presented on figure 1. It consists of 235 meshes (primary circuit plus secondary side of the steam generators).

The original physical model developed for the representation of the secondary side of the steam generator, and currently used in the 900 MWe and 1300 MWe configurations, is a 3-equation

homogeneous model. Nevertheless, this model was upgraded as part of the development of the 1450 MWe N4 configuration, with the addition of a drift equation and taking account of the special design of the N4 Steam Generator (with economizer).

The performances of the SIPA simulator are such that LOCA transients with break sizes up to 12 inches can be computed nearly in real time, either on a Cray computer (presently C98) or on a work station (SPARC 20).

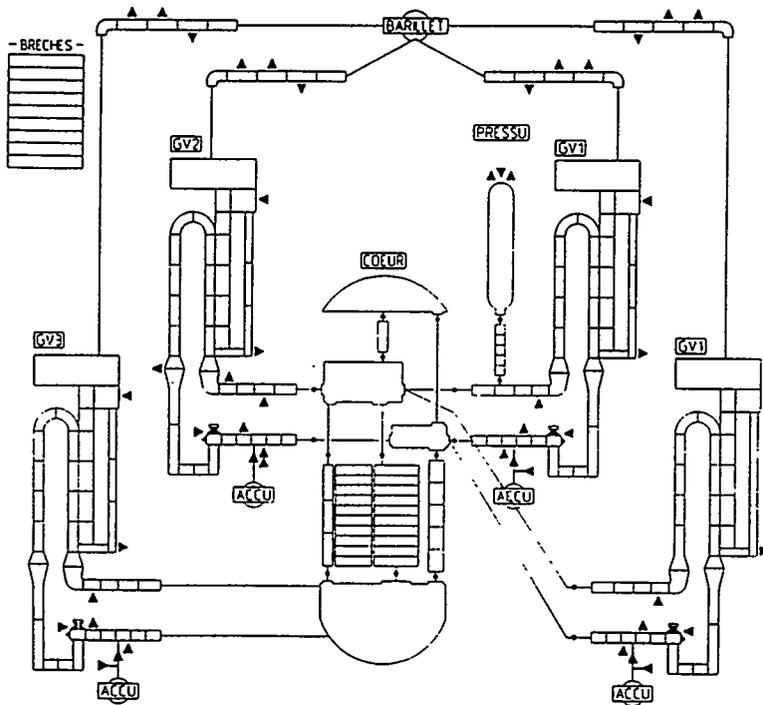


Figure 1 - CATHARE-SIMU nodalization scheme for the 1300 MWe configuration

II-2.2. Scope of Simulation

The physical range of the simulation goes from reactor in cold shutdown state to normal full power operation and accident conditions. The accidental scope includes, in particular :

- LOCA with break sizes up to 12 inches in every part of the different loops of RCS. Several breaks may be simultaneously simulated in combination with other failures (for instance, loss of external electrical sources, loss of Medium Head Safety Injection)
- steam line and feedwater line breaks,
- steam generator tube rupture (SGTR), up to 150 tubes (on the 1300 MWe configuration) in one or several steam generators,
- anticipated transients without scram (ATWS).

For the accidental scope, the relevance of CATHARE-SIMU is assessed against the CATHARE 2 last release, where validation includes a large experimental program (BARRE, 1995). The assessment procedure of CATHARE-SIMU consists of a comparison with CATHARE 2 over a wide range of accidental transients.

II-2.3. The SIPA Environment

As said previously, SIPA differs from the usual full-scale simulators, on some important points such as :

- the hardware and software structure which are capable of hosting various application programs,
- the ability to modify or upgrade easily the simulation software connected to the thermal-hydraulic code.

II-2.3.1. SIPA Standards

Assembling a set of codes in a single simulator implies that certain principles have been defined and fulfilled : these are the "SIPA standards". The objectives of these standards are to facilitate the coupling between codes, to ensure their portability on different machines and to optimize their maintenance.

These standards are, in particular, related to the interface between codes (normalized interfaces called "connection points"), and to the functional division inside a single code (data acquisition, steady-state calculation, transient calculation, post-processing).

II-2.3.2 The Target Computer and the Different Operating and Control Stations

The original target computer, which is still currently used is a CRAY machine (remote in the EDF computer centre near Paris). Otherwise, SIPA is now also running on local SUN SPARC 20 work stations (in particular, for the SIPACT simulators) with performances (in term of calculation and reaction times) which are quite close to those obtained with CRAY.

A main operating desk based on various SUN SPARC work stations is issued to control the simulator from interactive block diagrams and provides reports on the status of the facilities via various parameters and alarms.

An instructor station of the same type is used for the management of the training (e.g. simulation of a failure).

An additional station provides the real time display, with a sophisticated imagery, of the various phenomena that may occur inside the reactor coolant system and the secondary side of the steam generators. This system is called "*Pedagogical System*", to stress its teaching goal.

The connection and the animation of any computer system available in the actual control room are possible and have been achieved for the 900 MWe and 1300 MWe configurations (for instance, safety panel display system).

II-2.3.3. The "SWORD" Software Workshop

SWORD (Software Workshop Oriented towards Research and Development) is a fully integrated workshop. It includes code generators based on graphic and data inputs from P&ID and logic/control drawings : HYTHERNET generates simulation models for hydraulic networks (distribution of flows...), CONTRONET generates simulation models for I&C systems. SWORD also includes assembly generators which automatically link the different models involved in the simulation application (models manually generated or automatically generated by the code generators). These operations are based on the standardization of the "connexion points" (mentioned above).

II-2.4. The Different Configurations of SIPA

Currently, three main configurations have been developed : they represent the three main French NPP series : 900, 1300 and 1450 MWe. Each of them includes about thirty-five safeguard systems. The Pedagogical Station is available for the 900 and 1300 MWe configurations.

Moreover, the SWORD workshop has already been used to generate limited configurations (a few models were coupled) to study specific problems, for instance relative to coupling effects between containment and RCS (WEBER, 1996).

II-2.5 The Different Uses of SIPA

The main areas of use are :

- **Training** : SIPA aims at providing safety engineers and operating managers with advanced training so that they can successfully deal with any hypothetical accident and therefore prevent core damage. This is achieved thanks to the real time capability, the relevance of the physical models and the clear visualization of the physical phenomena. In 1995, there were 40 training sessions of 5 days each, either on the 900 MWe configuration or on the 1300 MWe configuration. Each session is displayed to about five trainees. Furthermore, foreign operators (Belgium, Korean and Czech) also participated in this training.

Every year, a specific training session is dedicated to the members of the French National Crisis Organization (in charge of crisis management in the case of any accidental situation that might occur). This training mainly emphasizes the physical phenomena occurring in a specific type of accidental transient (one different subject each year), and makes it possible to compare the diagnosis and prediction performed by the team to the simulated scenario.

While the training on SIPA was originally dedicated to shift safety engineers and operating managers, the aim of the SIPACT simulators (see §.II.1.2.4.), is to extend such knowledge to all plant operators. In order to do so, one instructor will be appointed to each of these simulators.

- Design and validation of operating procedures : the validation of operating procedures for a nuclear power plant requires long and costly inspections to guarantee the quality of the rules and instructions, given their criticality in terms of safety. Because of its capacities for real time calculation, and relevant simulation of the important physical phenomena, SIPA provides a good answer to this need, and moreover takes realistic account of the interactions between the Nuclear Steam Supply System (NSSS, which includes the RCS) and the other important safeguard systems.

A large effort has been made in this area to validate Emergency Operating Procedures, as part of the development of the French State Oriented Approach for the 1300 MWe plant.

Additionally, a tool (SCOOP, Simulation of Comportment of an Operator Observing Procedures) has been developed, which enables the operating procedures to be run in a batch calculation, by simulation of the operator actions. This tool increases the effectiveness of the validation, and moreover enables the sensitivity of the operator action to be assessed (time delay for instance). It has been used, connected to SIPACT, for the 1450 MWe EOP's assessment.

- SIPA is selectively used in various other situations, in particular when a quick answer is needed to a question regarding safety analysis (incident analysis, design sensitivity studies...). Moreover, some specific configurations have been generated through the SWORD workshop to investigate problems involving the RCS and different systems and their interaction.

II-3- THE APPLICATIONS OF SIPA IN THE VERY NEAR FUTURE

In this section, we are considering the further applications of the CATHARE-SIMU code. In section 4, we shall discuss the anticipated use of the CATHARE 2 code in the simulators.

II-3.1. The CP0 Full-Scale and Full-Scope Simulator

The CP0 plant series (six 3-loop 900 MWe plants at Fessenheim and Bugey) is equipped with a single, obsolete simulator. In addition the Fessenheim operators have no training simulator adapted to their own control room. So it was decided in 1993 to create a specific simulator for and at Fessenheim and to revamp the Bugey 2 simulator. Above all, these two simulators will be the first full-scale simulators built according to the SIPA principles : use of CATHARE-SIMU, SIPA standards, SWORD workshop...

Unlike SIPA, these simulators will be run on a local server, that is now available on the market at very reasonable cost. Moreover, the feasibility of running CATHARE-SIMU on parallel processors has been demonstrated, guaranteeing real-time relevant execution of all transients of the CATHARE-SIMU definition domain (i.e. LOCA up to a 12 inch break), with a cycle step of 100 ms.

These simulators will start in 1997.

II-3.2. The N4 Simulator

The N4 1450 MWe plant is characterized, in particular, by a fully computerized control room (KIC) and by programmable logic controllers for all logic and control operations. The new N4 training and engineering simulator will be built on the same principles as for CP0, and on the basis of the current SIPA 1450 MWe configuration, commissioned in October 1995. It will include in addition the present computerized control room. This simulator should be available, at Chooz, in 1998.

II-3.3. Upgrading Other Full-Scale Simulators

The other full-scale simulators will be progressively upgraded following the same principles as for CP0. Moreover, a thirteenth full-scale simulator will be devoted to the P'4 1300 MWe series, built according to the same principles.

II-3.4. Other Projects

Finally, SIP (Pedagogical Interface Simulator) should be installed on the eighteen NPP sites. These simulators are derived from the new CPO simulator, but are provided with an interface on screens instead of a full-scale control room replica. They should replace the current SIPACT simulators.

II-4. ANTICIPATED USE OF CATHARE 2 IN SIMULATORS

As discussed in the previous sections, CATHARE-SIMU has been incorporated into SIPA and SIPACT simulators and will be incorporated into the full-scale simulators in the very near future.

In the longer term, EDF's ambition is to incorporate CATHARE 2 in all of its simulators, in replacement of CATHARE-SIMU, so that there will be only a single code available to study, engineering and training. Adapting CATHARE 2 to real time simulators and extending the validity domain of its simulators to all transients occurring from any state, including situations with open primary circuit, are EDF's new objectives.

These objectives require developments in three directions : physics (especially for low pressure), real time capabilities, and automatic generation of the CATHARE modules. The foreseen simulation domain and the necessary developments, which constitute the SCAR (Simulator CATHare Release) project, are briefly presented below.

II-4.1. The simulation Domain

Figure 2. illustrates the scope of the current and future EDF simulators, in terms of complexity and seriousness of the accidents to be simulated and in terms of the initial states that have to be considered. In the future, the simulation domain will mainly extend to accidents starting from cold shutdown with open or vented primary circuit. Such extension requires a code like CATHARE 2 able to take into account non-condensable gases.

The need for extending the simulation domain to accidental transients occurring at cold shutdown (mid-loop operation in particular), is emphasized by the results of probability studies that have demonstrated that these situations contribute significantly to the risk of core melt. Consequently, the training of plant operators has become an important matter since the operator action (and the time delay in particular) is often determining all the more because automatic protections are not always available in these situations.

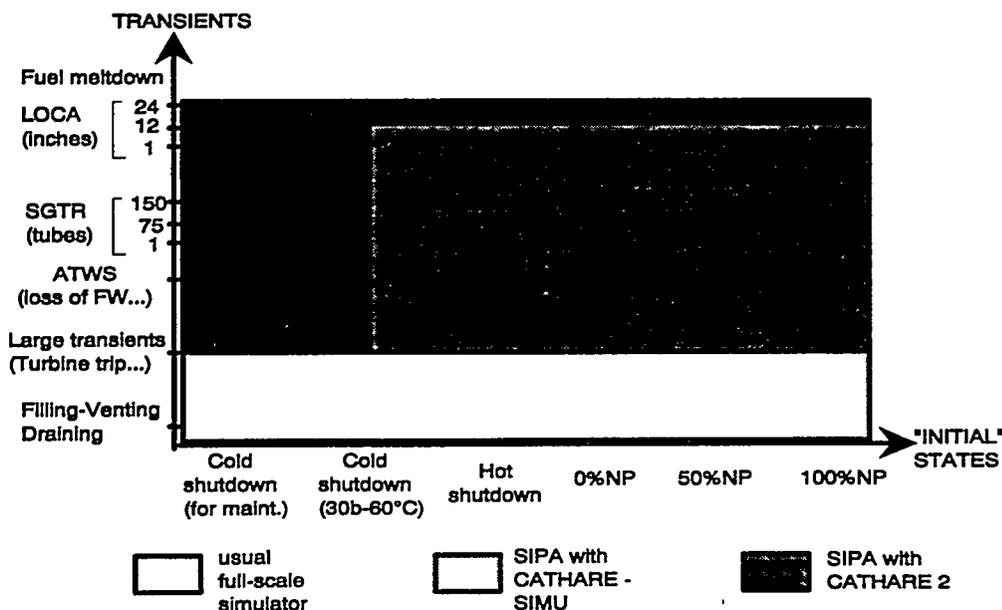


Figure 2 - Illustration of Simulator Topology

II-4.2. The SCAR Project

To manage the constraints inherent to a wide utilization of the CATHARE 2 code in the French simulators, various developments are planned as part of the SCAR project, mainly supported by EDF and CEA-IPSN. These developments are presented below.

II-4.2.1. Improving the Flexibility of the CATHARE Modules

By improving flexibility, we mean that

- modifications in the schematization of the reactor (geographical extent, connection points, topology, meshing...),
 - and integration of the possible evolution and improvement of the physical models
- should be quick and easy.

The developments aim at limiting the manual work performed by the user to only the traditional description of the reactor schematization, and the description of the connection points and their links with the CATHARE internal variables, on the basis of a simple syntax. The writing of the code dealing with the interfaces with the other modules of the simulator will be quite automatic.

II-4.2.2. Adapting CATHARE 2 to Real Time Calculations

The constraints are technical :

- a maximum time step of 100 ms,
- the need to integrate the representation of the Residual Heat Removal System (RHRS), and to simulate accidents starting with an open circuit (with non-condensable gases),

and economic : each simulator will be equipped with a dedicated computer machine. This machine will be chosen in the middle of the range, taking into account a forecast number of 31 such machines.

The different actions planned under the SCAR project mainly focus on the parallel running of the code : assessment of the different techniques for parallel computing (for instance, message passing), assessment of the different machines available on the market, verification of the non-impact on the single processor performances, minimization of the number of code subroutines to be modified. It will be remembered that the latest version of CATHARE 2 (V1.4) was designed to facilitate parallel computing : it has been demonstrated that an acceleration ratio of at least 5 should be expected (test performed on a CRAY computer with 8 processors).

II-4.2.3 Developments Regarding the Extension of the Simulation Domain

The needs for further developments in that area concern :

- improvement of calculation times at low pressure. A review of representative transients with convergence problems will be made in order to investigate the physical and numerical reasons for these difficulties, and assess the possible solutions.
- constraints resulting from running the code in a simulator environment : taking due account of the interaction between the CATHARE calculation and various sensors, actuators, valves, possibility to simulate one break or more at any mesh of the various circuits, etc...

These needs have been reviewed for the N4-1450 MWe plant and have led to the specification of a program of work.

II-5- CONCLUSION

To conclude this chapter, it will be useful to repeat that :

- the commissioning of the SIPA simulator, in 1991, was a key event in the simulator policy of EDF. This was the first time that an advanced thermohydraulics code, CATHARE-SIMU, derived from CATHARE, was implemented into a simulator. With respect to the older generation simulators, the simulation scope has been significantly increased and a wide range of accident situations (up to a 12 inch-break LOCA) can now be simulated nearly in real time. In the very near future, the SIPA principles and the use of CATHARE-SIMU will be extended to the whole French "full-scale simulator" network. Moreover, in 1996, compact versions of the SIPA simulator, named "SIPACT", and running on work stations, are being installed on each of the eighteen French NPP sites.

- In the longer term, the EDF objective is to extend the simulation domain of its simulators to low pressure, open primary circuit configurations, with non-condensable gases. In such situations, the

operator action is often determining for the mitigation of the accidents, and therefore the relevant training is necessary. Since non-condensable gases have to be represented, the last CATHARE 2 version (V1.4) has been chosen as the basic version for future simulators. This will provide a unique code available for safety studies, engineering and training, with a common development and maintenance structure. Under the SCAR project, some developments are already under way designed to adapt the CATHARE 2 code to simulators, both in terms of environment (interface with other modules) and real time capability throughout the whole simulation domain (use of parallel computers...).

SECTION III

SUMMARY OF THE FUTURE NEEDS

From the above-mentioned current or anticipated uses of CATHARE, either for Safety Studies or Simulators, some important requirements can be pointed out :

- Apart from the original LOCA frame, the simulation and validity range should now cover a much wider range of accident situations, extending from low pressure transients starting from cold shutdown with open RCS to the first stage of severe accidents. This implies a large variation range for RCS pressures, temperatures and flowrates, and relevant models to take into account non-condensable gases, fuel thermomechanics, neutronics, boron and radioactive product transport. There are also requirements resulting from running a code in a simulator environment, such as due account of the interaction between the thermohydraulic calculation and various items of equipment (captors, sensors, valves...).
- The determination of code uncertainty is a key element of any better or best-estimate methodology and should be systematically conducted during any qualification or verification process.
- The multidimensional capacity should be used to justify 0D or 1D approaches, provided that it itself benefits from sufficient qualification.
- The performances of the code, in terms of calculation time, should provide real-time calculations over the foreseen simulation domain of the French simulators (including transients starting from open RCS). The structure of the code should be flexible enough to take advantage of any hardware advance (e.g. parallel processing).
- In addition to the standard code documentation, accurate and exhaustive user guidelines should be available in order to minimize the user effect (for instance with respect to nodalization). User training, user clubs for mutual exchange of experience, also fit in with the same objective.
- Suitable pre-processing, visualization and analysis tools should be developed in order to facilitate the modification of data sets and the analysis of code results, especially for complex modelisations (e.g. 3D nodalization).
- The unicity of a code version, available for safety studies, engineering and training should be guaranteed. Last but not least, the role of code maintenance has to be emphasized : an efficient long-term maintenance structure should provide assistance to the users and ensure the appropriate code corrections and updates.

REFERENCES

- BARRE E.**, **BESTION D.** - 1995. "Validation of the CATHARE system code for nuclear reactor thermalhydraulics". ASME&JSME Fluid Engineering Conference - 13-18 August 1995 - Hilton Head
- WEBER O.**, **CHAZE J.L.**, **LOTZ M.**, **PENTORI B.**, **ROUSSET P.**, **VACHER J.L.** - 1996. " CATHARE 2 and PAREO 9 coupled onto SIPA". SMC'96 - 8-12 April - New Orleans

Current and Anticipated Uses of Thermal-Hydraulic Codes in Germany

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Abstract

In Germany, one third of the electrical power is generated by nuclear plants. ATHLET and S-RELAP5 are successfully applied for safety analyses of the existing PWR and BWR reactors and possible future reactors, e.g. EPR. Continuous development and assessment of thermal-hydraulic codes are necessary in order to meet present and future needs of licensing organizations, utilities, and vendors. Desired improvements include thermal-hydraulic models, multi-dimensional simulation, computational speed, interfaces to coupled codes, and code architecture. Real-time capability will be essential for application in full-scope simulators. Comprehensive code validation and quantification of uncertainties are prerequisites for future best-estimate analyses.

1 Introduction

In Germany, there are currently 19 nuclear power plants in commercial operation (13 PWR, 6 BWR), generating approximately one third of the country's electricity. More than half of this nuclear power comes from 8 reactors with 1300 MW nominal power and more. None of these powerful reactors is older than 12 years, i.e. the larger part of their lifetime lies still ahead. Although supporting the development of advanced reactors, the utilities have not announced any plan to add new nuclear capacity to their grid within the next years.

In spite of the fact that no nuclear power plants are under construction in Germany there is a need for continuous development and assessment of thermal-hydraulic codes in order to meet present and future needs of licensing organizations, utilities, and vendors.

2 Use of Thermal-Hydraulic Codes by Licensing Organizations

The ultimate responsibility for licensing and supervision of nuclear facilities lies with the Federal Government of Germany. The actual licensing and supervision functions are delegated, however, to the authorities of the individual states (Länder) where the plants are located. The state authorities ask the local Technical Inspectorates (TÜV) for expert's reports. Thermal-hydraulic calculations are performed by the TÜVs, most of them applying ATHLET. The federal ministry in charge of reactor safety (BMU) receives technical support from the GRS and other organizations.

The GRS has developed a complete system of computer codes for the analysis of transients and accidents. Development and assessment of these codes is sponsored by the Federal Ministry for Education, Science, Research and Technology (BMBF). For the reactor coolant system behavior in PWRs, BWRs, advanced reactors evolutionary design, Russian VVERs and RBMKs, the code ATHLET is applied. This code is described in a special paper for the Opening Session of this workshop [1]. ATHLET-CD is the extension of ATHLET for severe accidents with core degradation. QUABOX/CUBBOX and other 3D neutronic codes can be linked to ATHLET by an interface. Interface requirements for these codes are described in other papers during this Technical Session [2], [3].

The spectrum of applications for ATHLET comprises safety evaluations for the existing plants in Germany and abroad. Thermal-hydraulic calculations are performed by GRS and TÜVs on demand of licensing authorities for various purposes, e.g.

- evaluate the existing margin with respect to thermal shock on pressure vessels of older reactors,
- assess the feasibility of preventive accident management plans,

- check the effectiveness of backfitting measures, e.g. larger cross sections of pressurizer relief valves,
- evaluate the ECCS function for a core with new fuel elements. N. B.: The German acceptance criteria contain a special requirement concerning the allowable extent of core damage. It must be demonstrated in the licensing process that not more than 10% of the fuel rod cladding will rupture for design basis accidents.

There are a great number of support activities for countries in central and eastern Europe operating VVER and RBMK reactors. ATHLET is being used to analyze transients, design basis and beyond design basis accidents for these reactors.

3 Use of Thermal-Hydraulic Codes by Utilities

Electrical power in the different regions of Germany is supplied by several utilities, the major ones operating nuclear power plants alone or in common with other utilities. In the past, the utilities did not perform many thermal-hydraulic calculations themselves. They entrusted the calculations that were mandatory for license application to the vendors. Recently, the utilities have built up own capacities for thermal-hydraulic calculations. In the following, the code situation at PreussenElektra is described as an example.

3.1 Supply area of PreussenElektra and the nuclear power plants

The supply area of PreussenElektra (PE) is located in the northern part of the Federal Republic of Germany. PreussenElektra supplies one third of the area and one fifth of the total electrical consumption in Germany. The electrical power generated by PreussenElektra is mainly from coal fired and nuclear power plants. In 1994, 56% of PE's power production came from the following nuclear power plants. These stations are located in different federal states. The plant types, the net electrical power, the PE-share and the year of start-up are shown in Table 1.

Power station	Type	Federal State	Power MW	PE Share MW	Start-up year
<u>Brokdorf</u>	PWR	Schleswig-Holstein	1326	1061	1986
<u>Brunsbüttel</u>	BWR	Schleswig-Holstein	771	257	1986
<u>Krümmel</u>	BWR	Schleswig-Holstein	1260	630	1983
<u>Grohnde</u>	PWR	Lower Saxony	1325	663	1984
<u>Stade</u>	PWR	Lower Saxony	630	417	1972
<u>Unterweser</u>	PWR	Lower Saxony	1255	1255	1978
<u>Emsland</u>	PWR	Lower Saxony	1290	162	1988
Total			7857	4445	

Table 1: Nuclear power plants of which PreußenElektra is owner or shareholder

The underlined ones are those which are operated by PE. The plants at Brunsbüttel, Krümmel and Emsland are operated by other utilities. The power plant Grohnde has its own status; PE shares 50%, but there is a strong cooperation in technical matters. All nuclear plants operated by PE are PWR's. The oldest one is Stade (KKS) where the startup was in 1972, followed by Unterweser (KKU) with the startup in 1978. The power stations in Grohnde (KWG) and Brokdorf (KBR) started operation in 1984, respectively 1986, and belong both to the pre-Konvoi series of plants.

3.2 PreussenElektra's applications of transient analysis

PreussenElektra decided in 1992 to have the capability to perform transient analysis, because of the following reasons:

- to become independent of the vendor
- to perform transient analysis in the frame of periodic safety reviews
- to prove the relevance of findings with the consequences on backfitting measures for the running plants
- to answer questions raised in the licensing process

- to analyze events in the plant
- to assess the efficiency of modifications in the reactor protection and limitation system
- to optimize the concepts of preventive accident management

Consequently, a license to operate the ATHLET code was obtained from GRS in 1993. In the same year, a project to develop a data set for the Brokdorf plant (KBR) was started. This work was completed in the beginning of 1996.

Since KBR and KWG belong to the same class of plants (pre-Konvoi), it should be possible to extend the applicability of the KBR data set on the Grohnde plant (KWG) with only small modifications in operating parameters. After that, it is intended to enlarge the scope of data sets to the KKK plant. The following application is described in some detail in order to give an actual picture of an application typical for a utility.

3.3 Extent of simulation of the KBR data set

It was the objective of the KBR input modelling for ATHLET to arrive at a data set not restricted to a special transient but applicable to a wide range of transients and accidents.

In the data set which can be operated from the ATHLET Analysis Simulator ATLAS, the 4-loop plant KBR is simulated as a two loop plant. The modeling on the primary side of the plant consists of

- the reactor pressure vessel with the internals, simulated as thermo-fluiddynamic objects
- one loop representing 3 loops of the real plant (3 times mass flow rate of one loop, 3 times heat exchange capacity of one steam generator, etc.)
- one loop with the surge line and the pressurizer including the pressurizer spray system, pressurizer heating as well as the pressurizer relief valve and the two safety valves
- the chemical and volume control system and the additional boration system are for simplification simulated as fills with the appropriate mass and energy balance performed in the General Control Simulation Module (GCSM) of the ATHLET code.

The two loop modeling is continued on the secondary side:

- The steam generators with the two internal economizers, the downcommer, riser, separator and the dome as well as the complete secondary side pipe system are simulated as a two-loop system.
- The valves taken into consideration in the steam system are the main steam isolation valve, the relief valve, the safety valve, the turbine isolation valve, the turbine control valve and the main steam bypass valves.
- The flow rate and the enthalpy of the mass flow to the turbine is determined in GCSM and is coupled to the thermo-fluiddynamic system through fill components.
- The main feedwater system consists of the main feedwater tank, the feedwater pumps, the pre-heater track and the pipe system, all simulated as thermo-fluiddynamic objects. Three of the four main feedwater lines are according to the two-loop structure of the data set concentrated to one line. The other line is the feedwater line for the one-loop steam generator. In both injection lines the control and the isolation valve for the full mass flow train and the low mass flow train are simulated. The feedwater injected in the steam generators is divided into three lines with the flow rates 10%, 40%, 50%.
- The emergency feedwater system is simulated as a fill component with the appropriate mass flow rate and enthalpy computed in GCSM.
- The condensate system with its pre-heater section is simulated as mass and energy balances in GCSM.
- The components of the ECCS, e.g. accumulators, valves, coolers, pumps and storage tanks are simulated by thermo-fluiddynamic objects. The decay heat removal function is also considered in the modeling.

In the GCSM section of the data set for KBR the reactor protection system, the reactor limitations as well as the most important control systems are taken into account:

- reactor protection system
- control of the coolant temperature

- control and limitation of mass and pressure in primary circuit
- control and limitation of secondary side pressure
- level control of steam generators
- simulation of the turbine
- control of pressure in the main feedwater tank
- control of the condenser mass flow rate.

3.4 Spurious closure of a control valve in the main feedwater line

As an example for the capacity of the KBR data set the results of an event which is analyzed in the frame of the qualification process of the data set, is presented in this paper. The transient was initiated by a spurious closure of the full flow control valve in the main feedwater line due to an electrical defect (Fig. 1). Since the control valve in the low flow train did not open on demand because of the same electrical defect the feedwater supply of the one-loop steam generator was interrupted. Consequently, the water level in the steam generator decreases rapidly (Fig 2). As the steam generator level reached the 9 m elevation, which is a reactor protection threshold, reactor trip and turbine trip occurred.

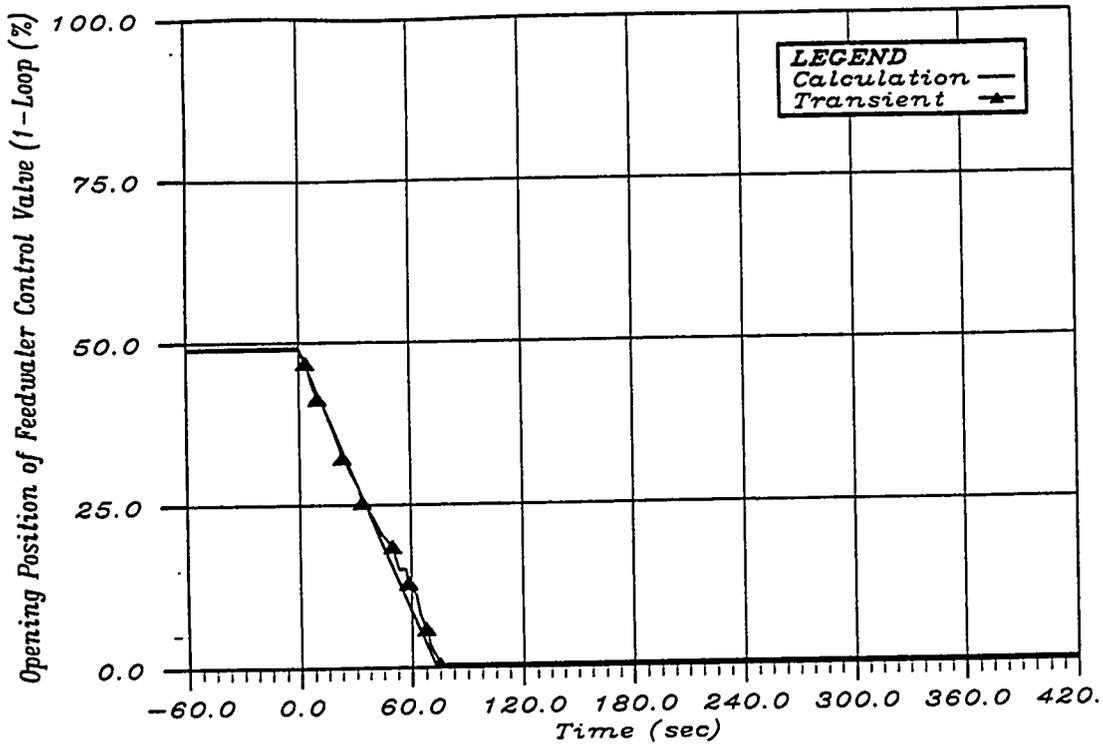


Fig. 1: Opening position of the feedwater control valve in single loop

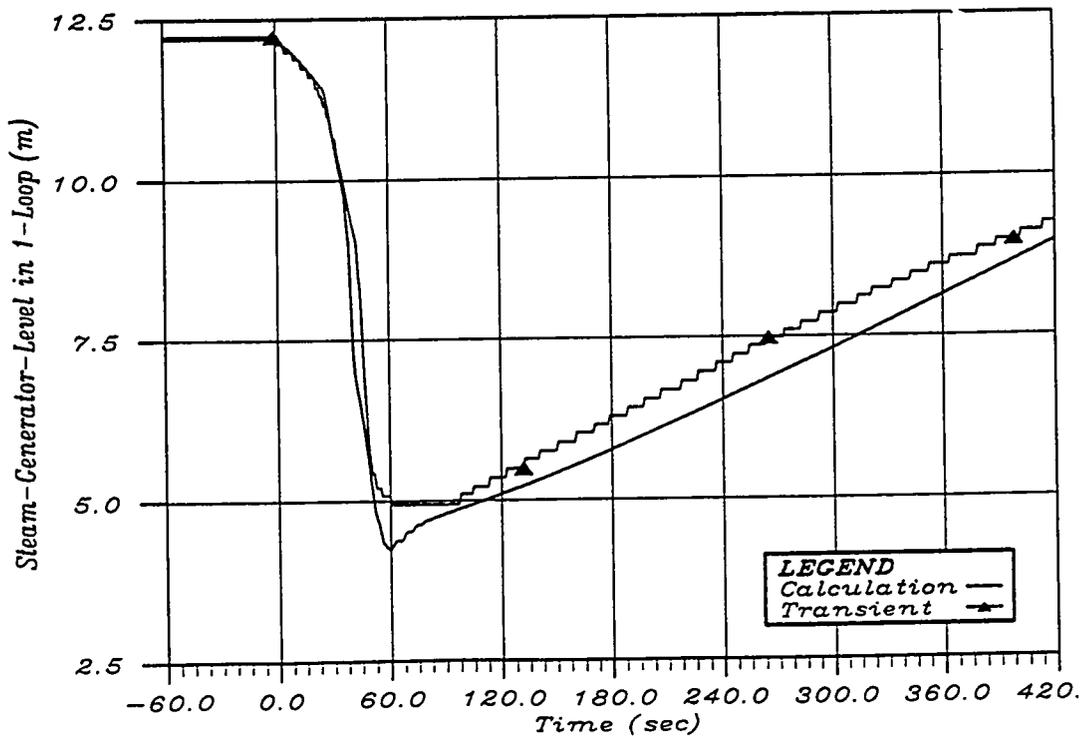


Fig. 2: Steam generator level in single loop

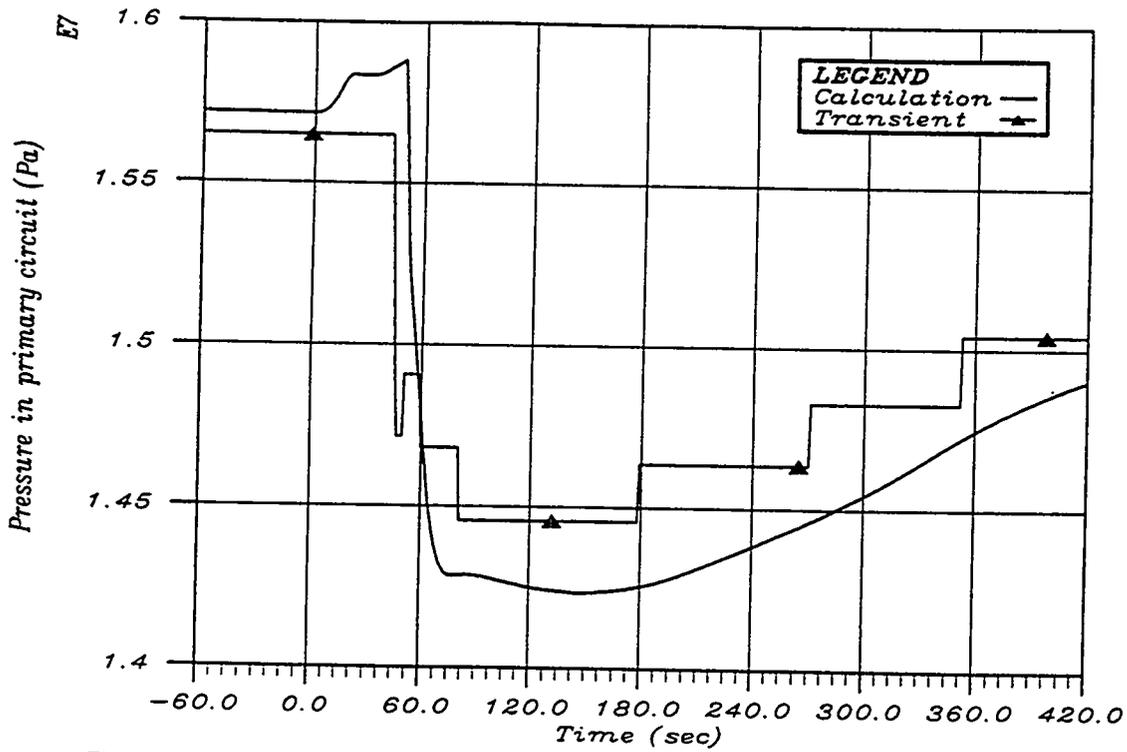


Fig. 3: Pressure in primary circuit

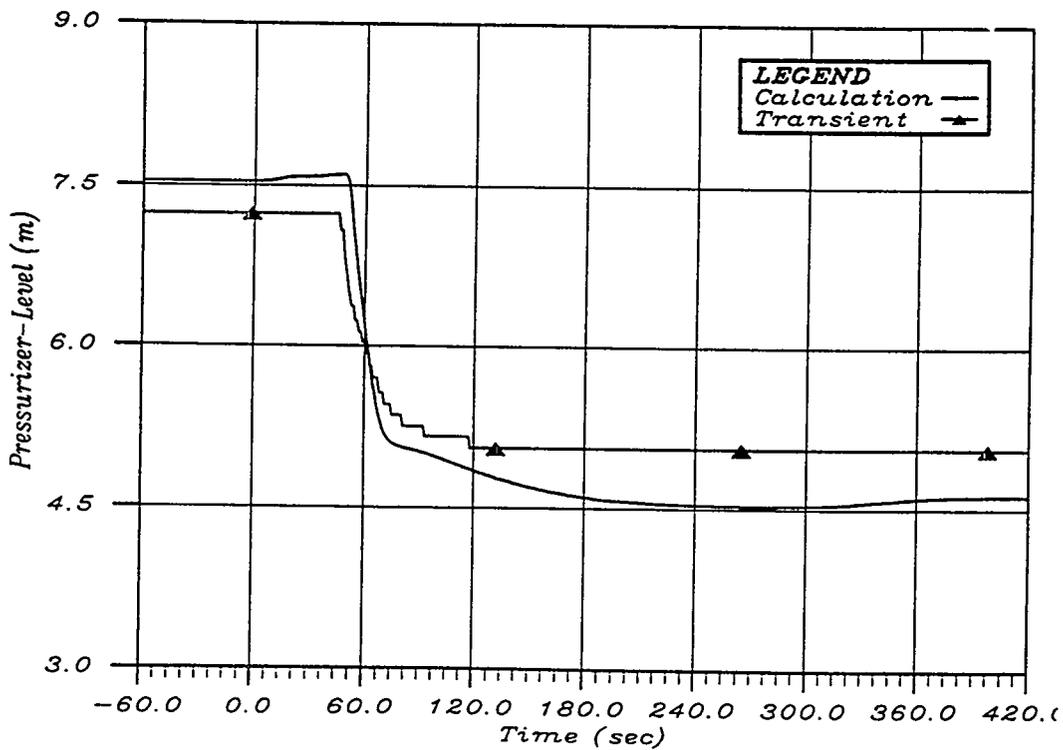


Fig. 4: Pressurizer level

The liquid level of the steam generator of the affected feedwater line decreases further. As this level reached 5 m, which is the set point of the emergency feedwater system, the emergency feedwater pumps of this train are activated and the level in the steam generator increases. On the primary side the pressure decreases immediately after reactor trip (Fig. 3). According to that the pressurizer level decreases too (Fig. 4) and is kept constant because of the removal of coolant into the CVCS. In summary, the relevant physical phenomena and plant actions are simulated well. This demonstrates that the input model and the code represent the plant behaviour properly.

3.5 Requirements to a transient analysis code

After the first experiences with the ATHLET data set for KBR the following items for a transient analysis code and the appropriate data sets from the view point of a utility were identified.

- The synthesis of a data set must be comprehensible, particularly for users not involved in the development of the data set.
- The structure of the control systems should be clearly arranged, so that the adjustment of operating parameters and thresholds can be modified easily.
- It must be possible to enlarge the data set without changing the complete structure of a data set, if there is a need to increase the extent of simulation.
- The numerical solver should be optimized to provide shorter computing times.
- The code models must be verified sufficiently. The range of application of the code models must be determined confidently.
- The code models must be documented in detail.
- It should be possible to operate the code and the appropriate post-processing and analyzing tools from a user platform. The necessary work on the level of the operating system of the computer should be minimized.

4 Use of Thermal-Hydraulic Codes by Reactor Vendors

Siemens is the principal vendor of nuclear power plants in Germany; one PWR was built by ABB. Siemens has also exported nuclear power plants to several foreign countries. It is engaged in the development of advanced reactors: EPR and SWR-1000.

ABB is applying ATHLET and RELAP5 in Germany. The following description of the vendors' code situation is restricted to current and future application of thermal-hydraulic codes at Siemens.

At Siemens AG Germany since 1995 S-RELAP5 has been the standard tool to perform analyses of the thermal-hydraulic plant behavior of NPP's during transients and accidents [4].

The S-RELAP5 code evolved from a modified RELAP5/MOD2 version, used at Siemens Power Corporation, USA (SPC), for performing PWR plant licensing analyses including small break LOCA analysis, steam line break analysis and PWR chapter 15 event analyses. The code structure for S-RELAP5 was modified to be essentially the same as that for RELAP5/MOD3, with the same code portability features. The coding for reactor kinetics, control systems and trip systems were replaced with those of RELAP5/MOD3. The following is a list summarizing major modifications and improvements in S-RELAP5:

Full two-dimensional treatment was added to the hydrodynamic field equations. The 2-D capability can accommodate the Cartesian and the cylindrical (z, r) and (z, θ) coordinate systems and can be applied anywhere in the reactor system. Thus far Siemens has applied 2-D modeling to the downcomer, core and upper plenum. If necessary, 3-D calculations can be approximated by 2-D plus one direction of cross flow. The application of a 2-D component in the downcomer is essential for simulating the asymmetric ECC water delivery observed in the Upper Plenum Test Facility (UPTF) downcomer penetration tests.

The energy equations were modified to conserve the energies transported into and out of a cell (control volume). Omission of some energy terms is still needed to make numerical

computation feasible. For analyses involving a containment volume, the new approach is more appropriate.

Computation of state relations for the steam noncondensable mixture at very low steam quality (i.e., the ratio of steam mass to total mass) was modified to allow the presence of a pure noncondensable gas below the ice point (0°C).

Significant modifications and enhancements were made to the RELAP5/MOD2 interphase friction and interphase mass transfer models. The constitutive models are flow regime dependent and are constructed from the correlations for the basic elements of flow patterns such as bubbles, vapor slugs (i.e., large liquid drops), liquid film and vapor film. A constitutive formulation for a particular flow regime may be composed of two different correlations. Transition flow regimes were introduced for smoothing the constitutive models. Partition functions for combining different correlations and for transitions between two flow regimes were developed based on physical reasoning and code data comparisons. The vertical stratification model was further improved.

The use of a different set of heat transfer correlations for the reflood model in RELAP5/MOD2 was eliminated. Some minor modifications were made to the selection logic for heat transfer modes (or regimes), single phase liquid natural convection and condensation heat transfer. The Lahey correlations for vapor generation in the subcooled nucleate boiling region were implemented.

The code S-RELAP5 can be coupled to a containment code via the Siemens coupling module EUMOD for LB-LOCA analysis. For reactivity transients S-RELAP5 can be linked to Siemens 3D-neutronic codes, such as PANBOX and HEXTIME, via the same module.

The code S-RELAP5 has been verified against a variety of experimental facilities via assessment. The assessment matrix includes tests from the following facilities: FLECHT/SEASET, LOFT, UPTF, CCTF, PKL and BETHSY.

The S-RELAP5 has been applied by Siemens to the following projects as an example:

NPP	Type of Analysis
Stade	Large and medium break LOCA analysis (licensing)
Goesgen	Small/medium/large break LOCA analysis (licensing), transient analysis (DNB, overpressurization)
Biblis A, B	Large break LOCA analysis (licensing), transient analysis (DNB)
Philippsburg 2	Large break LOCA analysis (licensing), transient analysis (DNB)
Grafenrheinfeld	ATWS, feed and bleed analysis for AM (design and licensing)
EPR	LOCA and transient analysis (design of ECCS)
Bohunice	LOCA analysis (design of ECCS)

Table 2: Application of S-RELAP5 by Siemens

The code S-RELAP5 will be used by Siemens in the foreseeable future to perform licensing analysis according to chapter 15 of a FSAR, but also for design purposes, such as the improvement of an ECCS system, or a modification of the reactor protection system.

5 Requirements for Future Applications

In the following, an attempt is made to collect some thoughts about the desired features of the codes that should become available within the next five years. These features are derived from deficiencies and limitations observed in the present codes. There is no absolute requirement to modify the existing codes if they are properly applied within their range of validity. Needs for further development are seen, however, with respect to certain applications for beyond design basis accidents and new reactor types. Reduction of the uncertainty range and of the user influence on calculated results are major goals for such a desired development.

Candidates for further development are the thermal-hydraulic models for reflood under low pressure and for low flow conditions during natural circulation. These phenomena are of special importance for passive cooling systems.

Increasing the number of field equations, e. g. by adding a droplet field, is not likely to improve code predictions in near future since additional closure relations would have to be

established and validated. However, a model for dynamic flow regime evolution, replacing the existing static flow regime maps, should be a promising approach.

Subcooling transients and boron mixing problems require the tracking of steep gradients. Future codes should offer spatial approximation schemes with less numerical diffusion.

Although the present codes are available for interactive use in plant analyzers, a logical further step should be to provide them as process models in full-scope plant simulators. This poses additional requirements on numerical robustness and real-time capability as well as on interfaces to BOP-models and simulator hardware. Computational speed by improving the numerics and by exploiting new computer architectures is a general requirement for all applications.

Multi-dimensional flow simulation with tolerable computing times could significantly reduce the user influence on results since a large part of the user influence stems from the practice to model the pressure vessel by a network of one-dimensional components. The sensitivity of 2D and 3D calculations to nodalization should be controlled, however, by applying sufficiently fine grid sizes. This again will require exploitation of new computer techniques.

The existing codes were built around a fluiddynamic model and its numerical solver. Heat conduction, neutron kinetics, and BOP models were then linked to this essentially fluiddynamic code. Future codes should find a more efficient balance between fluidynamics and the other processes.

For calculating extent of core damage for design basis accidents, detailed codes are available for hot spot temperature and clad behaviour calculations. Up to now, these codes have to be run off-line after the thermal-hydraulic system calculations are complete. It should be of advantage to have detailed mechanistic models for clad oxidation, variable gap heat transfer, strain and rupture of the cladding included in the system codes.

Reactor safety studies often require to calculate event sequences involving more than one code. This need has become obvious for accident management studies where transients may develop into severe accidents, and for new reactor concepts where the reactor coolant

system and the containment are closer linked, e.g. by the IRWST component. Interactive coupling or at least consecutive running is required for the thermal-hydraulic code with other codes that simulate containment behavior, core physics, fuel behavior, core heatup and melting, fission product release and transport during severe accidents. Purely informatic coupling approaches are not sufficient. Future coupling concepts have to consider the physical and numerical nature of the processes. Duplicated or even conflicting input between the different codes should be avoided.

For single phase multi-dimensional flows, the so-called Computational Fluid-Dynamic (CFD) codes are coming into use for calculations in components of the cooling circuit, e. g. for mixing of warm and cold fluid in pipes and plena. A strategy should be found to link CFD codes to system codes by an interface or even include them as 'local' codes.

Quality assurance should include tools and procedures for configuration control, i. e. to make sure that exactly the specified code version is applied. Portability to different computing platforms and the continuous maintenance are greatly facilitated by a clear code architecture and transparent data structure. FORTRAN 90 could be an element in such a strategy.

It was common practice in the past to have different input decks for the same plant. Lack of input convenience and long code running times led to input decks that were tailored just to the actual case to be calculated. This practice has yielded to a new approach which aims at a very comprehensive and detailed plant model, comprising all thermal-hydraulic components, heat slabs, neutronic data, and BOP-models that may be of significant influence for a transient or accident simulation. Construction and maintenance of such large data sets is accompanied by a quality assurance process with plant transient calculations and complete documentation. The effort to be invested for each plant specific data set is more than one man-year. This large investment should be preserved.

Further reduction of the user influence can be achieved by improved user guidelines and user training. Offers for user training should be preferred to formal user qualification. The user should be further supported by enhanced pre- and post processing tools, namely on-line graphics for visualization of input and results. Errors during input preparation could be diminished by more automatic diagnostics and context dependent help links to the manual.

The validation process has to be completed, considering integral experiments and separate effects tests of different scale with emphasis on large scale tests, like UPTF. In order to use the codes for best-estimate analyses, the methods for quantification of uncertainties have to be applied.

6 Conclusions

Although the codes ATHLET and S-RELAP5 are successfully applied in Germany today, there is a need for continuous development and assessment of thermal-hydraulic codes in order to meet present and future needs of licensing organizations, utilities, and vendors.

Desired improvements include the flow regime modeling, the modeling of natural circulation and the multi-dimensional capabilities.

Improved numerical techniques and new computer architectures should be exploited to gain the computational speed necessary for implementing the codes into full-scope simulators. Tracking of subcooling and boron concentration fronts requires non-diffusive numerical schemes.

The user influence should be reduced by improved guidelines and user training. Graphical and other pre- and post processing tools should support the user.

Quality assurance and code maintenance should be supported by transparent code structures and tools for configuration control.

Code validation will be completed and the methods for quantification of uncertainties will be applied.

References

- [1] Teschendorff, V., H. Austregesilo, G. Lerchl
Methodology, Status and Plans for Development and Assessment
of the Code ATHLET
OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes
Requirements, Annapolis, U.S.A., Nov. 5-8, 1996

- [2] Trambauer, K.
Interface Requirements to Couple Thermal-Hydraulic Codes to
Severe Accident Codes: ATHLET-CD
OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes
Requirements, Annapolis, U.S.A., Nov. 5-8, 1996

- [3] Langenbuch, S., et al.
Interface Requirements to Couple Thermal-Hydraulic Codes to 3D Neutronic
Codes
OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes
Requirements, Annapolis, U.S.A., Nov. 5-8, 1996

- [4] Kochskämper, K.
Validation of the Thermal-Hydraulic Computer Code S-RELAP5 for Performing
LOCA Analysis in PWRs
Conference: Nuclear Energy in Central Europe, Portoroz, Slovenia, Sept. 11, 1995

*Workshop on Transient
Thermal-Hydraulic and Neutronic Codes Requirements*

*Annapolis, MD
USA*

5 - 8 November 1996

**SUMMARY OF PAPERS ON CURRENT
AND ANTICIPATED USES OF
THERMAL-HYDRAULIC CODES**

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Papers Summarized

Country	Title	Authors
Japan	Current and Anticipated Use of T/H Codes for BWR Transient and Accident Analyses in Japan	J. Arai, S. Ebata
Switzerland	Current and Anticipated Uses of T/H and Neutronic Codes at PSI	S. Aksan, M. Zimmerman, G. Yadigaroglu
Japan	Current and Anticipated Uses of T/H Codes at the Japan Atomic Energy Research Institute	H. Akimoto, Y. Kukita, A. Ohnuki
Korea	Current and Anticipated Uses of T/H Codes in Korea	K. Kim, W. Chang
Italy	The Italian Experience on T/H Best-Estimate Codes: Achievements and Perspectives	A. Alemberti, F. D'Auria, E. Fiorine, G. Galassi, G. Marella, P. Marsili, P. Meloni, A. Naviglio
France	Current and Anticipated User of the CATHARE Code at EDF and FRAMATOME	JL. Gandrille, JL. Vacher, F. Poizat
Germany	Current and Anticipated Uses of T/H Codes in Germany	V. Teschendorff, U. Sommer, F. Depisch
United States	Capabilities Needed for the Next Generation of T/H Codes for Use in Real Time Applications	S. Arndt
Japan	Current and Anticipated Uses of T/H Codes in NFI	K. Tsuda, M. Takayasu
Spain	Current and Anticipated Uses of T/H Codes in Spain	F. Pelayo, F. Reventos

Current Code Applications

Country	Code	Application	Application Type
Japan	REDY, K2, RELAP-3B, NFI-1, COBRA-IIIC, BANDIX, FRANCESCA, MARVEL, TWINKLE,	Transient Analyses for Licensing	Licensing
	TOSDYN, TRACG, STAIF-PK, RETRAN02, TRAC-PF1	Operational Transient Analyses and Stability Analyses	Best-estimate
	SAFER, LAMB, APEX/SCAT, EUREKAN, SALUTE, LABEL, SATAN-M, BASH-M, LOCTA-M, COCO	LOCA, Reactivity-initiated Accidents	Licensing
	TRAC, TRAC-BD1, TRACG, WCOBRA/TRAC, RELAP5M2, RELAP5M3, RETRAN, MAAP	LOCA, PRA/PSA, Advanced Reactor studies, Accident management	Best Estimate
	JACOS	Coupled T/H (RELAP5) and operator model, for simulation of operator performance	Research
	REFLA/TRAC	PWR reflood phase studies	Research
	ARIES	Reactivity-initiated Accidents	Best-estimate

Country	Code	Application	Application Type
Switzerland	CASMO-4, SIMULATE	Steady-state core analyses	Best estimate
	RETRAN-3D, RELAP5, TRAC-BF1, RAMONA	Transient Analyses. BWR Stability, advanced reactor analysis	Best Estimate
	CONTAIN, GOTHIC, FLOW-3D	Containment response, advanced reactor analysis	Best Estimate
	TRANSURANUS, CORETRAN-01	Fuel behavior, core dynamics and sub-channel analysis	Best Estimate
Italy	RELAP5, TRAC, CATHARE2	Advanced reactor T/H analyses	Best estimate
	GOTHIC, FLOW-3D	Containment and 3D analyses	Best estimate
	MAAP4	Advanced reactor PSA	Best estimate
	QUANDY-EN	Advanced reactor reactivity analysis	Best estimate
	RELAP5, SCDAP, CATHARE, CONTEMPT, MELCOR, FUMO, ECART, ESTER, STCP	Investigation of experimental facility behavior, quantification of uncertainty	Research

Country	Code	Application	Application Type
Spain	RELAP5, TRAC-PF1, TRAC-BF1, RETRAN, TRETA, LAPUR	<p>LOCA , Transient and Accident Scenarios, Stability Analyses</p> <ol style="list-style-type: none"> 1. Independent calculations to verify licensing submittals 2. Support licensing reviews 3. Analyze real transients and potential scenarios not in design envelope 4. Verify emergency operating procedures 5. Operator training 6. Improve dialogue with industry 7. PRA/PSA 8. Evaluate Advanced Reactor characteristics 	Best Estimate

Country	Code	Application	Application Type
France	CATHARE, CATHARE-SIMU, SIPA	1. LOCA, transient, and accident analyses of existing reactors, especially determination of margin in earlier Appendix K calculations 2. Design of new reactors 3. Maintenance assistant for operating reactors analyses 4. VVER analyses 5. Simulators/training 6. Emergency Procedure validation	Best estimate
Korea	RETRAN-01, RETRAN-03	Plant transient analyses	Licensing
	RELAP5M3, CATHARE2	Plant transient analyses	Best estimate

Country	Code	Application	Application Type
United States	RELAP5, TRAC	Simulators, real-time simulation, emergency planning, PRA	Best Estimate
Germany	ATHLET, ATLAS simulator, RELAP5, S-RELAP5, PANBOX, HEXTIME,	<ol style="list-style-type: none"> 1. Licensing calculations for ECCS functions with new fuel designs 2. Evaluate margins in current designs 3. Determine the effectiveness of backfit measures 4. VVER and RBMK safety studies 5. Analytical capability independent of vendors (utilities) 6. Perform transient analyses for periodic safety reviews (utilities) 7. Plant design and licensing safety case submittals (vendors) 	Best Estimate

Future Needs

Country	Application Area	Specific Needs
Japan	BWR Transients	<ol style="list-style-type: none"> 1. Detailed analyses of BWR Core performance - Coupled T/H and Neutronics capability 2. Evaluate margins in current designs 3. Design codes for future reactor designs 4. Improve user interface 5. Improve numerics
Japan	<ol style="list-style-type: none"> 1. Passive system analyses 2. Best estimate evaluations for realistic operational management 3. Studies of aging-related phenomena 4. Fusion reactor design 	<ol style="list-style-type: none"> 1. Stable analytical capabilities at low pressure 2. Non-condensable gas treatment in two-phase flow 3. Treatment of more complex flow behavior (non-equilibrium, non-homogeneous) 4. Capability to couple T/H with neutronics, structural codes, and fuel 5. Better BOP capability 6. Replace current constitutive relation models with more mechanistic models

Country	Application Area	Specific Needs
Korea	<ol style="list-style-type: none"> 1. Analyses of operating reactors 2. Evaluations of future designs 3. Development of indigenous analytical capability 	<ol style="list-style-type: none"> 1. Code should have multipurpose capabilities, and be able to support analysis and simulator applications 2. KAERI considering internal code development effort, in order to enhance internal capabilities
Italy	<ol style="list-style-type: none"> 1. Evaluation of new generation reactors 2. Evaluation of VVER and RBMK reactors 	<ol style="list-style-type: none"> 1. Multi fluid capabilities, besides water-steam 2. Open interfaces to allow coupling of T/H codes with other codes, such as structural, neutronics, containment, and severe accident 3. 2-D and 3-D modeling capability, to provide for component-level modeling 4. Improved user interfaces 5. Improved guidelines for user qualifications

Country	Application Area	Specific Needs
France	<p>1. Improve fidelity and capability of simulations</p> <p>2. Bring together codes used for safety studies, engineering, and training into one code suite - create one unified code for multiple applications</p>	<p>1. Ensure that codes are validated for expanded ranges, beyond DBA conditions</p> <p>2. Need for systematic determination of code uncertainty as part of validation/verification program</p> <p>3. Multidimensional capabilities should be used to justify 0-D of 1-D approaches, provided that they can be validated.</p> <p>4. Improve runtime performance - real-time performance, or better</p> <p>5. Structure codes to be able to use future computer designs (e.g., parrallelization)</p> <p>6. Provide accurate and exhaustive user guidelines in order to minimize the user effect</p> <p>7. Improve the user interface so that it is easier to build models and to interpret the results, especially of complex models</p> <p>8. Design future codes so that they are easier to maintain - modularization and efficient code design with clearly understood program flow.</p>

Country	Application Area	Specific Needs
Switzerland	<ol style="list-style-type: none"> 1. Accident Management 2. Transients during plant startup and shutdown, especially for PRA/PSA applications 3. Estimates of uncertainty for plant analyses 4. Closer integration of various disciplines (e.g., reactor and containment, code neutronics and T/H) 5. Continuing trend to more realistic modeling 6. Advanced reactor modeling and new design options for existing plants 	<ol style="list-style-type: none"> 1. Choice of kinetics models 2. User-definable descriptions of nuclear cross-sections 3. Wider choices of fluid models, ranging from simple (HEM) to advanced 2-fluid (6 equation) 4. Optional 3-D T/H 5. Turbulence modeling 6. Improved fluid properties at low pressure (below atmospheric) 7. Open vessel T/H 8. Better treatment of physical discontinuities 9. Optional containment analytical capability 10. Optional BOP model 11. Faster running numerics 12. Code amenable to parallelization 13. Improved user interface 14. On-line documentation 15. Coupling between system codes and codes modeling local phenomena in specific components

Country	Application Area	Specific Needs
Spain	<ol style="list-style-type: none"> 1. Integrated Safety Assessment - coupled dynamic analysis and PSA 2. EOP Simulation 3. Uncertainty Methodology Studies 4. Safety of Advanced Reactors 5. Evaluate safety significance of scenarios not previously considered 6. Evaluate margins in current designs 	<ol style="list-style-type: none"> 1. Expand capabilities to deal with shutdown mode analyses 2. Asymmetrical neutron flux scenarios 3. Boron dilution 4. Thermal stratification and mixing 5. Reduce code uncertainties 6. Improve code speed and robustness 7. Improve treatment on non-condensables in liquid and vapor phases 8. 3-D neutronics 9. Reduce numerical diffusion 10. Include ability to model turbulence and thermal mixing 11. Advanced reactor capabilities

Country	Application Area	Specific Needs
United States	<ol style="list-style-type: none"> 1. Real-time Simulation 2. Emergency Planning 3. PRA 	<ol style="list-style-type: none"> 1. Improved code robustness 2. Improved code structure and numerics to support real-time and faster-than-real-time applications 3. Improve the user interface to allow a wider range of individuals to use the codes, especially PRA practitioners 4. Better configuration management and assessment 5. Improved, more detailed documentation that is easier to use 6. Ability to tailor models to particular phenomena in particular components
Germany	<ol style="list-style-type: none"> 1. Advanced EPR 2. Advanced BWR 3. Operating reactor analyses 	<ol style="list-style-type: none"> 1. Code should be capable of using one comprehensive input model to perform a wide range of analyses, so that different models do not have to be developed and maintained for different transients 2. Future codes need to include the capability to link the T/H capabilities to other codes, such as neutron kinetics, containment performance, fuel behavior, fission product behavior, and transport during severe accidents 3. Future T/H codes need to balance the fluid dynamics models with the models for heat conduction, and control systems so that fluid dynamics do not dominate design of code. The design of the code needs to be balanced among the different constituents

Common Recommendations

1. Improve the user interface so that more people can use the code, so that models are easier and less expensive to prepare and maintain, and so that the results are scrutable.
2. Design the code so that it can easily be coupled to other codes, such as core physics, containment, fission product behavior during severe accidents.
3. Improve the numerical methods to make the code more robust and especially faster running, particularly for low pressure transients.
4. Ensure that future code development includes assessment of code uncertainties as integral part of code verification and validation.
5. Provide extensive user guidelines or structure the code so that the "user effect" is minimized
6. Include the capability to model multiple fluids (gas and liquid phase).
7. Design the code in a modular fashion so that new models can be added easily. Provide the ability to include detailed or simplified component models.
8. Build on work previously done with other codes(RETRAN, RELAP, TRAC, CATHARE) and other code validation efforts (CSAU, CSNI SET and IET matrices).

The Italian experience on T/H best estimate codes: achievements and perspectives

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1-Introduction

Thermalhydraulic system codes are complex tools developed to simulate the power plants behavior during off-normal conditions. Among the objectives of the code calculations the evaluation of safety margins, the operator training, the optimization of the plant design and of the emergency operating procedures, are mostly considered in the field of the nuclear safety.

The first generation of codes was developed in the United States at the end of '60s. Since that time, different research groups all over the world started the development of their own codes. At the beginning of the '80s, the second generation codes were proposed; these differ from the first generation codes owing to the number of balance equations solved (six instead of three), the sophistication of the constitutive models and of the adopted numerics. The capabilities of available computers have been fully exploited during the years.

At present, four system codes are mostly diffused: Relap5 and TRAC originated from United States, Cathare and Athlet originated in France and Germany, respectively. A few additional system codes are also available in a restricted number of organizations.

The development of such codes implied a great research and experimental work in order to define and realize the mathematical model of the phenomena characterizing the physical process in the nuclear power plants. Then wide validation programs have been necessary to demonstrate the applicability of the codes to plants. These have been planned and carried out in national and international contexts at four levels, involving the use of data coming from:

- "fundamental" experiments;
- Separate Effects Test Facilities (SETF);
- Integral Test Facilities (ITF),;
- real plant.

Experimental data have been extensively compared with calculated data. Resources of the order of billion US \$ have been invested in this area during the time frame since the end of '60s till now. Investments in this area have been strongly reduced in the last five years with main regard to the experimental activities. However a very wide data base is currently available.

The present situation in relation to the development, validation and use of system codes, can be summarized as follows:

- the codes have reached an acceptable degree of maturity;

(1)-ANSALDO; (2)-University of Pisa; (3)-ENEL; (4)-ANPA; (5)-ENEA; (6)-University of Rome La Sapienza.

- the codes diffusion is fast growing especially in the Countries belonging to the former Soviet Union, in the East European and in the Far East Countries like Korea, China, etc.;
- the use of best estimate codes is more and more requested for assessing the safety of existing reactors in the former Soviet Union and in the East European Countries, and for designing advanced reactors;
- advancements in code capabilities in the past five years were mostly related to the applications for the new generation reactors;
- code validation criteria and detailed qualification programs are already in place, though not fully optimized or internationally agreed;
- methodologies to evaluate the 'uncertainty' (i.e. the error) in the prediction of nuclear power plants related scenarios by system codes, have been proposed and are being tested;
- problems like user effect (i.e. influence of code users on the predictions), nodalization qualification, quantification of code accuracy (i.e. ranking of the error in the comparison between measured and calculated trend), have been dealt with and are currently under investigation;
- relevant activities related to the best estimate codes have been recently completed (or will be completed in due course) in the frame of the OECD and the Committee on the Safety of Nuclear Installations (CSNI). These include:
 - the State of the Art Report on Thermalhydraulics of Emergency Core Cooling;
 - the set-up of the Integral Test Facility Code Validation Matrix;
 - the set-up of the Separate Effect Test Facility Code Validation Matrix;
 - the characterization of relevant plant status;

Stated that it appears quite reasonable to further develop the best estimate codes in order to take the advantage of the best available of technology and knowledge, but at the same time other aspects related the practical use of the codes such as the uncertainty evaluation of the results and their applicability to the specific plant type should be considered.

The latter is particularly important if it is we consider that the codes developed in the west countries are being used more and more in countries were there is limited specific experience.

2-Type and objectives of the code applications

Despite of the present situation (no nuclear power plants operating, no new nuclear power plants under construction) the best estimate codes, in Italy, have been used extensively during the past twenty years and are currently used.

In fact before the Chernobyl accident, in Italy, three nuclear power plant were operating, one double units (1000 Mwe each) was under construction and other two were committed.

Relating to that involvement a number of experimental facilities were constructed and operated. Based on their own specificity many Italian Organizations used the best estimated codes with different purposes, but all finalized to the safety as objective.

Stated that, areas like design and confirmation of design of Nuclear Power Plants (including components), characterization of complex transient scenarios, optimization of Emergency Operating Procedures, operator training and independent licensing represent

Historically, different codes were developed dealing with three different technical scenarios: "primary loop" (within DBA and beyond DBA before loss of geometric integrity of the core),

the "containment" (characterization of thermalhydraulic scenarios mostly in the same conditions as above) and the "severe accident" (in vessel and ex vessel system behaviour, corium behaviour, hydrogen production and diffusion, etc.). Limited links among the three areas existed till the advent of the advanced reactor where, among the other things, the consideration of a tight coupling between primary system and containment is necessary to predict the overall system performance.

Considering the above context four purposes can be distinguished in Italy for code development and use:

- A) characterization of transient scenarios in nuclear power plants;
- B) code assessment including the participation in International Programs;
- C) application of codes for investigating design and licensing issues for nuclear power plants;
- D) development of codes able to characterize the overall nuclear plant system behaviour and related developmental assessment.

It might be noted that most of the activities at items A), B) and C) have been conducted in Italy adopting codes developed abroad (a limited participation in the development occurred in a few cases), while activities specifically addressing the new reactor scenarios have been conducted in the frame of item D).

In the following a summarized description of the experiences and achievements of the Italian organization involved in the use, assessment and development of system codes is presented.

3-Italian Organizations Involved

Many Italian Organizations have made a quite large use of the best estimate codes. Some of them gained also a significant experience in the development area. As a consequence of the Chernobyl accident the overall activity in the nuclear field decreased in Italy and, in particular the number of the organizations still involved in the area of T/H is now reduced and in the following it will shortly described the mission and the specificity of the applications relating to such organizations.

3.1-ANPA

ANPA (National Agency for Environmental Protection) is the National Regulatory Body for Nuclear Power applications.

The mission of the ANPA, in the nuclear field, is to ensure the safety of the nuclear installations and an adequate protection of the public health and of the environment in Italy. The ANPA's scope of responsibility includes regulation of commercial nuclear power reactors; research reactors; fuel cycle facilities; medical, academic, and industrial uses of nuclear materials; and the transport, storage, and disposal of nuclear materials and waste.

ANPA (the former ENEA/DISP) in the past has been involved in several national and international safety research programs in the field of T/H and best estimate system codes validation process.

Among others it is worthwhile to mention that ANPA (as ENEA/DISP) participated in the past to the OECD-LOFT program, the ICAP and the SPES-1 test program making either directly or sponsoring T/H calculations using best estimate system codes [A3,A4]. At the same time ENEA/DISP accomplished the licensing activity for the nuclear power plants under construction

and the operating ones; in this frame ENEA/DISP performed independent safety evaluation using the best estimate codes (mostly Relap5).

More recently ANPA has been directly involved in the safety evaluation of the new generation reactors, as the AP600 and SBWR ;Relap5 and TRAC codes have been used for making T/H calculations.

Currently ANPA is participating to the validation process of Relap5/Mod3 code in the frame of the CAMP program.

3.2-ANSALDO

Beginning from the late sixties, Ansaldo has developed its capabilities and gained large experience in design, manufacturing, construction and servicing of nuclear power plant equipped with thermal and fast breeder reactors. The nuclear activities are organized under the Nuclear Division - Ansaldo DNU in Genoa and the Nuclear Components Unit - Ansaldo UCN in Milan. Currently, the Ansaldo main scope includes:

- development of advanced nuclear reactors
- engineering, construction and service of plants for the nuclear industry
- design and manufacturing of large components for NPPs
- marketing and sales of hi-tech nuclear technologies products outside the nuclear market

Manufacturing of nuclear components is performed in the Milan factory while other activities are conducted by the Nuclear Division.

Ansaldo DNU activities in the frame of best estimate system code calculations are at present essentially related to the use of Relap5/mod3 as well as of the Gothic (containment analysis) and Flow3D (three dimensional analysis). The knowledge on the use of such advanced codes has been growing during last years through application to a wide variety of plant and facilities both in the nuclear and conventional field.

DNU activities using Relap5 started in 1981 with the simulations of horizontal channels reflood experiments [A1,A2]. Calculations for the SPES-1 and SPES-2 facilities [A5-A10] were carried out while pre-test and post-test analysis for the OECD-LOFT SB3 have been performed [A3-A4].

ANSALDO DNU has been also involved in calculations for conventional systems where Relap5 was used to solve a number of problems. Examples of this extended range of applications are for example: the simulation of a Moisture Separator Reheater transient to understand the cause of unexpected high level drain tank signal, the prediction of the stagnation and corrosion for a tube boiler design (waste burner) and finally transient calculations of a turbo gas feed line pipe.

3.3-ENEA

ENEA is the Government Agency for Energy, New Technology and Environment and covers the institutional role for research and development of nuclear reactors; in particular ENEA-ERG-FISS has the responsibility for the activities concerning the nuclear fission.

In the past ENEA made a large use of T/H codes, as Relap and TRAC, for safety evaluation of Italian PWR-PUN that, before Chernobyl, was supposed to be realized in several units in Italy; at the same time ENEA was involved in the OECD-LOFT project and in this frame performed pre-test and post-test calculations for many tests. ENEA coordinated the design SPES1 integral test facility and led the activity of the related research program.

At present ENEA participates, in collaboration with Italian Industries and Universities, at design studies and experimental research programs, aimed, by providing analytical and experimental

results, to the design verification and performance evaluation of innovative safety systems and components.

Thanks to the participation in international programs of assessment and maintenance (ICAP, CAMP, CUC, CSARP), ENEA can use some T/H best estimate codes: RELAP5, CATHARE 2, TRAC, MELCOR.

The activities, which are being performed in ENEA, involve in particular the RELAP5 and CATHARE utilization.

These activities mainly concern:

- the evaluation of the codes capability to predict the physical phenomena related to innovative safety systems in the advanced reactors /B3,B4/;
- the development of the new models to take into account the behaviour of passive systems (in the frame of a ENEA-CEA co-operation on CHATARE);
- the design studies on innovative safety related components and systems for advanced BWR in collaboration with SIET Laboratories.

3.4-ENEL

ENEL is the National Utility for Electric Power Production.

After the Chernobyl accident and the related nuclear moratorium ENEL has been actively involved in the development and assessment of the advanced reactors with enhanced safety features.

In particular, ENEL cooperated with Westinghouse and General Electric to the assessment and development of the passive reactors AP600 and SBWR, with the responsibility to perform the Probabilistic Safety Assessment (PSA) studies for both the plants.

In this frame, the following analysis activities were in particular performed:

1. The thermal hydraulic behaviour of the AP600 reactor coolant system (RCS) during design basis, as well as degraded sequences was analyzed by the MAAP 4.0 code, to establish success criteria for the PSA.
2. Models of AP600 and SBWR were built with RELAP5 mod2 and mod2.5, in cooperation with Pisa University. Beyond-design-bases reactivity accidents were analyzed for both AP600 and SBWR, by the ENEL 3-D space-time code QUANDY-EN.

In the frame of AP600 design certification process, ENEL was one of the sponsors of the SPES-2 experimental test program. Pre-tests as well post-test analyses were performed, in cooperation with Pisa University, using different RELAP5 versions (2.5, , 3.1). Currently ENEL, together with other major European utilities and the industrial partners (Westinghouse and GENESI), is involved in the European Passive Plant Evaluation Program (EPP) which is aimed at designing a 1000 Mwe plant, acceptable for the European environment. In the frame of this activity, a model of the RCS has been prepared in cooperation with Pisa University, using RELAP5 3.1, and some accident sequences analyzed in a preliminary way.

Moreover, ENEL has in place a contract with EdF to participate to the basic development of the EPR reactor. In this frame, ENEL will evaluate the amount and rate of hydrogen production during degraded accident sequences using the RELAP/SCDAP code.

3.5-DCMN of University of Pisa

The Dipartimento di Costruzioni Meccaniche e Nucleari (DCMN) of Pisa University has been involved for more than thirty years in the system thermalhydraulics areas, i.e. all the three areas mentioned before, including the use and the development of codes and the design and

management of experimental facilities. The following system codes are in use at DCMN: Relap (different versions) and Relap5/Scdap, Cathare (different versions), Gothic, Melcor, Contempt (different versions), Fumo (see also below), Ecart (see also below), Ester and STCP (March, Merge and Naua).

The DCMN of University of Pisa has done activity aimed to characterization of transient scenarios specifically looking at data from ITFs. When available data from Counterpart or Similar Tests (CT or ST, respectively) have been exploited.

As examples of activities carried out in this frame at DCMN we mention the following:

- analysis of SBLOCA CT in BWR utilizing a data base from FIST, ROSA-III and PIPER-ONE, this last facility being built and operated at University of Pisa, ref. [P1];
- analysis of SBLOCA CT in PWR utilizing a data base from LOBI, BETHSY, LSTF and SPES, the experiment in this last facility being also designed at DCMN, refs. [P2] and [P3];

More recently, DCMN has been involved in the analysis of phenomena in experimental loops simulating new generation reactors, ref. [P17].

DCMN of Pisa University participated to all standard problems (ISP) organized by OECD in the primary circuit and containment fields. Participation in IAEA Standard Problem Exercises, EU and OECD/NEA-NSC Bechmarks, Phebus, LOFT, LACE, Marviken, SPES-2, HDR, PIPER-ONE, TMI and LOBI Programs can also be mentioned.

As a generic achievement, the capability to use the code at the best, can be emphasized. This also implies a direct understanding of the code limits and capabilities.

A significant specific achievement is the development of the UMAE (Uncertainty Methodology based on Accuracy Extrapolation), ref. [P9], that is a procedure to evaluate the uncertainty in the prediction of plant transients by system codes. The procedure is, and extensively makes use of the data base from ITF.

In order to answer the old question 'how good is good enough', the FFT based methodology has been proposed to quantify the level of agreement (disagreement) between a system code prediction and measured data. This method can be used, among the other things, to classify sensitivity calculations, to evaluate the improvements of a new code version, to judge a nodalization (or the code user), to accept calculations, ref. [P10]; The FFT based methodology has been requested and distributed to CEA (F, Centers of Cadarache and Fontenay-aux-Roses), GRS (G, Koln Center), IJS (Ljubljana, SLO), University of Zagreb (Croatia), NUPEC (J), JRC (Euratom, Ispra), ENEL (Roma, I), University of Lappeenranta (Lappeenranta, SF), CNEN (Rio-de-Janeiro, Brazil);

A procedure to qualify a nodalization has been proposed, ref. [P11].

In the same framework the user effect has been characterized, ref. [P12], while an attempt is in progress to fix acceptable criteria for the user qualification;

System codes have been applied to safety/licensing calculations and to confirm the design of advanced NPP. The activities have been done mostly under contracts with ENEA/DISP (now ANPA), ENEA, and ENEL.

A number of physically based models have been developed and qualified dealing with specific phenomena like critical flow, jet-thrust and jet impingement loads, CCFL, density wave in boiling channels and condensation also in presence of non-condensable gases.

Two system codes (different versions) have been developed and qualified at DCMN:

- a) FUMO including the integrated version, refs. [P14] and [P15]. FUMO allows the calculation of the containment behaviour of present generation (FUMO stand alone) and of advanced (Integrated-FUMO) reactors; SIMSIP is the primary module of the Integrated-FUMO;
- b) thermalhydraulic module of the ENEL ECART code aiming at the study of the fission product behaviour inside primary system and containment, ref. [P16].

3.6- DINCE of University of Rome "La Sapienza"

The thermalhydraulic staff of the Dipartimento di Ingegneria Nucleare e Conversioni di Energia (DINCE) of the University of Rome "La Sapienza" (up to 1989, Dipartimento di Energetica) has been involved, from the late 70's, in analyses related to experimental programs (SPES-1, [R1, R2]), accidental transients in power plants (TMI-2 Standard Problem, [R3], Italian 1000 MW PWR "PUN" plant design [R1, R2], Caorso 840 MW BWR plant design, etc.), pre- and post-test analyses (LACE, ACE and LOFT international programs). The computer programs used by the DINCE have been: Relap (different versions up to Relap5 mod. 2), Relap5/SCDAP, NAUA. In the 80's, several analyses have been performed on large and small break LOCA's, using LOBI and SPES data bases, and on core-concrete interaction calculations, using CORCON and VANESA computer codes.

Most of the activities have been performed in co-operation with ENEA, ENEA/DISP (now ANPA) and ENEL.

From 1984, the DINCE of the University of Rome has developed the conceptual design of a medium-size nuclear reactor, the MARS (Multipurpose Advanced Reactor inherently Safe), 600 Mwth PWR plant, characterized by the systematic use of passive safety systems and components. Quite a lot of accident scenarios have been evaluated using the Relap5 computer code [R4, R5, R6], and other computer programs developed for this purpose.

In the last years, the DINCE has been involved in the development of passive systems and components for innovative decay heat removal, also for new-generation-reactors, such as the AP600 and the SBWR [R7, R8, R9, R10].

In the area of development of codes, the DINCE has developed own design computer programs for steady-state and transient analyses, has participated in the development of CASTEM2000/TRIO series computer programs, and has developed and extensively used a thermalhydraulic code (CONSEN, [R11, R12]), able to analyze transients, also in cryogenic conditions, for the thermalhydraulic calculations related to break accidents in NET and ITER fusion reactors cooling systems.

4-Future needs

As mentioned before in Italy there are neither operating nor under construction nuclear power plants.

Nevertheless a significant involvement is still undergoing relating to the new generation reactors and the Assistance Programs of the Commission of the European Community to the East European Countries for the assessment and improvements of the safety of their former soviet technology nuclear power plants.

Moreover, the gained experience and the willingness (not only of the authors!) to survive in the Nuclear Arena, brought us to contribute to the future needs in the frame of system codes.

The following requirements have been identified as suitable features for a future code:

- **user model interfaces:** although a well established set of correlations and models has to be the basis for the system code, it is important to add an user interface to allow additional model/components to be tested. Some time the use of the code has been limited due to the lack of very simple models. The addition of this capability will extend greatly the fields of possible applications. In general the boundary conditions of the code should be opened to external access to gain the code flexibility needed for applications not limited to the nuclear field. User routines can then be added to the code to extend its capability. A user model interface should have also access to trip values and be able to modify the trip status as well as to access all the information needed from the code by the additional models.
- **multifluid capability:** the possibility to use multi components fluid mixtures will increase greatly the range of applicability of the code. New and advanced thermal cycles can be analyzed (as an example a mixture like H_2O/NH_3). Fluid properties should be accessed by the code in either the usual tabular or functional form using a subset of the user model interface. Tracing of the concentration is needed for both liquid and vapor phases while the addition of multi-noncondensable gases should be also included in the code modeling.
- **3D modeling capability:** during work in the last years for passive and/or inherently safe reactors design one of the main limit of the code was found to be the absence of a 3D modeling capability. Although the addition to a system code of a full 3-D simulation capability is anticipated to be outside the present available computing power the addition of a 3D (limited) capability inside the system code seems to be a desirable feature. Especially pool natural circulation and downcomer behavior have to be correctly handled by the code.
- **Parallel processing:** the diffusion of the parallel processing has been mainly limited by the absence of appropriate parallel numerical algorithms able to use the specific hardware advantages, the relatively high cost of parallel machines and generally by a non resolved doubt about the effectiveness of the parallel approach. Some experience in 3D parallel implementations is now available in Europe especially on w/s clusters using message passing interfaces. However it is not yet clear the real advantage for a system code to use such architecture. High real time computing ratios can be achieved only with a number of dedicated processors and this is not the usual situation available for example in industry.
- The use of message passing interfaces has been also proposed as an alternative way to code coupling. This solution can be considered very attractive taking into account the previously cited need for user model interface. Users models can be added easily to the code excluding any access to the source while parallel performances can be appropriately tested.
- **user guidelines:** adequate attention should be paid to user guidelines reports were suggestion, known problems and special applications as well as code limits and range of applicability should be exposed clearly. Providing courses on correct use is very important to solve known problems related to the dependence of the results from code user.
- **Code development:** a continuous development of the presently available computer codes is judged to be the preferred way to reach the above defined performances and capabilities. Development of completely new tools starting from scratch should be avoided since it present some relevant disadvantages: a complete stop of development on present code

version could result in the absence of a technology up-to-date computer code while the time needed by the new tool to reach the presently available capabilities is really difficult to be evaluated.

- **Graphical User Interface:** development of a code input GUI is anticipated to be a very important and useful point for the user, provided that: the input file will be still understandable by the common user, as soon as possible messages for input check is given and a complete control on code options is allowed. Code manuals should be on line either in a browse (print) or keyword search environment. No doubt exist that the post processing GUI like NPA now widely used is of fundamental importance to present and analyze the code results. New GUIs should solve the problem on how much the pre and post processing phase should be integrated and at what extent the previously developed interface can be still used or completely rewritten.

5-Conclusions

The best estimate system codes have reached an acceptable degree of maturity and their use is increasing as well as the field of application is expanding.

Furthermore it should be considered that even if a large amount of work has been accomplished in the area of code assessment, some questions still need a common answer from the scientific community in order to determine a common understanding and quality standards for the reactor safety evaluation; in particular further discussion is needed to more properly approach to the following issues:

- what is the meaning of best-estimate and what are the implications;
- when a code is adequate for NPP licensing applications;
- what is the acceptable error in a calculation (either accuracy or uncertainty);
- what are the conditions for a qualified nodalization;
- when improvement of a model is requested and new research is needed;
- what is the minimum number of calculations to judge the code quality.

Stated that we consider suitable to further develop the best estimate codes in order to take the advantage of the best available of technology and knowledge we support the effort of CSNI aimed to define the needs and the suitable feature of the future best estimate code.

REFERENCES

- A1. G.Proto, A.Alemberti, G.Bimbo, A.C.D. Wright, M.Z. Caplan**
 BLOWDOWN AND COLD WATER INJECTION EXPERIMENTS: COMPARISONS WITH THE
 FIREBIRD-III AND RELAP-5 CODES
 Proceedings of the International Meeting on Thermal Nuclear Reactor Safety
 Chicago, IL - August 29 - September 2, 1982
- A2. A.C.D. Wright, G.Proto, A-Alemberti, G.Bimbo, M.Z. Caplan**
 CANDU LOCA EXPERIMENTS: COMPARISONS WITH THE FIREBIRD-III AND RELAP-5
 IAEA - TC -427.5 (TC-SR-3) Proceeding of a specialists' meeting
 Budapest, Hungary, 3-7 October 1983
- A3. A. Alemberti**
 EXP. ANALYSIS AND SUMMARY REPORT ON OECD LOFT EXPERIMENT LP-SB-03
 OECD LOFT-T-3605 - December 1985
- A4. A. Alemberti**
 COMPARISON REPORT ON OECD LOFT EXPERIMENT LP-SB-03
 OECD LOFT-T-3606 - February 1987
- A5. A. Alemberti, C. Frepoli, G. Graziosi**
 COMPARISON OF THE SPES-2 PRE TEST PREDICTIONS AND
 AP600 PLANT CALCULATIONS USING RELAP5/Mod3
 Intern. Conference - New Trends in Nuclear System Thermohydraulics
 Pisa, May 30th- June 2nd - 1994
- A6. A. Alemberti, C. Frepoli, G. Graziosi**
 SPES-2 COLD BREAK EXPERIMENTS: SCALING APPROACH FOR DECAY POWER,
 HEAT LOSSES COMPENSATION AND METAL HEAT RELEASE
 Intern. Conference - New Trends in Nuclear System Thermohydraulics -
 Pisa, May 30th- June 2nd - 1994
- A7. A. Alemberti, C. Frepoli, G. Graziosi**
 SPES-2 RELAP5/Mod3 NODING AND 1" COLD LEG BREAK TEST S00401
 NRC 22nd Water Reactor Safety information Meeting - Washington D.C. October 1994
- A8. M.Bacchiani, C.Medich, M.Rigamonti, O.Vescovi, A.Alemberti, L.E.Conway** SPES-2, AP600
 INTEGRAL SYSTEM TEST S00706 -DEG BREAK OF DVI LINE
 ICONE-3 Kioto - Japan 23/27 April 1995 - Serial Number 141
- A9. A. Alemberti, C. Frepoli, G. Graziosi**
 RELAP5/Mod3 PRE-TEST PREDICTIONS FOR THE SPES-2 BREAK TEST S01613
 Technical Committee Meeting on Progress in Design, R&D and Testing of Safety Systems for
 Advanced Water Cooled Reactors - IAEA Conference Piacenza - Italy, May 1995
- A10. M.Bacchiani, C.Medich, M.Rigamonti, O.Vescovi, A.Alemberti, L.E.Conway**
 SPES-2, AP600 INTEGRAL SYSTEM TEST S01007 2" CL TO CORE MAKE-UP TANK
 PRESSURE BALANCE LINE BREAK NURETH-7 Saratoga Spring - New York - September 10/15
 1995
- B1. C.M. Antonucci, P. Meloni**
 "RELAP5/Mod2 analysis of the Station Blackout Experiment SP-ST-01, performed in SPES facility"
 ICONE-2 S. Francisco Ca. (USA) March 21-25, 1993
- B2. P. Meloni**
 "CHATARE 2 analysis of the Small Break LOCA Experiment SP-SB-03, conducted in SPES facility"
 X ENFIR/III ENAN Joint Nuclear Conferences on Reactor Technology and Nuclear Applications ;
 Aguas de Lindoia(Brazil) August 7-11, 1995.
- B3. C.M. Antonucci, P. Meloni**
 "Application of RELAP5/Mod3 to the testing of the AP600 Automatic Depressurization System."
 International Conference on New Trends in Nuclear System Thermohydraulics. Pisa(I) May 30- June 2,
 1994.

- B4. P. Meloni**
 "Evaluation of CATHARE VI.3 capability to simulate the performance of Automatic Depressurization System."
 ICONE-4 New Orleans Louisiana(USA) , March 10-14, 1996.
- C1. P. Marsili, A. Pasculli, P. Camiciola**
 " ATWS SCOPING CALCULATIONS FOR A BWR PLANT PERFORMED USING RELAP5/MOD3 AND CONTAINS CODES"
 Nuclear Engineering and Design 121(1990)
- C2. F. D'Auria P. Marsili,**
 " APPLICATION OF RELAP5/MOD 3 TO THE EVALUATION OF ISOLATION CONDENSER PERFORMANCE "
 ICONE-2- San Francisco March 21-24 1993
- C3. G. Bava, P. Marsili**
 " EVALUATION OF PWR POWER PLANTS POTENTIAL FOR ACCIDENT MANAGEMENT ACTIONS TO PREVENT CORE DAMAGE"
 International conference on << New Trends in nuclear Systems Thermohydraulics>> Pisa (Italy) May 30th- June 2nd. 1994
- C4. F. D'Auria, G. Galassi, P. Gatta, P. Marsili, L. Mastrantonio**
 "COMPARISON BETWEEN SMALL LOCA SCENARIOS IN EASTERN AND WESTERN TYPE PWRs"
 ICONE-4- New Orleans March 10-14,1996
- C5. G. Del Nero, A. Madonna G. Marella, A. Orazi**
 "Loss of Normal Feedwater Sensitivity Studies for AP600 Behaviour Characterization"
 International conference on << New Trends in nuclear Systems Thermohydraulics>> Pisa (Italy) May 30th- June 2nd. 1994
- C6. G. Marella**
 "A Simulation Program for Westinghouse PWR's"
 CSNI Specialist Meeting on Simulators and Plant Analyzers
 9-12 June 1992
- P1. Bovalini R., D'Auria F., De Varti A., Maugeri P., Mazzini M.**
 "Analysis of Counterpart Tests performed in BWR Experimental Simulators"
 XV Annual Meet. of Spanish Nuclear Society, Alicante (E), Oct. 23-25 1989
 J. Nuclear Technology. vol 97 Nr. 1 1992
- P2. D'Auria F., Galassi G.M., Ingegneri M.**
 "Evaluation of the data base from high power and low power small break LOCA counterpart tests performed in LOBI. Spes Bethsy and LSTF facilities"
 University of Pisa Report, DCMN - NT 237(94), Pisa (I), Nov. 1994
- P3. D'Auria F., Galassi G.M.**
 "Planning of Spes experiment SP-SB-03 counterpart to LSTF, Bethsy and Lobi- Mod2 experiments"
 University of Pisa Report, DCMN - NT 171(91), Pisa (I), May 1991
- P4. D'Auria F., Galassi G.M., Vigni P., Calastri A.**
 "Scaling of Natural Circulation in PWR Systems"
 EURO THERM Seminar N. 16: Natural Circulation in Industrial Applications,
 Pisa (I). Oct. 11-12 1990
 J. Nuclear Engineering & Design, vol 132 Nr. 2, 1992
- P5. D'Auria F., Galassi G.M.**
 "Characterization of Instabilities during Two-Phase Natural Circulation in PWR Typical Conditions"
 4th Int. Top. Meet. on Nuclear Reactor Thermalhydraulics. Karlsruhe (FRG), Oct. 10-13 1989
 J. Experimental Thermal and Fluid Science, Vol 3, Nr 90, 1990
- P6. A. Manfredini, F. Oriolo, S. Paci**
 "Gas Stratification in Containment Safety Analysis", International Conference on "Nuclear Containment", Cambridge (UK). 23-25 Settembre 1996.
- P7. Billa C., D'Auria F., Debrecin N., Galassi G.M.**
 "Application of Relap5/mod2 to PWR International Standard Problems"
 ANS Winter Meeting. San Francisco (Ca), Nov. 10-15 1991

- P8. F. Oriolo, S. Paci** "FUMO Thermal-Hydraulic Analysis of the VANAM M3 Test",
Dipartimento di Costruzioni Meccaniche e Nucleari, Università degli Studi di Pisa, RL 700 (96).
- P9. D'Auria F., Debrechin N., Galassi G. M.**
"Outline of the Uncertainty Methodology based on Accuracy Extrapolation (UMAE)"
OECD-CSNI Special Workshop on Uncertainty Analysis Methods, London (UK), March 1-3 1994
- P10. D'Auria F., Leonardi M., Pochard R.**
"Methodology for the Evaluation of Thermalhydraulic Codes Accuracy"
Int. Conf. on New Trends in Nuclear System Thermohydraulics - Pisa (I), May 30 - June 2 1994
- P11. Bonuccelli M., D'Auria F., Debrechin N., Galassi G.M.**
"A methodology for the qualification of thermalhydraulic codes Nodalizations"
8th Meet. of OECD-CSNI Task Group on Thermalhydraulic System Behaviour - Paris (F), June 30 - July 2, 1992 - 6th Int. Top. Meet. on Nuclear Reactor Thermalhydraulics, Grenoble (F), Oct. 5- 8, 1993
- P12. Aksan S. N. D'Auria F., Staedtke H.**
"User Effects on the Thermalhydraulic Transient System Codes Calculations"
CSNI Spec. Meet. On Transient Two-Phase Flow - System Thermalhydraulics, Aix-En-Provence (F), Apr. 6-8, 1992 J. Nuclear Engineering & Design, Vol 145, Nrs. 1&2, 1993
OECD 'Status' Report NEA/CSNI R(94)35, Paris (F) Jan. 1995
- P13. A. Manfredini, F. Oriolo, S. Paci, A. Villotti**
"Investigation on Gas Distribution Phenomena inside the Containment System of LWRs" III
International Conference on "Containment Design and Operation", Toronto (C), 19-21 October 1994.
- P14. A. Manfredini, M. Mazzini, F. Oriolo, S. Paci**
"FUMO Code Manual Volume 1: System Models." Dipartimento di Costruzioni Meccaniche e Nucleari. Università degli Studi di Pisa, RL 533 (92).
- P15. P. Barbucci, A. Manfredini, G. Mariotti, F. Oriolo, S. Paci**
"Development and qualification of FUMO code for the containment system simulation of advanced LWRs", IAEA Technical Committee Meeting on Progress in Development and Design Aspects of Advanced water cooled Reactors. Roma (I) 9-12 September 1991.
- P16. W. Ambrosini, G. Fruttoso, F. Oriolo, S. Paci, F. Parozzi**
"Assessment and Validation of ECART Code in Support to Severe Accident Radionuclide Transport". TCM IAEA "Advanced in and Experience with Accident Consequences Analysis", Vienna (A). 27-29 September 1995.
- P17. D'Auria F., Modro M., Oriolo F., Tasaka K.**
"Relevant Thermalhydraulic Aspects of New Generation LWR's"
CSNI Spec. Meet. On Transient Two-Phase Flow - System Thermalhydraulics, Aix-En-Provence (F), Apr. 6-8, 1992 J. Nuclear Engineering & Design, Vol 145, Nrs. 1&2, 1993
- R1. M. Biagioni, M. Caira, E. Cipollone, A. Naviglio**
"PWR-PUN and SPES facility cold leg 3" SBLOCA comparative analysis, using the RELAP4/mod 6 computer code" (In Italian)
Congresso ATI - L'Aquila 12-15 settembre 1984.
- R2. M. Biagioni, M. Caira, E. Cipollone, A. Naviglio**
"2" SBLOCA in cold leg: PWR-PUN and SPES facility" (In Italian)
Congresso ATI - Trieste 11-13 settembre 1985.
- R3. A. Buccafurni, G. Caruso, M. Colagrossi, G.P.C. Di Capua, A. Naviglio**
"Counter-current flow modeling and hydrogen generation influence on a PWR severe accident: the TMI-2 accident"
EUROTHERM Seminar on Thermal non-equilibrium in two-phase flow - Roma - Marzo 1989, pp.301-316
- R4. M. Caira, G. Caruso, E. Farello, A. Naviglio, L. Sorabella**
"Advancements in the design of safety-related systems and components of MARS nuclear plant"
Int. Conf. on Design and Safety of Advanced Nuclear Power Plants - October 25-29, 1992, Tokyo, Vol. II°, paper P5-5
- R5. M. Caira, M. Cumo, A. Naviglio**
"Thermal Hydraulic Features of MARS plant"
American Nuclear Society - Winter Meeting - 1989.

- R6. M. Caira, M. Cumo, E. Farello, L. Gramiccia, A. Naviglio**
"Safety analysis of the MARS IV nuclear plant"
Post SMIRT Seminar on Small and Medium Size Nuclear Reactor - San Diego, California; August 21-23 1989.
- R7. M. Caira, E. Farello, A. Naviglio, L. Sorabella**
"A High-Reliability primary coolant single loop PWR"
ASME-ANS-Winter Meeting - Dallas 25-30 Nov. 1990.
- R8. M. Caira, E. Farello, A. Naviglio, L. Sorabella**
"A passive system for decay heat removal from a double containment of a LWR"
American Nuclear Society, 1993 National Heat Transfer Conference.
- R9. M. Caira, M. Cumo, A. Naviglio, L. Sorabella**
"Unlimited cooling capacity of the passive-type emergency core cooling system of the MARS reactor"
3rd International Conference on Nuclear Engineering, Tokio 25 Apr. 1995.
- R10. M. Caira, E. Farello, A. Naviglio, L. Sorabella**
"Unlimited cooling capacity of the passive-type emergency core cooling system of the MARS reactor (II)"
4rd International Conference on Nuclear Engineering, New Orleans 10-14 Mar. 1996.
- R11. G. Caruso, L. Di Pace, T. Pinna, R. Meyder**
"Cryostat Pressurisation Accident Assessment Using a Computerised Model (CONSEN)"
18th Symp. on Fusion Technology - Paper PB-169 - Aug. 22-26, 1994, Karlsruhe
- R12. Caporali, G. Caruso, G. Franzoni, M.T. Porfiri**
"Parametric Analysis of an In-Vessel LOCA for the ITER Plant"
16th IEEE/NPSS Symp. on Fusion Engineering - Paper 0344 Sept. 30-Oct. 5, 1995 Illinois (USA)

CURRENT AND ANTICIPATED USES OF THERMAL HYDRAULIC CODES AT THE JAPAN ATOMIC ENERGY RESEARCH INSTITUTE

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I. INTRODUCTION

The Japan Atomic Energy Research Institute (JAERI) is conducting several research programs related to thermal-hydraulic and neutronic behavior of light water reactors (LWRs). These include LWR safety research projects, which are conducted in accordance with the Nuclear Safety Commission's research plan, and reactor engineering projects for the development of innovative reactor designs or core/fuel designs. Thermal-hydraulic and neutronic codes are used for various purposes including experimental analysis, nuclear power plant (NPP) safety analysis, and design assessment.

II. CODE USES IN LWR SAFETY RESEARCH PROJECTS

II.1 Code Applications

In the LWR safety research projects, thermal-hydraulic and neutronic codes are used in the areas of fuel safety research, structural safety research, risk analysis, evaluation of NPP events, human factors research, severe accident and accident management research, as well as thermal-hydraulic safety research. Typical examples of code application are as follows.

II.1.1 Man-Machine System Simulation

A man-machine system simulator JACOS (JAeri COgnitive Simulation system) has been constructed by combining RELAP5/Mod2 with other codes⁽¹⁾. JACOS consists of operator and plant models coupled dynamically. The operator model has been developed by employing artificial intelligence (AI) techniques of the distributed cooperative inference method with the so-called blackboard architecture. The plant model of a 3-loop PWR was developed using RELAP5/MOD2 combined with a conventional simulator software. The latter is used to simulate the BOP and plant control systems, and thereby to provide RELAP5 with boundary conditions in terms of, e.g., charging flow, letdown flow, FW flow, and main steam flow. JACOS runs on a SUN workstation two to three times slower than real time.

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II.1.2 Analysis of Abnormal Events in NPPs

Feedback of NPP operating experience to future reactor regulation and operation is sought for by analyzing safety significant events. The RETRAN02 and TRAC-PF1 codes were used for the analyses of events including the LaSalle-2 neutron flux oscillation event in March 1988, and the Mihama-2 steam generator tube rupture (SGTR) in February 1991^[2, 3]. The Mihama-2 analysis included an evaluation of pressurized thermal shock (PTS) based on the Mitsubishi ECC mixing model.

II. 2 Code Assessment and Improvement

In thermal-hydraulic safety research projects, codes have been modified and improved based on analysis of experiments conducted at JAERI and elsewhere.

II.2.1 PWR Reflood Research Program

The TRAC-PF1/Mod1 was modified into the REFLA/TRAC (see III.2.1) code in the PWR reflood phase research program where JAERI took part in the 2D/3D program.

As the second phase of the PWR reflood test program, demonstration tests are started in 1996 to assure the core safety at abnormal transients and accidents of PWR and BWR. Separate effect tests for CHF, post CHF and rewetting and natural circulation considering total power change due to void fraction change are planned to confirm the predictive capability of the REFLA/TRAC and COBRA-TF codes by the year of 2001.

II.2.2 ROSA-IV Program - Study on PWR small-break LOCAs and Transients

The ROSA-IV program conducted integral experiments on PWR small-break LOCA and abnormal transients followed by multiple failure of safety systems and/or delayed operator response to abnormal events^[4]. Typical scenarios simulated in these experiments include breaks on the cold leg, hot leg, cross-over leg, pressure vessel instrument tubes and steam generator U-tubes, ranging up to 8 inch in diameter, and abnormal transients initiated by station blackout and loss of feedwater. Abnormal transients initiated by loss of residual heat removal (RHR) system during mid-loop operation of RHR under reactor shutdown condition were also studied extensively^[5]. Data from these tests were used to assess the RELAP5/Mod1 and Mod2, TRAC-PF1/Mod1, and CATHARE-I and II codes.

One of the ROSA-IV experiment was chosen for CSNI international Standard Problem No. 26 (ISP-26) where 17 organization from 14 countries participated. As part of this ISP, JAERI collected input decks from the participating countries and conducted sensitivity calculations to evaluate the

nodding effects (user effects) on the results obtained with the same code. This effort was made for the RELAP5/Mod2 code which was used by the majority of the participants^[6].

The RELAP5/Mod2 code was modified by implementing interfacial drag models and a critical flow model which were developed on the basis of separate effects tests conducted in the ROSA-IV program^[7].

II.2.3 ROSA-V Program - Study on Accident Management Measures and Next-Generation PWR Safety

The current phase of the ROSA program, ROSA-V, is concerned with accident management measures for prevention of severe core damage. RELAP5/Mod2 and Mod3 are used for experimental analyses and are improved continually^[8, 9]. The CATHARE-II code is used for analysis of separate effects tests, for example full-scale pump test for two-phase flow.

Testing on the Westinghouse advanced passive reactor design (AP600) has been conducted since 1994 in cooperation with the US Nuclear Regulatory Commission (USNRC)^[10, 11]. These experiments are now analyzed using the RELAP5/Mod3 code. In parallel with system integral calculations which are conducted for a few selected experiments, many stand-alone calculations are also done for the response of the individual passive safety components.

New testing activity is being initiated for the candidate next-generation PWR designs developed by the Japanese industries. The RELAP5/Mod3 code has been used for post-test analyses of a couple of initial tests.

II.2.4 BWR Coupled Thermal-Hydraulic Testing Program and Analysis

Since 1991, JAERI has been conducting design studies for an experimental facility for simulation of the BWR coupled neutronic/thermal-hydraulic behavior in abnormal events. The design study has been conducted using the neutronic code EUREKA and the RELAP5/Mod2 code including its point kinetics model. Preliminary tests on coupled core response to inlet flow perturbations will begin in this fiscal year. Such inlet flow perturbations may occur in seismic events.

A TRAC-BF1 analysis is underway on seismically-induced excitation of nuclear-coupled thermal-hydraulic instability in BWRs^[12]. For this purpose, TRAC-BF1 has been modified to take into account the external acceleration to fluids due to earthquake. The modified version of TRAC-BF1 will be assessed against the experiments described above.

While the current facility geometry is one dimensional, with a single simulated bundle, plans are existing to build a smaller scale but multi-bundle facility to simulate 3D behavior. If realized, the testing will use a 3D coupled code which is now under development at JAERI (see III.2.4).

III. CODE USES IN REACTOR/CORE DESIGN STUDIES

JAERI has been developing LWR designs as well as core designs for future LWRs. Both foreign and in-house codes have been used.

III.1 Code Applications

III.1.1 High-Conversion PWR Core Design

High-conversion PWR core design, with tight-lattice, triangular fuel rod arrangement, was developed and assessed for safety in design basis events (DBEs). The JAERI-modified version of TRAC-PF1/Mod1 (REFLA/TRAC) and COBRA-IV-I codes were used for design assessment. Based on assessments against in-house and literature data for DNB in tight-lattice geometries, the KfK correlation was chosen for the design calculations^[13].

III.1.2 Passive PWR Designs

A medium-sized, integrated PWR design, named SPWR, which does not require control rods for reactivity control or shutdown was developed and assessed against DBEs using the RETRAN code^[14]. This reactor design relies on fluid density feedback effects for reactivity control, and on passive safety features for reactor shutdown, emergency core cooling and decay heat removal. For example, the reactor shutdown is achieved by a gravity-driven boron recirculation. Some application was also made of TRAC 3D calculation to address, for example, the boron mixing in the reactor coolant in emergency situations.

Another reactor design, named JPSR, is currently under development. This design again does not require control rods for short-term reactivity control. The core is characterized by a high density reactivity coefficient which is achieved by using boron-free reactor coolant. This design has been assessed against DBE scenarios using the REFLA/TRAC code^[15].

III.1.3 Plutonium Annihilation in LWRs

The feasibility of ²³⁸U-free rock-like oxide fuel, for annihilation of plutonium in LWRs, has been studied. The EUREKA-2 code has been used for reactivity-initiated accident (RIA) analyses, and the RETRAN/Mod3 code for the LOCA analyses for a PWR core design^[16]. Realistic analysis of RIA is crucial for the feasibility of such core design.

III.2 Code Assessment and Development

The major codes assessed and developed for the design studies at JAERI are as follows.

- (a) 3D System analysis code for accidents and transients
 - i) REFLA/TRAC code for PWR

- ii) TRAC-BF1 code for BWR
- (b) Subchannel code for core design
 - i) COBRA-TF code for PWR and BWR
- (c) Couple 3D neutronics/thermal-hydraulics code
 - i) 3D neutronics code using node method coupled with REFLA/TRAC code and TRAC-BF1 code
- (d) two-phase flow code with a $k-\epsilon$ turbulent model for continuous medium

The assessment and improvement on these codes are summarized in the following paragraphs.

III.2.1 REFLA/TRAC Code

The REFLA/TRAC code was constructed on the framework of the TRAC-PF1/MOD1 code by installing physical models developed at JAERI^[17-24]. The code has been verified for various transients and accidents in PWRs, especially for LB and SB LOCAs.

The assessment calculation was performed for the tests shown in Table 1. The assessment results show that the REFLA/TRAC code can predict major phenomena during SBLOCA and LBLOCA in PWRs^[25-33]. Figure 1 shows an example of assessment results for heat transfer enhancement phenomena during the reflood phase in a PWR LBLOCA using SCTF test data^[28, 29]. The REFLA/TRAC code predicts a higher liquid velocity in higher-power bundles and thus predicts a recirculating flow in the core (see Fig. 1(a)). The magnitude of the heat transfer enhancement is well predicted by the 3D model of the REFLA/TRAC code as shown in Fig. 1(b).

The assessment calculation also made clear the limitations and problem areas of the code listed below.

1) CHF prediction during transients

The DNBR in the rod bundle is overestimated by the REFLA/TRAC code. In the REFLA/TRAC code, the DNBR is predicted assuming uniform distributions of void fraction and fluid temperature over the horizontal cross-section of a rod bundle. Subchannel analysis is required for more accurate prediction of DNBR in the rod bundle with local power peaking.

2) Post CHF core heat transfer at high pressure

The models, listed below, were developed based on data at low pressure.

- i) Film boiling HTC
- ii) Minimum film boiling temperature

iii) Quench front propagation model

More assessment of these models is required using data at high pressure.

3) Multi-dimensional flow in a large open volume

Diffusion of momentum and energy is not modeled in the REFLA/TRAC code. Thus, phenomena affected by 3D effect should be modeled using empirical correlation.

i) Downcomer CCF,

ii) Tie plate CCF,

iii) Direct contact condensation, etc.

To perform safety analyses of advanced PWRs such as the high conversion PWR and the JAERI Passive Safety Reactor, the REFLA/TRAC code was used for the analysis of LBLOCA, SBLOCA, pump seizure accident, control rod ejection accident, steam generator tube rupture accident, and ATWS induced by station blackout³³⁻³⁵. The application results demonstrate that the REFLA/TRAC code can be used for the analyses of various transients in PWRs. This code is used for the design work of the passive safety reactor at present.

III.2.2 TRAC-BF1 Code

The TRAC-BF1 code is used for the analyses of transients and accidents in BWRs. The assessment calculations were performed for SBLOCA and LBLOCA simulation tests with ROSA-III test facility and Two Bundle Loop test facility. The results confirmed that the TRAC-BF1 code can predict the peak clad temperature and major phenomena during LOCAs. The BWR plant analysis was performed for the recirculation pump seizure accident, the recirculation pump trip accident, and the load rejection without turbine bypass valve. The code worked well for these analyses. The assessment results showed that some modifications were required for separator and jet pump component models, and the level tracking model.

It was tried to unify the system analysis code for BWR and PWR by the installation of the BWR component models into the REFLA/TRAC code in early of 1990s. Although the component models such as JETP, CHAN, SEPD, were successfully installed into the REFLA/TRAC code, the predictive capability of the code was poor for BWR analyses because of the poor predictive capability of the PWR constitutive package against BWR transients. It was given up to unify the BWR and PWR system analysis codes because huge assessment work was required for the verification of the unified code.

III.2.3 COBRA-TF Code

For the core design of LWRs, it is important to analyze the cooling limit during abnormal transients. Although TRAC codes have 3D option for core

thermal hydraulic analysis, it is difficult to model the core channel by channel because of the limitation of the computational cost. It is also difficult to model the annular dispersed flow because the liquid phase is represented by one-velocity and one-temperature in TRAC codes. To analyze the core thermal hydraulics in detail, especially for DNB and dry-out phenomena, the COBRA-TF code is being assessed^{137, 381}. The code uses the subchannel formulation based on three-field model of the two-phase flow. This code is expected to be used not only for BWRs but also for PWRs. Assessment work for DNB prediction in PWRs is under way through comparison with test data and COBRA-IV results. Preliminary results show that the DNB in a PWR bundle can be predicted within an error of 10 % by the COBRA-TF code. Assessment work for dry-out phenomena in BWRs is also under way through comparison with test data. The development of grid spacer model is also under way.

III.2.4 3D Neutronics Code Coupled with System Analysis Code

The coupling of the CITATION code with the REFLA/TRAC code was performed in 1992. However, the code was not practical because huge computational cost was required. Now, a 3D neutronics code is being developed using the node method to reduce the computational cost. The code is expected to be coupled with the REFLA/TRAC and TRAC-BF1 code on a super computer with parallel processing. The 3D neutronics code is expected to be completed in 1997 and be coupled with TRAC codes in 1998. The code is expected to be used for the design of the advanced LWRs to make clear the two-phase flow stability limit under natural circulation and the quantitative evaluation of the safety margin of core cooling limit with a high local power peaking.

III.2.5 3D Two-Phase Flow Code with a $k-\epsilon$ Turbulence Model

A 3D thermal hydraulic code with a $k-\epsilon$ turbulence model is developed to analyze the natural circulation behavior in a large volume of the passive safety reactors¹³⁹¹. This code is expected to be used for the analysis of the thermal stratification phenomena and natural circulation phenomena in a water pool of a passive water reactor system. This code is also expected to be used for the calibration of constitutive equations in the system codes such as the REFLA/TRAC code.

IV. ANTICIPATED USES OF CODES IN FUTURE PROGRAMS

In future, the LWR thermal-hydraulic research programs at JAERI will focus more on advanced reactor and core designs, on aging-related phenomena, and on operational safety. For thermal-hydraulic systems codes, demands will increase for better coupling with or inclusion of 3D neutronic code, better coupling with structural and fuel, more flexible coupling with 3D thermal-hydraulic modules, and better modeling capability for BOP and plant control systems.

There will be increasing interest in replacing the current constitutive relation models with more mechanistically or micromechanistically-based models. The inclusion of these models into system codes would not be straightforward. The outputs from system codes include combined effects of various models and numerics; improvement of a single model often results in worse results. So, there have been lots of iterations between physical and practical models. JAERI has developed a code named MINCS⁽⁴⁰⁾ dedicated to benchmarking of physical models in combination with various numerical schemes. Such a code may provide a useful bridge between model development and application to system codes.

The code applications to non-reactor systems will increase in future. Past applications at JAERI include a RELAP5/Mod2 analysis of a LOCA in the divertor cooling system of the experimental fusion reactor ITER⁽⁴¹⁾. For this analysis, the code was coupled with a 2D (radial + azimuthal) conduction model. The heat transfer package was replaced. Greater flexibility in physical properties, geometries, environmental conditions (gravity, centrifugal force, etc.) would be required for future code to facilitate such applications.

REFERENCES

- (1) Yoshida, K. et al., "Development of AI-Based Simulation System for Man-Machine System Behavior in Accidental Situations of Nuclear Power Plant," J. Nucl. Sci. Technol., 33-2, 110-118 (1996).
- (2) Hirano, M. and Watanabe, T., "Analyses of the Mihama-2 SGTR Event and ROSA-IV Experiment SB-SG-06 to Simulate the Event," Proc. 5th Int. Topical Mtg. on Nuclear Reactor Thermal Hydraulics, Salt Lake City, U.S.A., Vol.1 (1991) 165-173.
- (3) Araya, F., et al., "Analysis of a Neutron Flux Oscillation Event at LaSalle-2," Nucl. Technol. Vol.93, No.1 (1991).
- (4) Kukita, Y., Anoda, Y. and Tasaka, K., "Summary of ROSA-IV LSTF First-Phase Program: Integral Simulation of PWR Small-Break LOCAs and Transients," Nucl. Engrg. Des., 131-1 (1991) 101-111.
- (5) Chataing, T., Nakamura, H. and Kukita, Y., "Code Analyses of Multi-Dimensional Phenomena in a ROSA-IV/LSTF Experiment Simulating a Loss of Residual Heat Removal Event during PWR Mid-Loop Operation," Proc. 2nd JSME-ASME Joint Intl. Conf. on Nucl. Engrg. (1993).
- (6) Kukita, Y. et al., "OECD/NEA/CSNI International Standard Problem No. 26 Comparison Report," NEA/CSNI R(91)13 (1992).
- (7) Asaka, H. et al., "Computer Code Simulation of Large-Scale Integral Experiments on PWR Thermal-Hydraulic Responses during Accidental Conditions," Proc. 1st Int. Conf. on Supercomputing in Nuclear Applications

- (SNA '90), Mito, Mar. 12-16, 1990.
- (8) Watanabe, T. and Kukita, Y., "Experimental Simulation of PWR Station Blackout Transient Involving Pump Seal Leak," Proc. 6th Intl. Topical Mtg. on Nuclear Reactor Thermal Hydraulics, Oct. 5-9, 1993, Grenoble.
 - (9) Nakamura, H., Anoda, Y. and Kukita, Y., "Steam Generator Multitube Rupture Experiments at ROSA-IV/LSTF," Proc. 6th Intl. Topical Mtg. on Nuclear Reactor Thermal Hydraulics, Oct. 5-9, 1993, Grenoble, pp. 993-1001.
 - (10) Kukita, Y. et al., "ROSA-AP600 Testing: Facility Modifications and Initial Test Results," J. Nucl. Sci. Technol., 33-3 (1996) 259-265.
 - (11) Rhee, G.S., Kukita, Y., and Schultz, R.R., "NRC Confirmatory AP600 Safety System Phase I Testing in the ROSA/AP600 Test Facility," Proc. U.S. Nuclear Regulatory Commission 23rd Water Reactor Safety Information Mtg., Bethesda, MD, Oct. 23-25, 1995.
 - (12) Hirano, M. and Tamakoshi, T., "An analytical study of excitation of nuclear-coupled thermal hydraulic instability due to seismically induced resonance in BWR," Nucl. Eng. Des. 162 (1996) 307-315.
 - (13) Suemura, T. et al., "Safety analysis of double-flat-core high conversion light water reactor. :Large break LOCA and station blackout ATWS," JAERI-M 90-047 (1990).
 - (14) Sako, K. et al., "Passive Safety Reactor SPWR," Proc. Int. Conf. on Design and Safety of Advanced Nuclear Power Plants, Tokyo (1992).
 - (15) Murao, Y. et al., "A concept of JAERI passive safety light water reactor system (JPSR)," Proc. 7th Int. Mtg. on Nuclear Reactor Thermal-Hydraulics (1995).
 - (16) Akie, H., et al., "Pluronium Annihilation in Rock-Like Fuel LWR," to be presented at the 10th Pacific Basin Nuclear Conf. (10-PBNC), Kobe, Oct. 20-25, 1996.
 - (17) Akimoto, H. and Murao, Y., J. Nucl. Sci. Technol., 29(4), 642 (1992)
 - (18) Akimoto, H. et al., JAERI-Data/ Code 94-006, (1994), (in Japanese).
 - (19) Akimoto, H., Ohnuki, A. and Murao, Y., J. Nucl. Sci. Technol., 33(4), 290 (1996).
 - (20) Abe, Y., Akimoto, H. and Murao, Y., J. Nucl. Sci. Technol., 28(3), 208 (1991).
 - (21) Ohnuki, A., Akimoto, H. and Murao, Y., J. Nucl. Sci. Technol., 29(3), 223 (1992).
 - (22) Abe, Y. et al., J. Nucl. Sci. Technol., 30(12), 1214 (1993).
 - (23) Abe, Y. et al., "Proc. of The International Conference on Multiphase Flows '91-Tsukuba", 373 (1991).
 - (24) Akimoto, H. et al., JAERI-M 90-122, "Implementation of an Implicit Method into Heat Conduction Calculation of TRAC-PF1/MOD2 Code" (1990).
 - (25) Akimoto, H., Ohnuki, A. and Murao, Y., JAERI-M 93-240, (1993) (in

Japanese).

- (26) Ohnuki,A., Akimoto,H. and Murao,Y. , J. Nucl. Sci. Technol., 30(3), 187 (1993).
- (27) Akimoto,H., Ohnuki,A. and Murao,Y. , Proc. 2nd Int. Conf. on Multiphase Flow '95, Vol.2 p2-37~p2-44, April (1995).
- (28) Ohnuki, A. , Akimoto, H. and Murao, Y. , "Proc. Int. Conf. On New Trends in Nuclear System Thermohydraulics," Vol.1 231 (1994).
- (29) Ohnuki, A. and Akimoto, H. , "Assessment of REFLA/TRAC Code for Heat Transfer Enhancement Phenomena during Reflood Phase of PWR-LOCA," to be presented at NUTHOS-5 , (1997).
- (30) Akimoto,H., Ohnuki,A. and Murao,Y., ASME FED-Vol. 223, Validation of Systems Transients Analysis Codes, Book No. G00973, pp.1-8, (1995).
- (31) Akimoto, H., Ohnuki, A. and Murao, Y. , JAERI-M 94-037, (1994), (in Japanese).
- (32) Akimoto,H. et al., , Proc. of the Fifth International Topical Meeting on Reactor Thermal Hydraulics, Vol. VI pp.1797-1803, (1992).
- (33) Ohnuki,A., Akimoto,H. and Murao,Y. , J. Nucl. Sci. Technol., 32(3), 245 (1995).
- (34) Heat Transfer and Fluid Flow Laboratory , JAERI-M 91-055, (1991), (in Japanese).
- (35) Okubo, T. et al. , ANS Sixth Proceedings of Nuclear Thermal Hydraulics, pp. 79-86, (1990).
- (36) Iwamura, T., et al. , ASME HTD-Vol. 150, 31 (1990).
- (37) Okubo, T. , Ezzidi, A. and Murao, Y. , JAERI-M 93-069, (1993).
- (38) Ezzidi, A. , Okubo, T. and Murao, Y. , JAERI-M 93-133, (1993).
- (39) Ohnuki, A., Kamo, H. and Akimoto, H. , " Development of Multidimensional Two-Fluid Model Code ACE-3D for evaluation of Constitutive Equations," to be published as JAERI-Data/Code report, (1996)
- (40) Watanabe, T. et al., "Two-Phase Characteristics Analysis Code, MINCS," JAERI 1326 (1992).
- (41) Yonomoto, T. et al., "Loss-of-Coolant Accident Analysis for ITER Divertor System," Proc. 6th Intl. Topical Mtg. on Nucl. Reactor Thermal Hydraulics, Oct. 5-9, 1993, Grenoble, pp. 807-814.

Table 1 Assessment matrix for REFLA/TRAC code

(a) Basic test

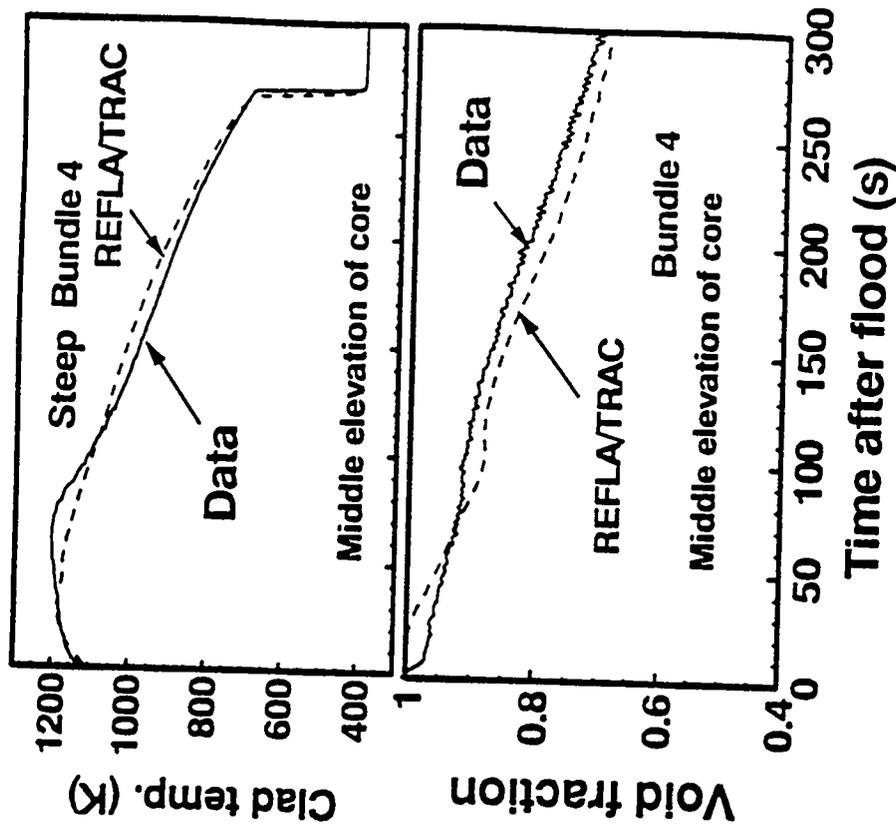
Item	Test name
Wall friction	Isbin, Inoue-Aoki, Janssen
Void fraction	Sudo, Currier, Smissaert, Hughes, Petrick, CISE

(b) Large Break LOCA simulation tests

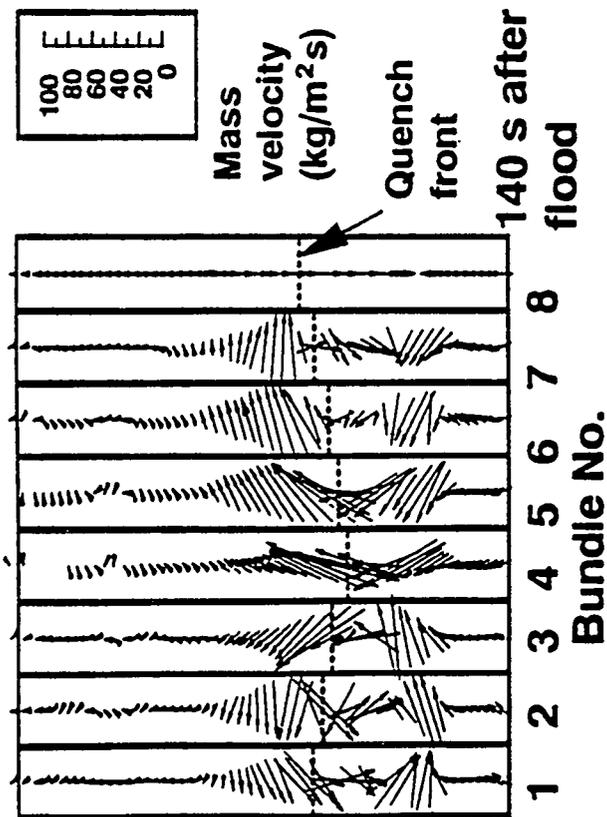
Item	Test name
Critical flow test	Marviken, Super MOBY DICK, MOBY DICK, BNL nozzle test, Super CANNON
Counter current flow test	CREARE 1/15-scale downcomer test, Single pipe tests at Dartmouth courage
Condensation test	ECC mixing test at Tokyo Institute of Technology, Cold leg flow test with Cylindrical Core Test Facility, Cold leg flow pattern test with Upper Plenum Test Facility
Reflood test	Cylindrical Core Test Facility, Slab Core Test Facility, JAERI's small scale reflood test, FLECHT SET, FLECHT SEASET
Integral test	LOFT L2-3, LOFT L2-5, LOFT LP2-6, Semiscale S-06-3

(c) Small Break LOCA simulation tests

Item	Test name
Core boil-off test	NEPTUN test
Counter current flow at hot leg	CCF test by Ohnuki, et al. CCF test by Richter, et al. CCF test with Upper Plenum Test Facility
Integral test	ROSA-IV LSTF 5% cold leg break test



(b) Clad temperature and sectional void fraction



(a) Liquid mass velocity

Fig.1 Assessment results of 3D model of REFLA/TRAC code with SCTF test data

Current and Anticipated Uses of Thermal-Hydraulic Codes in NFI

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Abstract

This paper presents the thermal-hydraulic codes currently used in NFI for the LWR fuel development and licensing application including transient and design basis accident analyses of LWR plants. The current status of the codes are described in the context of code capability, modeling feature, and experience of code application related to the fuel development and licensing. Finally, the anticipated use of the future thermal-hydraulic code in NFI is briefly given.

1. Introduction

The current trend of the LWR fuel design is to increase the fuel burn-up in order to reduce the volume of spent fuels and the fuel cycle costs [1]. Development of such fuel designs requires reliable computer codes which accurately predict the thermal-hydraulic performance of the reactor core. The pressure drop and thermal margin are the most important parameters for fuel thermal-hydraulic design and analysis. The primary objective of the thermal-hydraulic design of the LWR fuel is to predict these parameters as accurately as possible. The NFI computer codes for the fuel thermal-hydraulic design have been qualified against the results of experiments conducted using large scale test loops and applied to the actual fuel and core design [2], [3]. In order to use the thermal-hydraulic computer codes for the reactor safety analysis with the new fuel design, they must cover a wide variety of phenomena such as transient critical power or DNB (Departure from Nucleate Boiling), CCFL (Counter Current Flow Limiting) during LOCA, density wave oscillations in the BWR core stability, film boiling in RIA (Reactivity Initiated Accident), etc. Thermal-hydraulic codes applied to the design and analysis of the LWR fuel are more or less based on the one dimensional two-phase flow model which are supplemented by empirical parameters such as the drift flux parameter and the critical power or DNB correlation which have been obtained experimentally. This has led to the development of several individual codes to cover the wide range of applications. The following description gives an overview of the NFI computer codes with regard to each thermal-hydraulic topic related to the LWR core and plant dynamics. In the last section of this paper, the anticipated use of the future computer codes in NFI is briefly described.

2. Description of NFI Computer Codes

Summary of the NFI main computer codes is shown in **Table 1** and **Table 2** in which each computer code is described with regard to its capability, modeling features, application and qualification levels, and the interrelation between the events to be simulated.

2.1 DNB Correlation and Critical Power Correlation

The DNB correlation for PWR fuel and the critical power correlation for BWR fuel are the common bases of all thermal-hydraulic analyses to be described in the following Sections. The NFI-1 correlation (DNB correlation) and the COBRA-IIIIC code [4] are used for the evaluations of the NFI PWR fuel design (14×14 , 15×15 and 17×17 type). The NFI-1 correlation has been developed using the test results obtained at Columbia University. This correlation was recently verified against the test data obtained at the NUPEC facility [5]. The result of statistical evaluation from 362 points of DNB data shows a standard deviation of 0.088.

For the NFI 9×9 BWR fuel, a critical power correlation (boiling length vs. critical quality) has been developed based on the test data taken at the Siemens 15 MW test loop [3]. The statistical evaluation of this correlation from 371 data points shows a standard deviation of 0.022. The FRANCESCA code [6] is used by NFI for the prediction of the boiling transition. This code has been originally developed by EURATOM.

2.2 PWR Systems Transient Analysis Code

The RELAP-3B code has been originally developed by USNRC [7]. The NFI improved version of this code includes the PWR systems model (i.e. system component model, control and safety protection systems models), and some improved features (e.g., the pressurizer thermal-hydraulic model). The use of this code for the licensing analysis has been authorized by the Japanese regulatory body (MITI) for all non-LOCA transient analyses of the PWR systems. The hydraulic model employs a one dimensional homogeneous equilibrium model (3 equations), a bubble rise model for the steam separator, and a special model for the pressurizer. The DNB prediction is performed for given core parameters using the NFI-1 DNB correlation and the COBRA-IIIIC code.

2.3 BWR Systems Transient Analysis Code

The precursor of the NFI BANDIX code for the BWR systems transient analysis has been originally developed by Siemens for the Siemens plant. This code has been verified against the BWR transient test data such as the Peach-Bottom-2 turbine trip test [8]. The use of this code for the licensing analysis has been authorized by MITI for most of the system transient analyses of the

BWR systems excluding LOCA and RIA [9].

2.4 BWR Core Stability Analysis Code

The STAIK-PK code is the NFI frequency-domain stability analysis code. The DYNAS-2 code is the time-domain version of the STAIK-PK code and it employs a three dimensional neutron kinetics model instead of the point kinetics model of the STAIK-PK code. The base of these two codes has been developed by Siemens. Both codes have been extensively verified by NFI against reactor stability test data including regional stability [10]. The STAIK-PK code has been authorized by MITI to use for the reactor licensing analysis.

2.5 RIA Analysis Code

The EUREKA-N code is the NFI RIA analysis code which has been improved from the original EUREKA code developed by JAERI [11]. The thermal-hydraulic conditions are calculated with a one-dimensional homogeneous model. For the neutron kinetics, a point kinetics model with the adiabatic approximation is used. The shape function is updated at several time steps by the 3-dimensional coarse-mesh diffusion calculation. Usually for the licensing application, credit is taken for the Doppler reactivity feedback only, and the void reactivity feedback is neglected. With this conservative assumption, the predicted maximum enthalpy becomes significantly higher than would be predicted by taking void reactivity into account.

2.6 BWR LOCA Analysis Code

The SALUTE and LABEL codes are used for the BWR LOCA analysis [12]. The original base codes have been developed by Siemens. The main code, SALUTE, calculates the long term system responses during LOCA including system pressure, flow rate, water level, CCFL at the core top and bottom or bypass, and peak cladding temperature. The LABEL code predicts the short term system response during the blowdown phase of the large break LOCA. These codes have been approved by MITI and are used for the reactor licensing.

3. Anticipated Use of Thermal-Hydraulic Codes in NFI

The current reactor safety analysis methodology is the result of a long history of development in the past several years. As a result of this historical development, combinations of relatively simple thermal-hydraulic models for individual events have been established individually for each computer code. This situation may continue for the next several years. On the other hand, rapid advance of the computer technology allows highly sophisticated methods in the thermal-hydraulics analysis of the two-phase flow. For example, a three field model has been already in use in the advanced code. Vapor, water film, and water droplet are modeled explicitly by first principle conservation equations

[13]. Our development goal is a single general-purpose code, based on the first principles, that allows for a unified approach to perform the wide range of safety analyses. Another goal for computer thermal-hydraulics is to reduce the cost of testing. The high cost of large scale experiments, such as CHF testing, may be replaced by the accurate computer simulations using an advanced code.

References

- [1] K. Sato et al., High Burnup Step III Fuel Development for Japanese BWRs (Design and Development of the NFI Type 9×9 Fuel), *Proc. ANP' 92 Conf.*, Tokyo, (1992).
- [2] Nuclear Fuel Industries, Ltd., : Thermal-Hydraulic Test of NFI Design PWR Fuel, *NFI Topical Report NFK-8027 Rev. 5* (in Japanese), (1985).
- [3] Nuclear Fuel Industries, Ltd., : Thermal-Hydraulic Design Method of NFI Design BWR Fuel, *NFI Topical Report NLR-04* (in Japanese), (1994).
- [4] D.S.Rowe, COBRA IIC : A Digital Computer Program for Steady-State and Transient Thermal-Hydraulic Analysis of Rod Bundle Nuclear Fuel Elements, *BNWL-1695*, (1973).
- [5] M. Akiyama et al., Reliability Proving Test on Maximum Thermal Loading of PWR Fuel Assembly, *J. At. Ener. Soc. Japan*, Vol. 36, No.1, pp. 47-59 (1994).
- [6] G. Forti, A Dynamic Model for the Cooling Channels of a Boiling Nuclear Reactor with Forced Circulation and High Pressure Level, *EUR-4052e*, (1968).
- [7] User's Manual for RELAP-3B-MOD101, A Reactor System Transient Code, *NUREG-0004*, (1976).
- [8] L.A. Carmichael et al., Transient and Stability Tests at Peach Bottom atomic power Station Unit 2 at End of Cycle 2, *EPRINP-564*, (1978).
- [9] Nuclear Fuel Industries, Ltd., : BWR Plant Transient Analysis Method, *NFI Topical Report NLR-07* (in Japanese), (1990).
- [10] Nuclear Fuel Industries, Ltd., : BWR Stability Analysis Method, *NFI Topical Report NLR-06* (in Japanese), (1994).
- [11] M. Ishikawa, et al., EUREKA : A Computer Code for Uranium-Oxide Fueled, Water Cooled Reactor Kinetics Analysis, *JAERI 1235*, (1974).
- [12] Nuclear Fuel Industries, Ltd., : BWR ECCS Performance Analysis Method, *NFI Topical Report NLR-10* (in Japanese), (1994).
- [13] M.J. Thurgood, et al., COBRA/TRAC - A thermal Hydraulic Code for Transient Analysis of Nuclear Vessels and Primary Coolant Systems, *NUREG/CR-3046*, (1983).

Table 1 Summary of NFI Thermal-Hydraulic Code (Transient and Stability)

Code Name	Licensing Applications	Thermal-Hydraulics & Neutronics	Qualification
RELAP-3B	PWR Systems Transient Analysis (non-LOCA)	<ul style="list-style-type: none"> • One dimensional homogeneous flow model • Non-equilibrium two-phase model for pressurizer • Bubble rise model for steam separator • Point kinetics • Special models for reactor vessel components, control systems, and reactor protection systems 	<ul style="list-style-type: none"> • Qualified against reactor startup tests
BANDIX	BWR Systems Transient Analysis (non-LOCA)	<ul style="list-style-type: none"> • One dimensional homogeneous flow model • 4 system pressure nodes (core, vessel dome and 2 steam lines) • Void sweep model in the core node • Point kinetics • Special models for reactor vessel components, control systems, and reactor protection systems 	<ul style="list-style-type: none"> • Qualified against reactor startup tests, plant stability and transient tests of typical BWR/4 and BWR/5
STAIIF-PK	BWR Core Stability	<ul style="list-style-type: none"> • One dimensional two-phase drift flux model • 5 equations (2 mass and 2 energy and 1 momentum) • Subcooled boiling model • Multiple channel types with distinct geometry and power distributions • Point kinetics for critical (core stability) mode or subcritical mode (regional stability mode) • Recirculation system model (from upper plenum to lower plenum / pump models for external recirculation, jet pump and internal pump) • Frequency-domain analysis 	<ul style="list-style-type: none"> • Qualified against thermal-hydraulic stability test data for parallel channel stability simulation • Qualified against reactor core stability data including regional stability data: <ul style="list-style-type: none"> - Core stability data: jet pump plant, internal pump plant, external pump plant
DYNAS-2	BWR Core Stability	<ul style="list-style-type: none"> • One dimensional two-phase drift flux model • 5 equations (2 mass and 2 energy and 1 momentum) • Subcooled boiling model • 3 dimensional kinetics (one group coarse mesh diffusion equation) • Recirculation system model • Time-domain analysis 	

Table 2 Summary of NFI Thermal-Hydraulic Code (RIA and LOCA)

Code Name	Licensing Applications	Thermal-Hydraulics & Neutronics	Qualification
EUREKA-N	Design Basis RIA Analysis	<ul style="list-style-type: none"> • One dimensional homogeneous flow model • Film boiling heat transfer coefficient <ul style="list-style-type: none"> - Dougall-Rohsenow correlation (hot standby) - NSRR experimental correlation (cold startup) • Point kinetics with adiabatic approximation • 3 dimensional coarse-mesh diffusion equation for the recalculation of the shape function • Doppler feedback and with /without moderator feedback 	<ul style="list-style-type: none"> • Qualified against SPERT III reactivity accident test results
SALUTE	Design Basis LOCA Analysis (Long Term System Response)	<ul style="list-style-type: none"> • One pressure node in reactor vessel • 9 nodes for mass and energy equations in the reactor vessel • Core model with one hot channel and average channel • Multi-dimensional flow model based on separate effect experiment (SSTF) • Heat transfer coefficients based on multi-region flow regime • Core spray-heat transfer model based on experiment (BWR FLECHT) • CCFL at the top and bottom of core and bypass region • Lumped heat slab model for the vessel and internals • Metal-water reaction model (Baker-Just model) 	<ul style="list-style-type: none"> • Qualified against ROSA III integral experiment data
LABEL	Design Basis LOCA Analysis (Short Term System Response)	<ul style="list-style-type: none"> • 9 pressure nodes in reactor vessel • 3 equations homogeneous flow model • Recirculation pump model: external recirculation pump, jet pump or internal pump • Critical flow model (Moody or Homogeneous Equilibrium Model) 	<ul style="list-style-type: none"> • Qualified against ROSA III integral experiment data

Current and Anticipated Use of Thermal-Hydraulic Codes for BWR Transient and Accident Analyses in Japan

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1. Introduction

This paper summarizes the current and anticipated use of the thermal-hydraulic and neutronic codes for the BWR transient and accident analyses in Japan. The codes may be categorized into the licensing codes and the best estimate codes for the BWR transient and accident analyses.

Most of the licensing codes have been originally developed by General Electric. Some codes have been updated based on the technical knowledge obtained in the thermal hydraulic study in Japan, and according to the BWR design changes.

The best estimate codes have been used to support the licensing calculations and to obtain the phenomenological understanding of the thermal hydraulic phenomena during a BWR transient or accident. The best estimate codes can be also applied to a design study for a next generation BWR to which the current licensing model may not be directly applied.

In order to rationalize the margin included in the current BWR design and develop a next generation reactor with appropriate design margin, it will be required to improve the accuracy of the thermal-hydraulic and neutronic model. In addition, regarding the current best estimate codes, the improvement in the user interface and the numerics will be needed.

2. Transient and Stability Analysis Model

BWR transient and stability analysis codes are shown in Table 1.

2.1 Licensing Analysis Model

(a) Transient Analysis Model

From the safety analysis viewpoints, major evaluation item of the BWR transient analysis is the MCPR (Minimum Critical Power Ratio) decrease (Δ MCPR) and reactor peak pressure during the operational transients such as turbine trip with bypass failure. In Japan, REDY code(2-1), which was originally developed by General Electric, has been used for such transient analysis. REDY code simulates reactor core, recirculation system, vessel dome, steamline, safety/relief valves and the major control systems. The latest REDY version can simulate the reactor internal pump system for ABWR plant as well as the jet pump system. Reactor core model is based on neutron point kinetics with six delayed neutron groups. This model is rather simple compared with the three-dimensional code described in the following section. However, analysis conservatism is applied in the parameters such as void coefficient for the licensing evaluation.

Besides the licensing analysis, REDY code also applied to the control system design such as the feedwater control, recirculation control and pressure control system. For this purpose, REDY code is tuned to the plenty of the actual plant data obtained in the plant start-up tests.

In the calculation of the Δ MCPR, SCAT code has been used in the licensing analyses. SCAT code calculate transient MCPR using the REDY results as the boundary condition to simulate the hottest bundle in the core. SCAT code employs the single channel thermal hydraulics node model in the axial direction, solving the mass, momentum and energy conservation equations and fuel rods heat conduction equations in the radial direction. MCPR is calculated based on the GEXL correlation.

(b) Stability Analysis Model

K2 code(2-2), developed by Toshiba, has been used in the licensing analysis in Japan. This code is based on the frequency domain analysis with the

Laplace transformed functions of linearized equations, employing one-point reactor neutronics model and axially one-dimensional and multi-parallel channel model. The fuel heat conduction model is based on a radially one dimensional equation.

K2 code has a capability of regional stability (out-of-phase core oscillation mode) analysis which is based on the neutron higher mode transfer function using subcriticality and the higher mode flux shape (normally first azimuthal mode) calculated by the other 3-D harmonics analysis code.

K2 code calculates the decay ratio, which is used in index to show the stability margin, for core (global core oscillation), channel and regional stability.

The qualifications of channel stability model were performed with the thermal-hydraulic test data of the BWR channel mock-up test loop. The core and regional stability qualifications were also performed with the actual plant stability test data, such as Vermont Yankee and Caorso test data.

2.2 Best Estimate and Detailed Analysis Model

The three-dimensional core transient codes, TOSDYN and TRACG, have been used for the detailed analysis of the BWR transient and stability performance.

(i) TOSDYN code(2-3) is developed by Toshiba, mainly for the use of analyzing the spatial effect on BWR transient and stability. To treat the spatial change of reactor power and coolant flow redistribution, three-dimensional neutronics model and a parallel channel thermal hydraulic model are incorporated. The time domain model of the overall BWR system, including the model of ex-core components and recirculation system and major control system, is the same as that used in REDY code. TOSDYN code consists of four component model. They are the neutronics model of one bundle mesh size, the channel thermal-hydraulics model for maximum twenty parallel channel groups, the heat transfer model and ex-core model. Major application of this code is the evaluation of the thermal-hydraulic behavior in the core during the regional instability which cannot be evaluated by the frequency domain stability analysis code.

(ii) TRACG code(2-4) is based on the BWR version of TRACG(Transient Reactor Analysis Code) code which had been originally developed by INEL(Idaho National Engineering Laboratory) and modified as the best-estimate

model of thermal-hydraulic condition in a BWR system by General Electric. The three-dimensional neutron kinetics model developed by Toshiba has been implemented into TRACG code as the collaborative work between GE and Toshiba. The extensive work of the qualification analyses were jointly performed by GE, Toshiba and Hitachi to complete the TRACG code.

TRACG has the three-dimensional neutron kinetic model solving the modified one-group, time dependent diffusion equations, which is consistent with the 3-D BWR core simulator. The thermal-hydraulic model is two fluid model solving the conservation equations for mass, momentum and energy for gas and the liquid phases. TRACG employs a flexible system component building model with a node-junction method to simulate the BWR systems.

Major application of this code is the detailed analysis of the thermal-hydraulics coupled with neutronics such as regional stability, long-term transient of reactor depressurization due to steam condensation, and other complicated thermal-hydraulic phenomena which other code cannot simulate.

Qualification analysis is also performed for the thermal-hydraulics tests and actual plant data.

3. Design Basis Accident Analysis Model

3.1. Licensing Analysis Model

In the BWR licensing analysis for an accident, several analysis codes have been utilized in Japan, as shown in Table 2, according to the accident type of interest.

(a) LOCA Analysis Model

The SAFER code (3-1) is a licensing code to calculate long term reactor vessel inventory and peak cladding temperature following a BWR LOCA. SAFER has been jointly developed by General Electric, Hitachi and Toshiba.

SAFER employs the homogeneous equilibrium two-phase model as the basic thermal hydraulic model. The basic equations in SAFER are the conservations equations of mass and energy for the two-phase mixture. It also includes the drift flux model and the bubble rise model to calculate the relative velocity of the vapor leaving from a water level surface. In the SAFER model, the reactor pressure vessel is divided into eight nodes, which represents the major regions of the pressure vessel.

The SAFER model has several specific models to simulate the physical phenomena which occur in the course of a LOCA transient and have the impact on the core cooling characteristics and the inventory transient. Those are for instance the CCFL and CCFL breakdown models, multi-channel effect model and heat transfer model in the refill-reflood phase. The correlations for these models have been determined based on the separate effect test results conducted in the Japanese utilities and vendors joint study program as well as in Toshiba.(3-2 to 3-5)

The SAFER model has been extensively qualified in both Japan and the United States. In Japan, the TBL (two bundle loop) LOCA simulation tests jointly conducted by the Japanese BWR utilities and vendors, and the ROSA-III LOCA simulation tests conducted by the JAERI have been used for the SAFER qualification.(3-6 & 3-7) Those tests have covered a wide range of break spectra and ECCS combinations. The SAFER simulation results for the system behavior have been generally compared well with those test results and the peak clad temperatures (PCT) have been predicted 20 - 150 K higher than those obtained in the TBL and ROSA test results.

The LAMB code originally developed by GE is used to calculate the thermal-hydraulic transient in reactor pressure vessel during a blowdown phase of a LOCA, mainly for several tens seconds following a LOCA. The basic equations of LAMB are the conservation equations of mass, momentum and energy for the two-phase mixture. The outputs of LAMB are the core flow transient, the pressure transient and the break flow rate. The core flow transient and the pressure transient are used in the SCAT code which models the thermal-hydraulics in a single fuel channel to calculate the timing and location of the boiling transition occurred in a high power fuel channel. The break flow rate calculated using LAMB is used to estimate the release of the radio-activity to the environment following a LOCA.

(b) Reactivity Initiated Accident (RIA) Analysis Model

A reactivity initiated event is a design basis accident for the BWRs. The dynamic nuclear analysis code APEX simulates the reactivity initiated events caused by a postulated drop of the control rod from the reactor core. The core-average power transient is calculated using the point kinetic model and the power distribution in the reactor core is calculated with the R-Z two dimensional diffusion model. APEX employs an conservative assumption in which the moderator feedback effect is neglected.

The SCAT code, which simulates the thermal-hydraulics transient in a single fuel channel, calculates the fuel enthalpy change following a RIA using the power transient from the APEX calculation. APEX/SCAT calculation results are considerably conservative compared with a realistic model like ARIES stated below.

3.2 Best Estimate Model

(a) LOCA Analysis Model

The best estimate models have been used to support licensing calculation model or to obtain a detailed phenomenological interpretation about LOCA related phenomena.(3-7 & 3-8) The best estimate codes are mainly the BWR versions of TRAC, TRAC-BD1 and TRACG (TRAC GE version).

TRAC has been also applied to the development study for a next generation reactor with a passive system. In the passive containment cooling system (PCCS) development study, an integral system test GIRAFFE has been conducted to demonstrate the feasibility of the PCCS. The PCCS performance analysis model has been developed using TRAC with some modification to the heat transfer model in the presence of noncondensable. The TRAC model has been verified by conducting the GIRAFFE test analysis and applied to the PCCS design analysis for a next generation BWR.(3-9 & 3-10)

(b) RIA Analysis Model

The Japanese BWR utilities and vendors have jointly developed a realistic analysis code ARIES for a RIA analysis.(3-11 & 3-12) ARIES has a three dimensional neutronic model coupled with multi-channel thermal hydraulic model and can simulate strong space dependent feedback effect associated with the local power increase due to control rod movement. The basic thermal-hydraulic model is a non-equilibrium separated two-phase flow model which uses the drift flux correlation.

The ARIES model has been verified with the benchmark problem posed by OECD/NEACRP/CSNI and the test data from the SPERT III E-core.

4. Severe Accident Analysis Model

The MAAP code has been extensively used to develop the accident management strategy for a severe accident (SA) in the current BWRs in Japan. In addition, for a next generation nuclear reactor like the ABWR evolutionary plant for which the Japanese BWR utilities and vendors have conducted the development program, the countermeasures for a SA are considered in the design stage.(4-1) The passive containment cooling system has been introduced to the ABWR evolutionary plant for SA countermeasures.(4-2) The PCCS model has been incorporated to the MAAP code, which calculates the PCCS performance in the presence of noncondensable and aerosol and applied to the ABWR evolutionary plant analysis.(4-3)

5. Anticipated Use of Analysis Codes

The current licensing codes have been used to design a BWR with sufficient design margin. From the viewpoint of the rationalization of the design, more sophisticated analysis models may be necessary.

(a) Transient Analysis Model

The current licensing analysis has been based on the conservative methodology with the relatively simplified thermal-hydraulic models. The requirement of much detailed methodology and model is increasing from the viewpoint of more relaxed restriction in design and operation and more accurate simulation of the sophisticated thermal-hydraulic phenomena. The three-dimensional code TRACG has been developed for this purpose and will be one of candidates as a future licensing code for transient evaluation.

(b) Accident Analysis Model

In order to rationalize the margin included in the current BWR design and develop a next generation reactor with appropriate design margin, it will be required to improve the accuracy of the thermal-hydraulic and neutronic model.

In addition, the improvement in the user interface and the numerics will be needed in order to extensively use the current best estimate codes. The parallel processing will be used in the best estimate calculation.

REFERENCES

- (2-1) Linford, R.B., "Analytical Methods of Plant Transient Evaluations for the General Electric Boiling Water Reactor", NEDO-10802, Feb. 1973.
- (2-2) Toshiba Licensing Report, "BWR plant stability analysis method (in Japanese)", TLR-010 Rev.1 (1996).
- (2-3) Y.Takigawa et al., "Caorso Limit Cycle Oscillation Analysis with Three-Dimensional Transient Code TOSDYN-2", Nucl. Technol., 79, 210,(1987).
- (2-4) Y.Takeuchi et al., "TRACG Transient Analysis Code - Three-Dimensional Kinetics Model Implementation and Applicability for Space-Dependent Analysis", Nucl. Technol., 105, 162, (1994).
- (3-1) Chan, K.C., et al., "The GESTR-LOCA and SAFER Models for the Evaluation of the Loss-of-Coolant Accident Volume II SAFER - Long Term Inventory Model for BWR Loss-of-Coolant Analysis", NEDO-23785-1-A, Feb., 1985.
- (3-2) Nagasaka, H., et al., "Qualitative Evaluation of ECCS Capability during Refill-Reflood Phase for BWR LOCA", J. Nucl. Sci. Technol., 28[3], 258-267, 1991.
- (3-3) Nagasaka, H., et al., "18 Degree Sector System Test (ESTA-II)", NUREG/CP-0058, Vol.3, 706-721, 1984.
- (3-4) Nagasaka, H., et al., "BWR Core Cooling in Refill/Reflood Phase", *ibid.*, Vol.3, 706-721, 1984.
- (3-5) Nagasaka, H., "New Japanese Correlation on Core Cooling and CCFL Characteristics during BWR LOCA", NUREG/CP-0072, Vol.5, 55-75, 1985.
- (3-6) Itoya, S., et al., "Assessment of SAFER03 Code using ROSA-III Break Area Spectrum Tests on Boiling Water Reactor Loss of Coolant Accidents", J. Nucl. Sci. Technol., 24[8], 639-652, 1991.
- (3-7) Itoya, S., et al., "SAFER03 and TRAC-BD1 Analysis of TBL Experiments on a BWR LOCA", 2 nd International Topical Meeting on Nuclear Power Plant Thermal Hydraulic and Operations, 1986..
- (3-8) Abe, N., et al., "Analyses of Upper Plenum Level Oscillatory Phenomena by TRAC-BD1", Nucl. Technol., 70, 335-342, 1985.
- (3-9) Yokobori, S., et al., "GIRAFFE Test Results Summary", NUREG/CP-0149, Vol.1, 165-176, 1995.
- (3-10) Arai, K., "TRAC Qualification for Passive Containment Cooling System Performance Prediction against the GIRAFFE Tests", 3rd JSME/ASME Joint Int.

Conference on Nucl. Eng. (ICONE-3), 1041-1047, 1995.

(3-11) Uematsu, H., et al., "Development of a Three-Dimensional Transient Code for Reactivity-Initiated Events in Boiling Water Reactors - Models and Code Verifications", Nucl. Technol., 88, 87-97, 1989.

(3-12) Izutsu, S., et al., "Development of a Three-Dimensional Transient Code for Reactivity-Initiated Events in Boiling Water Reactors - Two Rod Drop Accident Analyses", *ibid.*, 89, 92-102, 1990.

(4-1) Ishikawa, M., et al., "The Japanese Utilities' Requirements for a Next Century BWR", 3-rd JSME/ASME Joint Int. Conference on Nucl. Eng. (ICONE-3), 637-644, 1995.

(4-2) Omoto, A., et al., "Advanced Reactor Containment Design Approach", 4-th JSME/ASME Joint Int. Conference on Nucl. Eng. (ICONE-4), 1996.

(4-3) Kubokoya, T., et al., "Safety System Considerations for ABWR Evolutionary Program", 3-rd JSME/ASME Joint Int. Conference on Nucl. Eng. (ICONE-4), 1995.

Table 1 Computer Code for BWR Transient and Stability Analysis in Japan

Code	Application	Model
REDY	Operational Transient Analysis(Licensing Calculation) - Turbine Trip (Pressurization transient) - Recirculation Pump Trip (Flow transient) Control System Design Analysis ATWS Analysis	Point neutron kinetics Reactor vessel, core, downcomer model Jet-pump/internal pump model Steamline model and safety/relief valve model Major control system (feedwater, pressure, recirculation)
K2	Stability Analysis (Licensing Calculation) - Core, Channel, Regional Stability (Decay Ratio)	1D multi-parallel channel thermal-hydraulics Point neutron kinetics Frequency domain analysis to calculate decay ratio
TOSDYN	Operational Transient Analysis - Spatial effects in core during transient Stability Analysis - Regional instability - MCPR evaluation during instability - Detectability evaluation of instability	3-D neutronics modified one-group diffusion model - four or one bundle/mesh size (option) - axial 24 nodes 1-D parallel channel core thermal-hydraulics - multi-channel with axial 24 nodes Ex-core component modeling
TRACG	Operational Transient Analysis - Long Term Analysis Stability Analysis - MCPR evaluation during instability - Detectability evaluation of instability ATWS Analysis	Modified one-group diffusion in 3D geometry 1D parallel channel thermal-hydraulics simulation of core 3D thermal-hydraulic simulation of the vessel Detailed description of reactor, piping and BOP

Table 2 Computer Code for BWR Accident Analysis in Japan

Code	Application	Model
SAFER	LOCA Analysis (Licensing Calculation) <ul style="list-style-type: none"> • Long-term water level transient & peak cladding temperature calculation 	<ul style="list-style-type: none"> • Homogeneous Equilibrium Two-phase Model • Drift Flux and Bubble Rise Model for Nonhomogeneous Effect • Mass and Energy Conservation Equations for Two-Phase Mixture • Fixed Nodalization (8 Nodes for Reactor Pressure Vessel)
LAMB	LOCA Analysis (Licensing Calculation) <ul style="list-style-type: none"> • Core flow and pressure transient calc. in blowdown phase • Break flow rate calc. in main steam line break accident 	<ul style="list-style-type: none"> • Homogeneous Equilibrium Two-phase Model • Mass, Energy & Momentum Equations for Two-Phase Mixture • Fixed Nodalization (9 Nodes for Reactor Pressure Vessel)
SCAT	Thermal-Hydraulic Transient Analysis for Single Fuel Channel (Licensing Calc.) <ul style="list-style-type: none"> • Boiling transition calculation • Fuel enthalpy calc. in a RIA 	<ul style="list-style-type: none"> • Homogeneous Equilibrium Two-phase Model • Mass and Energy Conservation Equations for Two-Phase Mixture
APEX	Reactivity Initiated Accident Analysis (Licensing Calculation) <ul style="list-style-type: none"> • Power transient calculation 	<ul style="list-style-type: none"> • Point Kinetic Model • R-Z Two Dimensional Diffusion Model • Adiabatic Assumption • No Moderator Feedback

Table 2 Computer Code for BWR Accident Analysis in Japan (Continued)

Code	Application	Model
TRAC-BWR	<p>LOCA Analysis (Best Estimate Calculation)</p> <ul style="list-style-type: none"> • Thermal-hydraulic calculation in reactor pressure vessel and primary containment vessel 	<ul style="list-style-type: none"> • Full Two-Fluid Nonequilibrium, Nonhomogeneous T/H Model • Noncondensable Gas Model • Mass, Energy & Momentum Equations for Two Phase • Mass Conservation Equation for Noncondensable • Constitutive Equations • Three Dimensional Modeling Capability • Flexible Nodalization
ARIES	<p>Reactivity Initiated Accident Analysis (Best Estimate Calculation)</p> <ul style="list-style-type: none"> • Neutronic coupled with thermal-hydraulic calculation for reactor power transient 	<ul style="list-style-type: none"> • Three Dimensional Neutronic Model • One Dimensional Multi-Channel Thermal Hydraulic Model • Non-Equilibrium Separated Flow Model with Drift Flux Model • Mass and Energy Conservation Equations for Two Phase Momentum Conservation Equation for Mixture • Space Dependent Feedback Model

Current and Anticipated Uses of Thermal Hydraulic Codes in Korea

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Abstract

In Korea, the current uses of thermal hydraulic codes are categorized into 3 areas. The first application is in designing both nuclear fuel and NSSS. The codes have usually been introduced based on the technology transfer programs agreed between KAERI and the foreign vendors. Another area is in the supporting of the plant operations and licensing by the utility. The third category is research purposes. In this area assessments and some applications to the safety issue resolutions are major activities using the best estimate thermal hydraulic codes such as RELAP5/MOD3 and CATHARE2.

Recently KEPCO plans to couple thermal hydraulic codes with a neutronics code for the design of the evolutionary type reactor by 2004. KAERI also plans to develop its own best estimate thermal hydraulic code, however, application range is different from KEPCO developing code. Considering these activities, it is anticipated that use of the best estimate hydraulic analysis code developed in Korea may be possible in the area of safety evaluation within 10 years.

I. Introduction

The first Korean nuclear power plant, Kori unit 1, began commercial operation in 1978. It had been built based on a turn-key base. It is 600 MWe, 2-loop, Westinghouse PWR. At that time thermal hydraulics had not matured enough to cover overall reactor analysis. RELAP4 and updated RELAP5 series codes have been introduced since 1980 but general applications like safety issue resolutions, were somewhat limited until 1985. Intensive

thermal hydraulic activity was initiated as KAERI(Korea Atomic Energy Research Institute) developed joint projects on both PWR fuel and NSSS designs with KWU and ABB-CE, respectively, in 1985 for the purpose of localization of nuclear engineering technology. The uses of the thermal hydraulic codes provided by nuclear vendors as KWU and ABB-CE in the design areas, were the major activities in this period. In addition, CATHENA code has been introduced under the technology transfer agreement between KAERI and AECL since 1983 for CANDU analysis.

As USNRC developed ICAP(International Code Assessment & Application Program) for 5 years starting from 1986, Korea participated in ICAP for RELAP5 version assessments. Korea could enhance technical capability in the area of the best estimate thermal hydraulic safety analysis through various types of informations on the code developmental assessment. Korea also has maintained the membership of CAMP (Thermal- hydraulic Code Applications and Maintenance Program) based on the achievements from ICAP. The CAMP members are organized by KINS (Korea Institute of Nuclear Safety) in a way of efficient cooperation. KAERI uses CATHARE2 code for enhancement of analysis reliability in addition to RELAP5/MOD3.

The utility KEPCO(Korea Electric Power Company) holds a membership of RETRAN and it also uses Westinghouse analysis codes concerning plant operation analyses. KNFC(Korea Nuclear Fuel Company) which is a daughter company of KEPCO, has been using the Westinghouse codes for RTSR(Reload Transit Safety Report) on Westinghouse-type PWR since 1993.

Therefore the uses of various thermal-hydraulic codes are applied to three major areas, i.e. design uses, analyses of plant by the utility, and best estimate purposes. Within the next 10 years, it is expected that most of foreign codes will probably be replaced by the Korean developed codes.

II. Current uses of thermal-hydraulic codes in Korea

1. In the design areas

As an effort of nuclear design technology localization in Korea, KAERI implemented two joint design projects on nuclear fuel design and NSSS design

with KWU and ABB-CE, respectively, including the technology transfers from 1986. The purpose was to learn the know-how in the nuclear designs and to develop Korea's own types of both fuel and a nuclear power plant. Foreign vendor codes were first introduced during the technology transfer period. Among these codes, thermal hydraulic codes have usually been used for the description of FSAR as well as RTSR. The first plant constructed under a joint design program is Younggwang unit 3 & 4 (YGN 3/4) which are 1000 MWe, 2-loop, ABB-CE type reactors and began commercial operations in 1995 and 1996, respectively. Those ABB-CE codes applied to YGN 3/4 are still being used in the designs of successive units, Ulchin 3, 4, 5, and 6, and YGN 5&6. In 1994 KEPCO decided to replace the KWU fuel with a Westinghouse designed fuel in all Westinghouse PWR. In result KNFC has carried out analyses for RTSR using Westinghouse codes instead of KWU codes ever since.

2. In utility

The KEPCO joined RETRAN-01 code development program in 1980 and now holds the membership of RETRAN-03 users club. KEPCO has also used Westinghouse codes for Non-LOCA analysis since 1989. The codes are usually used for both plant transient analyses and licensing purposes. It plans to develop a new integrated system code recently by coupling proven individual codes like a 3-D neutronics code, a 3-D core thermal hydraulic code, and a system analysis code as an effort to reduce foreign dependency in plant management. This option seems to be chosen to save costs for validation efforts because the individual code development is unlikely to be economical [1]. KEPCO aims at its application to the design of the evolutionary type reactor in 2004, however, the most probable application will be limited in Non-LOCA analysis. In this manner KEPCO would establish its own technology in thermal hydraulic analysis.

3. The use of best estimate thermal hydraulic

Korea has used the best estimated thermal hydraulic code actively since KINS(Korea Institute of Nuclear Safety) concluded the agreement on participation of the research program, ICAP(International Code Assessment & Application Program) with USNRC in June 1986 for 5 years. Korea should submit a total of 15 assessment reports to USNRC using RELAP5 series code under the agreement and thus organizations such as KAERI, KEPCO, etc. joined the assessment program under management of KINS. This activity contributed to Korean nuclear technology in experiencing the intensive assessments of a best estimate thermal hydraulic code using data from large scale test facilities like LOFT, BETHSY, LSTF, and so on. Korea could also have opportunities to join the international research collaborations like ISP-26 and 27 and to obtain the updated code manuals, the users guidelines and the QA documents, NPA(Nuclear Plant Analyzer) through this agreement. Table 1 summarizes major assessments carried out for ICAP[2].

Korea was officially offered by USNRC to join the CAMP (Thermal-Hydraulic Code Applications and Maintenance Program) in the 3rd Joint Standing Committee on Nuclear and Other Energy Technologies between Korea and United States which was held on the May 17th 1991 in Seoul. Since Korea recognized that the achievements gained from ICAP, must be beneficial to both sides, KINS as the Korean representative concluded the agreement on CAMP with USNRC in August 1993. In order to achieve the successful outcomes, KINS has systematically been organizing the research teams in several related organizations such as KAERI, KEPCO, Universities, etc. Figure 1 illustrates such cooperation. Assessment status related with CAMP is shown in Table 2. The most recent version available in Korea is RELAP5/MOD3.2

In addition to RELAP5 Korea concluded another agreement, 'CATHARE Software Agreement' with CEA, France in Nov. 1988. The purpose was to enhance the reliability in thermal hydraulic analysis for the accident management because there was no integrated test facility for confirmations of physical assumptions included in the accident scenarios. The most updated version installed is CATHARE2 1.3U. These days assessments of both codes, i.e. RELAP5/MOD3 and CATHARE2, are also being carried out. Status of the activities regarding CATHARE2 are shown in Table 3.

III. Anticipated uses of thermal hydraulic codes in Korea

It is no doubt that best estimate methodology will be adopted not only to future designs of reactors but also to analyses of operating plants. In this regard, KAERI has studied an uncertainty quantification method for the RELAP5/MOD3 in cooperation with KEPCO using experimental data available within Korea to develop KAERI-REM(Realistic Evaluation Model). Since it is a primitive attempt and available experimental data are limited in Korea, a complete methodology has not been set up so as to cover all licensing accidents so far. This method has been applied to the actual reactor Kori 3&4, 900 MWe, 3-loop, Westinghouse PWR but the calculated safety margin for LBLOCA has not increased as much as expected comparing with the result calculated by the existing method. For this reason Korea requires its own developed code to achieve the estimate thermal hydraulic analysis goal as an extension of previous work. Meanwhile, applications of well proven existing codes or modified vendor codes would be dominant trends until completion of the developing code. This code development is not likely to start from the beginning. It will be carried out in the manner that minimizes efforts by combining models and methodologies that are well proven in existing codes. The code should be used for multipurposes, so its applications will not be limited in the accident analysis [3]. For an example, it may replace the simulation software of the future full scope simulator. KEPCO has already been discussing the feasibility of using the most updated best estimated thermal hydraulic code in the simulator. KAERI considers a new thermal-hydraulic code whose application ranges are similar to those of current best estimate thermal hydraulic codes but with the most updated code architectures. To provide necessary data for the code developments as well as to confirm the future Korean reactor design, KAERI is planning construction of a integrated test facility.

Therefore the uses of existing codes with minor modifications may be dominant within the next 10 years, however, it is anticipated that the use of the best estimate thermal hydraulic code developed in Korea will be most probable in safety analysis after 2007.

IV. Conclusions remarks

Even though 10 PWR and 1 CANDU are operating and 4 PWR and 3 CANDU are under construction in Korea, all codes provided by foreign organizations are still used. The royalty problems concerning the codes are seriously raised in design applications and the utility also experiences the difficulty in code maintenance due to the foreign dependency these days.

Therefore Korea should develop its own methodology in best estimate thermal hydraulic safety analysis, in order to promise confidences in both the design and the safety for the future competitions. It is believed that the recent Korean potentials in technology and economics make the development possible.

V. References

- [1] Zoran Stosic, 'Enhancing the Scope of Applications of Standard Thermal Hydraulic Codes by Linking with Others', International Conference on Nuclear Engineering, Vol 1 - Part B, pp 517-531, ASME 1996
- [2] M. Reocreux, 'Current and Future Trends in Nuclear Reactor Thermal-hydraulics', International Conference on 'New Trends in Nuclear System Thermalhydraulics', Pisa, Italy, 1994
- [3] S.Y. Kim, et al., 'Best Estimate Regulatory Audit Code Development', KINS/GR-078, KINS Report

Table 1. The Status of RELAP5 Code Assessments for ICAP

Application	Simulating Accident/ Experiment	Test Facility	Status	Used Code version
PWR Plant Transient	• Loss of Offsite Power Incident at June 1981	Kori unit 1 (1981.6)	NUREG/IA- 0030	RELAP5/ M2/C36.04
	• Net Load Trip Test	YGN unit 2	Submitted	M2/C36.02
	• Natural Circulation Test	YGN unit 2	0125	M2/C36.02
	• Inadvertant Safety Injection	Kori unit 3	0105	M3/5m5
Integral Effect Test	• LBLOCA Test L2-3	LOFT	0070	M2/C36.04
	• LBLOCA Test L2-5	LOFT	0032	M2/C36.04
	• LBLOCA Test L2-5	LOFT	Submitted	M3/5m5
	• SBLOCA Test L3-7	LOFT	0031	M2/C36.04
	• IBLOCA Test L5-1	LOFT	0069	M2/C36.04
	• Total Loss of Feedwater and Recovery Test, L9-1 /L3-3	LOFT	0114	M3/5m5
	• SBLOCA Test S-NH-1	Semiscale	0099	M2/C36.04
	• FLB Test S-FS-11	Semiscale	0104	M3/5m5
• LBLOCA Test SB-CL- 18	LSTF	0095	M3/5m5	
• SBLOCA Test 9.1b	BETHSY	0104	M3/7j	
Separated Effect Test	• Critical Flow Test #15,24	Marviken	NUREG/IA- 0086	M2/C36.04 M3/5m5
	• Direct-Contact Condens- ation in Horizontal Co- current Stratified Flow	Northwestern University	0077	M2/C36.04 M3/5m5
	• CCFL Test in Simple Vertical Tubes and Rod Bundle Tests	KAERI CCFL	0100	M3/5m5 M3/7j
	Completed 17 Assessment Reports (4 NPP, 10 IETs, 3 SETs)		14 Published 2 Review 1 Publishing	11 : MOD2 9 : MOD3

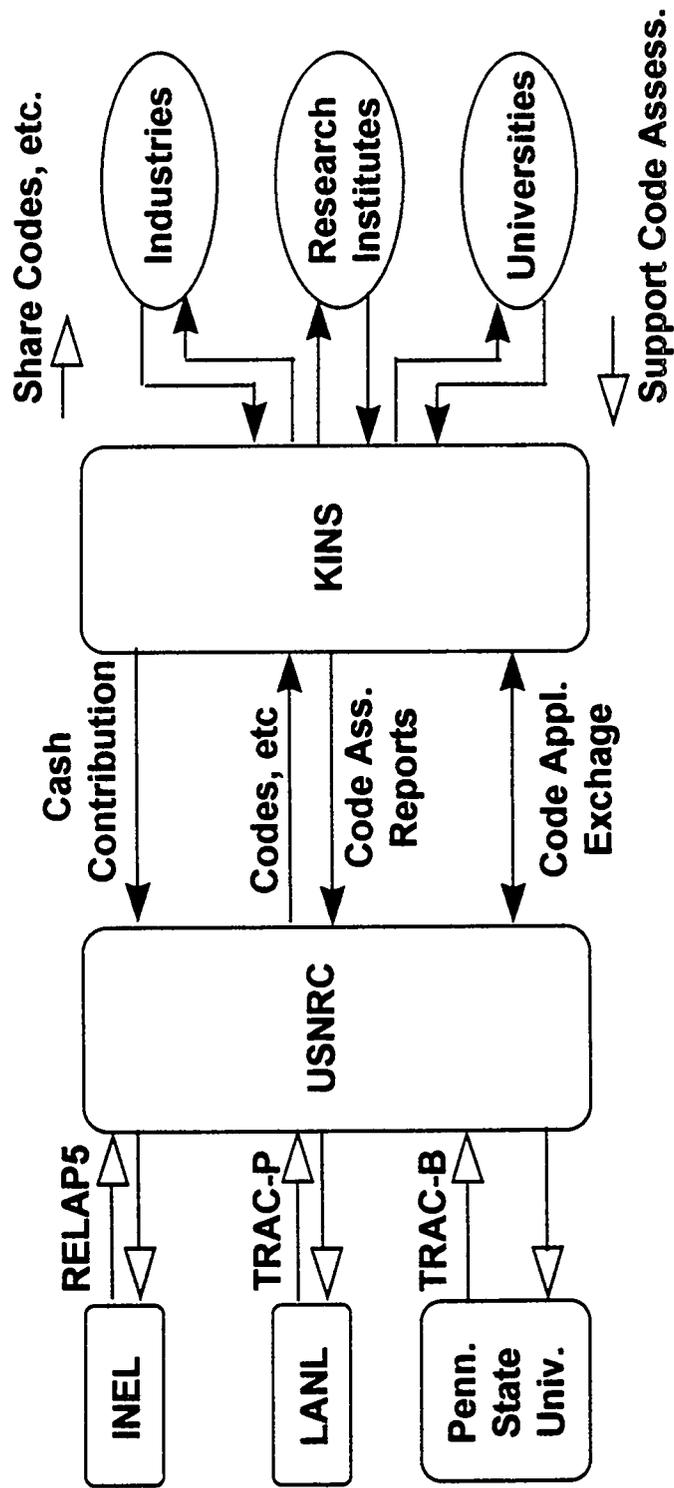


Figure 1. CAMP Operation System

Table 2. The Status of CAMP Activities

Test Facility	Simulating Accident/Exp.	Status (Organization)	Used Code version
LSTF	• SGTR Simulation Test SB-SG-06	Submitted at May 95	RELAP5/ M3.0
	• Loss of RHR During Mid-Loop Operation	Base Calculation Completed	M3.1 M3.0
	• Steam Line Break Test SB-SL-01	Base Calculation Completed (KOPEC)	M3.1 M3.1
Semiscale	• SBLOCA Natural Circulation Test S-NC-8B	To be submitted	M3.1 M3.0
	• Two-phase NC and Reflux Condensation Test, S-NC-3 & 4B	Base Calculation Completed (Kyounghee Univ.)	M3.1
BETHSY	• SBLOCA Test 6.2tc	Submitted in Feb. 95	M3/7J
	• Loss of RHR during Mid-loop (PRZ manway open) Test 6.9a	Undergoing	M3.1 or Later Version
LOFT	• Natural Circulation Test 3.4a	Under consideration	(KAERI/KINS)
	• SBLOCA Test L3-1	Undergoing (Kyounghee Univ.)	M3.1
	• TLOFW and Recovery Test L9-1/L3-3	To be calculated	M3.1 or Later Version
FLECHT-SEASET	• SBLOCA Test LP-02-6	Undergoing (KNFC)	M3.1
	• Improvement of RELAP5 Reflood Model	Submitted in Feb. 95	M3.1-KAERI Improved
Kyunghee Univ. Facility	• Natural Circulation Test	To be calculated in 97	
Seoul National Univ. Facility	• Natural Circulation Test		
KAIST Facility	• Isolation Condenser Test	New Item(KAIST)	
KAIST CMT Facility	• Direct Contact Condensation Test	Submitted in Nov. 95 (KAIST)	M3.0 M3.1
Kori unit 2 (W/H, 600 MW)	• PRZ-SI Incident	New Item(KEPCO)	
	7 Submitted 7 Undergoing(Under consideration) 2 New Item		

Table 3. Status of CATHARE2 Uses at KAERI

Test	Test Description	Status	Remarks
BETHSY 3.4a	<ul style="list-style-type: none"> • Single phase NC - Unbalanced loops 	Completed	
6.2tc	<ul style="list-style-type: none"> • SBLOCA - 6" Cold Leg Break 	Completed	Also RELAP5/M3/7j
6.9	<ul style="list-style-type: none"> • Loss of RHR during Mid-loop Operation 	Completed	Also RELAP5/M3.1
a	<ul style="list-style-type: none"> - PRZ manway open 	To be calculated in '97	
b	<ul style="list-style-type: none"> - PRZ manway and SG Inlet Plenum open 		
c	<ul style="list-style-type: none"> - PRZ manway and SG Onlet Plenum open 	Calculation Completed	ISP-38
d	<ul style="list-style-type: none"> - Vents open and Sight Gage Broken 	Undergoing	
e	<ul style="list-style-type: none"> - Upper Head/PRZ Vents open 	To be calculated in 97	
7.2c	<ul style="list-style-type: none"> • Reflux Condensation with noncondensable gas 	Completed	Also RELAP5/M3.1
9.1b	<ul style="list-style-type: none"> • SBLOCA - 2" Cold Leg Break with delayed ultimate procedure 	Completed	ISP-27
Younggwang 3/4	<ul style="list-style-type: none"> • LBLOCA/SBLOCA - SIT Capacity Evaluation 	Completed	
	<ul style="list-style-type: none"> • Loss of RHR during Mid-loop Operation - No vent - Upper head/PRZ/Letdown Line Vents - PRZ manway open w/wo SG 	Completed	

CURRENT AND ANTICIPATED USES OF THERMAL-HYDRAULIC CODES IN SPAIN

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Abstract.

Spanish activities in the field of Applied Thermal-Hydraulics are steadily increasing as the codes are becoming practicable enough to efficiently sustain engineering decision in the Nuclear Power industry.

Before reaching this point, a lot of effort has been devoted to achieve this goal. This paper briefly describes this process, points at the current applications and draws conclusions on the limitations. Finally it establishes the applications where the use of T-H codes would be worth in the future, this in turn implies further development of the codes to widen the scope of application and improve the general performance.

Due to the different uses of the codes, the applications mainly come from the authority, industry, universities and research institutions.

The main conclusion derived from this paper establishes that further code development is justified if the following requisites are considered:

- 1.-Safety relevance of scenarios not presently covered is established.
- 2.-A substantial gain in margins or the capability to use realistic assumptions is obtained.
- 3.-A general consensus on the licensability and methodology for application is reached.

The role of Regulatory Body is stressed, as the most relevant outcome of the project may be related to the evolution of the licensing frame.

1. INTRODUCTION.

Spanish activities in the field of Applied Thermal-Hydraulics are steadily increasing as the codes are becoming practicable enough to efficiently sustain engineering decision in the Nuclear Power industry.

Before reaching this point, a lot of effort has been devoted to achieve this goal, and a lot is left. The participation in different international programs (CAMP, CSNI-ISP, ICAP^{1,2}, LOFT³) has resulted in the creation of different groups of qualified users and well tested models of all the Spanish plants.

The Consejo de Seguridad Nuclear (CSN), as the Regulatory Body, has played a relevant role in the promotion of the activities in this context.

This paper points at the current applications, and draws some conclusions on the observed limitations. Finally, it establishes the applications where the use of T-H-codes would be valuable in the future. This, in turn, implies a further development of the codes to widen the scope of application and improve the general performance. The role of Regulatory Body is stressed, as the most relevant outcome of the project may be related to margin reductions, use of realistic assumptions in licensing assessments, and eventually affecting the licensing bases.

2.-PRESENT USE OF CODES.

Spanish authority responsible for the nuclear safety is the Consejo de Seguridad Nuclear (CSN). The CSN coordinates the accessibility of thermalhydraulic codes that are used within the CSN itself, the industry (NPP and engineering organizations), research institutions and universities.

Due to the different uses of the codes, the applications mainly come from the authority, industry and universities. The activities where codes are currently being used are the following:

- 1.-Licensing related activities.
- 2.-Research.
- 3.-Probabilistic Safety Assessment.
- 4.-Plant support and Emergency operations.

To perform these activities a panoply of codes is currently used:

TH codes: RELAP, TRAC-PF1, TRAC-BF1, RETRAN, TRETA^a, LAPUR.

Severe Accident codes: RELAP-SCDAP, MELCOR, MAAP.

Subchannel Codes: COBRA.

Neutronic Codes: CASMO-SIMULATE, SCALE, SIMTRAN^b.

^aTRETA is a modular code developed by CSN and configured to model a PWR plant.

^bSIMTRAN is an integrated neutronics-thermalhydraulics code for 3-D dynamics of PWR cores, part of the SEANAP Core Analysis System.

2.1.-Licensing related activities.

Through the licensing process, if needed, both, the Authority and the Applicant make use of the codes to support their positions.

The main activities follows:

1.-Perform independent calculations.

Independent calculation is not intended to bypass the evaluation process, which is in any case necessary and previous to decide the use of TH codes.

The capability to contrast results from different sources is very valuable as a mean to rise potential areas of concern. Some examples are given in following points.

2.-Independently verify the adequacy of the different hypothesis used in the transient and LOCA analyses.

Example of applications in this context have occurred in the analyses of transients during the licensing process of plants with new design steam generators. Specific transients evaluated were: The inadvertent ECCS actuation, in which the impact of the efficiency of pressurizer spray was evaluated; steam Generator Feed-Water line break, in which the details of the accident were evaluated; locked rotor in a single loop spanish plant was also explored, though the code (RELAP) was unable to approach the critical pressure.

The evaluation of new methodologies is a field in which the use of the TH codes plays an important role. This is currently being done as applications are on the desk, covering transient and accident (LB&SB-LOCA) analyses.

3.-Support questions, final requirements and help in NPP-CSN dialogue.

The aforementioned feed-water line break was an example in which the use of codes was very useful in the support of questions from the Authority and the final determination of some analyses requirements. Also the Inadvertent ECCS actuation accident served as an example in which dialogue between NPP and CSN was supported by code applications.

4.-Analyze real transients and potential scenarios not necessarily under the design envelope.

The use of TH codes finds its most direct application in the analysis of real plant transients, where first, they allow to gain insight helping to understand the plant evolution and to ascertain the driving phenomena, and second, simple modifications of code inputs help to explore 'what if' questions relative to the transient.

An example of this application of the codes was the evaluation of a Reactor coolant pumps runout in a PWR⁴.

Extensive use of codes was also required for the analysis of the BWR instabilities issue⁵ and barrel cracking.

5.-Check of Emergency Operating Procedures.

EOPs evaluation have required the use of codes in order to perform an exploratory work on the different scenarios corresponding to a specific EOP. An example of this application⁶ resulted in a very valuable experience. Extension of this strategy of EOP evaluation will be described later.

6.-Support in the process of operator and supervisor training and licensing.

CSN and industry responsibility in the operators and supervisor qualification has resulted in the use of TH codes. This application is specially relevant as the use of best estimate codes is essential, at least, in simulators training. At the present time, a real time running version of a best estimate code is used for the training of the crews of most spanish plants in the TECNATOM (spanish training company) facilities.

CSN is making extensive use of TH codes to develop a Data-Base for use in the examinations. The simulated scenarios are introduced as questions in which the integral perception of licensees is assessed.

7.-Help in the relationship between NPP and engineering companies.

The NPP capability to dialogue in levelled terms with the engineering companies performing licensing calculations is notably enhanced by the use of the current TH codes.

2.2.-Research

Spanish research activities in the field of nuclear Thermal-Hydraulics is mainly focused to applications. The main areas of study in the context of this paper are the following:

- 1.-Integrated Safety Assessment.
- 2.-EOP simulation.
- 3.-Postprocessing TH codes.
- 4.-Development of tools for the assessment of Severe Accident Management Guides.
- 5.-Uncertainty Methodology Study.
- 6.-Analysis of usual and unusual occurrence of heat transfer modes.
- 7.-Safety Features of Advanced Reactors.

2.3.-Probabilistic Safety Assessment.

PSA activities involve the use of TH codes. Besides the usual analysis of PSA sequences and the checking of thermalhydraulic early steps of severe damage progressions, a project to evaluate the use of TH codes in shutdown modes is underway⁷. Part of the project implies the participation of the universities in ISP-38.

2.4.-Plant support and Emergency Operations.

From the plant operation support point of view, different activities are developed mainly by NPP's teams and/or engineering organisations:

- 1.-Creating and improving NPP models.
- 2.-Analysis of scenarios involving EOP's
- 3.-Solving engineering general questions related to process, or protections and controls (discussing setpoints, dynamic behaviour of interactive systems,....)
- 4.-Analysis of actual plant transients.

5.-Help in clarifying eventual discrepancies between codes used by the different organisations related with the design.

6.-Adjusting Nuclear Plant Analyzers models in order to assume that their predictions are consistent with the analyst's model.

7.-Any other related with plant dynamics.

The use of fast running codes in the environment of an emergency is actively pursued in the CSN. To validate this tools, best estimate codes are used as a reference.

3.-FUTURE APPLICATIONS.

Future applications are considered in the following paragraphs. These applications are the result of needs not currently fulfilled by the codes, outcome of research projects, and expected evolution of licensing activities due to either external or internal regulatory initiatives.

3.1.-Current needs not fulfilled.

From the experience acquired in the different uses so far mentioned, some code limitations become apparent. These limitations are well known by the community, and they not only cover capability limitations but also difficulties to qualify the application itself (i.e.uncertainty,...). These needs can be summarized as follows:

1.-Expanding of capabilities to deal with shut-down modes.

2.-Transients with high asymmetrical neutron flux variation.

3.-Boron dilution scenarios.

4.-Thermal stratification and mixing.

5.-Near and above critical pressure scenarios.

6.-Efficient generation of methodology to deal with the uncertainty problem.

7.-Code speed, robustness and numerics reliability.

8.-Capabilities required from advanced reactor characteristics.

To cope with these problems some code extensions are required covering the following items:

1.-Improve the treatment of noncondensables, either dissolved or in the vapour phase.

A well known limitation of present codes is the modelling of the presence of noncondensables in the system. This options has not been thoroughly validated and some effort should be allocated. The usual consideration of the absence of noncondensables dissolved in the liquid phase may prove to be relevant in situations in which some dilution is expected. Also the present correlations available in presence of noncondensables are very limited and poorly validated.

2.-Introduction of 3-D neutronics.

The introduction of the capability to model transient 3-D neutronics will be useful in different scenarios dominated by large asymmetric neutronic fluxes. This is the case of Steam Line Breaks, Rod Ejections, Fast boron dilutions, etc.... In these situations, the use of Point or even 1-D Kinetics may be misleading as unrealistic transient evolution may be expected, not necessarily conservative as eventual local criticality may be skipped.

This capability is present in some codes like TRAC/NEM, SIMTRAN, etc... A problem on the use of this capability is the difficulty to handle the whole lot of information needed to feed the code and also the machine requirements to run efficiently.

3.-Reduce numerical diffusion and improve capability of tracking fronts.

Numerical diffusion is a problem rooted in the present numerical schemes used by the codes. This affects the code capability to deal with those transients in which the capability to track some local variable is of importance. An example in which this problem appears is the fast boron dilution accident, but also the slow ones provided the driving flow is small enough.

4.-Capability to model turbulence and thermal mixing.

Turbulence and thermal mixing are specially relevant in situation in which streaming may be present. Situations like the aforementioned fast boron dilutions, ECCS injection and downcomer redistribution, distortion on local plant measurements, pressurizer dynamics, are examples where this capability would be helpful. A problem arises as the mesh size usually required in Fluid-Dynamic codes is small in comparison to the system codes, thus some work should be required to overcome this difficulty.

5.-Capability from field and constitutive equations to approach and go beyond critical pressure.

Though somehow an academic question, the approach to the critical pressure limit from six equations codes is not currently solved. This problem is specially critical in dealing with the locked rotor transient in which the capability to model the whole transient (transient and recovery actions) requires the use six equations. Also the qualifications of correlations and flow regimes maps in the vicinity to this limit is scarce. ATWS is another scenario where for the same reasons present six equation codes may run into difficulties.

6.-Consideration of the code uncertainty problem.

Codes application is affected by the difficulty to state the confidence and probability of the results for a given boundary condition (boundary uncertainty is not considered in this discussion). This problem is specially important in dealing with licensing application related to accident analyses, but also APS could benefit in the determination of a realistic success criteria.

The consideration of the uncertainty during code development is important as it is believed that the feedback between model development and overall uncertainty reduction may drive, in a objective way, the need for model changes. Also the code uncertainty should be a previous requirement in developing a code, not a consequence.

7.-Use of efficient programming and improvement in code numerics.

This point is related to the efficiency of the code to run in a satisfactory way, that is, fast, robust and reliable.

Code speed is a requisite that is relevant as applications become more demanding. Sensitivity analyses, long time spans, phenomenological complexity and large systems require these characteristics.

8.-Capabilities required from advanced reactor characteristics.

Advanced reactors design have introduced the need for an improvement in the modelling of different components so that gravity driven injections, pools and condensers, dry wells or containments are properly modelled.

3.2.-Research outcomes.

From the results of our present research projects several future applications are expected:

1.-Integrated Safety Assessment⁸.

From Integrated Safety Assessment (ISA), a valuable aid to estimate the safety level in the plant will be available. ISA will be able to couple dynamic analysis and PSA results in such a way that the impact of software (protection demand criteria) as well as of design modifications will be reflected in changes in the risk quantification. In the context of ISA, the concept of risk comes from the joint consideration of damage, represented by selected damage variables, and probability of damage occurrence. Extension of ISA methodology to Accident Sequence Precursor Studies is also foreseen. This may include the associated operator actions.

2.-EOP simulation.

From the EOP simulation, a coupling between computerized operator actions and TH codes will be available. This will notably enhance the capability to analyze the effectiveness of different procedures to cope with emergencies and accident management. This project, though independent, will be also incorporated in the already mentioned ISA to allow for procedure assessment from the safety point of view. The extension into the safety assessment domain has been recently undertaken.

3.-TH codes postprocessing⁹.

By capability to postprocess TH codes, we understand the ability to rigorously evaluate the consistency of the results obtained from the code calculation. The consistency will look at the TH balance equations in such a way that the different contributors to the balance are evaluated. The balance can be checked at the node, component and system level. Incorporation of this capability as a benefit for the user should be considered.

4.-Development of tools for the assessment of Severe Accident Management Guides.

This project may be considered as a natural extension of EOP simulation and also integrated in the ISA methodology with the peculiarity that the TH code to be used is a severe accident code. Currently some work is being done on MAAP.

5.-Uncertainty Methodology Study.

Spain is participating in the CSNI international exercise on Uncertainty Methodology Study. The approach is basically that of the NUREG-CR-5249 but for the use of GRS like approach for combining the uncertainties for high ranked parameters instead of the use of a response surface. The selected code is RELAP5/MOD3 and the work is performed by ENUSA (Spanish fuel and services company).

6.-Analysis of usual and unusual occurrence of heat transfer modes.

The Politechnical University of Catalunya (UPC) is currently working on the evaluation of the impact that different recovery actions for the SBLOCA scenario have on the Heat Transfer modes.

7.-Safety Features of Advanced Reactors.

Also UPC is working on the ESBWR technology evaluating the modelling capabilities of the safety features of this kind of reactor.

UPC, CIEMAT (spanish research institution) and the Politechnical University of Valencia are participating on the TEPS (Technology Enhancement of Passive Safety Systems) programme.

From these projects it is expected that some areas of improvements for the codes will be observed.

3.3.-Regulatory evolution.

Regulation cannot be considered a static element and its evolution must be considered when it becomes obsolete to satisfy the goals it was intended to achieve. This obsolescence may come from different areas. In what we are concerned, the future applications of codes may be impacted by the regulatory position.

Reduction of conservative hypothesis, or analysis assumptions based on code accuracy is expected. Reluctancy to take credit of these, may derive in a marginal benefit from code development in the licensing area. Also, the move towards risk based licensing actions and its probable impact in the present deterministic accident analysis orientation, will require an effort to define the requirements of future development on TH codes.

Licensability of the final product, as well as a consensus on the general terms for its application methodology should be addressed. Efforts in this direction have resulted in the general acceptance of Best Estimate codes but with heterogeneity between different countries in the licensing approach.

As a final conclusion it is considered that a clear statement from the Regulatory Body community on which is going to be the frame for future acceptance of licensing applications of these codes is essential to drive or allocate resources for code development.

4.-CONCLUSIONS.

- 1.- Present codes satisfactorily serve in current applications they were designed to deal with.
- 2.- Some needs not currently fulfilled will require from code development.
- 3.- Current research in other areas than Thermal-Hydraulic should be considered in the requisites definition for a code development.
- 4.- Justification for code development must consider, among others:
 - a) Safety relevance of scenarios not presently covered is established.
 - b) A substantial gain in margins or use of realistic assumptions
 - c) General consensus on licensability and methodology for application.

5.-REFERENCES.

- 1.'Segundas Jornadas Técnicas ICAP-ESPAÑA. Experiencia Adquirida como resultado del proyecto ICAP-ESPAÑA.', Comité de Coordinación ICAP-ESPAÑA ICSP-01-92 Noviembre-1991
- 2.'Segundas Jornadas técnicas ICAP-ESPAÑA. Aplicaciones del proyecto ICAP-ESPAÑA.', Comité de Coordinación ICAP-ESPAÑA noviembre 1991
- 3.'Proyecto OECD-LOFT. Memoria de la participación española.', A.Alonso et.al. Mayo-1990
- 4.'Development and validation of the 3-D PWR core Dynamics SIMTRAN code.', F.Merino, C.Ahnert, J.M.Aragónés. International Conference M & C + SNA'93 Mathematical methods and Supercomputing in Nuclear Applications Karlsruhe, Germany, 19-23 April 1993
- 5.'Coupled Thermohydraulic-neutronic instabilities in boiling water nuclear reactors: a review of the state of the art.', José March-Leuba, José M.Rey. Nuclear Engineering and Design 145(1993)97-111.

6. 'Análisis de los procedimientos de emergencia asociados a la rotura de tubos en el generador de vapor de C.N. José Cabrera y su comparación con otras plantas españolas.', Julio Pérez SEP/PPTT/IN/64/91

7. 'Análisis Termohidráulico de Escenarios Transitorios en condiciones de parada mediante el código RELAP-5.', Departamento de Ingeniería Química y Nuclear. Universidad politécnica de Valencia Mayo-1996

8. 'Extending PSA to Accident Management (AM). The case of Steam Generator Tube Rupture (SGTR) Emergency Operating Procedures (EOP) Assessment.', M. Sánchez Perea et al, ICONEIV March 10-14, 1996 New Orleans, USA

9. 'Implementation of a Thermalhydraulic postprocessor for RELAP5/MOD3.2', Roberto Herrero Internal CSN Report. June 1996.

CURRENT AND ANTICIPATED USES OF THERMALHYDRAULIC AND NEUTRONIC CODES AT PSI

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Abstract

The thermalhydraulic and/or neutronic codes in use at PSI mainly provide the capability to perform deterministic safety analysis for Swiss NPPs and also serve as analysis tools for experimental facilities for LWR and ALWR simulations. In relation to these applications, physical model development and improvements, and assessment of the codes are also essential components of the activities.

In this paper, a brief overview is provided on the thermalhydraulic and/or neutronic codes used for safety analysis of LWRs, at PSI, and also of some experiences and applications with these codes. Based on these experiences, additional assessment needs are indicated, together with some model improvement needs.

The future needs that could be used to specify both the development of a new code and also improvement of available codes are summarized.

1 Introduction

Thermalhydraulic codes for the transient behavior of nuclear reactor systems are in use at PSI (Paul Scherrer Institute, previously Swiss Federal Institute for Reactor Research EIR), for about twenty five years. In Switzerland the research and application activities in relation to the thermalhydraulics and neutronics in accident analysis of Light Water Reactors (LWRs) and Advanced LWRs (ALWRs) are mainly concentrated at the Paul Scherrer Institute. The Swiss Nuclear Safety Authority (HSK) and Swiss Utilities provide also support and partial financing for the activities in this area. In addition, HSK has some ongoing work in support of the review of Probabilistic safety assessment studies, mainly in the area of severe accidents.

At PSI, in the Nuclear Engineering and Safety Research Department, the Laboratory for Reactor Physics and Systems Engineering (LRS), the Laboratory for Thermal Hydraulics (LTH) and the Laboratory for Safety and Accident Research (LSU) pursue activities that

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use transient thermal hydraulics and/or neutronic codes. Currently, the majority of LWR accident analysis applications are mainly performed and integrated into the following projects: STARS (Transient analysis for Swiss nuclear power plants (NPP), ALPHA (a program to assess the containment-behavior of passive LWRs), CAMP (Code Assessment and Maintenance Program), and severe accident source-term analyses for Swiss nuclear power plants. The field of severe accidents will not be covered in this paper.

2 Description of current activities and current use of codes

2.1 Thermal-hydraulic and/or neutronic codes used for safety analysis

The thermal-hydraulic and/or neutronic codes which are used at PSI mainly provide the capability to perform deterministic safety analysis for Swiss NPPs and also serve as analysis tools for experimental facilities for LWR and ALWR simulations. To this aim, the necessary computer codes have been installed and tested on a cluster of UNIX workstations and very few are also installed on a CRAY computer. To date, input models for these codes have been developed for some major experimental facilities, both our own and from other countries. These were used for physical model development and improvements, and also code assessment. In addition to these, most of the Swiss NPPs are simulated with models, which are tested using available plant data or results of vendor analyses. The following codes are currently being used for these types of simulations:

- CASMO-4 and SIMULATE for steady state core analysis,
- RETRAN-3D for BWR and PWR transient analysis with integrated three-dimensional neutronics, including limited Small-Break Loss-of-Coolant Accident (SB-LOCA) analysis; Large Break (LB) - LOCA analysis is excluded,
- RELAP5 for PWR LOCA analysis and thermalhydraulic transient analysis for LWRs and ALWRs,
- TRAC-BF1 for BWR transient analysis,
- RAMONA 3.9 for BWR-stability,
- CONTAIN for thermal hydraulic analysis of the containment,
- GOTHIC for ALWR containment thermal-hydraulic problems,
- FLOW-3D for mixing problems in large ALWR containment compartments,
- TRANSURANUS for fuel behavior,
- CORETRAN-01 for core-dynamics and subchannel analysis,
- RELAP5/SCDAP for severe accident analysis.

In general, whenever possible, the policy of using well maintained and validated codes with a significant user base is followed. This ensures an efficient exchange of user experiences and also considerably reduces the necessary extensive validation effort needed for the codes.

The scope of the simulations and analysis includes design base accidents, and, with increasing weight, beyond-design-base transients such as anticipated transients without

scram (ATWS), and also some selected severe accident cases. Some of the codes listed above are also used for the safety analysis of the passive ALWR designs.

2.2 Some experiences on selected cases in relation to thermalhydraulics of LWRs

PSI has participated in the international thermalhydraulics LWR research program with extensive system safety analysis code validation, code model improvements and plant applications. Code validation and model improvement were performed within the framework of the International Code Assessment and Applications Program (ICAP) and the successor, Code Application and Maintenance Program (CAMP), both led by the United States Nuclear Regulatory Commission (US NRC). This collaboration provided access to the internationally used codes such as RELAP5 and TRAC-BF and their various versions (written by US organizations) in exchange for code validation work performed at PSI. In addition, participation in the Committee for the Safety of Nuclear Installations (CSNI) International Standard Problems (ISPs) also provided access to experimental data in addition to code validations.

Research work in this area is related to two-phase flow and heat transfer problems encountered in LWR and ALWR accident analysis. Principal objectives are the realistic modeling of relevant phenomena and "best estimate" prediction of operational transients and accidents for the safety analysis of LWRs. Thus, the activities range from experimental and analytical research of fundamental phenomena to experimentation, code assessment, and finally analysis of Swiss nuclear power plants. In this paper, the main emphasis will be on the current use of the thermalhydraulic codes in relation to assessment and application. Some selected examples are given for various uses of the thermal-hydraulic system codes, as follows:

- Code validation work within the frameworks of the ICAP and CAMP programs:
 - Post-test analysis of OECD-LOFT small and large break LOCA experiments, e.g. LP-SB-03, LP-02-6 and LP-LB-1, using the RELAP5/Mod2 and Mod3 codes (e.g., ref. [1]).
 - Developmental and independent assessment of various versions of the RELAP5 and TRAC-BF codes using the PSI-NEPTUN reflooding and boil-off tests,
 - Independent assessment of various versions of RELAP5 using Westinghouse FLECHT and Lehigh University reflooding tests and ORNL-THTF boil-off tests (e.g., ref. [2]).
 - Developmental assessment of TRAC-BF using TLTA BWR large break LOCA tests and FLECHT reflooding tests.
- Code improvements and implementation of some models into the RELAP5 and TRAC-BF codes cover flow regime maps with interfacial drag, CHF and post-CHF models, blowdown and reflooding quench phenomena, proposals for addressing mass error problems in long transients [3], corrections to critical flow model, etc. In addition some analytical model development for certain key thermalhydraulic phenomena, e.g. rewetting, inverted annular film boiling and dispersed flow heat transfer, were accomplished (e.g., ref. [4]).
- Code assessment work for the DOE Physical Benchmark Exercises was performed using both the RELAP5 and TRAC-B codes.

- Extensive participation in International Standard Problems (ISP) organized mainly by the CSNI to assess the safety analysis system codes also led to additional code assessment work and provided experience at international level. Here, only some of the ISPs calculated and analyzed with RELAP5/Mod2 and Mod3 versions will be mentioned. Some examples are: LOBI-MOD2-A2-81 small break LOCA test (ISP 18, CEC, Ispra, Italy), ACHILLES reflooding test with nitrogen injection from accumulators (ISP 25, AEA Winfrith, UK), LSTF-SB-CL-18 small break LOCA test (ISP 26, ROSA-IV program, JAERI, Japan), BETHSY 9.1.b small break LOCA with accident management measures (ISP 27, CEA, Grenoble, France), PACTEL VVER-440 natural circulation test (ISP 33, VTT, Finland), (e.g., [5]).
- Building on the extensive experience with the use of the transient system codes, e.g., RELAP5, TRAC-B, RETRAN, safety analyses for Swiss NPPs are being performed. These analyses and calculations cover both PWRs (Westinghouse and SIEMENS-KWU type) and BWRs (GE, BWR-I and BWR-III type). Some selected examples of transients analyzed are:
 - Large and small break LOCA in PWRs with emergency core cooling (ECC) systems in operation or with limited ECC and/or restricted heat removal from the steam generator (longest transient case, about 10 hours), (e.g., ref. [6]),
 - Station blackout cases for PWRs,
 - Rod ejection analysis (REA) in PWRs [7],
 - Core response after main steam line break (MSLB) in a PWR (with 3D-kinetics) and also related containment analysis,
 - Large and small break LOCA in BWRs with various availability of ECC systems, e.g. core spray line break, loss of feed water and stuck open safety relief valve transients, etc.,(e.g., [8]),
 - BWR stability analysis,
 - A spectrum of ATWS scenarios in BWRs (e.g., ATWS with MSIV closure), (e.g., [9]),
 - Rod drop analysis (RDA) in BWRs (for design basis and beyond design basis conditions), (e.g., [10]).

In order to calculate this wide spectrum of transients and overcome some of the difficulties encountered in the analysis, e.g. mass errors, modeling of reflooding, critical flow, steam separators, etc., there is a strong need to introduce some model improvements supported by code assessment, as indicated earlier. In addition, beyond-design-basis transients leading to severe accidents provide input to the source term analysis codes. These studies indicate the need for close connection between thermal-hydraulic transient analyses, and the neutronics, severe accident and source term codes.

2.3 Validation base (at PSI)

2.3.1 RETRAN-3D

In the opinion of the authors, the validation base for RETRAN-3D is limited for conditions at low flow and low pressures which lead to high void situations. These conditions are typical for the later phases of BWR-ATWS scenarios. Consequently, some work was performed to provide more data in this range of conditions for the Chexal-Lellouche void correlation that is used in one form or the other in both RETRAN-3D and RELAP5 [11].

More recently, work has started to assess the performance of the void modeling in RETRAN-3D using void data that previously has not been used in its validation process [12].

The treatment of natural circulation by RETRAN-3D has been tested in the past based on data from an instrumented thermal-hydraulic test loop, jointly constructed by Institute of Nuclear Energy Technology (INET, Beijing, China) and PSI, that was operated in natural-circulation, two-phase conditions (system pressure around 2.0 MPa). This work will be continued using more recent data from a different loop.

During BWR-ATWS scenarios, under natural circulation conditions, reverse flow through the core bypass is established. The amount of void carry-under from the upper plenum into the core bypass affects the flow rate through the core. To the authors' knowledge, this phenomenon was not addressed in any validation process (also for other codes).

2.3.2 RELAP5

As already mentioned above, extensive code assessment work within the ICAP and CAMP and also by participating in the NRC-LOFT and, OECD-LOFT programs has been performed at PSI in addition to other assessment activities, such as the CSNI-ISPs. These activities have resulted in proposals for code improvements and several of these were implemented or are being implemented [13]. In general, the RELAP5 code has a wide assessment basis, even though this may not be true for a specific version of the code. Major changes in a new version of the code may require repetition of most of the earlier assessment cases. With the computing facilities available today, this is not a major problem, though it requires systematization of both the developmental and independent assessment processes. Detailed proposals have been provided in CAMP presentations [2, 3 and 13] about the areas where improvements are needed, e.g. reflooding, flow regime maps with interfacial drag coefficients, CHF, post-CHF, the blowdown quench process, the mass error seen during long transients at low mass flow and low pressure conditions.

2.3.3 TRAC-BF1

The assessment work with TRAC-BF1, is limited. This is also the case within the CAMP program, due to the limited number of countries interested in a BWR system code. A few assessment cases and applications of this code indicate that there are limitations in some areas, e.g. reflooding, spray cooling, component models such as separator model, 1-D neutronics model, etc.

3 Future Needs

3.1 Analyses to be performed and future applications

It is natural to derive the requirements of future code capabilities from the anticipated needs of applications for the next 3-4 years. At PSI, future applications are mainly driven by the needs of the Swiss Nuclear Safety Authority, the Swiss nuclear industry (e.g. Swiss Utility groups) and analytical needs of PSI research programs. The following observations may provide some insights about the necessarily not fully defined medium- and long-term needs:

- The trend to use realistic modeling will continue.
- Answering questions related to accident management (mitigation) will require analysis of ever longer lasting sequences. A more detailed representation of the balance of plant will also be required.
- Transient analysis for scenarios during the start-up and shut-down phases may be needed in support of the Swiss Nuclear Safety Authority review process of PSA's for Swiss NPPs.
- Estimation of the uncertainties for plant analyses performed will most likely require a computational effort, at least an order of magnitude larger.
- A trend to integrate several disciplines into one single analysis code becomes more evident with ever increasing computer capacity. Examples are:
 - * Integration of core dynamics (3D-kinetics) into thermalhydraulic system analysis codes,
 - * Integration of containment analysis capability into thermalhydraulic system analysis codes,
 - * Integration of elements of subchannel and/or fuel analysis to obtain data on the most severely loaded fuel pin for the LOCA-analysis.
- Use of the codes for ALWR safety analysis and simulation of related experimental facilities.

In relation to ALWR safety analysis, new design options are currently being considered to improve the safety of the new generation nuclear plants. As a consequence, various new reactor concepts with passive safety features are being developed. Many of these designs rely on depressurisation of the primary system in order to allow gravity driven injection systems to discharge water into the core region and avoid the risks of high pressure core melting. Low pressure phenomena tend, therefore, to be characteristic of ALWR designs. In addition, in many designs, the primary system is closely coupled with the containment. Thus, computational tools need to be developed to calculate the integral response of ALWRs. The new components which are included in these designs also need to be integrated into the codes. The new passive ALWRs introduce new challenging analytical efforts for the modeling of particular phenomena and the computation of system effects. Existing codes such as RELAP5 must be augmented with models describing certain particular features of the new passive systems and validated again.

The ALPHA project at PSI aims at the experimental and analytical investigation of the long-term decay heat removal and resultant containment response of passive ALWRs. For the analysis of the experimental data obtained in this project, e.g. the PANDA experiments, uses of both system thermal-hydraulics codes such as RELAP5, a containment code such as GOTHIC and also of general purpose CFD codes like FLOW-3D for specific mixing problems in large tanks are underway. Eventhough these codes were not originally designed and developed to be used for ALWR conditions, their use for these experiments will indicate their additional applicability ranges, performance, and will also provide some input in relation to the needed improvements for their extended application to ALWRs.

3.2 Long-term code development

It is important to identify to what extent, for which transients, and how the improvements can be achieved, and discuss the prospects for improvements. To this end, it is probably better to start by having an agreed upon list which shows the present-day limits in relation to: numerical methods (e.g. low flow, low pressure anomalies and related numerics), computing techniques, closure relations, specific component models, jump conditions, discontinuity tracking, etc. This may then lead to a decision to take a new path, e.g. new code development or continue developing the available codes. In the later case, it is very important to use the best available know-how and establish strict configuration control, assessment and a maintenance program.

One or another version of the thermalhydraulic codes, e.g., RELAP5, TRAC-BF, RETRAN, can be used for most of the transients that they have been designed to calculate. If only one version contains the necessary capability, there should be very strict configuration control and also a very systematic developmental and independent code assessment process.

3.3 Some requirements for an ideal new code

Based on the anticipated future needs and applications at PSI, and also profiting from the experience gained in code assessment and applications throughout many years at PSI, some desirable features of the ideal new code, for which work might be done during the next 3 to 5 years, can be derived. By doing so, it is generally assumed that the relevant features of the codes such as RELAP5, TRAC-BF1 or RETRAN-3D (these are the codes that the authors are most familiar with) will also be available in the new code. Consequently, only enhancements are proposed below:

- Choice of (integrated) kinetics model: 0D, 1D, 3D consistent by providing the possibility to collapse to 1D and 2D. The 3D-kinetics option would typically be based on a nodal two-group representation of the 3-D diffusion equation. The core reflectors would be represented explicitly. In addition, a capability for transient pin-power reconstruction is desirable for a best-estimate analysis, in relation to assessing the fuel related limits.
- User-definable description of the nuclear cross-sections. It would give the experienced analyst the opportunity to represent some details which were not considered at the time cross-sectional models were integrated by the code developers into the codes.
- Choice of the fluid model possibly ranging from as simple as the homogenous equilibrium model to a more advanced two-fluid model (may be full 6-equation model); and eventually to multi-fluid models. A model with an intermediate degree of sophistication is very helpful (e.g., 4 equations with dynamic slip). The input requirements to these different flow models should be incremental, using the most simple fluid model as the starting point.
- Optionally 3D-thermal hydraulics (e. g., for the RPV or limited areas of special interest, such as areas where the mixing of fluid streams in plena is of importance).
- Turbulence modeling (for mixing).
- Fluid properties valid down to below-atmospheric pressure.
- Optional modules for the tracking of non-condensable gases.

- Open vessel thermalhydraulics (free surface).
- Discontinuity tracking in general (boiling boundary, improved water level tracking).
- Optional model for containment thermalhydraulics for integrated system analysis.
- Optional model for balance of plant (BOP).
- Optional fuel model with a degree of sophistication similar to the current standard fuel behavior codes (e.g. TRANSURANUS, FRAP-T6) for damage assessment, allowing the representation of the few critical pins.
- Fast-running numerics (implicit).
- Code structure amenable to parallelization.
- Component oriented user interface with minimal data requirements, with optional link to a data base system containing the plant data. Ideally, one would start the preparation of input by setting up the noding diagram which would help to organize the remaining input. The topology of the diagram would automatically be transformed into the necessary code input. Input data required by the user interface should represent a minimum set. Duplication of the input data (if necessary) should be performed by the user interface.
- Optimization in relation to user effects [14], e.g. support for nodalization studies.
- On-line manual in hypertext format.
- Providing coupling and feedback between system codes and codes modeling some of the local phenomena in detail using mechanistic models, e.g. mixing, turbulence, natural convection and circulation, etc. This coupling can also be extended through this interface to some alternative codes, e.g., 3D-kinetics code based on a transport theory for benchmarking, containment code, CFD code.
- It may also be desirable to have the capability to perform burnup calculations which will help to establish the initial conditions (prior to the transient) in a consistent way, also from the point of view of reactor physics.
- Post-processing can be organized in a stand-alone code. This would allow for high flexibility, as the graphic analysis requirements are expected to reach a new level of complexity and sophistication with the more frequent use of 3-dimensional kinetics analysis or 3-dimensional thermalhydraulics.

It is quite likely that the listed code features will lead to conflicting design goals. Hence, a careful design study would be needed to clearly define priorities.

3.4 Upgrade requirements

3.4.1 Shortcomings of the validation base

The work performed for evaluation of the CSNI-Separate Effect Test (SET) Matrix provides useful input for the needed assessment base [15].

Low-power low-pressure transients and ALWR transient cases need a validation basis.

For all the transient system-codes considered, conditions with reverse flow through the core bypass such as expected during BWR-ATWS are not included in the validation base. This clearly limits the degree of confidence in the results of such analyses.

3.4.2 Improvements for the existing codes

It is very important and vital to use the accumulated know-how presently available and to establish a strict configuration control, assessment and maintenance program for the existing codes.

New released versions should contain major proven improvements relative to the earlier versions. The code development strategies used for the CATHARE and RETRAN codes or certain vendor licensing codes are good examples for the code development process. Following this step, it is then possible to decide to integrate user interfaces for model preparation, output interpretation, even include very specific user guidelines in preparing input data. This type of well controlled codes could possibly also be interfaced with other codes, e.g. for containment, fuel behavior, severe core damage, 3D neutronics, etc.

Specific code improvement and extension needs can be specified by considering the future application needs outlined in Section 3.1 in combination with shortcomings noted during our post code assessment efforts (Section 2.3). All the additions needed for an ideal code were listed in Section 3.3; some of these could also be incorporated in existing codes.

References

- [1.] Luebbesmeyer D., "Post-Test Analysis and Nodalization Studies of OECD-LOFT Experiment LP-02-6 with RELAP5/Mod2 CY 36-02", NUREG/IA-0088, 1992.
- [2.] Aksan N., Sencar M., "Evaluation and Assessment of Reflooding Models in RELAP5/Mod2.5 and RELAP5/Mod3 Codes Using Lehigh University and PSI/NEPTUN Bundle Experimental Data", 7th International Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH-7), Saratoga Springs, New York, USA, Proc. Vol. 3, NUREG/CP-0142, September 1995.
- [3.] Analytis G. Th., "Effect of Wet-Wall Interfacial Shear Correlations on the Mass-Error of RELAP5/Mod3.1", Trans. Am. Nucl. Soc., Vol. 73, 1995.
- [4.] De Cachard F., "Development, implementation an assessment of specific closure lows for inverted-annular film-boiling in a two fluid-model", NUREG/IA-0133, 1992.
- [5.] De Pasquale F., Sencar M., Aksan N., "Analysis of the BETHSY 2" Cold Leg Break Experiment Using the RELAP5/Mod2.5 Code at PSI", 6th International Topical Meeting on Nuclear Reactor Thermalhydraulics (NURETH-6), Grenoble, France, 1993.
- [6.] Luebbesmeyer D., "Small Break LOCA Analyses as Basis of Severe Accident Cases for a 3-Loop PWR Using RELAP5/Mod3.1", 1996 RELAP5 International Users Seminar, Dallas, Texas, USA, 17-21 March, 1996.
- [7.] Knoglinger E., Belblidia L. A., Skoff G., Kalfelz J. M., "Spatial Effects of a Rod Ejection Accident in a PWR", Trans. Am. Nucl. Soc., Vol. 61, 1990.
- [8.] Analytis G. Th., "Analysis of a Hypothetical LB-LOCA in a BWR-4 Using TRAC-BF1", Trans. Am. Nucl. Soc., Vol. 73, November, 1995.
- [9.] Coddington P. and Wand H., "Analysis of a Main Steam Line Isolation Valve Closure Transient without Scram for a BWR/6 Mark III plant", Jahrestagung Kerntechnik 96, Mannheim, Germany, May 1996.
- [10.] Holzgrewe F., Kalfelz J.M., Zimmermann M.A., Maeder G and Schmocker U., "Investigations Related to Increased Safety Requirements for Reactivity Initiated Accidents", to be published in Proceedings OECD Specialists' Meeting on Transient Behaviour of High Burn-up Fuel, CEA, Centre d'Etudes de Cadarache, France, Sept. 12-14, 1995.
- [11.] Aounallah Y., Dreier J., "Experimental Assessment of the Chexal-Lellouche Void Correlation for Low-Flow Conditions and Tight-Lattice Geometry", Trans. Am. Nucl. Soc., Vol. 70, 1994.
- [12.] Maier D. and Coddington P., "Validation of RETRAN-03 Against a Wide Range of Rod Bundle Void Fraction Data", paper submitted to the 1996 ANS/ENS Winter Meeting, Washington D. C., USA, November 1996.
- [13.] Analytis G. Th., "Developmental Assessment of RELAP5/Mod3.1 with Separate Effect and Integral Test Experiments: Model Changes and Options", PSI report no. 96-09, April 1996.

- [14.] Aksan N., D'Auria F., Städtke H., "User effects on the transient system code calculations" CSNI report, NEA/CSNI/R (94)35, January 1995.
- [15.] Aksan N., D'Auria F., Glaeser H., Pochard R., Richards C., Sjoeborg A., "Separate Effects Tests Matrix for Thermal-Hydraulic Code Validation", Vol. I and II, CSNI report, OECD/NEA/GD (94)/82, 1994.

Capabilities Needed for the Next Generation
of Thermo-Hydraulic Codes for Use in Real Time Applications

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KEYWORDS

Simulators, Real-time simulation, Emergency planning, PRA

ABSTRACT

The real-time reactor simulation field is currently at a crossroads in terms of the capability to perform real-time analysis using the most sophisticated computer codes. Current generation safety analysis codes are being modified to replace simplified codes that were specifically designed to meet the competing requirement for real-time applications. The next generation of thermo-hydraulic codes will need to have included in their specifications the specific requirement for use in a real-time environment. Use of the codes in real-time applications imposes much stricter requirements on robustness, reliability and repeatability than do design and analysis applications. In addition, the need for code use by a variety of users is a critical issue for real-time users, trainers and emergency planners who currently use real-time simulation, and PRA practitioners who will increasingly use real-time simulation for evaluating PRA success criteria in near real-time to validate PRA results for specific configurations and plant system unavailabilities.

INTRODUCTION

The real-time reactor simulation field is currently at a crossroads in terms of the capability to perform real-time analysis using the most sophisticated computer codes. Rapid advances in computer hardware have provided the capability of running the most complicated engineering codes such as RELAP5, TRAC, and their successor codes at real-time speeds. Additional improvements in the next few years will remove most of the requirements for use of coarse grid sizes, limits on time steps and other simplifications currently needed to use any of these codes as real-time simulators. Most of the real-time simulator vendors are now working to produce a real-time version of one of the advanced codes. However, simply running the most advanced codes quickly does not, by itself, make them useful or appropriate for real-time applications such as training simulators or emergency planning aids. The use of the codes in real-time applications imposes much stricter requirements on robustness, reliability and repeatability than do design and analysis applications.

Additional requirements will be imposed by the fact that the traditional users of real-time codes are not analysts who have a good understanding of the basics of computational thermo-hydraulics and the limitations of the code's applicability. Implementation of these codes will be done by simulator instructors, emergency planners, and system engineers who are not familiar with issues associated with stopping and restarting analysis codes. This will

require the new code to have very little user effects even for novice users. Use of the codes for near real-time, real-time and faster than real-time calculations for emergency planning will also require them to handle the initial event (usually very severe) as well as the long term effects (often with very small hydraulic pressure differences) without the user stopping and restarting the run.

In addition to the trainers and emergency planners who currently use real-time simulation, the movement toward real-time and near real-time use of PRA tools by both licensees and the regulators will require regulators and plant staff using real-time or near real-time PRA tools to include real-time thermo-hydraulic codes. New versions of the codes will need to be capable of evaluating PRA success criteria in near real-time to validate PRA results for specific configurations and plant system unavailabilities. This will potentially call for codes and models that can be used by novice users to do near real-time FSAR level safety reviews for unanalyzed configurations of plant systems, structures and components. This implies a requirement for codes to permit the novice users to renodalize models, without rebenchmarking the code. This further implies a time step and nodalization insensitivity that is far more robust than the current generation of codes.

CURRENT STATE-OF-THE-ART IN REAL-TIME REACTOR SIMULATION

Currently real-time reactor simulators are being fielded with thermal-hydraulics models with a drift-flux or two fluid formulations with three-dimensional, 1.5 or 2 group neutronics, and fully coupled coarse node containment modes. In the past, hardware has limited the computational capability of real-time simulations. Since the current cost of hardware for real-time simulators is a small fraction of code development, the memory size is expanding rapidly, and CPU speed improvements are remarkable, the restrictions on code complexity have, for the most part, been removed. This has resulted in a change in the way real-time simulation is developed and evaluated. In the past, the trade-offs in real-time simulation have included the cost of the computers, the ability of the codes to accurately simulate the plant in steady state and normal operations, the ability of the codes to adequately run the set of transients needed for the defined application, and the completeness of the simulation (and cost). In the 1980s, the number of additional systems that were defined as needed to fulfill the requirement of real-time simulation grew a great deal as a result of the NRC Simulator Certification process and requirements for simulation in areas that had not yet been addressed by simulation (shutdown operations, emergency preparedness, accident management, etc.). This has expanded the scope of real-time simulation both in terms of the scope of applications and in the breadth of modeling that needs to be included. The primary thermo-hydraulic codes must also provide inputs to all of the other models now required for the different areas of simulation.

Today, the trades-offs for real-time simulation are based primarily on the ability to provide stable, robust, reliable, and repeatable models that are tailored to the requirements of the application but flexible enough to handle new requirements as they become known. The use of the most complicated "best estimate" codes in real-time applications is now becoming a reality. Safety analysis codes like RELAP5, TRAC, and CATHARE have real-time versions and are beginning to be used as practical real-time applications. Most of the

real-time simulator vendors are now working to produce real-time versions of one of the advanced codes. The use of these codes will solve some of the problems while potentially introducing new problems. Since the current generation "best estimate" codes were developed to solve safety analysis questions on older computer platforms, they were optimized around different requirements. The next generation of thermo-hydraulic codes will need to be optimized based on a much wider set of requirements relating to the need for a more robust and flexible tool.

REQUIREMENTS FOR THE NEXT GENERATION OF THERMO-HYDRAULIC CODES

The primary justification for any major project such as the development of a new generation of thermo-hydraulic codes needs to be the resolution of unmet user needs. One class of real-time applications for next generation code requirements will be event analysis. The next generation of codes will need to be able to better simulate events such as BWR oscillations, steam generator tube ruptures, PWR reactor coolant pump seal failure, cooldown by natural circulation, station blackout, BWR vessel thermal stratification, boron mixing during ATWS, pressurized thermal shock, and inter-loop blowdown. The current generation of thermo-hydraulic codes have been generally unable to analyze these and similar transients for which they were not designed. The next generation of thermo-hydraulic codes will need to be better at prediction than the current generation has been. The application of event analysis using near real-time simulation will likely expand in the future. The need to be able to run an event without modifying the code input deck or the code itself will require a more robust code that will be less dependent on "helping it through" the difficult parts of the transients. These event analyses will most likely be done by less experienced users that will require a more user friendly Graphic User Interface (GUI).

Another class of real-time application will be the expanded scope training simulator. As was discussed in the previous section, the current and next generation simulator will be used by reactor operations, emergency preparedness groups, accident management, maintenance planning, and any number of other plant organizations. The Japanese "IMPACT Super Simulator" project that is now under development has a specification that calls for a flexible system that can simulate any plant component or system at any time during an event. To do this, the plan is to have a flexible structure that will readily accommodate changes in calculational degree of detail, function and range of scale. The next generation of thermo-hydraulic code as a part of simulators like this will be required to provide information on a greatly expanded list of plant systems and parameters. The primary thermo-hydraulic codes must provide inputs to all of the other models required for the different areas of simulation (for example, much more detailed radiation tracking models, noncondensable gas models, and more explicit coupling to core, containment, and severe accident models).

Another class of requirements will come from the faster than real-time use of the code for emergency planners and severe accident users. These users require codes that will provide them with information on the state of the primary system at much greater than real-time speeds, so that long time frame transients can be evaluated both off line and in faster than real-time mode to provide the decision maker with information to assist them in making

decisions. These users require that the code to be capable of various levels of complexity (depth as well as breadth of the models) to suit the needed levels of accuracy and speed for the application.

Another class of requirements will come from the PRA practitioners who will increasingly use real-time simulation for evaluating PRA success criteria in near real-time to validate PRA results for specific configurations and plant system unavailabilities. With enhanced use of PRA in plant operations, many plants are now using real-time risk meters as a tool in planning the on-line maintenance for the plant. As more and more real-time operational decisions are based on these risk-based tools, the need to understand and evaluate the thermo-hydraulic assumptions and criteria used by them will be expanded for both the plants and the regulator. The users of these analysis tools will be much less experienced than the traditional users, and the requirements that they will impose on the codes for evaluation of new plant configurations will call for time step and nodalization insensitivity that is much greater than the current generation of codes.

Some of the key requirements for the next generation of thermo-hydraulic codes should include:

- Robustness, reliability and repeatability to permit code runs that can run to completion with high reliability without the need for prior knowledge of the unique aspects of the transient,
- Much improved user interface that will permit all classes of users to obtain technically defensible results,
- Large improvements in time step and nodalization insensitivity over the current generation of codes,
- Improved time step control,
- Better configuration management and assessment,
- Strong and easy to understand documentation,
- Ability to model important phenomena that the current generation of code can not, and
- Ability to tailor the level of detail and speed of the code to the application.

CONCLUSIONS

Development of the next generation of thermo-hydraulic codes will require a strong commitment to identify and address all important user needs. For this reason, user input and evaluation should be done in a continuous manner and also be built into any plans for development at important discussion points. The needs for a new generation of thermo-hydraulic codes are clear. The efforts of the thermo-hydraulic community in developing these new generation codes should be clearly focused in meeting the requirements that have been and will be set forth by the users.

REFERENCES

S. A. Arndt, "Simulations and Simulators—Their Role in Science and Society" Encyclopedia of Microcomputers, Volume 15, Marcel Dekker, Inc. 1995

K. Vierow, et al, "The IMPACT Super Simulator - Basic Framework", Proceedings of the Society for Computer Simulations, Volume 27, Number 3.

K. D. Nguyen, et al, "The Use of Transient Simulations to Resolve Control Systems Issues at the Palo Verde Nuclear Generating Station", Proceedings of the Society For Computer Simulations, Volume 27, Number 3.

R.J. Beelman and A. Ashok, "RELAP5/MOD 3.2 R/T: Real-Time Best-Estimate Neutronics/Thermal-Hydraulics for Simulators", Proceedings of the Society For Computer Simulations, Volume 28, Number 2.

C. M. Allison and D. L. Hagrman, "SCDAPSIM Reactor Systems Analyzer for Design and Beyond Design Bases Accident Conditions", Proceedings of the 5th International Conference on Simulator Methods in Nuclear Engineering, Montreal, Canada, Sept. 8-11, 1996.

OECD/CSNI

Workshop on Transient Thermal- Hydraulic and Neutronic Codes Requirements

*Annapolis-MD-USA-
5-8 Nov. 1996*

SUMMARY OF PAPERS ON INTERFACE REQUIREMENTS TO COUPLE THERMAL-HYDRAULICS CODES

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OUTLINE

- 1. INTRODUCTION : Coupling why ? how ?
- 2. REVIEW OF DIFFERENT DOMAINS :
 - 2.1 T/H - REACTOR PHYSICS
 - 2.2 T/H - SEVERE ACCIDENTS
 - 2.3 T/H - CONTAINMENT
 - » Data exchange
 - » Coupling schemes
 - » Time synchronization
- 3. REQUIREMENTS FOR INTERFACES
- 4. COMMON SCHEMES
- 5. CONCLUSIONS

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COUPLING : WHY ?

■ **COMPLEX PROBLEMS INVOLVING SOLUTION OF THERMAL-HYDRAULICS WITH OTHER DISCIPLINES :**

- Reactor physics.
- Chemistry, metallurgy and mechanics (severe accidents)

OR BETWEEN ADJACENT DOMAINS (PRIMARY SYSTEM AND CONTAINMENT)

■ **DIFFERENT DISCIPLINES → DIFFERENT RESOLUTION METHODS :**

- Physical models
- Spatial resolution
- Time discretization
- Algorithms
- Validation matrices

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COUPLING : HOW ?

■ **THE "OLD" WAYS :**

- EXTERNAL ITERATIONS BETWEEN CODES : TIME CONSUMING → LIMITED NUMBER OF ITERATIONS.
- INTEGRATED CODE :
 - » Large inertia to new developments
 - » Low reusability
 - » Maintenance

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THERMAL-HYDRAULICS REACTOR PHYSICS

NEEDS : ANALYZE SPECIFIC ACCIDENT SEQUENCES

- PWR, VVER :
 - » Boron Dilution Accidents
 - » Anticipated transients without scram
- BWR : Nuclear coupled T/H instabilities induced by seismic waves (HIRANO,JAERI)
- RBMK

COUPLING WHAT ?

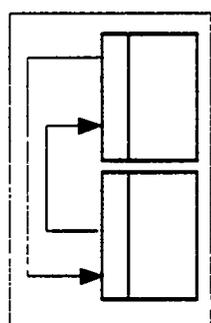
- Thermal-Hydraulics system code
- Reactor physics code :
 - » Neutron diffusion equation
 - » Multigroup
 - » 3D
- Thermal-Hydraulics : Detailed subchannel analysis

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COUPLING : HOW ?

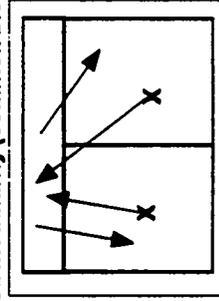
THE NEW TENDENCIES :

- MERGING SEPARATE PROCESSES :
 - » Minimizes code modification
 - » Generates data exchanges between processes
 - » Parallel execution possible



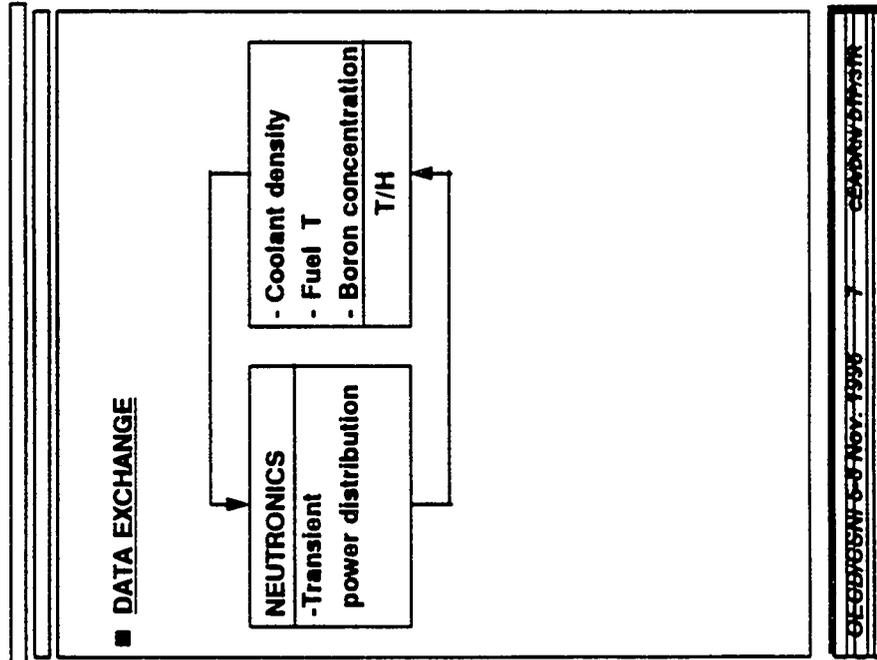
STATIC LINKING :

- » Avoids large data transfers
- » Reduced modularity (common blocks)



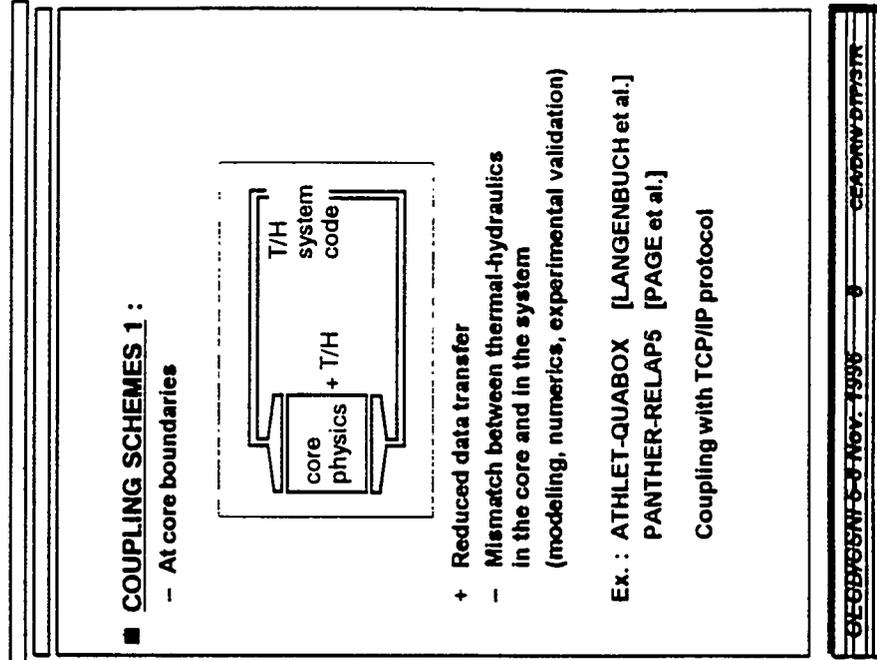
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THERMAL-HYDRAULICS REACTOR PHYSICS (2)



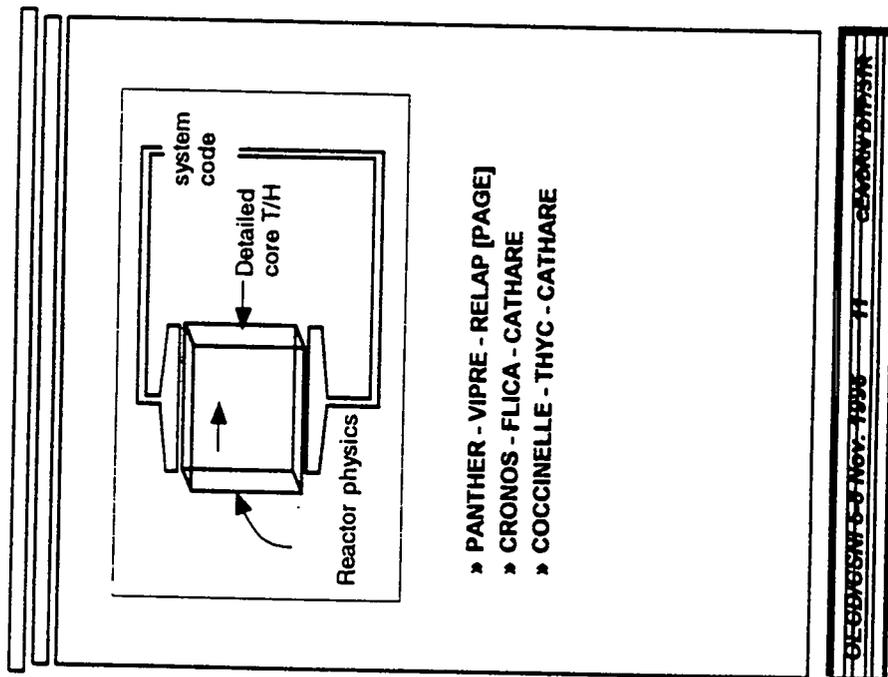
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THERMAL-HYDRAULICS REACTOR PHYSICS (3)



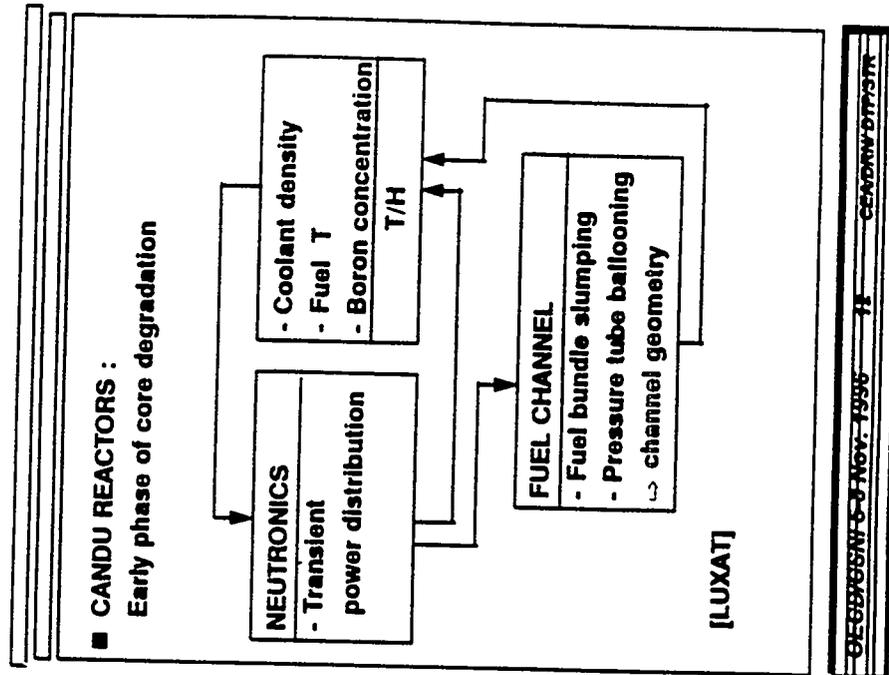
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T/H - REACTOR PHYSICS DETAILED CORE T/H



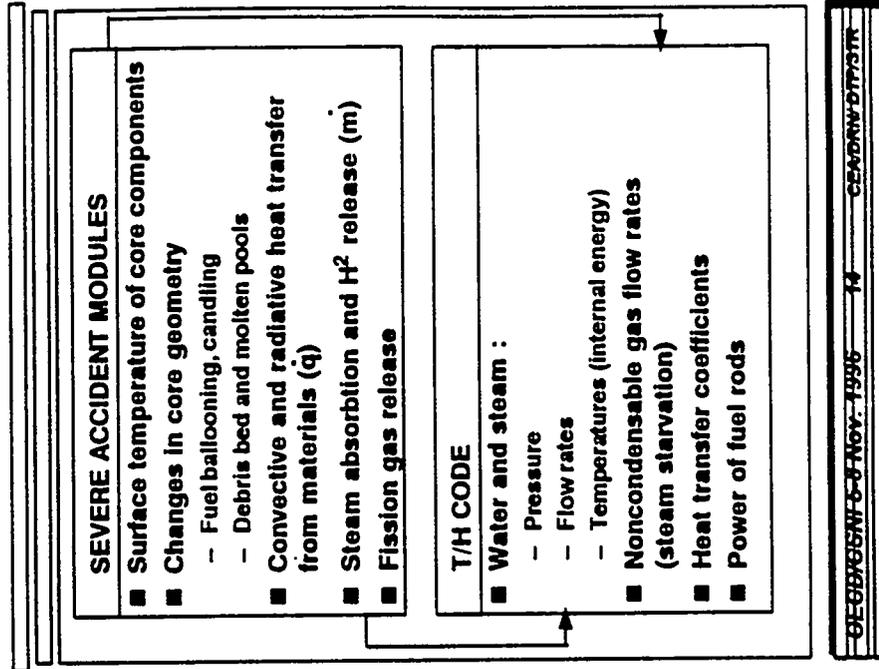
DESIGN/5-3 Nov. 1996 11 GEN/04/07/37A

T/H - REACTOR PHYSICS FUEL CHANNEL



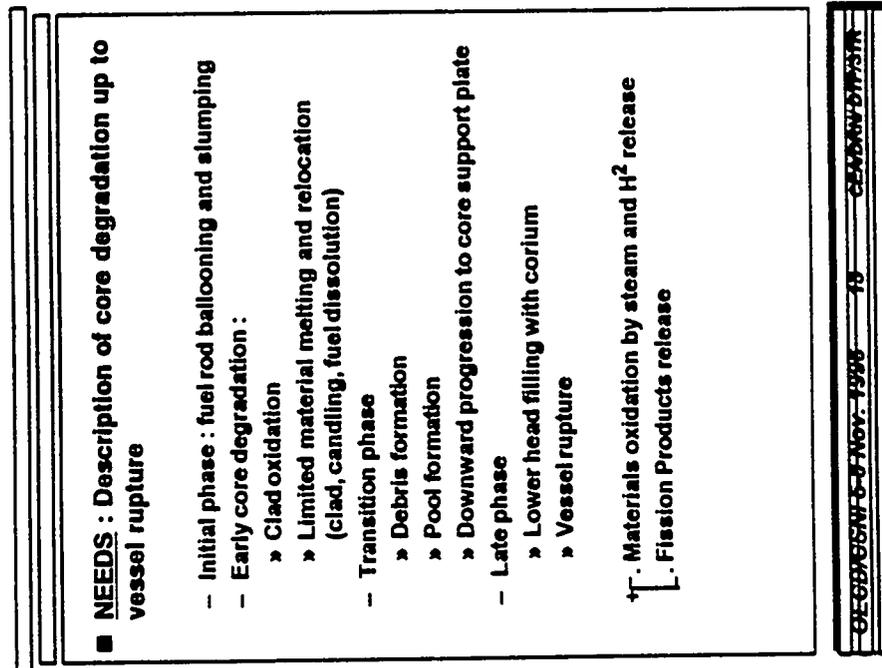
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DATA EXCHANGE (VERY SIMPLIFIED)



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T/H - SEVERE ACCIDENTS



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T/H - SEVERE ACCIDENTS

COUPLING SCHEMES

- SCDAP/RELAP [ALLISON] :
 - SCDAP : core degradation and material progression down to support plate
 - COUPLE : corium behavior in lower head and vessel failure
 - RELAP : transport of fluid & reactor kinetics
- DATA Exchange :
 - Via common blocks

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T/H - SEVERE ACCIDENTS (2)

COUPLING SCHEMES

- ATHLET CD [TRAMBAUER] :
 - ECORE : Core degradation (heat up, oxidation, melting)
 - EFIPRE : Fission products emission
 - TRAPG [SOPHAEROS] Fission products transport
- DATA EXCHANGE
 - Common blocks
 - Jacobian matrix for system including T/H variables and tightly coupled functions

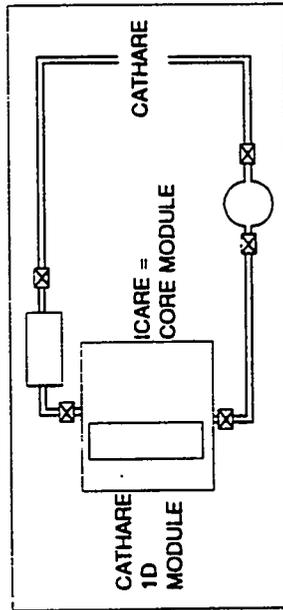
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T/H - SEVERE ACCIDENTS (3)

COUPLING SCHEMES

■ ICARE/CATHARE (CAMOUS) :

Nest of Russian dolls :



■ DATA EXCHANGE

- Static link :
- CATHARE 1D ↔ materials (ICARE code module)
- "Compression" of Jacobian matrix of each module → relation between variables at junctions
- Solution of the Jacobian matrix of junction variables
- Solution of the internal variables

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T/H - SEVERE ACCIDENTS (4)

TIME SYNCHRONIZATION

- Ensure mass and energy conservation
- Loose coupling : data exchange at each time step
- Tight coupling : inclusion in the Jacobian matrix

	TC
RELAP/SCDAP	• Oxidation rates (energy)
ATHLET CD	• Convective HT • Oxidation rates
ICARE/CATHARE	• Heat transfer • Oxidation rates • Geometry changes

- Time control by T/H module
- Time-step reduction imposed by ICARE module for high rates (tight coupling)
- Subcycling and time-step reduction (ATHLET)

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CONTAINMENT CODE

- **NEEDS :**
 - Containment = ultimate heat sink
 - LOCA in PWR and BWR
 - Inadvertent operation of safety relief valves

- **DATA EXCHANGE**

CONTAINMENT
 - Pressure at breach
 - Heat flux to RCS

↑
 ↓

T/H
 - Mass flow rate
 - Enthalpy flow rate
 ... at breach

- **[BARATTA]**
 - ↗ Spatial refinements
 - ↗ Time scales (larger in containment with 0D models)

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RCS-T/H - CONTAINMENT CODE

COUPLING SCHEMES

- **1 SEPARATE PROCESSES (PSU)**
 - SCDAP/RELAP and CONTAIN
 - Interface routines by PVM (process management, data transfer)
 - Modification of routines in CONTAIN to enable communications (no change of physical models)

- **2 INTEGRATION**
 - RELAP and COCO] (SIEMENS)
 - RELAP (EUMOD (COCO))]
 - ↙ interface
 - CATHARE - Containment (CEA)

- **3 TIME SYNCHRONIZATION**
 - RCS - T/H time step
 - CPU time containment << CPU time RCS

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REQUIREMENTS ON INTERFACE

→ FOR SOFTWARE DEVELOPMENT

- **Minimize code modifications - Ensure code independence**
 - Modularity (local modifications)
 - Rules for data access
 - Gestion of algorithm conflicts
- **Minimize overhead for data transfer**
- **Allow parallel code execution (parallel computers, networked computers)**
- **Control interprocesses communications (Q/A)**
- **Avoid redundancy and ensure coherence of :**
 - Geometrical data
 - Physical properties
 - Models

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REQUIREMENTS ON INTERFACE

→ FOR USER

- **Pilot initialization (input deck, ...)**
- **Control iterations (steady state) or time integration**
- **Specify to external codes :**
 - WHICH variables to transfer
 - WHEN
- **Process the data transferred**
- **Change when appropriate**
- **Handle software exceptions**

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REQUIREMENTS ON INTERFACE

- **FOR THE PHYSICAL RELEVANCE OF SIMULATION**
- **Conserve mass and energy**
- **Transfer data in a temporally consistent manner ($\psi = h\Delta T$)**
- **Respect relevant frequencies (oxidation rates)**
- **Accurate projections between different meshes**
- **Take into account geometry changes in T/H**
 - Severe accidents

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COMMON SCHEMES

- **STATIC LINKING :**
 - No overhead for data transfer
 - But
 - » reduced modularity
 - » Local change requires understanding module architecture
 - » Exponential increase of complexity with module size
 - » Much cross-checking required (algorithms conflicts, data storage)
- **MERGING SEPARATE PROCESSES**
 - Minimal code modifications
 - Parallel code execution
 - Time step management required
 - But :
 - » overhead for data

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COMMON SCHEMES

→ "MERGING SEPARATE PROCESSES"

as far as possible

- Limit : phenomena involving
- Tight coupling
 - and
 - large volumes of data transfer

Ex. :

- T/H neutronics coupled on a core-wide basis
- Some phenomena in severe accidents :
oxidation, ...

→ STATIC LINKING OF THESE PHENOMENA :

- Modified modules
- Modified iterative solution

Ex. :

- Simplified core physics included in T/H
- ICARE = new core module of CATHARE
- ATHLET - CD = inclusion in Jacobian matrix

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CONCLUSIONS (1)

■ Applications involving different disciplines :

Best estimate approach → coupling of different codes

■ Requirements 1 : Optimization :

- Computer time overhead
- Development and maintenance costs
- User's efficiency (tools, ergonomy)

■ Requirements 2 : Physical relevance of coupling :

- Conservation of mass, energy, momentum
- Respect of relevant frequencies

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THERMAL HYDRAULIC-SEVERE ACCIDENT CODE INTERFACES FOR SCDAP/RELAP5/MOD3.2^a

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ABSTRACT

The SCDAP/RELAP5 computer code is designed to describe the overall reactor coolant system thermal-hydraulic response, core damage progression, and fission product release during severe accidents. The code is being developed at the Idaho National Engineering Laboratory under the primary sponsorship of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission.

The code is the result of merging the RELAP5, SCDAP, and COUPLE codes. The RELAP5 portion of the code calculates the overall reactor coolant system (RCS), thermal-hydraulics, and associated reactor system responses. The SCDAP portion of the code describes the response of the core and associated vessel structures. The COUPLE portion of the code describes the response of lower plenum structures and debris and the failure of the lower head.

The code uses a modular approach with the overall structure, input/output processing, and data structures following the pattern established for RELAP5. The code uses a building block approach to allow the code user to easily represent a wide variety of systems and conditions through a powerful input processor. The SCDAP portion of the code uses a similar approach. The user can represent a wide variety of experiments or reactor designs by selecting fuel rods and other assembly structures from a range of representative core component models, and arranges them in a variety of patterns within the thermal-

a. Work supported by the U.S. Nuclear regulatory Commission, Office of Research, under DOE Contract No. DE-AC07-76IDO1570

hydraulic network. The COUPLE portion of the code uses two-dimensional representations of the lower plenum structures and debris beds.

The flow of information between the different portions of the code occurs at each system level time step advancement. The RELAP5 portion of the code describes the fluid transport around the system. These fluid conditions are used as thermal and mass transport boundary conditions for the SCDAP and COUPLE structures and debris beds. In turn, the SCDAP and COUPLE portions of the code describe the geometry of the core and other vessel structures, heat transfer to the fluid, and mass transfer between the fluid and the structures.

INTRODUCTION

The SCDAP/RELAP5 computer code is the result of merging the RELAP5,¹ SCDAP, and COUPLE² models. The objective of this coupling is to provide the capability in a single mechanistic code to calculate the complex physical phenomena that can occur during a severe core melt accident in a nuclear reactor. The resulting code is capable of describing the overall reactor coolant system (RCS) thermal-hydraulic response, core damage progression, and fission product release during severe accidents.

The RELAP5 portion of the code calculates the overall RCS system response including the transport of fluid through the system, control system behavior, reactor kinetics, and heat conduction in lower temperature vessel structures and RCS piping and structures. The SCDAP portion of the code calculates the heatup and damage progression in the core and surrounding structures including the upper plenum structures, shroud, and lower core plate. This portion of the code describes the (a) heating, deformation, oxidation, and melting of fuel rods, control rods/blades, and other structures, (b) formation, heating, and melting of debris, and (c) the formation, growth, and relocation of molten pool materials. The COUPLE portion of the code describes (a) the accumulation, heating, and melting of debris and associated lower plenum structures, (b) the formation and growth of molten pools, and (c) the failure of the lower head due to thermal and creep rupture mechanisms. The code is being developed at the Idaho National Engineering Laboratory (INEL) under the primary sponsorship of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission (NRC). The currently released version of the code is SCDAP/RELAP5/MOD3.1.³ Work is underway on a developmental version of the code, SCDAP/RELAP5/MOD3.2.⁴

GENERAL CODE CAPABILITIES

SCDAP/RELAP5 is capable of modeling a wide range of system configurations from single pipes to different experimental facilities to full-scale reactor systems. The configurations can be modeled using an arbitrary number of fluid control volumes and connecting junctions, heat structures, core components, and system components. Flow areas, volumes, and flow resistances can vary with time through either user-control or models that describe the changes in geometry associated with damage in the core. System structures can be modeled with RELAP5 heat structures, SCDAP core components, or SCDAP/COUPLE debris models. The RELAP5 heat structures are one-dimensional models with slab, cylindrical, or spherical geometries. The SCDAP core components are two-dimensional structures and include representative light water reactor (LWR) fuel rods, Ag-In-Cd and B₄C control rods and/or blades, electrically heated fuel rod simulators, and general structures. The SCDAP debris models are used in the core region and use a lumped parameter approach to describe the behavior of the debris within a thermal-

hydraulic volume. The COUPLE debris model uses two-dimensional, finite elements with a user-defined mesh to include any structures and thermal-hydraulic volumes within the RCS. However, the model is typically used to represent the lower plenum regions of the vessel and the accumulation of debris from the core and upper regions of the vessel. Models to describe selected processes, such as reactor kinetics, control system response, and tracking non-condensable gases, can be invoked through user control.

SCDAP/RELAP5/MOD3.1 was released in 1995. This version contained a number of significant improvements since the initial version of SCDAP/RELAP5/MOD3 was released. These improvements included the addition of several new models to describe the earlier phases of a severe accident, changes in the late phase models to provide more "physically intuitive" behavior for full plant calculations, and changes to improve the overall reliability and usability of the code. The improvements in the early phase models included the addition of models to treat (a) the effects of grid spacers including the effects of Inconel spacer grid-zircaloy cladding material interactions, (b) BWR B₄C control blade-zircaloy channel box material interactions, and (c) accelerated heating, melting, and hydrogen generation during the reflood of damaged fuel rods. The most significant changes to the late phase models included an extension to the molten pool models to treat the sporadic growth of the boundaries of the molten pool into adjacent regions and structures. Improvements in overall reliability and usability of the code for plant calculations included changes in the overall code numerics to enhance numerical stability and reduce code failures, and changes in the codes input/output processors. The most noticeable of these for the code users was the conversion of the SCDAP input to a form more compatible with the RELAP5 style. In addition, SCDAP/RELAP5/MOD3.1 was also subjected to (a) an intensive effort of verification testing to identify and resolve outstanding code errors, and (b) a systematic assessment of the code to quantify uncertainties in the predicted results.

SCDAP/RELAP5/MOD3.2 is the current developmental version of the code and will contain several late phase modeling improvements recommended by an NRC established independent review group which published its final recommendations in January 1993.⁵ The MOD3.2 late phase model improvements include: (a) molten pool formation, growth, and crust failure, (b) the melting and failure of upper plenum structures, and (c) improvements in the modeling by COUPLE of lower plenum debris behavior and the potential for failure of the lower head. In addition, the MATPRO material properties library⁶ and associated physical models will be updated to include the effects of several material interactions not currently considered.

MODULE INTERFACES

Common blocks are used to exchange information between COUPLE, SCDAP, and RELAP5. The exchange of information occurs at every time step.

The variables calculated by SCDAP and COUPLE and passed on to RELAP5 are: (a) surface temperatures of SCDAP core components and COUPLE combined debris beds and structures, (b) heat transferred to the fluid by radiation from intact heat structures, (c) changes in flow area and hydraulic diameter, (4) rate of consumption of steam and the corresponding production of hydrogen, (5) release of fission gases such as Xe and Kr, and (6) heat transferred from porous debris to fluid in contact with the porous debris, heat transferred from a molten pool to fluid, and heat transferred from slumping core material to fluid.

The surface temperatures of core components and lower plenum debris beds and structures are used by RELAP5 to calculate the convective heat transfer between the structure/debris bed surfaces and the vapor and liquid phases of the vapor. These, in turn, are used to compute the volumetric vapor generation rate at each surface. The surface temperatures of core components are passed to RELAP5 for each axial node of each component of the reactor core. The surface temperatures of the lower plenum debris and structures are passed for each finite element in contact with the fluid. The heat transferred by radiation from the surfaces of SCDAP and COUPLE heat structures to the fluid interfacing with these heat structures is also calculated by SCDAP and COUPLE. This energy is then included in calculation of the internal energy and temperature of the fluid interfacing with these structures.

The degradation of the reactor core has a significant impact on the flow of coolant through the region of the reactor core and the region of the lower head. The flow areas, volumes, volume lengths, and hydraulic diameters of RELAP5 control volumes in the core region and lower head are adjusted by SCDAP to account for the changes in geometry caused by fuel rod ballooning, fuel rod and control rod meltdown, fragmentation of embrittled fuel rods, and slumping of core material to the lower head of the reactor vessel. The junction areas in both the axial and lateral directions are adjusted.

The RELAP5 volumetric source term for steam and non-condensable gases is adjusted in the SCDAP core component routines to account for the production of hydrogen by the oxidation of the reactor core, the removal of steam by the same process, and the release of fission gases from fuel rods. These source terms are updated by SCDAP at each time step for each axial node of each core component.

The SCDAP debris bed models modify the hydrodynamic conditions in associated thermal-hydraulic volumes to account for the heat transferred from porous debris to fluid, the heat transferred from the outer surface of a molten pool to the fluid in contact with the molten pool, and the heat transferred from slumping debris that breaks up.

RELAP5 calculates several variables that are transferred to SCDAP to calculate the behavior of the reactor core including (a) the power in each fuel rod component, (b) the heat transfer coefficient for the vapor and liquid phases, (c) the vapor and liquid temperatures, (d) the rate of mass transfer of steam through the boundary layer at the surface of SCDAP components, (e) the volume fraction of liquid, (f) vapor and liquid specific enthalpy and other thermodynamic and transport properties, and (g) pressure. Fuel rod power has three components - (a) fission, (b) fission product decay, and (c) actinide decay. The mass transfer rate of steam is used by the SCDAP oxidation routines to establish a vapor diffusion limit for oxidation. The liquid volume fraction and fluid thermodynamic and transport properties are used by SCDAP to calculate the heat transfer from porous debris to fluid, heat transfer from a molten pool to fluid, and heat transfer from slumping material to fluid. The fluid pressure is used by SCDAP to define a boundary condition in the fuel rod ballooning model and to define a boundary condition in the model for creep rupture of the lower head and other structures.

The RELAP5 portion of the code was extended in several areas in order to treat unique conditions associated with severe accidents - (a) fluid properties were extended to account for temperatures above the melting point of the fuel and the presence of non-condensable gases, (b) fluid conservation and constitutive models were modified to account for the transport of hydrogen, fission gases, and aerosols, time-dependent changes in the geometry of the vessel structures, the transport of molten core material, and the presence of porous debris beds, and (c) models were added to account for the diffusion of steam through a gas

boundary layer and for surface-to-surface and fluid radiation heat transfer. The reactor kinetics models were also modified to incorporate the feedback from the heatup of SCDAP fuel rod components in the core.

CODE ARCHITECTURE

The code is developed using a modular approach with the overall structure, input/output processing, and data structures following the pattern established for RELAP5. These features are discussed in the following subsection.

Code Structure

SCDAP/RELAP5 is coded in a modular fashion using a top-down structure. The various models and procedures are isolated in separate subroutines. Figure 1 shows an overview of the code structure by major subroutine name. Input processing is performed in INPUTD and associated lower level subroutines. Transient control is performed by TRNCTL and associated subroutines. The STRIPF routine extracts data from the restart plot file for use in other computer programs. Because of their complexity, the input processing and transient control routines are described in more detail in the following paragraphs.

The input processing is performed in three phases. In the first phase, the input data is read and checks are made for typing and punctuation errors (such as multiple decimal points and letters in numerical fields), and stores the data keyed by line number so that the data are easily retrieved. A listing of the input data is provided, and punctuation errors are noted. During the second phase, restart data from a previous simulation are read if necessary and all input data are processed. Some processed input is stored in fixed common blocks, but the majority of the data are stored in dynamic data blocks that are created only if needed by a problem and sized to the particular problem. Extensive input checking is performed on the new input data being processed. The third phase of processing begins after all input data have been processed. Because all data have been placed in common or dynamic data blocks during the second phase, complete checking of interrelationships can proceed. An example of cross-checking is a check on the existence of hydrodynamic volumes referenced in junctions and heat structure boundary conditions. The initialization required to prepare the model for start of transient advancement is done at this level.

The transient routines controlled by TRNCTL performs the following functions. TRNSET sets up dynamic blocks required for transient execution, performs final cross-linking of information between data blocks, sets up arrays to control the sparse matrix solution, establishes scratch work space, and returns unneeded computer memory. TRAN controls the transient advancement of the solution. The subroutine TRNFIN releases space for the dynamic data blocks that are no longer needed and prints the transient timing summary. Table 1 describes selected lower level routines controlled by TRAN.

CONCLUSIONS

The merging of SCDAP, RELAP5, and COUPLE has been accomplished by maintaining close control and rigor in adhering to the established architecture of the combined code. The modular approach used has been successful in ensuring that code modifications and additions are accommodated without negatively impacting code performance or introducing unnecessary errors. In the process of merging the codes, however, some valuable lessons were learned that should be considered in future development

efforts. During the initial code development, close attention was paid to ensure clean and consistent interfaces between modules. Individual modules were developed by a relatively small core group of developers who worked closely together and received direct feedback on code errors and performance anomalies from code users at the INEL. The result of this early process was a state-of-the-art general purpose code that included mechanistic models incorporating the latest available experimental information from thermal-hydraulic and severe accident programs being conducted around the world. However, limited funding and the emphasis on model development and code performance resulted in less attention being paid to code usability and the user interface.

As the user base increased, the importance of the user interface became increasingly apparent. In particular, since the SCDAP and RELAP5 codes used different style input, a great deal of effort was spent in resolving user problems associated with errors or misinterpretation of differences in input and output between the two codes. These difficulties ultimately led to the conversion of the SCDAP portion of the input to a form more compatible with the RELAP5 input style. In addition, code reliability and usability was improved by incorporating much more intensive input error checking to verify input consistency and input data ranges.

Expansion of the code user community also resulted in more individuals and organizations contributing to the development of code models. To maintain code integrity, a very rigorous code configuration control system was established at the INEL, and formal guidelines for developing and modifying individual code modules were defined. These guidelines were published in a SCDAP/RELAP5 programmers manual⁷ describing acceptable practices for implementing new models into the code. Examples of acceptable practices included ensuring all material properties correlations were defined within the MATPRO code library, accessing data directly from common blocks, recomputing local variables for each call of a subroutine, providing restart capability for all new models, and ensuring all new models were able to utilize the code time step repetition capabilities. These guidelines have clarified code development requirements for individuals and organizations developing models outside the INEL, and have made it easier for the INEL code development staff to implement and assess these new models.

Finally, expansion of the code modeling capabilities also involved some tradeoffs between simplification of code interfaces and code robustness. In some cases, changes in the numerical solution techniques or additional constraints on time step size and advancement were imposed when variables passed between SCDAP and RELAP5 were found to produce unstable or non-convergent results. These improvements in code numerics significantly lowered the cpu-time needed to perform a calculation. SCDAP/RELAP5/MOD3.1 is a faster running, more reliable version of the code than any previously released version. In addition, comparisons of predicted and measured results from numerous international experiments simulating the early phases of severe accidents show that the variation between the calculated and measured behavior is typically less than ~ 20%. Similarly, full plant calculations and sensitivity studies performed in support of NRC direct containment heating and steam generator tube rupture issue resolution have demonstrated the robustness and reliability of the code over a wide range of severe accident conditions.

REFERENCES

1. RELAP5/MOD3 Code Manual, Volumes I through IV, NUREG/CR-5535, EGG-2596, DRAFT, June 1990.

2. E. C. Lemmon, COUPLE/FLUID A Two-Dimensional Finite Element Thermal Conduction and Advection Code, EGG-ISD-SCD-80-1, February 1980.
3. SCDAP/RELAP5/MOD3.1 Code Manual, Volumes 1-5, NUREG/CR-6150, EGG-2720, Idaho National Engineering Laboratory, June 1995.
4. SCDAP/RELAP5/MOD3.2 Code Manual, Volumes 1-5, Revision 1, NUREG/CR-6150, INEL-95/0609 (Formerly EGG-2720), Idaho National Engineering Laboratory, To be Published.
5. SCDAP/RELAP5 Independent Peer Review, Los Alamos National Laboratory report, LA-12481, January 1993.
6. SCDAP/RELAP5/MOD3.2 Code Manual, MATPRO-A Library of Materials Properties for Light-Water-Reactor Accident Analysis, Volume 4, Revision 1, NUREG/CR-6150, INEL-95/0609 (Formerly EGG-2720), Idaho National Engineering Laboratory, To be Published.
7. E. W. Coryell, L. J. Siefken, and R. J. Wagner, SCDAP/RELAP5 Programmers Manual, EGG-SSRE-9283, May 1994.

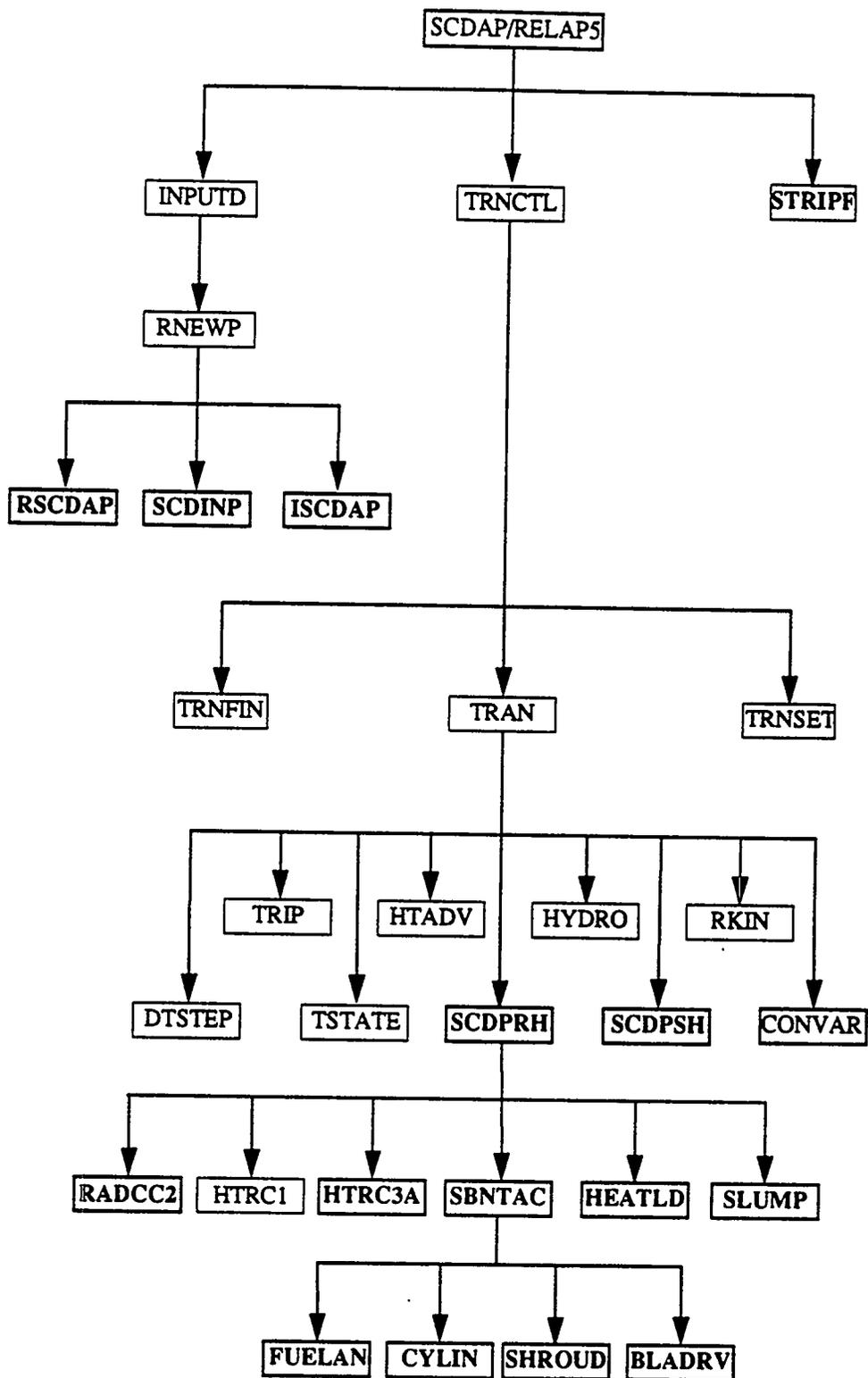


Figure 1. SCDAP/RELAP5 architecture with SCDAP specific routines highlighted.

Table 1. Selected transient subroutine functions.

Routine	Function
DTSTEP	Determines the time step size, controls output editing, and eliminates whether transient advancements should be terminated
TRIP	Evaluates logical statements. Each trip statement is a single logical statement that has a true or false result. The decision of what action is needed resides within the components in other modules.
TSTATE	Calculates the thermodynamic state of the fluid in each hydrodynamic user-defined time-dependent volume.
HTADV	Advances heat conduction/transfer solutions using previous-time-step reactor kinetics power and previous-time-step hydrodynamic conditions for computing heat transfer coefficients.
SCDPRH	Advances the heat conduction, mechanical response (including changes in geometry), and fission gas release models using previous-time-step hydrodynamic conditions. It is in this block that nearly all the SCDAP core components routines are exercised.
HYDRO	Advances the hydrodynamic solution.
SCDPSH	Drives the COUPLE subcode.
RKIN	Advances the reactor kinetics of the code.
CONVAR	Provides the capability of simulating control systems typically used in hydrodynamic systems. It consists of several types of control components.
RADCC2	Calculates the radiation heat transfer in a fuel bundle.
HTRC1	Computes heat transfer coefficients for the fluid.
HTRC3A	Calculates heat transfer from debris to coolant.
SBNTAC	Drives all SCDAP components.
HEATLD	Calculates the heatup of circulating liquefied debris contained by hardpan. The subroutine also calculates the thickness of the hardpan and spreading of the molten pool.
SLUMP	Determines whether a new unique slumping of core material into lower vessel region occurred during a time step. It calculates the total mass of material that will end up eventually falling into the lower vessel region due to this slumping.
FUELAN	Calculates the response of a LWR fuel rod component.
CYLIN	Calculates the response of an Ag-In-Cd control rod component.
SHROUD	Calculates the response of a shroud component.
B;ADRV	Calculates the response of the B ₄ C control blade/channel box component.

INTERFACE REQUIREMENTS TO COUPLE THERMAL HYDRAULICS CODES TO SEVERE ACCIDENT CODES : ICARE/CATHARE

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1. Introduction

In order to describe with the same code the whole sequence of severe LWR accidents, up to the vessel failure, the Institute of Protection and Nuclear Safety has performed a coupling of the severe accident code ICARE2 [1] to the thermalhydraulics code CATHARE2 [2]. The resulting code, ICARE/CATHARE, is designed to be as pertinent as possible in all the phases of the accident.

This paper is mainly devoted to the description of the ICARE2-CATHARE2 coupling.

2. Objective of the ICARE2-CATHARE2 coupling

In the frame of the PHEBUS SFD and FP programs and of the LWR severe accident safety analysis, IPSN has been working since 1988 on the development and validation of the mechanistic ICARE2 code.

This code is able, at present time, to describe - both in reactor cores and in experimental bundles - all the phenomena occurring during the early phase of the core degradation : thermal and mechanical behavior of the fuel and control rods (melting, ballooning,...), chemical interactions (Zr oxidation, UO₂ dissolution,...), thermalhydraulics (parallel multi-channels without cross flows), fission product release. For the late degradation phase, development of models for debris beds and molten pools is in progress.

The code has been validated on in-pile (PHEBUS SFD, PBF, ...) and on out-of-pile experiments (CORA) [3]. Moreover, calculations have been performed for the TMI2 reactor core degradation phase [4].

However, the ICARE2 description is limited to the core zone and the initial and boundary conditions at core inlet and outlet for an ICARE2 calculation of the degradation phase have to be provided by a system code.

The thermal hydraulics code CATHARE2 has been developed by CEA, IPSN, EDF and FRAMATOME since 1980 for PWR safety analysis. An extensive assessment work has been performed applying a two steps methodology : qualification of the closure laws on analytical experiments (more than 1000) including separate effects tests and component tests and verification calculations of integral tests (more than 30). This code is able to perform best estimate calculations of all thermalhydraulics transients involved by LWR accidental situations considered in safety studies. However its range of application is limited to transients involving no severe damage of fuel rods.

In order to overcome these limitations, it was decided to couple ICARE2 to CATHARE2.

3. Principle of the coupling

In the phenomenology of severe accidents, the accidental sequences can be divided into three phases : the initial phase where no severe damage of fuel or control rods and structures occurs, the early core degradation phase where limited material melting and relocation takes place and the late core degradation phase during which substantial material relocation happens, molten pools and debris beds can form and corium can fall into the lower plenum and, in case of vessel failure, come into the containment.

CATHARE2 is a system code which has been developed to describe the thermalhydraulics behavior of a whole PWR circuit during the first of these three phases of an accidental transient. It is a modular code. A circuit is represented by different elements which are connected to each other by junctions. In the present version, CATHARE2 V1.3U, the following modules are used to describe the circuit : a 1D pipe module (used to describe pipes or core channels), a 0D volume module (used to describe large size elements like the pressurizer, the accumulator, the steam generator dome or the lower plenum), a tee module to describe connections of pipes, a 1D pump module and a 2D downcomer module. In the next version, CATHARE2 V1.4, to be released before the end of 1996, a 3D module will be available to describe the vessel or the containment thermalhydraulics.

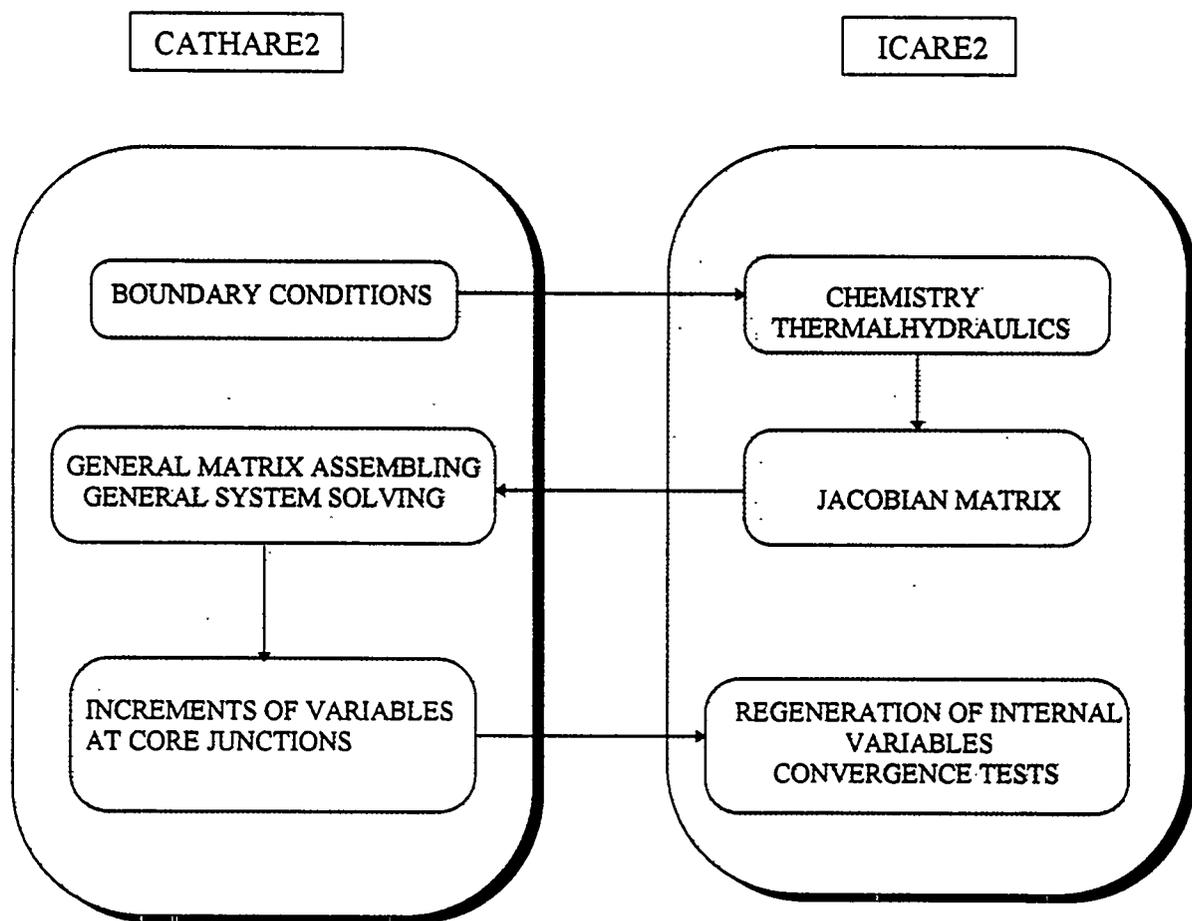
The two phase flow is calculated using a two fluid approach (6 equations for the 1D module, 10 equations for the 3D, plus if necessary transport equations for non condensable gases, boron and fission products).

A multi-layer wall module calculates radial conduction in the structures. A fuel pin module is used to calculate the thermo-mechanics of the fuel and clad. But the variation of the channel cross section induced by the deformation of the rods as well as chemical interaction are not taken into account in the thermalhydraulics calculation.

ICARE2 is aimed at the description of the core degradation phases.

The first versions of ICARE2, up to V2 mod 2, were mainly devoted to the description of the early core degradation phase. The following models were included : multichannel thermalhydraulics of a steam-non condensable mixture without cross flows (in case of channel blockage, flow redistribution is calculated only at the bundle inlet), thermal and mechanical behavior of fuel and control rods (with a detailed calculation of clad ballooning and rupture), clad and structures oxidation, chemical interactions (in fuel, control rods and spacer grids), conductive and radiative heat transfer between the materials at high temperature, melting and relocation of materials, fission product release, simplified description of a debris bed. The present version, V3 mod 0, also deals with molten pools and debris beds, thus allowing to calculate part of the late degradation phase. However, for the moment, the lower plenum is not described, so the corium fall into the lower head cannot be calculated.

ICARE2 (V3 mod 0) has been introduced into CATHARE2 (V1.3U) as a new CATHARE2 module. The ICARE2 "CORE" element (composed of one or several channels) is connected to adjacent CATHARE2 elements through junctions (2 for each core channel). A global description of the coupling principle is given in the scheme below.



CATHARE2 drives the calculation, giving to the ICARE2 channels like to the other elements the inlet and outlet boundary conditions. For each iteration of the Newton-Raphson method used to solve the global non linear system, the equations of each element are linearized. For the ICARE2 core, in which the CATHARE2 1D two phase 6 equations thermalhydraulics model has been implemented, this leads - like for the CATHARE2 core - to a block tri-diagonal system. Mass and energy equations applied between two (vector) nodes lead to a 4 (lines) \times 16(columns) block ; momentum equations applied between two (scalar) nodes lead to a 2 (lines) \times 16(columns) block. Then, in each CATHARE2 element and therefore in the ICARE2 core, the internal variables are eliminated and the contribution of each element to the general assembling matrix is calculated in terms of variations of junction variables. Thus the ICARE2 Jacobian matrix is calculated and sent to CATHARE2 which, after assembling the general matrix and solving the general system, returns to ICARE2 the variation of the main variables at core junctions (pressure, liquid and gas enthalpies, void fraction, non condensable gases fractions and liquid and gas velocities). The following phase is the regeneration phase where internal variable increments of each module are calculated from the junction variables increments. All the variables are then updated and convergence tests are performed.

The Jacobian matrix sent by ICARE2 to CATHARE2 and the CATHARE2 general assembling matrix are similar whatever the core module may be. The main differences come from the fact that ICARE2 uses temperatures instead of enthalpies, which implies changes in the derivatives and from terms in ICARE2 accounting for geometry changes and oxidation.

At each time step, the mass transfers (candling, chemical reactions) in ICARE2 are calculated once at the first iteration and a semi implicit solution of the thermalhydraulics is performed, in order to predict possible starvation effects knowing the oxygen shortage. Then, using known values of the mass transfers, the wall energy equations and the thermalhydraulics equations are simultaneously solved (by a Newton-Raphson method), giving the Jacobian matrices involving fluid variables increments at any core junctions. This procedure has been chosen, instead of performing all the calculations (chemistry, candling, thermics, thermalhydraulics) totally implicitly, to save computing time. This method works well except when large relocation or high oxidation rates take place during the time step. In this case a sub-cycling technique is used in order to reach successfully the end of the global time step (condition already fulfilled by both candling and chemical phases). For each sub-time step the Newton Raphson iterations are performed.

The ICARE2 wall to fluid coupling is totally implicit but thermics and thermalhydraulics are calculated in two separated modules, which, in principle, allows to replace easily the ICARE2 thermalhydraulics module by any other.

Convergence is declared when the increments of the wall temperatures and internal fluid variables are lower than threshold values.

At the end of the time step, ICARE2 calculates the final temperature, mass and chemical composition fields along with the final states of the walls, the new physical properties and fission products release. At last, a proposal is made for the value of the next time step. The criteria used to make this proposal are based on temperature variations during the last time step, number of necessary iterations to converge, ...

4. Work required by the coupling and difficulties encountered

As a first step in the coupling work, the CATHARE2 (V1.2E) 1D two phase thermalhydraulics model has been implemented into ICARE2, with three main differences. In ICARE2, the channel cross section is variable, to take into account the deformation and degradation of the structures. The enthalpies are replaced by the temperatures as main unknowns because these latter are considered as more convenient to test the convergence of the Newton-Raphson method. Additional terms have been added in the mass and energy balance equations to describe mass and energy exchanges between the fluid and the walls, due to oxidation. However, in ICARE2, the energy equations are written under the conservative form like in CATHARE2 V1.3U.

In CATHARE2, which is now the driver for the ICARE2 calculation, the time step management has been modified to take into account the possibility to activate a sub-cycling technique in ICARE2 in case of convergence problems.

It was also necessary to extend the CATHARE2 vapor and structures material properties to high temperatures.

The main difficulties, which were encountered during the coupling process, concerned :

- * the thermal coupling between walls and fluid : in CATHARE2, it is implicit. In the original ICARE2 single phase (vapor) thermalhydraulics model, explicit convective heat exchange coefficients were used. When the CATHARE2 two phase model was implemented into ICARE2, numerical problems were encountered using these explicit coefficients in the case of high void fraction changes during a time step. It was thus necessary to adopt implicit heat exchange coefficients.

- * the consideration of mass transfers (due to oxidation chemical reactions) and geometry changes (due to candling) in the thermalhydraulic calculation : the original CATHARE2 equations had to be modified to take such transfers into account. Convergence difficulties were met for high oxidation rates (in particular in the conditions of starvation) and important geometry changes (with a possible occurrence of channel blockages). These difficulties were solved by reducing the time step (imposing to CATHARE2 the ICARE2 time step proposal).

- * the treatment of the (liquid) residual phase : convergence problems were encountered when the void fraction α is very near to 1, specially with high fractions of non condensable gases. Convergence criteria had to be changed.

- * vapor properties at high temperatures : the CATHARE2 V1.3 laws were extended to high temperatures, but numerical difficulties were encountered when using these laws. Some work remains to be done on that problem.

- * management of sub cycling techniques.

- * consistency in convergence criteria (on temperature or enthalpy on both sides of the channel junctions).

5. Current status of the coupling and future work

At present time, a preliminary version of ICARE/CATHARE is available. Several tests in Large Break-LOCA situation have been performed to check the operability of this version and the relevance of its results during the whole accidental sequence. Some results are given in figures 1 to 6.

A comparison has been made, for the LOCA phase, between ICARE/CATHARE and CATHARE2 V1.3U results (figures 1 to 3). Differences appear, mainly on the gas temperatures, as soon as the void fraction exceeds 0.9. These differences are under examination at that time. The slightly different values of the void fraction calculated by the two codes are a consequence of the difference in numerical methods to calculate wall to fluid exchanges. This may lead to high differences in the critical flux which varies strongly when the void fraction goes from 0.9 to 1. This in turn results in different values of the wall to fluid heat fluxes and thus in different gas temperatures.

On figures 4 and 5, void fraction, hydrogen mass fraction and temperature profiles are shown for the whole duration of the accident.

An example of fuel and clad relocation is given in figure 6.

Future work will be performed in two directions :

- * development of a new ICARE/CATHARE version with an improved two phase thermalhydraulics model (CATHARE2 V1.4 3D model instead of the 1D, treatment of porous media (debris bed)). This version will allow to calculate the whole degradation phase of vessel structure, up to the possible vessel failure.

- * development of a simplified ICARE/CATHARE version (parallel multi-channel model without cross flows in the core, ICARE2 0D "VOLUME" based on the CATHARE2 0D "VOLUME", in order to calculate the corium fall into the lower plenum). This simplified version will allow to perform rapid calculations and thus for example sensitivity studies and uncertainty analysis.

A first version of this simplified version of ICARE/CATHARE, able to calculate the whole sequence of a severe accident in a LWR, without reflooding of the damaged core, is foreseen to be released in 1998.

To validate this version, calculations will be performed for the TMI2 accident (phases 1 and 2) and the LOFT FP2 test.

6. Structure and contents of thermalhydraulics codes required for coupling

Our present experience in coupling the severe accident code ICARE2 with the thermalhydraulics code CATHARE2, allows us to lay down some recommendations, concerning both structure and contents of the thermalhydraulics code, aimed at making easier further similar couplings.

A non-exhaustive list of requirements, to be taken into account in future specifications of thermalhydraulics codes, is supplied below:

6.1 Informatics and numerics

- * code modularity, allowing to easily access to the core zone, without affecting the other parts of the primary circuit,
- * use of standard programming languages (and simple programming rules), in order to insure code portability and distribution on any kind of computer,
- * robust numerical methods supporting the treatment of chemical interactions, starvation phenomena and residual phases, whatever the temperature (and partial pressures) range,
- * ability to use a sub-cycling technique in order to reach an imposed final time,
- * convergence tests performed on temperature increments instead of enthalpy ones (easier management in presence of non-condensable gases),
- * ability to solve the problem of implicit coupling between non-neighboring fluid cells (radiative heat transfers may couple fluid cells located in the core center with fluid cells located at other elevations in core periphery),
- * source terms (mass and energy) for the balance equations calculated in an independent routine (provision for an easy substitution of convective exchanges, addition of extra terms like those linked to oxidation processes, ...).

6.2 Physics

- * thermalhydraulics model dealing with any variation of fluid cross section versus time (ballooning, candling, ...) and occurrence of channel (or fluid cell) blockages,
- * balance equations written under the conservative form and using extensive variables (total mass, total energy),
- * balance equations able to deal with porous media,
- * suitable vapor and material physical properties operating satisfactorily at high temperatures,
- * vapor properties taking into account steam dissociation (above 2000 K), with a possible feedback on the calculation of heat transfer coefficients with walls.

7. Conclusion

A coupling of the thermalhydraulics code CATHARE2 with the severe accident code ICARE2, in order to be able to describe satisfactorily, with a unique code, the whole sequence of severe LWR accidents, up to the vessel failure, is under progress.

A preliminary version of this coupling is available at present time and tests are being performed to check the operability of this version and its pertinence during the whole accidental sequence. Validation work is underway.

Recommendations concerning structure and contents of future thermalhydraulic codes have been provided in this paper in order to make easier further similar couplings.

8. References

[1] R.GONZALEZ, F.JACQ, P.CHATELARD, F.FICHOT
ICARE2 : a tool for making fast running calculations on LWR core degradation
Workshop on Super Simulators
Tokyo, Japan, November 1994

[2] CATHARE TEAM
This Meeting

[3] R.GONZALEZ, B.ADROGUER, P.CHATELARD, J.C.CRESTIA
Status of the ICARE2 V2 code and overview of its validation
NURETH 6 Meeting, Grenoble, October 1993

[4] F.FICHOT, R.GONZALEZ, P.CHATELARD, B.LEFEVRE, N.GARNIER
ICARE2 late phase degradation models : application to TMI-2 accident
International Seminar on Heat and Mass transfer in Severe Reactor Accidents
Cesme, Turkey, May 1995

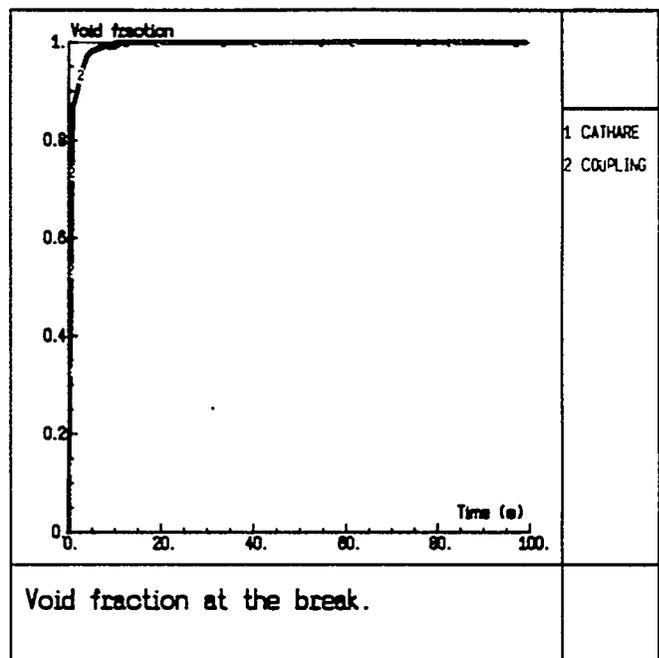
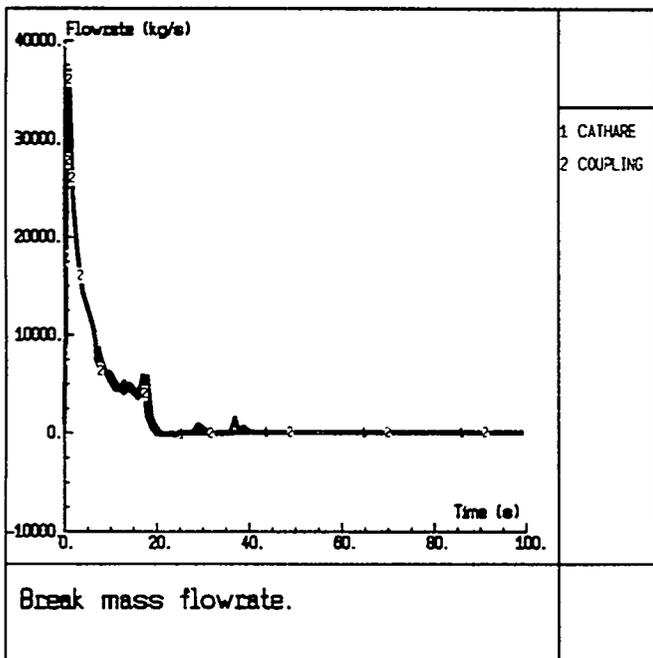
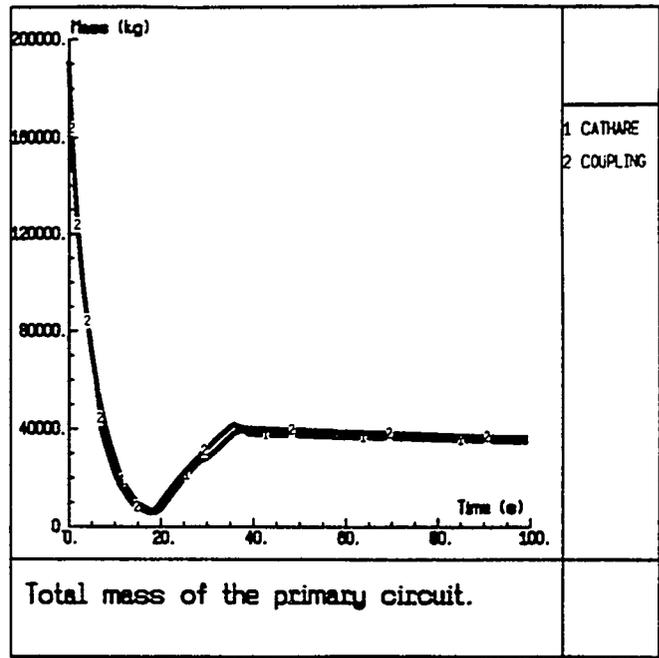
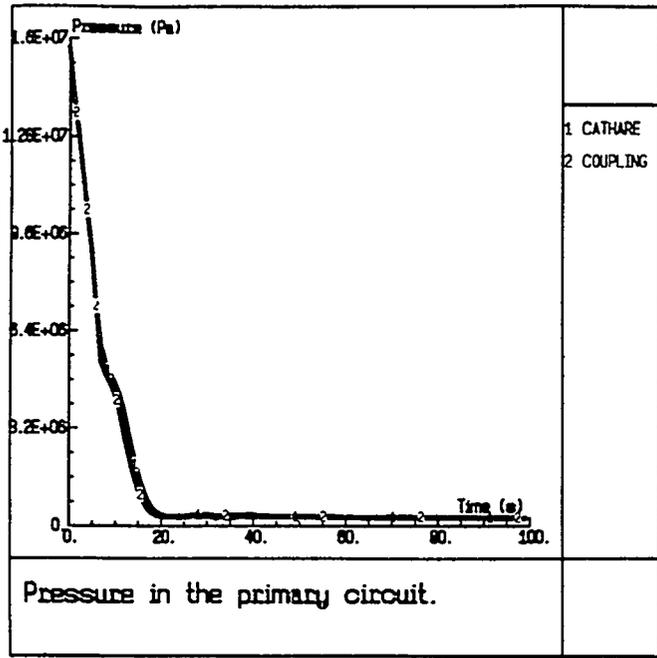


Fig. 1 : Large Break LOCA – Comparison of ICARE/CATHARE and CATHARE V1.3U results during the LOCA phase

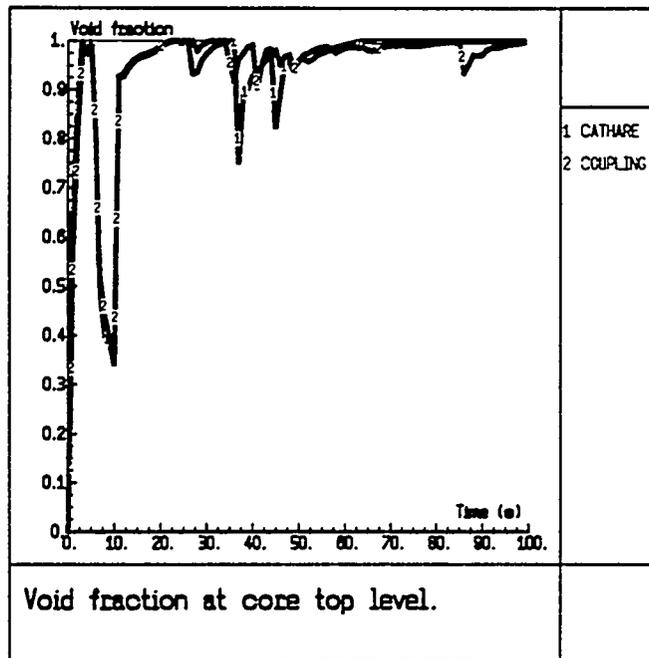
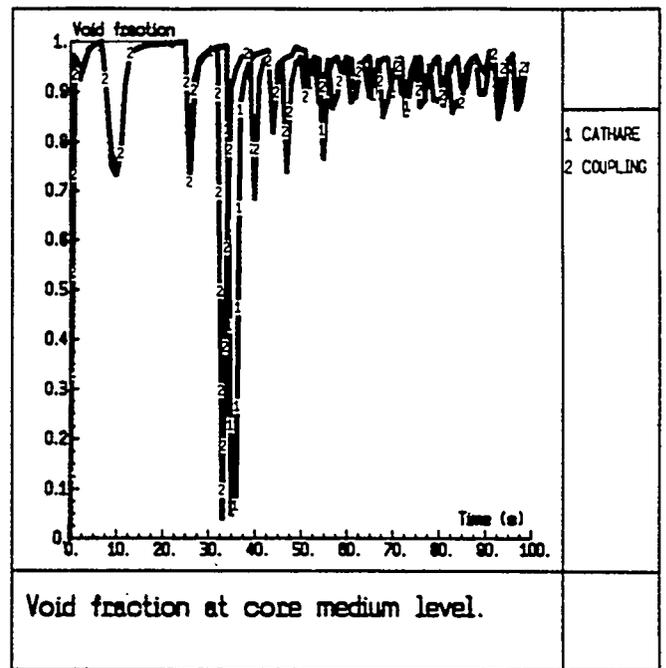
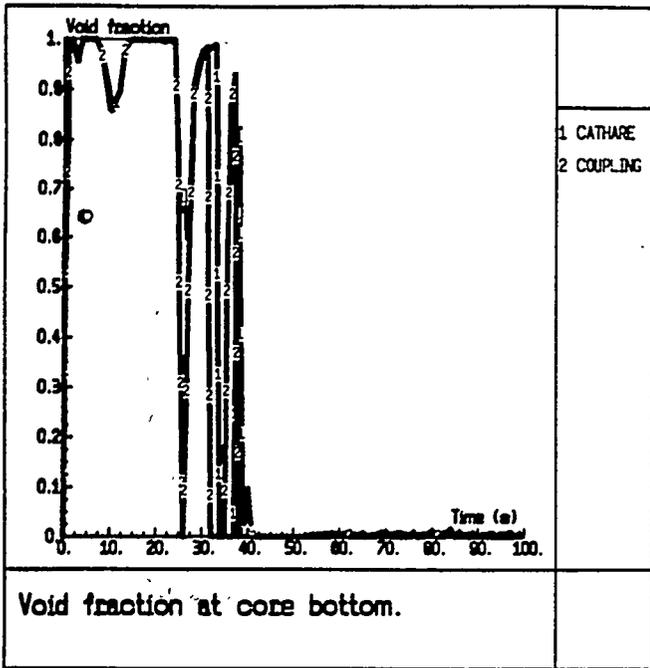


Fig. 2 : Large Break LOCA – Comparison of ICARE/CATHARE and CATHARE V1.3U results during the LOCA phase

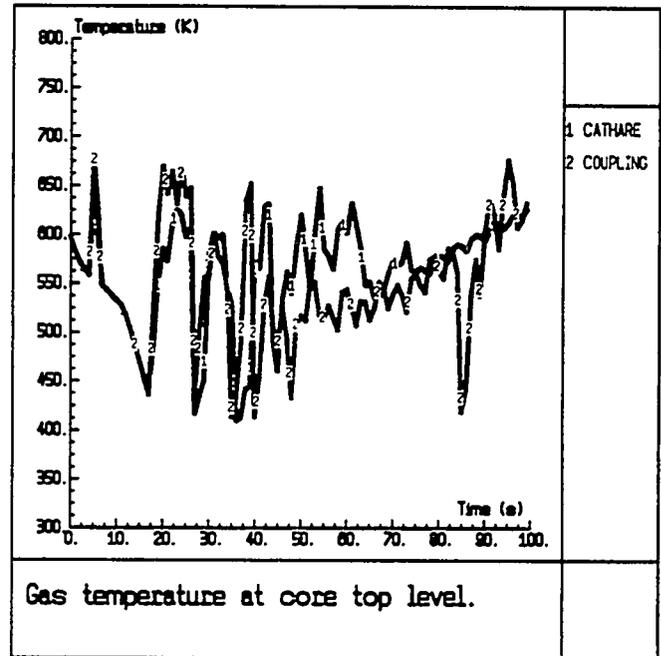
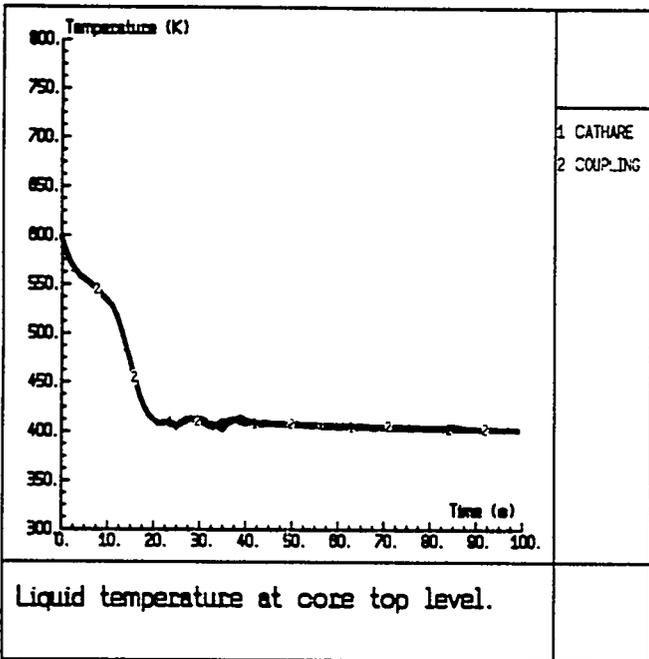
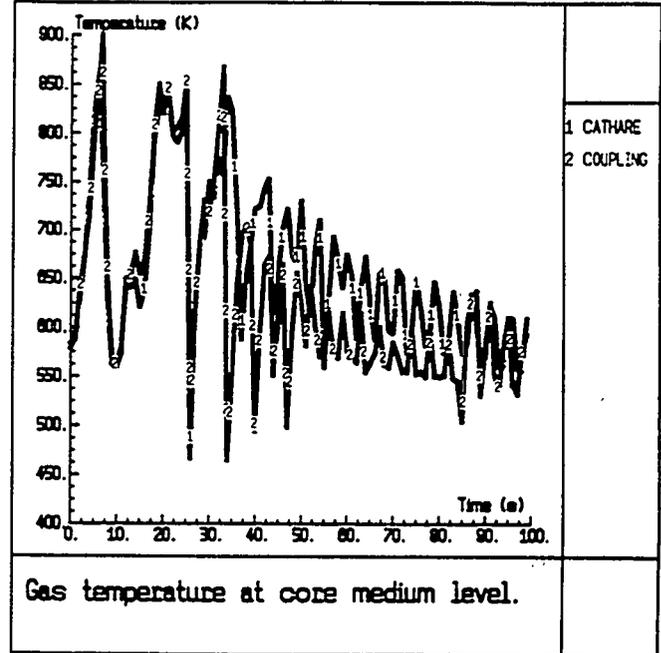
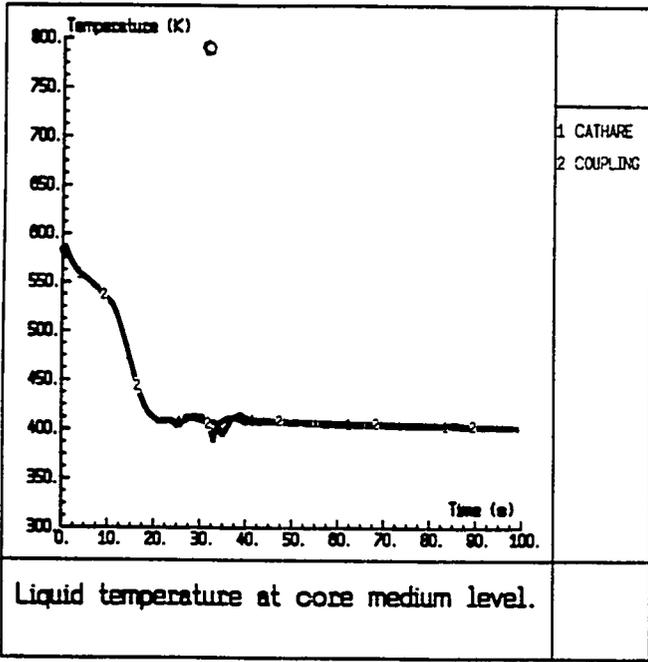


Fig. 3 : Large Break LOCA – Comparison of ICARE/CATHARE and CATHARE V1.3U results during the LOCA phase

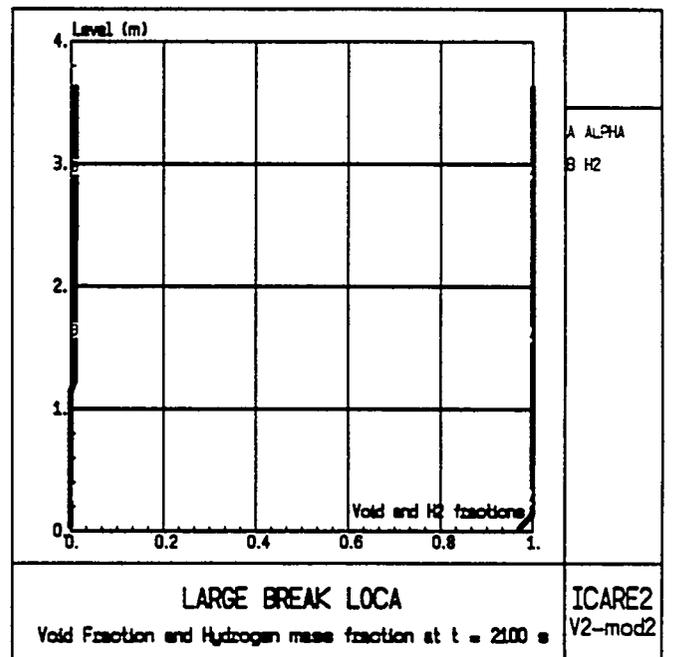
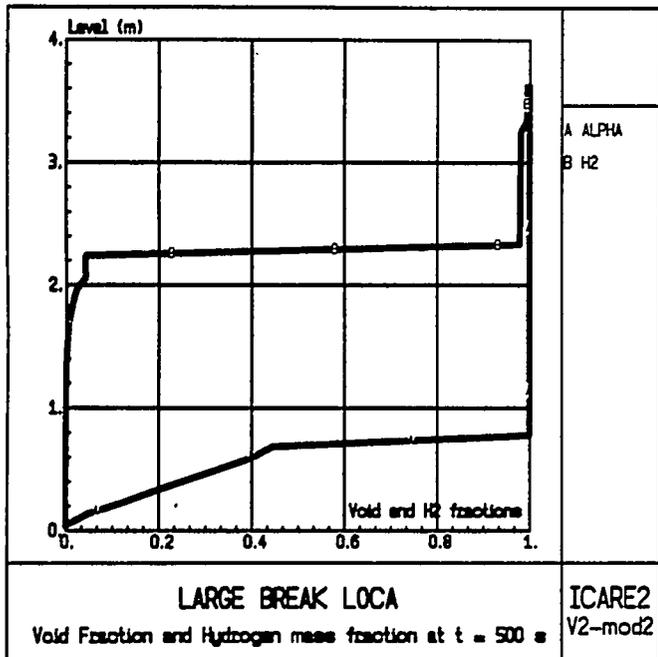
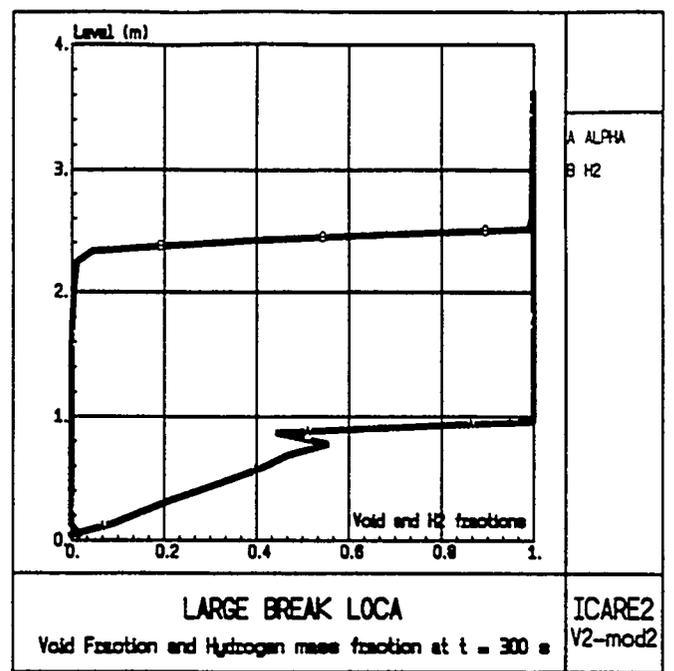
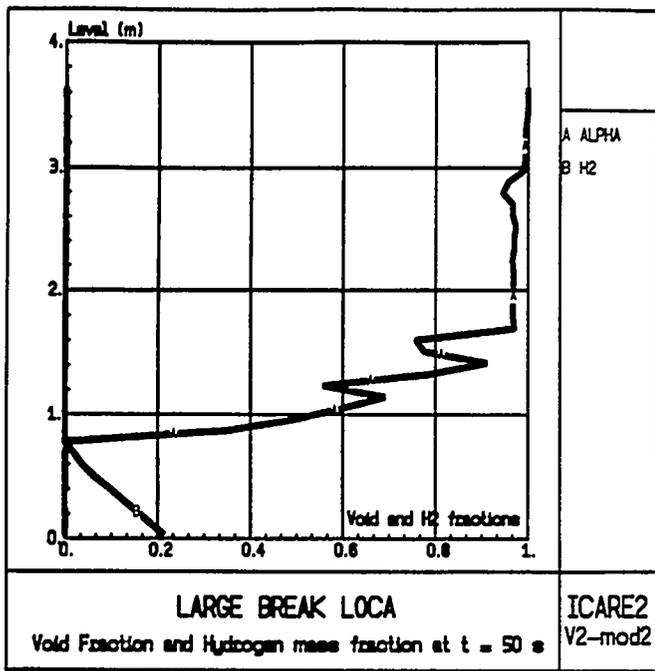


Fig. 4 : Large Break LOCA – ICARE/CATHARE results
Void fraction and Hydrogen mass fraction

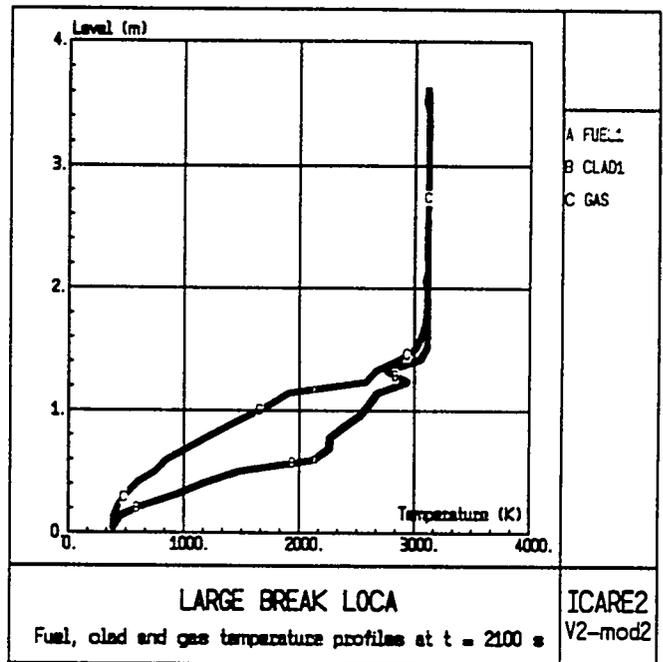
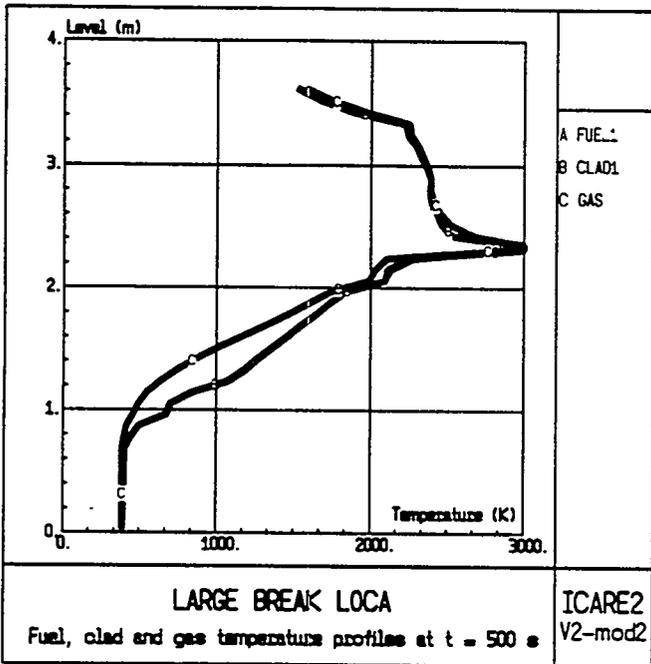
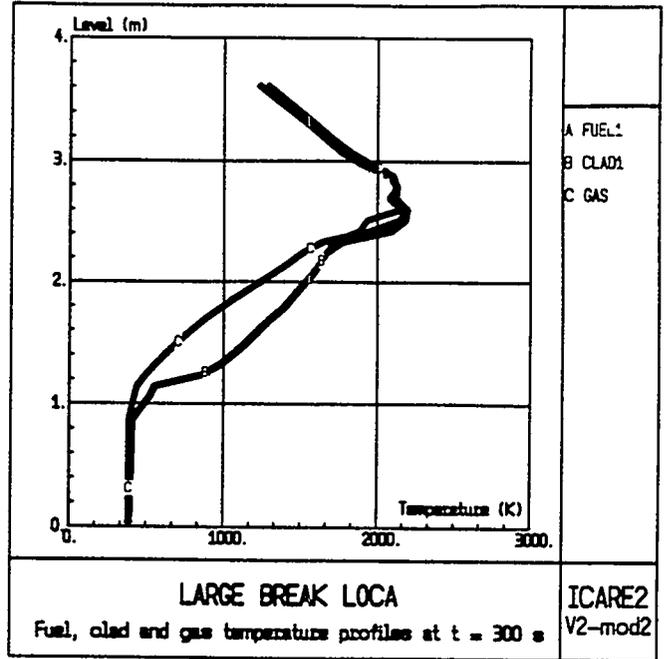
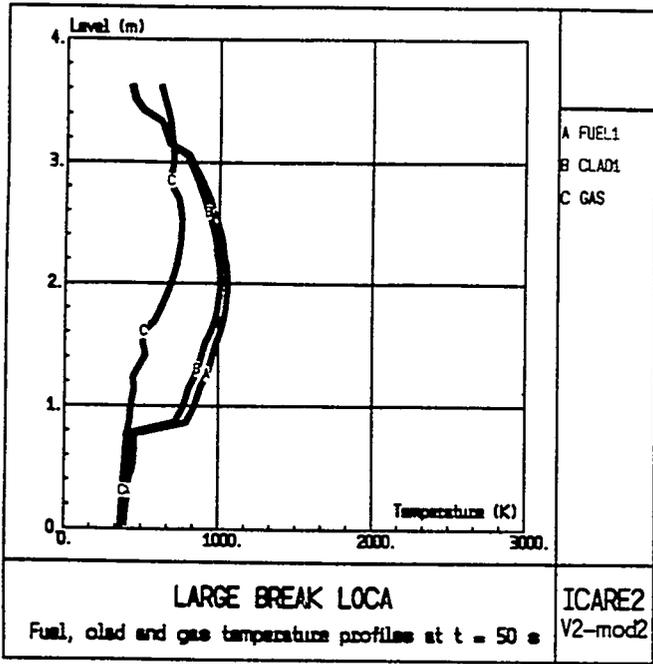


Fig. 5 : Large Break LOCA – ICARE/CATHARE results

Temperature profiles

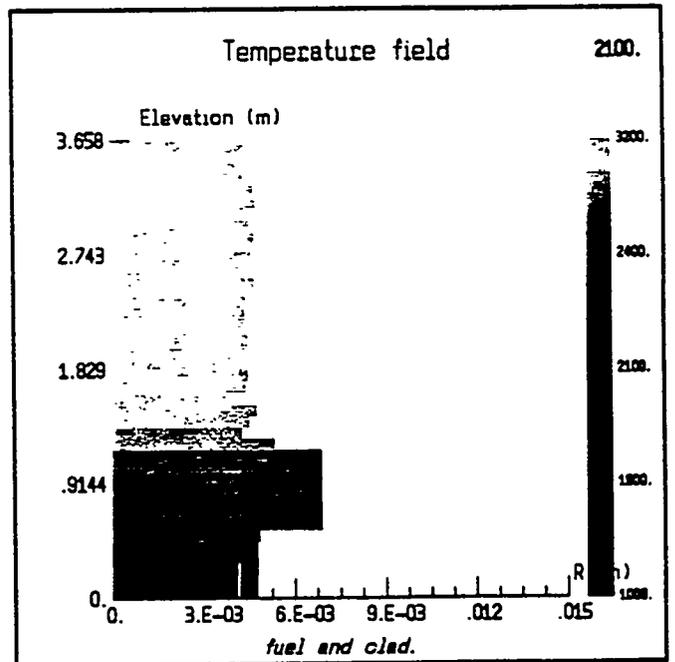
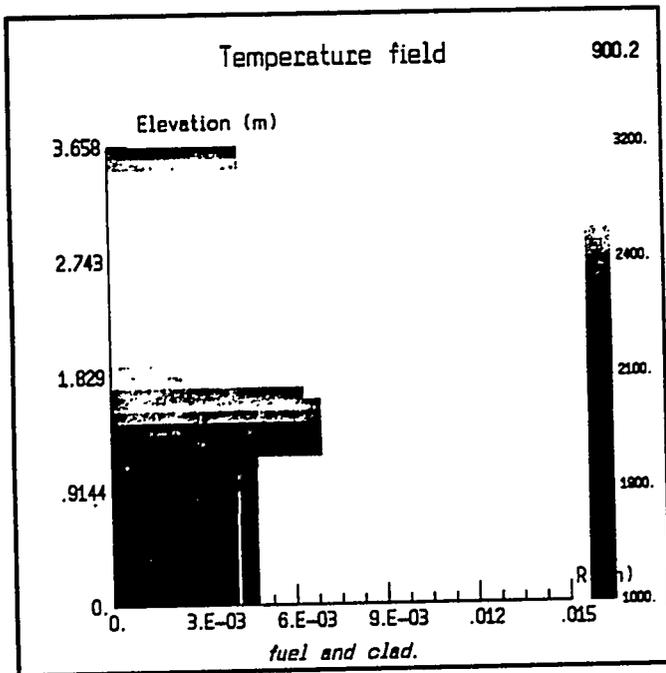
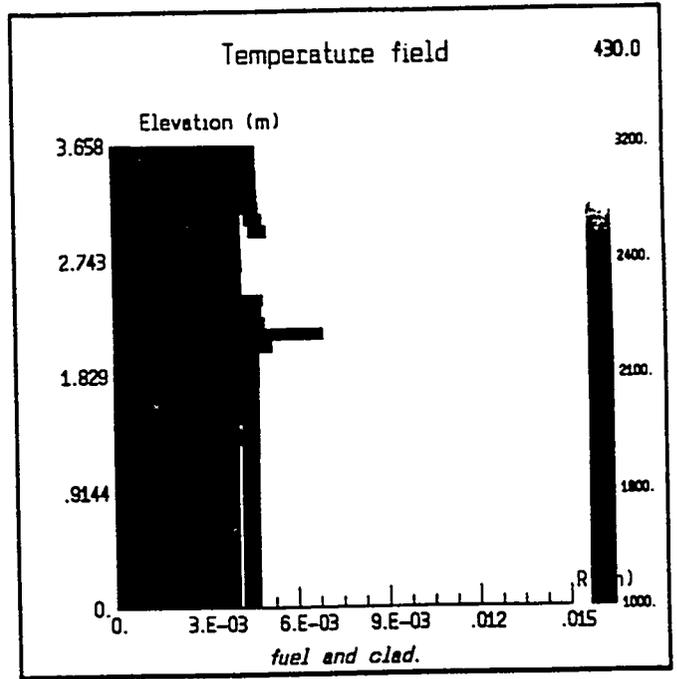
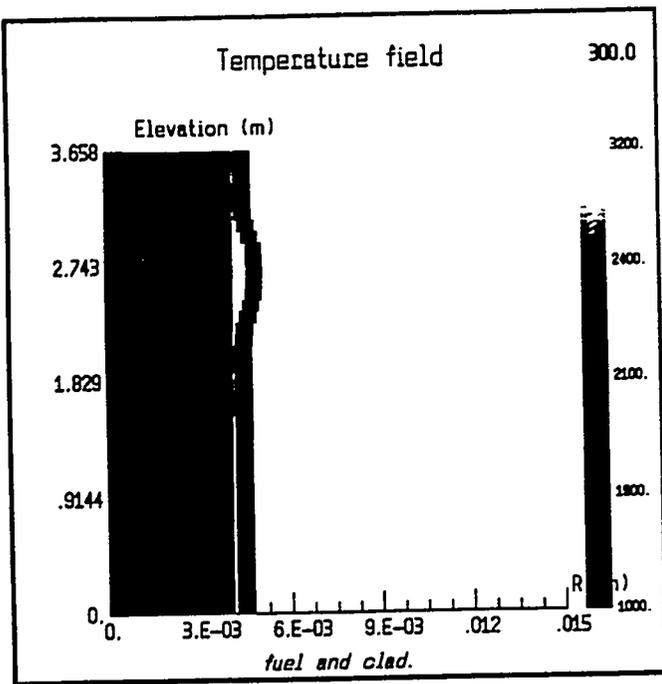


Fig. 6 : Large Break LOCA - ICARE/CATHARE results
Core degradation phase

Interface Requirements to Couple Thermal-Hydraulic Codes to Severe Accident Codes: ATHLET - CD

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Abstract

The system code ATHLET-CD is being developed by GRS in cooperation with IKE and IPSN. Its field of application comprises the whole spectrum of leaks and large breaks, as well as operational and abnormal transients for PWRs, BWRs, and VVERs. At present the analyses cover the in-vessel thermal-hydraulics, the early phases of core degradation, as well as fission products and aerosol release from the core and their transport in the Reactor Coolant System. The aim of the code development is to extend the simulation of core degradation up to failure of the reactor pressure vessel and to cover all physically reasonable accident sequences for western and eastern LWRs including RBMKs.

The ATHLET-CD structure is highly modular in order to include a manifold spectrum of models and to offer an optimum basis for further development. The code consists of four general modules to describe the reactor coolant system thermal-hydraulics, the core degradation, the fission product core release, and fission product and aerosol transport. Each general module consists of some basic modules which correspond to the process to be simulated or to its specific purpose. Besides the code structure based on the physical modelling, the code follows four strictly separated steps during the course of a calculation: (1) input of structure, geometrical data, initial and boundary condition, (2) initialization of derived quantities, (3) steady state calculation or input of restart data, and (4) transient calculation.

In this paper, the transient solution method is briefly presented and the coupling methods are discussed. Three aspects have to be considered for the coupling of different modules in one code system. The most important point is the conservation of masses and energy in the different subsystems as there are fluid, structures, and fission products and aerosols. The second aspect is the convergence of the numerical solution and stability of the calculation, concerning above all the fluid-dynamic models. The third aspect is related to the code performance, running time, and code handling.

The coupling strategy of ATHLET-CD is based on a compromise of these three aspects under consideration of the specific demands of the integration technique used for the fluid-dynamics. It has important advantages: (1) the error control by the integration routine allows for an optimized time step size, (2) the energy and masses are conserved within acceptable margin, (3) the use of common variables instead of data bank application saves considerable computing time.

The development and validation of ATHLET-CD is sponsored by the German Federal Ministry for Education, Science, Research and Technology (BMBF).

1. Introduction

The system code ATHLET-CD (Analyses of Thermal-Hydraulics of LEaks and Transients with Core Degradation) is being developed by GRS in cooperation with the Institut für Kernenergetik und Energiesysteme (IKE), University of Stuttgart. ATHLET-CD comprises also the aerosol and fission product transport code SOPHAEROS which is being developed by the Institut de Protection et de Sûreté Nucléaire (IPSN) and GRS.

Its field of application comprises the whole spectrum of leaks and large breaks, as well as operational and abnormal transients for PWRs, BWRs, and VVERs. At present the analyses cover the in-vessel thermal-hydraulics, the early phases of core degradation, as well as fission products (FP) and aerosol release from the core and their transport in the Reactor Coolant System /BES95/. The aim of the code development is to extend the simulation of core degradation up to the failure of the reactor pressure vessel, and to cover all physically reasonable accident sequences for western and eastern LWRs including RBMKs.

The code is used for reactor safety studies and to evaluate accident management measures and procedures. Therefore a systematic validation is being performed by means of post test calculations of integral tests and separate effect tests. These tests are proposed by the CSNI validation matrices and cover thermal-hydraulic tests (e.g. LOFT, UPTF, PKL, and LOB1), in-pile and out-of-pile bundle degradation tests (e.g. LOFT-FP, PHEBUS, and CORA) as well as fission product and aerosol transport tests (e.g. FALCON, DEVAP, and STORM).

2. Code Structure

The ATHLET-CD structure is highly modular in order to include a manifold spectrum of models and to offer an optimum basis for further development. The code consists of four general modules as shown in figure 1: (1) reactor coolant system thermal-hydraulics module **ATHLET**, (2) core degradation module **ECORE**, (3) fission product core release module **EFIPRE**, and (4) fission product and aerosol transport module **TRAPG**. Each general module consists of some basic modules which correspond to the process to be simulated or to its specific purpose.

The module ATHLET is employed for the analyses of thermal-hydraulics of leaks and transients without core degradation /TES95/. It consists of: (1) thermo-fluid dynamics module **TFD**, (2) heat transfer and heat conduction module **HECU**, (3) neutron kinetics module **NEUKIN**, (4) general control simulation module **GCSM**, and (5) TFD differential equation system solver **FEBE**. The TFD has two different fluid-dynamics equation systems: (1) four equation model (liquid mass, vapour mass, mixture momentum and mixture energy with enthalpy as integration variable) and (2) five plus N equation model (liquid mass, vapour mass, N gas masses, mixture momentum, liquid energy, and vapor/gas energy with temperature as integration variable). Specific models for pumps, valves, separators, mixture level tracking, critical flow etc. are contained in the TFD module.

ECORE contains among others: (1) core heat-up, melting, and relocation module **EHEAT**, (2) module for the radiative heat transfer to the surroundings of the core **ERAD** and (3) fuel rod power generation module **EPOWER**. ECORE calls the same heat transfer package as HECU and EPOWER uses the same point neutron kinetics as NEUKIN. With ATHLET-CD the fuel rods are simulated by ECORE, HECU is used only for the simulation of structures outside the core. ECORE has models to describe the behaviour of fuel rod, PWR control rod (with silver, indium, and cadmium (AIC) or with boron carbide (B_4C) as absorber), and BWR channel box and control elements (with B_4C). ECORE includes the models for (1) cladding oxidation (rate equation approach), (2) clad ballooning, burst and embrittlement, (3) fuel dissolution by molten Zircaloy, and (4) simplified candling of metallic melt UO_2 / α Zr or AIC / stainless steel or B_4C / stainless steel. EPOWER consists of models for (1) point neutron kinetics and decay heat, (2) electrical heater rod, and (3) user defined power generation.

EFIPRE embodies: (1) module for FP release based on rate equations **EFPRAT**, (2) module for FP diffusion in fuel grain **EFGAIN**, (3) module for FP diffusion in fuel pellet **EFFUEL**, and (4) FP gap release module **EFGAP**. The release of 35 different species can be modelled and expressed in terms of mass, activity and decay power. The initial inventory can be defined by user input or calculated by a preprocessor (ORIGEN).

TRAPG contains besides the fission product and aerosol transport module of **TRAPMELT** the new module **SOPHAEROS** to describe simultaneously transport, deposition, agglomeration, resuspension and chemical reactions of FP and aerosols.

The general modules serve mainly as control and interface routines, while the basic modules are kept as far as possible in the original form to facilitate their maintenance. The transfer of variables between the modules is shown in table 1. Besides the code structure based on the physical modelling, the code follows four strictly separated steps during the course of a calculation: (1) input of structure, geometrical data, initial and boundary condition, (2) initialization of derived quantities, (3) steady state calculation or input of restart data, and (4) transient calculation.

Input, as well as output (formatted print and unformatted plot and restart file), are uniform for all modules. During the input each module has its own section with a minimum set of data, since common data are input only once and transferred to the other modules. The input is structured by module and model specific unique control words and key words as well as by module specific objects or components. The output is structured by four identifiers, (1) the module specific object name, (2) the model name, (3) the name of physical variable, and (4) the index which corresponds to the length coordinate. The name of the physical variable can be extended by a second qualifier or index for two-dimensional discretisation or multi-component systems.

All basic modules listed above have their own time integration techniques which are fitted to the individual processes. The link and data exchange between the modules is not controlled by a general

data bank system (e.g. RSYST, SIGAL) but by means of common blocks and specific interface routines under consideration of the feedback between the different physical quantities. In the following the coupling between these basic modules will be illustrated.

3. Steady State Calculation

Before the transient calculation starts, steady state conditions for the fluid system and the heat conduction elements have to be established. They are iterated by the use of explicit algebraic equations in the modules TFD, ECORE and HECU in the following structure:

- **Module TFD - thermo-fluiddynamics**
 - Determination of heat sources and sinks for the fluid system
 - Calculation of specific energy distribution in the fluid system
 - Iteration of pressure distribution
 - Adjustment of friction and form loss coefficients
 - Iteration of enthalpy and steam mass fraction
 - Adjustment of the pump speed
- **Module ECORE - core degradation**
 - Calculation of radiative heat transfer to core surroundings
 - Calculation of heat transfer coefficients in core region,
 - Calculation of temperature distribution and heat conduction in the core
- **Module HECU - structure heat conduction**
 - Calculation of heat transfer coefficients for structures,
 - Calculation of temperature distribution and heat conduction in structures
 - Adjustment of axial power profile in heat exchangers
 - Update of energy balance with adjusted heat sources for the fluid system
- **Module GCSM - simulation of control and balance of plant systems**
 - Update of GCSM signals
- **Module EPOWER or NEUKIN - nuclear power generation**
 - Calculation of axial power profile in the core (only 1D-kinetics)
 - Balancing of the reactivity
- **Go to second step.**

The iteration is completed if all convergence criteria are fulfilled or a limited number of outer iteration loops have been performed and the inner loop convergence criteria are fulfilled. The residual imbalance decays during a "zero-transient" calculation prior to the real transient.

4. Transient Calculation

The method used for integrating the overall thermal-hydraulic problem in time is called FEBE (Forward Euler, Backward Euler) /HOF81/. It provides the implicit solution of a general non-linear ODE system of first order. The differential equation system is based on a semi-discrete approximation (method of lines). The physical models provide the time derivatives of the integration values

$$\frac{dy}{dt} = f(y, t)$$

The implicit solution in the time interval $[t^n, t^n + \Delta t]$ results from the backward step in time:

$$\frac{y^{n+1} - y^n}{\Delta t} = f(y^{n+1}, t^{n+1})$$

The Taylor expansion of the right hand side at point y^n and t^n , the so called linear-implicit Euler's method, yields

$$\frac{y^{n+1} - y^n}{\Delta t} = f(y^n, t^n) + \left\{ \frac{\delta f}{\delta y} \right\}^n \cdot (y^{n+1} - y^n) + \frac{\delta f^n}{\delta t} \cdot \Delta t$$

with the Jacobian matrix:

$$\left\{ \frac{\delta f}{\delta y} \right\}^n = \{ a_{i,k} \} = \left\{ \frac{\delta f^i}{\delta y_k} \right\}^n$$

This method provides the increment of the integration variables $\Delta y = y^{n+1} - y^n$, along the step from t^n to $t^n + \Delta t$ by solving the linear equation system:

$$\left[I - \Delta t \cdot \left\{ \frac{\delta f}{\delta y} \right\}^n \right] \cdot \Delta y = \Delta t \cdot f(y^n, t^n) + \Delta t^2 \cdot \frac{\delta f^n}{\delta t}$$

To control the convergence of the solution and to optimize the time step size, FEBE uses a variable time step, variable order (>2) method with an extrapolation to infinitely small time steps; i.e., the total time step Δt is subsequently replaced by $\Delta t_K = \Delta t / n_K$ with $n_K = \{1, 2, 3, 4, 6, 8, 12, 16, 24, 32\}$. In order to improve the robustness of the code, the sub-division is limited to three sub-time steps. If this sub-division does not fulfill the accuracy criteria, the overall time step size is reduced.

The solution requires the evaluation of (1) the Jacobian matrix and (2) the partial time derivatives. The numerical calculation of the Jacobian matrix is performed by the approximation of the partial derivatives by difference quotients:

$$\left\{ a_{i,k} \right\} = \left\{ \frac{\delta f^i}{\delta y_k} \right\}^n = \left\{ \frac{f^i(\dots, y_k^n + \Delta y_k, \dots, t^n) - f^i(\dots, y_k^n, \dots, t^n)}{\Delta y_k} \right\}$$

Also the partial time derivative is approximated by a difference quotient

$$\frac{\delta f^n}{\delta t} = \frac{f(y^n, t^n + \Delta t) - f(y^n, t^n)}{\Delta t}$$

There are three different ways to tie up the other models in this integration method, each one with advantages and disadvantages:

- Fully implicit coupling, i.e. all other integration variables are included in the solution vector y . This would be theoretically the optimal solution, but the expansion of the solution matrix would cause numerical problems and the computing time would be unacceptable.
- Loose coupling, i.e. each module has its own integration method and common data are transferred only once per time step. This would be the optimal way in terms of computing time, but it would result in instabilities in case of strong feedback between distinct models.
- Intermediate coupling, i.e. each module has its own integration method, modules without or only minor feedback are coupled loosely but models with significant feedback are integrated into the solution method of the thermo-fluid dynamics (tight coupling). This is an acceptable compromise in terms of accuracy and computing time. This method was chosen for ATHLET-CD and will be explained in the following (see figure 2).

The tight coupling is chosen for all of the modules which contribute significantly to the variation of the integration variables y during the evaluation of the Jacobian matrix or the partial time derivative. They are synchronized with the FEBE integration schema. The interaction between two different modules is shown by two examples.

First example: EHEAT calculates the thermal behaviour of the fuel rod, which yields the heat source to the fluid. This interface data are transmitted from ECORE to TFD. On the other hand, the heat source depends on the fluid quantities. The interface data transmitted from the TFD to ECORE are the following fluid properties of liquid phase and vapor/gas phase: pressure, temperature, mass flow, velocity, and mass fraction.

The heat source to the fluid Q_i depends on the difference between structure and fluid temperature $T_s - T_f$, the heat transfer coefficient α , and the surface area A :

$$Q_i = A \cdot \alpha \cdot (T_s - T_f)$$

The heat transfer coefficient itself is function of structure temperature and the fluid quantities $\alpha(y, T_s)$. The structure quantities (temperature etc.) vary only with time evolution, i.e. by the in-

tegration in time of the module EHEAT which is called by ECOPE. Their effect to the heat source is taken into account by the current value at the beginning of the time step or sub-time step at y^n and t^n :

$$Q_i(y^n, t^n) = A \cdot \alpha \cdot (T_s - T_f)$$

as well as by the evaluation of the partial time derivative at y^n and t^{n+1} :

$$Q_i(y^n, t^n + \Delta t) = A \cdot \left(\alpha + \frac{\delta \alpha}{\delta T_s} \cdot \Delta T_s \right) \cdot (T_s + \Delta T_s - T_f)$$

The feedback of the fluid quantities to the TFD regarding the heat source is considered during the evaluation of the Jacobian matrix. For $y_k = T_f$ the value of the heat source at $y_k^n + \Delta y_k$ and t^n yields:

$$Q_i(y_k^n + \Delta y_k, t^n) = A \cdot \left(\alpha + \frac{\delta \alpha}{\delta T_f} \cdot \Delta T_f \right) \cdot (T_s - T_f - \Delta T_f)$$

In this step only the interface routine of ECOPE is called to recalculate the heat transfer coefficient and to update the heat source. However the call and integration of the module EHEAT is not required during the evaluation of the Jacobi matrix due to the clear separation of heat transfer package and core heat-up simulation.

Second example: EHEAT calculates also the oxidation of the cladding, which results in additional heat source as well as in hydrogen generation and steam consumption and subsequently in a change of the fluid volume. The hydrogen generation rate is transmitted as interface data from ECOPE to TFD.

The oxidation and hydrogen generation \dot{m}_h depends on the structure temperature T_s , the oxide layer thickness s and the surface area A :

$$\dot{m}_h = A \cdot x(T_s) / s$$

To consider the effect of steam starvation on the oxidation rate in a similar way as the effect of fluid quantities to the heat source Q_i which depends linearly on the heat transfer coefficient, the oxidation and hydrogen generation are reduced by a multiplicative term $g(p_s)$ as function of the relative partial pressure of steam p_s . With this approximation, the feedback between fluid-dynamics and oxidation rate follows the same procedure as for the heat source. The hydrogen generation rate at the beginning of a time step or sub-time step at y^n and t^n is:

$$\dot{m}_h(y^n, t^n) = A \cdot g(p_s) \cdot x(T_s) / s$$

In the evaluation of the partial time derivative at y^n and t^{n+1} the progression of the oxide layer thickness is taken into account, but not the progress of the structure temperature since the oxidation model is called before the integration of the structure temperature:

$$\dot{m}_h(y^n, t^n + \Delta t) = A \cdot g(p_s) \cdot x(T_s) / (s + \Delta s)$$

In the evaluation of the Jacobian matrix the hydrogen source yields as function of the relative partial pressure of the steam if $y_k = p_s$:

$$\dot{m}_h(y_k^n + \Delta y_k, t^n) = A \cdot g(p_s + \Delta p_s) \cdot x(T_s) / s$$

This can be calculated generally for different hydrogen sources in one fluid volume in terms of the present partial pressure and the hydrogen source at the beginning of the time step:

$$\dot{m}_h(y_k^n + \Delta y_k, t^n) = \dot{m}_h(y_k^n, t^n) \cdot g(p_s + \Delta p_s) / g(p_s)$$

In this step only the interface routine of ECORE is called to recalculate the term $g(p_s)$ and to update the hydrogen source.

To summarize, for the correct coupling of the fluid-dynamics and the fuel rod behavior, the module ECORE is called not only at the beginning of the time step or sub-time steps of the TFD but also for the calculation of the Jacobian matrix and the partial time derivative to provide the TFD with the necessary data. A progress in time requires the integration of EHEAT. During the evaluation of the Jacobi matrix the feedback of the fluid quantities to the TFD source terms is determined by means of the interface routines of ECORE only. In the first example ECORE calls only the heat transfer package to calculate the new heat transfer coefficient as function of the fluid quantities and recalculates the heat source to the fluid. In the second example the time consuming call of the module EHEAT is avoided by the linear approximation of the dependency between the hydrogen source and the fluid quantities. The recalculation of the hydrogen source is performed in the interface routines in ECORE.

Besides the integration methods, another aspect must be also considered. For all processes which are driven by differences of physical quantities, e.g. convective heat transfer

$$Q_i = A \cdot \alpha \cdot (T_s - T_f)$$

or radiative heat transfer driven by temperature differences, which are calculated in different modules, special attention has to be given to the correct synchronization in time. To conserve the energy, the temperature difference must be calculated in the different modules either at the beginning or at the end of the time step but never in a mixed mode, i.e. one temperature at the beginning and the other at the end of the time step. For the integration of the TFD module, Q_i is used as initial condition at t^n :

$$Q_i(t^n) = A \cdot \alpha(t^n) \cdot (T_s(t^n) - T_f(t^n))$$

When the module ECORE is called after the integration of TFD, the fluid temperature is given at the end of the time step $T_f(t^n + \Delta t)$ but the structure temperature is still given for the beginning

of the time step $T_s(t^n)$. To reach agreement between the heat transfer and the driving temperature difference at the end of the integration of both modules, in module ECORE the temperature difference at the end of the time step is used for the implicit integration of the structure temperature:

$$\bar{Q}_i(t^n + \Delta t) = A \cdot \alpha(t^n) \cdot (T_s(t^n + \Delta t) - T_f(t^n + \Delta t))$$

After the integration of the structure temperature, the heat transfer coefficient is determined for the end of the time step and the final convective heat transfer is calculated:

$$Q_i(t^n + \Delta t) = A \cdot \alpha(t^n + \Delta t) \cdot (T_s(t^n + \Delta t) - T_f(t^n + \Delta t))$$

which is used in the TFD module at the beginning of the next time step. With this approach the overall energy balance is fulfilled within an acceptable error margin, the calculation results are in the first order independent of the time step size, and the calculation is stable. The same approach is considered for the coupling of the modules TFD and HECU (convective heat transfer) and the modules EHEAT and HECU (radiative heat transfer).

The same holds true for the coupling of the FP diffusion in fuel grain and fuel pellet (modules EF-GAIN and EFFUEL). In this case the FP concentration corresponds to the temperatures and the diffusion coefficient to the heat transfer coefficient. It is mandatory that in one component, i.e. in one representative fuel rod, both modules are evaluated with the same time step size to fulfill the mass balance of the FPs.

The evaluation of the point neutron kinetics requires the actual fluid quantities and fuel temperature to get the correct total reactivity. Therefore, the module EPOWER is called after the integration of TFD and EHEAT, with the result that for the subsequent evaluation of TFD the actual heat source is not available and the feedback is delayed by one sub-time step. This is generally not significant for severe accident condition. For full power or partial load operation, the time step size has to be limited, if the total reactivity increases, in order to avoid non-physical instabilities.

Modules without or with minor feedback to the fluid-dynamics are coupled loosely, this means the modules are evaluated only once per TFD time step (module EFIPRE and SOPHAEROS). An overview about the coupling between the different modules and the main processes which are affected by the coupling is given in table 2.

5. Conclusion

Three aspects have to be considered for the coupling of different modules in one code system. The most important point is the conservation of masses and energy in the different subsystems as fluid (liquid, vapor, gases), structures (fuel rods, control assembly, walls etc.), and fission products and aerosols, as well as, but with less priority the conservation of momentum in the fluid system. The

second aspect is the convergence of the numerical solution and stability of the calculation, concerning above all the fluid-dynamic modules. The third aspect, which is probably more important for the the code user, is the code performance, running time, and code handling.

The coupling strategy of ATHLET-CD is based on a compromise of these three aspects under consideration of the specific demands of the integration technique used for the fluid-dynamics. The procedure for integration and coupling described above appears complex and time consuming, but it has important advantages: (1) the error control by FEBE allows for an optimized time step size, (2) the energy and masses are conserved within acceptable margin, (3) the use of common variables instead of data bank application saves considerable computing time.

6. Literature

BES95 Beste J., K. Trambauer

Status of ATHLET-CD Development Shown by the LOFT-FP-2 Analysis as an Example
Heat and Mass Transfer in Severe Reactor Accidents, International Symposium, Cesme,
Turkey, May 1995

HOF81 Hofer E.

An $A(\alpha)$ -stable variable order ODE-solver and its application as advancement procedure
for simulation in thermo- and fluid dynamics.

Proceedings of the International Topical Meeting on Advances in Mathematical Methods
for the Simulation of Nuclear Engineering Problems, München, April 1981

TES95 Teschendorff V., H. Gläser, F. Steinhoff

ATHLET Validation Using Accident Management Experiments

Proceedings of the 7th International Meeting on Nuclear Reactor Thermal-Hydraulics
NURETH-7, NUREG/CP-0142, September 1995

TFD ⇒ EHEAT Liquid temperature Vapour temperature Pressure Gas mass fraction Vapour partial pressure Mass flow rate		EHEAT ⇒ TFD Heat source to liquid Heat source to vapour and gas Vapour mass sink Hydrogen mass source Flow blockage
TFD ⇒ HECU Liquid temperature Vapour temperature Pressure Gas mass fraction Vapour partial pressure Mass flow rate		HECU ⇒ TFD Heat source to liquid Heat source to vapour and gas Vapour mass sink Hydrogen mass source
EHEAT ⇒ ERAD Cladding temperature HECU ⇒ ERAD Structure temperature	ERAD ⇒ EHEAT Structure temperature Heat transfer coefficient	ERAD ⇒ HECU Cladding temperature Heat transfer coefficient
EHEAT ⇒ EPOWER Fuel temperature	TFD ⇒ EPOWER Fluid temperature Fluid density Boron concentration	EPOWER ⇒ EHEAT Heat source to fuel
EHEAT ⇒ EFIPRE Fuel temperature Absorber temperature Cladding oxidation Component failure Material distribution	EFIPRE ⇒ EPOWER Decay power reduction	EFIPRE ⇒ SOPHAEROS Fission product release rate Aerosol release rate
EFGAP ⇒ EFFUEL FP concentration	EFFUEL ⇒ EFGAIN FP concentration	EFGAIN ⇒ EFFUEL Fission product source
TFD ⇒ SOPHAEROS Fluid temperature Pressure Vapour mass fraction Fluid velocity	EHEAT ⇒ SOPHAEROS Cladding temperature HECU ⇒ SOPHAEROS Structure temperature	SOPHAEROS ⇒ TFD Decay heat suspended FPs SOPHAEROS ⇒ EHEAT Decay heat deposited FPs SOPHAEROS ⇒ HECU Decay heat deposited FPs

Table 1: Variablen transfer between the modules.

Process common to different modules	Module coupled	Type of Coupling
Convective Heat Transfer in the Core	TFD \Leftrightarrow EHEAT	tight
Convective Heat Transfer to Structures	TFD \Leftrightarrow HECU	tight
Oxidation of Core Components	TFD \Leftrightarrow EHEAT	tight
Oxidation of Structures	TFD \Leftrightarrow HECU	tight
Radiative Heat from Core to Structures	EHEAT \Leftrightarrow ERAD \Leftrightarrow HECU	loose**
Point Neutron Kinetics and Fission Power	TFD + EHEAT \Leftrightarrow EPOWER	loose**
Fission Product Core Release / Decay Power	EHEAT \Leftrightarrow EFIPRE	loose
Fission Product Diffusion Grain/Pellet	EFGAIN \Rightarrow EFFUEL	loose**
Fission Product Core Release	EFIPRE \Rightarrow SOPHAEROS	loose
Fission Product Transport / Decay Power	TFD \Leftrightarrow SOPHAEROS	loose
Fission Product Deposition / Decay Power	HECU \Leftrightarrow SOPHAEROS	loose

Table 2: Type of coupling of different modules.

Loose: Coupling based on TFD time step.

Loose**: Coupling based on TFD sub-time step.

Loose+*: Coupling based on minimum of TFD time step and EFGAIN sub-time step.

Figure 1: ATHLET-CD code structure

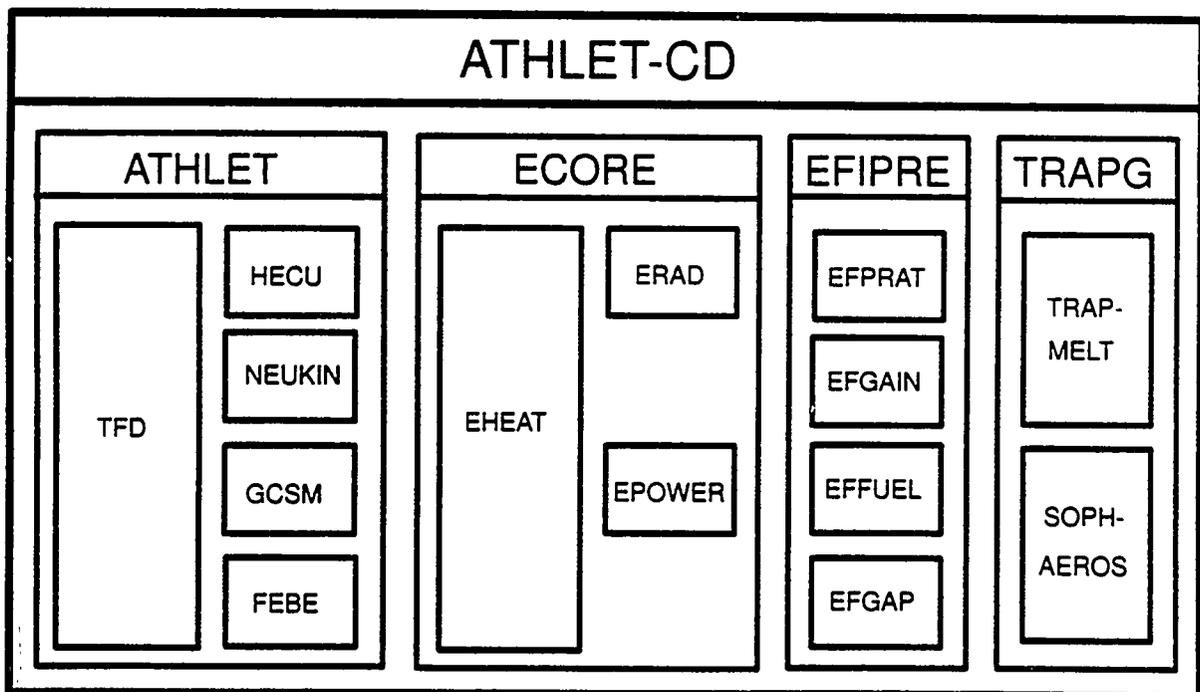
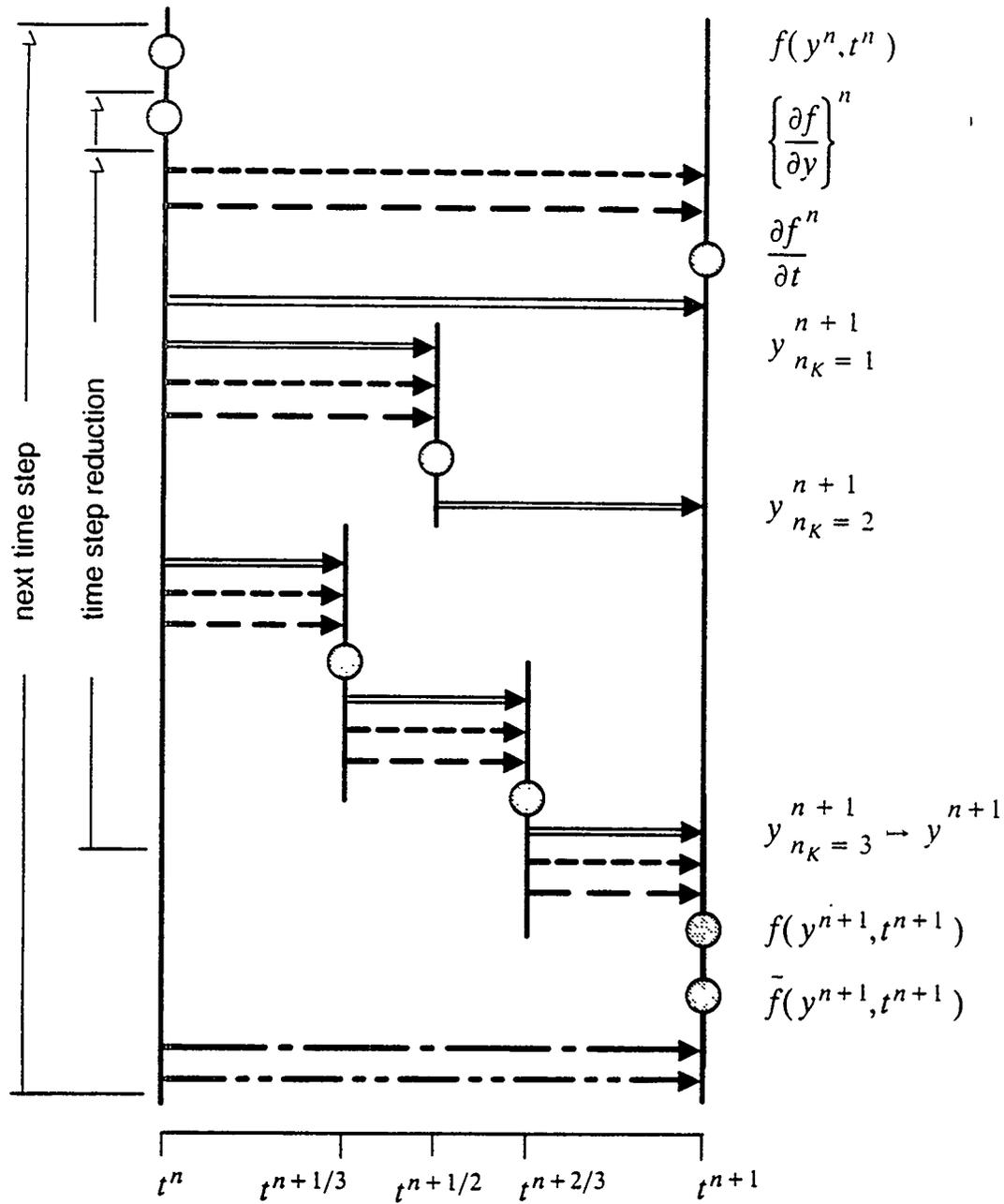


Figure 2: Solution of linear TFD Equation System (TFD - ES) in ATHLET-CD



$$\text{TFD - ES : } \left[I - \Delta t \cdot \left\{ \frac{\partial f}{\partial y} \right\}^n \right] \cdot \Delta y = \Delta t \cdot f(y^n, t^n) + \Delta t^2 \cdot \frac{\partial f^n}{\partial t}$$

Module: TFD EHEAT HECU EFIPRE SOPHAEROS

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Neutronic Codes Requirement
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**Interface Requirements to Couple Thermal-Hydraulic Codes to 3D
Neutronic Codes**

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Abstract

The present situation of thermalhydraulics codes and 3D neutronics codes is briefly described and general considerations for coupling of these codes are discussed. Two different basic approaches of coupling are identified and their relative advantages and disadvantages are discussed. The implementation of the coupling for 3D neutronics codes in the system code ATHLET is presented. Meanwhile, this interface is used for coupling three different 3D neutronics codes.

1 Introduction

The analysis of global plant transient and accident behaviour and the analysis of 3D neutronics behaviour have been developed as separated and complementary fields of safety analysis for NPPs. The plant transient analysis is performed by system analysis codes which comprise very detailed models of coolant flow, heat transfer and components but usually only simplified neutronics models based on point kinetics or 1D-kinetics. The 3D reactor core behaviour is analyzed by neutronics codes solving 3D neutron diffusion equations representing each fuel assembly of the core loading and describing feedback effects by fuel rod and coolant flow models corresponding to each fuel assembly. Meanwhile, the interest to couple 3D neutronics models to system codes has been growing continuously. Such improved models are required to analyze

specific accident sequences like boron dilution accidents, which were identified by safety research, and to analyze more realistically ATWS sequences with complete or partial failure of reactor scram. All these accident sequences are determined by a strong coupling between neutronics and thermo-fluid dynamics in the reactor core. Additionally, the coupling of 3D neutronics models reflects the permanent effort to increase accuracy of simulations and to use more realistic models by reducing limiting model assumptions.

The different approaches of coupling are discussed and the implementation of various 3D neutronics models in the system code ATHLET is described.

2 General considerations

It is worth to remember that currently applied codes in both areas of safety analysis are the result of a long period of code development which contributed to develop efficient numerical solution methods for fluid dynamics and neutronics. Each code uses structures optimally adapted for its specific purposes. Generally, available fluid dynamic codes and also neutronic codes are strongly related to specific programs of code development in research institutes. Additionally, the application of these codes in safety analysis is based on a great effort of code validation against separate effects tests, integral tests and plant data. The validation of fluid dynamics codes is usually determined by validation matrices. The analysis of this experimental data base determines the fundamental basis of code acceptance. For neutronics codes there is a strong relation to analytical methods and codes used to generate nuclear data for fuel assembly design. These procedures are also based on practical experiences and validation by nuclear measurements for critical facilities and for operational core conditions. Therefore it should be accepted that a single approach of coupling a 3D neutronics model to a thermalhydraulic code may be not the only solution. The main objective should be to provide a frame or a strategy for coupling such codes.

3 Discussion of coupling strategies

The available basis of thermalhydraulic system codes and 3D neutronics codes can be described as follows:

The core models in thermal-hydraulic codes consist of point kinetics models or 1D neutronics models which are coupled to an average fluiddynamic channel of the core region described by a pipe component and to a corresponding average fuel rod model. Feedback variables are nodal coolant temperatures and densities determined by the average coolant channel and the fuel temperature determined by the fuel rod model. In most codes, also in ATHLET, the pointkinetics can be related to several parallel coolant channels and corresponding fuel rod models describing parts of the reactor core.

The 3D neutronics models for core analysis have been expanded to full reactor core models which comprise complete models of the thermal-hydraulics in the core region. Usually the core thermal-hydraulics is modeled by a parallel coolant channel model without cross flow mixing. This describes completely the conditions in a BWR core, but can be used also as a first approximation of a PWR core. In some reactor core models are implemented subchannel thermal-hydraulics codes including cross-flow between fuel assemblies.

Starting from this situation two basically different approaches of coupling seem to be reasonable:

1. Coupling of 3D neutronics models to the system code which models completely the thermal-hydraulics in the primary circuit including the core region
2. Coupling of 3D reactor core models describing neutronics and thermal-hydraulics in the core region to the system code which models only the thermal-hydraulics in the primary circuit exclusive the core region.

The advantages and disadvantages of these two different approaches are the following:

With respect to neutronics no essential differences exist. The efficient numerical solution methods for neutronics are kept. Usually the feedback models have been added to the neutronics models and can be separated easily.

With respect to thermal-hydraulics great differences between both approaches exist. In the first approach the thermalhydraulic equations in the primary circuit and the core region are consistently solved by the physical models and numerical methods applied in the system code. This is important because fast pressure disturbances or the transport of enthalpy step changes can be treated correctly by the time-integration methods. In ATHLET the thermal-fluiddynamic equations are integrated by the FEBE-algorithm which includes a series of fractional time-steps including an extrapolation scheme. Thus the time-integration scheme is fully controlled by the specified degree of accuracy.

Generally, the thermal-hydraulic models in system codes are more complete and detailed than those of reactor core models and no limitations for counter current flow or high void content exist. Also any refinement in modeling downcomer and lower or upper plenum respectively will be part of the thermal-hydraulic system code.

A relevant disadvantage of this approach could be that the implemented general purpose time-integration schemes used in system codes may be inefficient or very computer time consuming to solve problems with a great number of coolant channels in the core region. But optimizations can be performed within the existing numerical algorithms because in the core region the matrix coefficients will get a regular structure.

Another aspect could be that the reactor core model includes some peculiar features like a very detailed fuel rod model adjusted for fast reactivity initiated accident conditions. However, such specific models can be also transferred and implemented as a model of the system code.

4 Implementation of coupling 3D neutronics codes in ATHLET

As a general strategy to couple 3D neutronics models to ATHLET the first approach is recommended and it was implemented for coupling three different neutronics models. The chosen implementation will be described in the following chapter. In one case also the second approach was implemented and practical experience was obtained what will be discussed.

4.1 Coupling approach modelling fluid dynamics completely by system code

In the system code ATHLET an interface to 3D nuclear codes has been implemented which is applied now to couple three different neutronics codes. As discussed before this interface is based on the approach to couple only the 3D neutronics model to the thermalhydraulic code. The neutronics codes available are BIPR-8 for VVER with hexagonal fuel assemblies from Kurchatov-Institut, the code DYN3D for VVER from Research Center Rossendorf and the GRS-Code QUABOX/CUBBOX for LWR with rectangular fuel assemblies.

The interface structure is designed in a very general way, corresponding to the main tasks of coupled calculations.

1. Reading input data consisting of the input data of independent codes and an additional part describing the relation between fluid dynamic channels and core loading.
2. Data exchange between fluid dynamic system code and neutronics, namely the transfer of power density distribution and feedback parameters between models.
3. Controlling for static solutions the iterations between fluid dynamics and neutronics to obtain steady state conditions.
4. Controlling for transient calculations the synchronization of time integration by determining time-step size and the sequence of calculational steps

It is supposed that the neutronics code is adjusted to these main tasks. Practically, the experience was that this structure was available in all codes studied.

The main features of these tasks are discussed.

The additional input defines the relation between fuel assemblies in the core loading and the flow-channels. Therefore the relation can be defined very flexible by grouping of fuel assemblies or by a 1 to 1 correspondence. Also the axial mesh width in neutronics and thermalhydraulics calculations may be different, this will be taken into account in the step of data exchange.

The main physical parameters, which must be exchanged between fluiddynamic models and neutronics choosing this coupling approach, are the following:

- The power density distribution
It is the result of the neutronics calculation and must be transferred to fluidynamics
- The distributions for fuel temperature, the coolant density and coolant temperature as well as the boron concentration. These parameters are the result of the fluiddynamic model including the boron transport model and must be transferred to neutronics.

Generally, following approach is taken:

In static calculations the calculation of parameters in fluidynamics and neutronics is performed iteratively till steady state conditions are reached. In transient calculations the solution of fluidynamics and neutronics is done subsequently accepting a delay of one time-step between power density values and feedback parameter values in solving equations. This doesn't affect the accuracy of solution, as long as the time-step size is small relative to the time-constant of the fuel.

From the programming aspect the interface is structured such that three levels exist.

This structure mainly contributes to limit the interference between fluiddynamic system code and neutronics code to a minimum. In order to maintain the independence of data between the codes, an additional set of arrays was defined for the interface level for each parameter to be exchanged. This allows that each code can keep its own indexing methods. The mapping of values is performed within the interface. This specific feature will also be useful developing a code version for distributed computing as the

main data arrays for exchange are completely separated from the programs and the control over their distribution can be performed in the interface level.

The levels of the interface are described as follows:

The first level consists only of general calls from ATHLET for main program functions of the interface. In this layer all program control is performed by ATHLET. It also includes the data exchange between ATHLET arrays and the interface arrays as explained above.

The second level consists of subroutine calls for the interface subroutines of the specific neutronics models. In this level will be decided which neutronic model will be used.

The third level is specific for each neutronics model and necessary adaptations can be implemented. This level contains also the data exchange between interface arrays and data sets of neutronic models.

For static calculations it is only necessary to control the iterations between fluid dynamics and neutronics in an appropriate way. That is to determine the accuracy of power density distribution calculated in neutronics before starting the next fluid dynamic solution.

Attention must be paid to the time-integration, because a strategy must be implemented, which considers all possible relations between time-step size in fluid dynamics and neutronics. The time-step size in fluid dynamics may be larger than, equal to or smaller than the optimum time-step size in neutronics. Dependent on this relation the number of time-steps and the time-step size itself must be chosen for neutronics.

4.2 Coupling approach modelling fluid dynamics exclusive core region by system code

As indicated the coupling of the 3D core model DYN3D was also implemented using the second approach, in which the fluid dynamics in the core region is modeled within the reactor core model. The interface variables are in that case located at the bottom and at the top of the core. The values of pressure, mass-flow rate, enthalpy and boron concentration at these locations must be transferred. Thus only a few number of

parameters have to be exchanged, which is effectively supported by a specific feature of the General Control and Simulation Module (GCSM) of the ATHLET code. As expected difficulties were caused by numerical reasons. The coupling of the two thermo-hydraulic parts is done explicitly and very small time-step sizes, lower than 10 ms, were needed for stable calculations. The observation was that the pressure drop over the core and the core mass-flow rates oscillate in a random manner caused by numerical effects. These oscillations were successfully damped by adding a low pass filter of first order for the pressure drop representing the boundary condition for the mass-flow calculations in the fluiddynamic model of DYN3D. This additional damping was applied for various transients obtaining good results. Further investigations are needed to evaluate consequences of this approach for fast transients.

5 Summary

Experience with the described coupling strategy has been obtained by coupling three different 3D neutronics models. This proves that the approach is general and flexible enough. Test calculations have been performed up to now for reactivity initiated accidents by control rod withdrawal, ATWS-transients and boron dilution transients. Applications will be presented in a companion paper. The next step will be to validate the coupled codes for the range of applications.

Acknowledgement

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6 References

- /LAN 96/ S. Langenbuch et al.
3D Neutronic Codes coupled with Thermal-Hydraulic System Codes for PWR, BWR and VVER Reactors
Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Nov. 5 - 8, 1996

DEVELOPMENT OF AN INTEGRATED THERMAL-HYDRAULICS CAPABILITY INCORPORATING RELAP5 AND PANTHER NEUTRONICS CODE

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Introduction

Ensuring that safety analysis needs are met in the future is likely to lead to the development of new codes and the further development of existing codes. It is therefore advantageous to define standards for data interfaces and to develop software interfacing techniques which can readily accommodate changes when they are made. Defining interface standards is beneficial but is necessarily restricted in application if future requirements are not known in detail.

Code interfacing methods are of particular relevance with the move towards automatic grid frequency response operation where the integration of plant dynamic, core follow and fault study calculation tools is considered advantageous.

This paper describes the background and features of a new code TALINK (Transient Analysis code LINKage program) used to provide a flexible interface to link the RELAP5 thermal hydraulics code with the PANTHER neutron kinetics and the SIBDYM whole plant dynamic modelling codes used by Nuclear Electric. The complete package enables the codes to be executed in parallel and provides an integrated whole plant thermal-hydraulics and neutron kinetics model. In addition the paper discusses the capabilities and pedigree of the component codes used to form the integrated transient analysis package and the details of a calculation of a postulated Sizewell 'B' Loss of offsite power fault transient.

Interfacing techniques

Separate codes can be coupled in a number of ways including :

- By merging the separate programs into one with linkage via subroutine or function calls (referred to as static linking below).
- By running the codes as separate processes and exchanging data between the processes.

Both of these linkage methods have relative advantages and disadvantages:

Static linking

- Using statically linked codes, a more complex coupling can be accommodated without unacceptable speed reduction or large data transfer files. This is beneficial where for example fluid thermal-hydraulics data are being transferred to the neutronics code on a core node-wise basis (rather than just core inlet conditions).
- Many older engineering codes written in FORTRAN frequently make extensive use of global variable storage and data transfer via common blocks. The widespread use of common blocks frequently reduces the data flow modularity of the code (although the code might still have reasonable functional modularity). Thus the results of algorithms in one part of the code can be strongly coupled to behaviour in other part(s) of the code. In codes of this type understanding the behaviour of one part of the code can involve at least a detailed appreciation of the code architecture and probably the details of the code as a whole. Such problems will increase in a non-linear fashion as the size of the code increases. Further development problems can arise if the format of related common blocks differs between routines. These type of development problems form one of the reasons why object oriented design (OOD) methods are now becoming widely used for modern software engineering to enforce rules for data access and to improve the localisation of data and the associated methods (functions). At present however thermal-hydraulics and neutron kinetics codes using OOD techniques are not widely used or available.

Linking older codes of the type discussed above into a single code can therefore involve extensive cross checking to prevent and eliminate variable and algorithm conflicts and hence is very costly. Even linking modular codes written to modern

software engineering quality standards, such as PANTHER, may involve some cross-checking if global data storage is used. Moreover if one or more of the linked codes is (separately) modified to any great extent subsequently then much of the cross checking work may need to be revisited to update the integrated code. Much of this work is eliminated if the codes are executed as separate processes with separate address spaces.

Separate processes

- The use of inter-process communications involves an overhead on the total code execution time. However the use of parallel code execution permits the codes to be executed on different processors either in a single machine using symmetric multi-processor (SMP) technology (for example) or distributed across more than one computer. Such a client-server architecture provides a flexible means of utilising a number of networked computers.

However, in order for parallel code execution speed advantages to be obtained, the code linkage must ensure that processes are not held waiting for data for a significant period. Various techniques may be adopted to achieve parallel operation in an explicitly coupled thermal-hydraulics and neutron kinetics codes system. For example, if the core model calculation normally uses the core inlet temperature from the circuit thermal-hydraulics model as a boundary condition then Lagrangian extrapolation along the solution characteristics could be used in some circumstances. This would allow the neutron kinetics calculation to be run prior to the time pertaining for a purely sequential explicit coupling of codes.

- The inter-process communication linkage process is likely to lead to a range of new files containing details relating to the links created. This data must be controlled with appropriate QA so that ad-hoc alterations are not adopted. Using statically coupled codes alterations are unlikely to be introduced once testing has been completed satisfactorily, unless required by other developments. Thus for statically linked codes the extra documentation and QA would be limited to

that for the initial development and for input revision.

- Debugging codes executing in parallel separate processes is usually more complex than for a single process particularly if the code originating the problem(s) is unknown.
- If codes linked by inter-process communications are to be transferred to another hardware platform the communications routines may need to be rewritten.

Thus the choice of linkage method adopted will depend upon the weighting applied to the relative advantages of each method for the circumstances involved. If separate processes are used for several codes then the use of an interfacing code becomes beneficial to simplify overall control of the calculations.

Interface code features

To limit the extent of alterations needed to the codes being interfaced and provide a flexible and user friendly integrated code package, a number of features should be considered for inclusion in the interface code:

- A means of specifying to the external codes which variables need to be transferred, their types and in which direction the transfers are to be performed.
- A means of specifying when the variables are to be transferred.
- A means of processing the data being transferred between the external codes.
- A means of changing the details listed above during the analysis if appropriate.
- A means of handling software exceptions and shutting down all processes tidily.
- A means of recording a subset or all of the data transferred to facilitate debugging activities or to provide a QA audit trail.

In addition, operations performed by the interface code should involve minimal overhead and should cause the minimum delay to the external codes. TALINK meets these requirements by pooling data

from the client codes in an internal database. The client codes can then request any database items and are requested to supply data to TALINK as required. TALINK also uses a simple command interpreter to manipulate database items, for units conversion for example. A number of features are included to provide portable and flexible control of data transfer operations:

- TALINK input is read which specifies a series of external code data transfer operations to be considered at each TALINK iteration.
- One or more data transfer operations can be associated with each external code.
- Tables correlating the TALINK database variable names with external data table names are input to identify the data to be transferred for each operation.
- Data can flow in either direction for each data transfer operation as specified by input to TALINK.
- The TALINK internal database supports multiple variable types. Data transfers with external codes can include type conversion between compatible types if requested.
- To facilitate the ordering and synchronisation of data transfers, the data read from external codes into the TALINK database can be accessed to allow conditions for data transfers to be input to TALINK. These conditions are checked at each TALINK iteration, for example to check the TALINK code record of the transient time. Such a check could be used to determine if another RELAP5 time step calculation should be initiated by this TALINK iteration, for example.
- Data transfer operations are split into two groups which are performed before and after specified operations on the TALINK database are performed. Thus information read in to TALINK from the analysis codes at the start of the TALINK step can be processed to provide data for output at the end of the step.
- A specified subset of the TALINK database

contents can be written to a logfile for debugging or to provide a QA audit trail.

- Data transfers between TALINK and the analysis codes are performed using the industry standard TCP/IP protocols.

The interface is therefore not code specific. Furthermore the command interpreter input, defining TALINK operations can even be overwritten during operation, so that the variables transferred and the processing operations carried out can change during a calculation. For example, data on a valve position need only be sent if the valve moves.

Safety analysis codes linked in the present package

The Nuclear Electric core neutronics and thermal-hydraulic code PANTHER has been linked initially with an improved version of RELAP5/MOD-2 and the whole plant dynamics code SIBDYM using the new interface code TALINK. Now that the original development phase of the integrated package has been completed the linkage with RELAP5/MOD-2 will be replaced by a link with RELAP5/MOD-3 once the required RELAP5/MOD-3 input decks are available. The capabilities of the analysis codes are discussed below.

PANTHER

PANTHER provides a general-purpose whole-reactor calculation capability based on multigroup neutron diffusion and core thermal-hydraulics models for thermal reactor analysis.

Development of PANTHER started in 1986, led by CEGB with contributions from the UKAEA (now AEA Technology). The development of PANTHER stems from the need to provide a general, flexible and easy to use code to replace a number of earlier plant specific codes. The original development concentrated on applications relating to PWR and AGR studies (the code name is an acronym derived from PWR and AGR Neutronics and Thermal-Hydraulics Evaluation Route) but the generic nature of the models has made it capable of analysing almost any thermal reactor. It has now been applied to the analysis of PWR, AGR, MAGNOX, VVER, RBMK and BWR.

PANTHER allows a comprehensive range of calculations to be performed including :

- steady-state performance
- fuel management
- safety transient analysis including PCI assessment
- operational support including on-line core follow.

PANTHER is part of a larger development (Ref 1) of a comprehensive, integrated package of core performance codes.

PANTHER is based upon a modular design which uses a natural control language to specify the required operations providing ease of use coupled with great flexibility in the range and specification of the analysis to be performed. The control language provides the facility to store and reuse sets of operations by the inclusion of a macro facility.

The PANTHER code provides the capability to perform neutron kinetics calculations in 0, 1, 2 or 3 dimensions for rectangular or hexagonal assemblies.

The multigroup neutron diffusion equations are solved using either the analytic nodal method or the finite difference approximation. The numerical iteration used for the two methods is essentially the same but in the nodal case the node-to-node coupling coefficients are periodically updated through the iteration by solving subsidiary 1-dimensional nodal equations for each direction.

Different calculational meshes can be used for the flux, thermal feedback and irradiation.

These features allow the code to be run accurately with a coarse mesh: eg for a 4-loop 193 assembly PWR using one mesh per assembly and eight axial meshes.

The steady-state, K-effective eigenvalue, neutron diffusion equations are solved using an efficient, robust iterative solution requiring no inner iterations. The solution is accelerated using the method based upon Chebyshev polynomials.

The transient solution uses the same spatial approximations and iteration method as the steady-state solution and has essentially the same

convergence behaviour coupled with the use of an exponential transformation of the neutronics solution to allow the use of large time steps.

Extensive verification and validation of PANTHER has been performed using both calculational benchmarks and plant data. Accurate solutions have been published for a range of standard LWR benchmark problems including the NEACRP rod ejection benchmarks for which the PANTHER code is taken as the reference solution. Validation using plant data has been performed with data measurements from Callaway, Wolf Creek, Zion II, Tihange, Doel and Sizewell 'B' PWRs, the Kozlodoy VVER-440 and Kaliningrad VVER-1000, an RBMK and all of the UK AGRs.

RELAP5

At present, the Nuclear Electric Sizewell 'B' Project version of RELAP5/MOD-2 has been linked via TALINK. RELAP5/MOD-2 has been extensively developed and validated by Nuclear Electric. In addition it has been used in the independent assessment of the transient analysis fault studies for the Sizewell 'B' Pre-Operational Safety Report (POSR) performed by NNC using Westinghouse proprietary codes. RELAP5/MOD-2 was therefore selected as providing a stable basis for the original development phase of the integrated thermal-hydraulics and neutron kinetics transient analysis code package.

The Nuclear Electric Sizewell 'B' Project version of RELAP5/MOD-2 is based on cycle 36.05 and was developed by UKAEA Winfrith for use on SUN workstations and incorporates a number of model revisions which were subsequently incorporated in RELAP5/MOD-3.

The linkage with RELAP5/MOD-3 in the near future is expected to be a straightforward step since only a small quantity of code needs to be introduced in RELAP5/MOD-3 and much of this is likely to be the same as that used for the RELAP5/MOD-2 link.

SIBDYM

The Sizewell 'B' total plant model SIBDYM (Sizewell 'B' Dynamics Model) models all of the major items of plant including the reactor core, reactor coolant loops, pressuriser, steam generator and turbines. The Station Automatic Control Systems are modelled as digital (sampled) systems.

Versions of SIBDYM are available which allow the modelling of all four plant loops independently. Using this capability allows, for example, feed system instability situations in which cyclic behaviour with the steam generators out of phase might occur to be analyzed. (Such events have been reported at the Wolf Creek and Callaway plants).

SIBDYM has been used in the Sizewell 'B' POSR. It is currently used for the analysis of operational transients and as part of the plant dynamic analyzer (PDA) where plant transients are examined in real time.

Linkage of the safety analysis codes with TALINK

The PANTHER code already incorporates the facility to interact with external codes using the TCP/IP protocol so this facility was utilised for the interface with TALINK. This involved the modification of the natural language PANTHER control input to include the necessary instructions.

The RELAP5/MOD-2 coding interface is based on the minor edit processing code modified to call a new interface routine. When first called this routine retrieves a table of minor edit variable names. This table is interrogated by subsequent code, which compares variable name character strings from TALINK with the minor edit variable names to establish a pointer table to the values to be transferred at each time step.

Only a limited number of variables need to be transferred to and from the SIBDYM balance of plant model coding. In view of this the SIBDYM coding has been modified to directly access data in a new internal table of values which may be referenced/updated for TALINK data transfers.

All codes advance over a specified time interval before exchanging data and no iteration takes place.

Transient Analysis Model

The transient analysis codes package formed with the aid of the TALINK interface code has been used to analyze the behaviour of an example transient detailed validation against plant data is under way. The demonstration transient selected is a postulated bounding fault analyzed for the Sizewell 'B' reactor safety case using the NNC Sizewell 'B' Project version of the Westinghouse intact circuit transient analysis code LOFT-5. The principal initiating fault

is a loss of off-site power (taken to occur at time zero).

Other failures modelled include:

- SG overpressure transient to beyond design but with some relief available.
- Failure of 3 or more RCCAs to insert on reactor trip - ATWT.

As a consequence of these faults the following failures are assumed:

- RCPs trip at time zero.
- Main feed is lost (at 0.2 seconds).
- Turbine stop governor valve closed at 3.0 seconds.
- The Emergency Boration System (EBS) is initiated in loops 1, 3 and 4 at 10 seconds.
- No auxiliary feed flow.

In addition the pressuriser heaters and sprays are assumed to be disabled.

Transient Analysis Results

The first 50 seconds of the transient were analyzed using the integrated transient analysis package with a number of system parameters being passed on a dynamic basis between PANTHER and RELAP-5 using the TALINK code. These parameters included the quadrant power calculated by PANTHER

The original safety case analysis used the results of both 3-D and point kinetics LOFT-5 calculations. Conservatism was incorporated to allow for uncertainties in the data needed to predict the results of asymmetric boron injection and facilitate performance of analysis which would simultaneously bound the first three fuel cycles of the Sizewell 'B' reference fuel cycle. The TALINK results demonstrated its use as a fault study tool.

The new integrated code package enables Nuclear Electric to perform best-estimate 3-D neutronics based calculations of, for example, fuel degradation arising from the fault transient being analyzed for specific times in cycle. The accuracy of the calculation results is then constrained by the accuracy of models such as that used to calculate the effects of

fluid mixing in the downcomer and lower plenum.

Benefits of the combined code package and future development

Nuclear Electric now has the capability to perform best-estimate transient analysis involving multi-dimensional neutronic kinetics reactor core calculations with coupled primary and secondary circuit thermal hydraulics and balance of plant calculations.

Using the integrated thermal-hydraulics and neutronics package enables complex fault transients to be analysed using the best-estimate neutron kinetics capabilities of PANTHER removing the need for pessimisms inherent in simpler analysis. This could be used to provide greater flexibility for certain aspects of plant operation in a plant safety case, for example.

In addition the introduction of the SIBDYM balance of plant models has enabled the RELAP5/MOD-2 turbine model to be removed. This revision was considered to be necessary since the RELAP5 model did not conserve energy and had been found to cause pressure solution fluctuations.

The integrated code package is linked flexibly. Thus, if a different primary and secondary circuit thermal-hydraulic code were adopted, for example, then the new integrated code package could be setup without substantial additional effort.

The integrated code package will be revised shortly to incorporate RELAP5/MOD-3 instead of RELAP5/MOD-2. The package is also likely to be extended in future to incorporate the Battelle North-West/EPRI VIPRE-01/MOD-2 code to enable detailed sub-channel analysis to be performed.

Acknowledgements

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References

1. Hutt P.K., Gaines N., Halsall M.J., McEllin M., White R.J., The UK core performance code package. Nucl. Energy, 1991, 30, No5, pp291-298.

An Analytical Study on Excitation of Nuclear-Coupled Thermal-Hydraulic Instability Due to Seismically Induced Resonance in BWR

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Abstract

This paper describes the results of a scoping study on seismically induced resonance of nuclear-coupled thermal-hydraulic instability in BWRs, which was conducted by using TRAC-BF1 within a framework of a point kinetics model. As a result of the analysis, it is shown that a reactivity insertion could occur accompanied by in-surge of coolant into the core resulted from the excitation of the nuclear-coupled instability by the external acceleration. In order to analyze this phenomenon more in detail, it is necessary to couple a thermal-hydraulic code with a three-dimensional nuclear kinetics code.

1. Introduction

An analytical study was performed for a seismically-induced instability in BWR⁽¹⁾. The primary objective of the study is to supply quantitative information helpful to determine whether or not further research is necessary on this topic. This paper reviews the methods and models applied and the major results obtained in the study for the purpose to supply a material to discuss the interface requirements to couple a thermal-hydraulic code with a nuclear kinetics code.

A seismically-induced sloshing of fluid in a tank or reservoir is one of the important research themes to assure structural integrity, where the focal point may be a resonance of the motion of water level with seismic acceleration. In BWR, there exist inherent frequencies related to so-called nuclear-coupled thermal-hydraulic instabilities. In fact, neutron flux oscillation events occurred at several BWRs, for example, at Caorso in Italy in 1982⁽²⁾, at LaSalle-2 in U.S.A. in 1988⁽³⁾ and recently at WNP (Washington Nuclear Project)-2 in U.S.A. in 1992⁽⁴⁾. The oscillations which occurred at LaSalle-2 and WNP-2 are understood as a core-wide (in-phase) oscillation, where the neutron flux over the whole core oscillates in the same phase. The oscillation observed at Caorso, on the other hand, has been recognized as a regional (out-of-phase) one, where the neutron flux in one part of the core oscillates in a different phase from that in the rest of the core.

Concerning earthquakes, several minor but interesting events took place at Japanese BWRs. Most recently, the reactor tripped on high neutron flux at Onagawa in November, 1993. Although the mechanism of the trip might not directly be linked to the topic mentioned above, this event apparently raised an incentive to initiate this study. The recent earthquake at Kobe, of course, formed a part of the motive force.

The period of the oscillation observed at LaSalle-2 was reported to be 2 to 3 seconds. Although the power spectrum of seismic waves with this range of periods may be

all cases, the built-in values in TRAC-BF1 are applied for the kinetic constants and coefficient for void feedback reactivity.

The degree of stability can be characterized by the decay ratio R, which was evaluated by calculating the power response to a step change in the pressure at the steam outlet. As shown in Fig.2, the decay ratios were defined as the ratio of the second peak to the first one and were evaluated to be 0.44, 0.63 and 0.74 for Cases 1, 2 and 3, respectively. The inherent periods were also evaluated from Fig.2 as approximately 5 seconds.

2.3. Modeling of seismic acceleration

The external acceleration in vertical direction was modeled simply by a sine curve as

$$\theta = 0(\text{vertical direction}) \text{ and } a_z = a^*g \cdot \sin\left(\frac{2\pi t}{\tau}\right) \quad (2)$$

in Eq.(1), where τ is a period. It is difficult to define a realistic range of the seismic amplitude a^* , since the power spectrum of the amplitude quickly decreases as the period increases to several seconds and insufficient reliable data exist in this range of period. In the study, it was assumed that $a^* = 0.1$ as a base case. This value may be much larger than the power spectra corresponding to a period of 5s of recorded data in large earthquakes.

3. Major calculated results

Using the input data for Case 3, the most unstable one, sensitivity calculations on τ were performed setting $a^* = 0.1$ in Eq.(2). The calculated core power transients are shown in Fig.3, where the reactor scram was neglected in order to see the maximum power in case without scram. The resonance is clearly shown in this figure. Namely, the case with $\tau = 5s$, which is the inherent period of the core-wide instability, gives the highest power peak. The periodic reactivity insertion was caused by periodic in-surge of coolant into the core and subsequent collapse of voids.

The calculated core power transients assuming $\tau = 5s$ with $a^* = 0.1$ are shown in Fig.4 for Cases 1, 2 and 3. As expected, the highest peak was calculated to occur in Case 3. The heights of the first, second and third power peaks are plotted as a function of the decay ratio in Fig.5. It is shown that the peak heights are largely dependent on the decay ratio. This figure implies that if the decay ratio is nearly one or more, significantly large reactivity insertion could happen.

The calculated peak power for Case 3 is shown in Fig.6 as a function of the amplitude a^* of the sine curve. It is shown that the peak power also largely depends on the amplitude.

4. Concluding Remarks

Since the realistically possible maximum amplitudes of seismic waves with long periods greater than 1s are quite uncertain, the absolute values of the calculated power peaks shown in Figs.3 to 5 may have less meaning. The value of 0.1g used in

all cases, the built-in values in TRAC-BF1 are applied for the kinetic constants and coefficient for void feedback reactivity.

The degree of stability can be characterized by the decay ratio R , which was evaluated by calculating the power response to a step change in the pressure at the steam outlet. As shown in Fig.2, the decay ratios were defined as the ratio of the second peak to the first one and were evaluated to be 0.44, 0.63 and 0.74 for Cases 1, 2 and 3, respectively. The inherent periods were also evaluated from Fig.2 as approximately 5 seconds.

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The external acceleration in vertical direction was modeled simply by a sine curve as

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in Eq.(1), where τ is a period. It is difficult to define a realistic range of the seismic amplitude a^* , since the power spectrum of the amplitude quickly decreases as the period increases to several seconds and insufficient reliable data exist in this range of period. In the study, it was assumed that $a^* = 0.1$ as a base case. This value may be much larger than the power spectra corresponding to a period of 5s of recorded data in large earthquakes.

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this study may be extremely large for such seismic waves. In the next step, therefore, it is necessary to evaluate the realistically possible maximum amplitude with the help of the experts in the area of seismology. However, it was clarified in this study that there exists a mechanism that could lead to relatively large reactivity insertion.

The problem was well simplified in this study, namely only the in-phase oscillation excited by vertical seismic wave was taken into account. In reality, a seismic wave is three-dimensional and consists of full range of frequency spectra for all directions. In the case of in-phase oscillation, there exists only one oscillation mode. In the case of regional oscillation, i.e. out-of-phase oscillation, however, various oscillation modes exist and some of them could be excited depending on the direction, period and amplitude of the seismic wave. In some modes, the inherent frequencies could be higher, and thus the amplitudes of the corresponding seismic wave could be larger. In order to well understand such complex phenomena, it is necessary, first of all, to well understand the mechanism of the regional oscillation itself. It is obvious that numerical tool to couple a thermal-hydraulic code with a three-dimensional nuclear kinetics code is necessary.

In addition, the applicability of the constitutive relations in TRAC-BF1 to transient two-phase flow phenomena under time varying acceleration field may be questionable. Further research efforts are required to this area.

A test program has been launched at JAERI for investigation of nuclear-coupled thermal-hydraulic phenomena in BWR including nuclear-coupled instability and nuclear-coupled response to seismically-induced changes in the core inlet flow rate. The tests will be run at prototypical pressure and temperature. The neutronic feedback will be simulated by controlling the electric power to the simulated fuel rods based on real-time neutronic calculation performed using the temperatures and void fractions measured in the test section. Preliminary tests using a single-bundle test section will be initiated in 1996. Whereas the test section itself is one-dimensional, it is planned to conduct tests in future for boundary conditions determined by a system code coupled with a 3-dimensional kinetics model, which is currently being developed at JAERI.

References

- (1) Hirano, M. and Tamakoshi, T., "An analytical study of excitation of nuclear-coupled thermal hydraulic instability due to seismically induced resonance in BWR," Nucl. Eng. Des. 162 (1996) 307-315.
- (2) E.Gialdi, et al., Core stability in operating BWR: Operating experience, Prog. Nucl. Energy, Vol.15, 1985, pp.447-459.
- (3) G.A.Murphy, Selected safety-related events, Nuclear Safety, Vol.29, No.3, 1988, pp. 356-362.
- (4) WPPSS, Unusual reactor scram due to core instability, LER 92-037, 1992.
- (5) Shaug, J.C. et al., "Analysis of fluid dynamics in a boiling water reactor in a varying acceleration field, Forum on Unsteady Fluid Flow, ASME Winter Annual Meeting, Boston, USA, October, 1987.
- (6) Weaver, W.L., et al., TRAC-BF1 manual: Extensions to TRAC-BD1/MOD1, NUREG/CR-4391, EGG-2417, 1986.

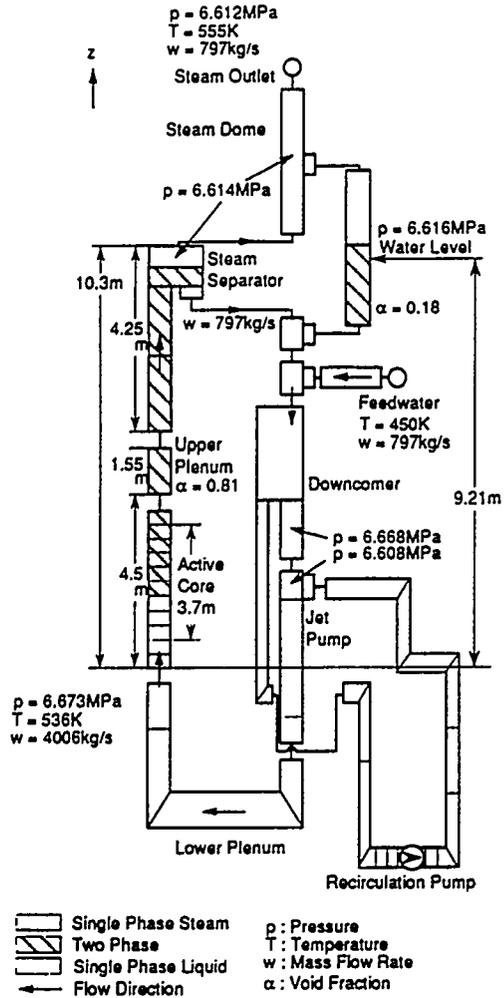


Table 1 Summary of initial steady state conditions

Items	Case 1	Case 2	Case 3
Operation Condition	N.C. ¹⁾	N.C.	N.C.
Core Power(%Rate) ²⁾	49.0	49.0	54.0
Core Mass flow Rate(%Rated) ³⁾	30.0	30.0	28.2
Power-to-Flow Ratio (%/%)	1.63	1.63	1.91
Axial Power Distribution	Cosine	Flat	Flat
Core Inlet Temperature(K)	536	536	534
Core Outlet Void Fraction	0.814	0.812	0.844
Decay Ratio	0.44	0.63	0.74
Inherent Period(s)	5	5	5

¹⁾ N.C.: Natural Circulation

²⁾ Rated Power: 3293 MWt

³⁾ Rated Core Mass Flow Rate: 1.34×10^4 kg/s

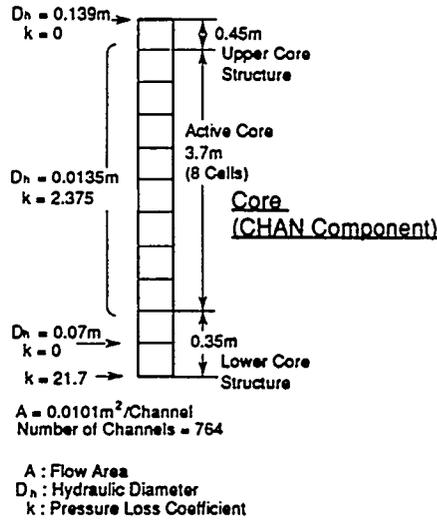


Fig. 1 Nodalization scheme and initial steady state of Case 1

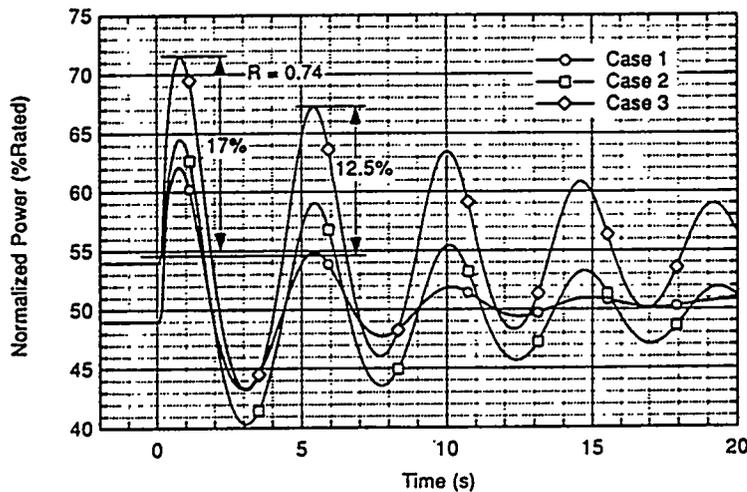


Fig.2 Core power transients after step change in pressure

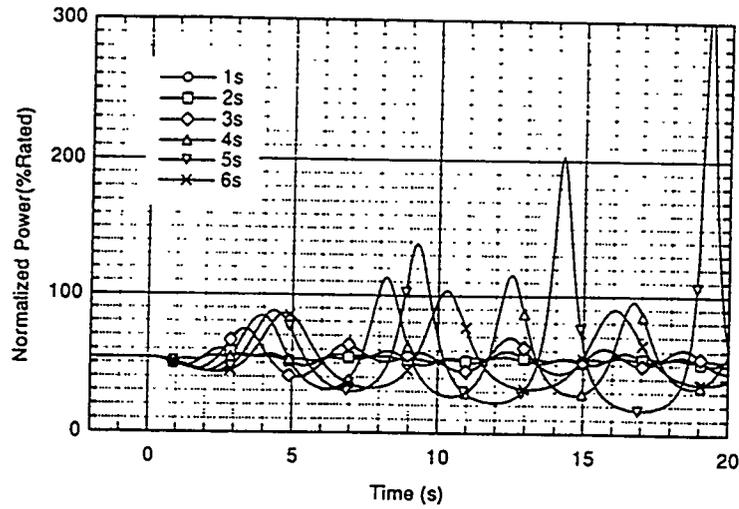


Fig.3 Core power transients in sensitivity calculations on period of external acceleration

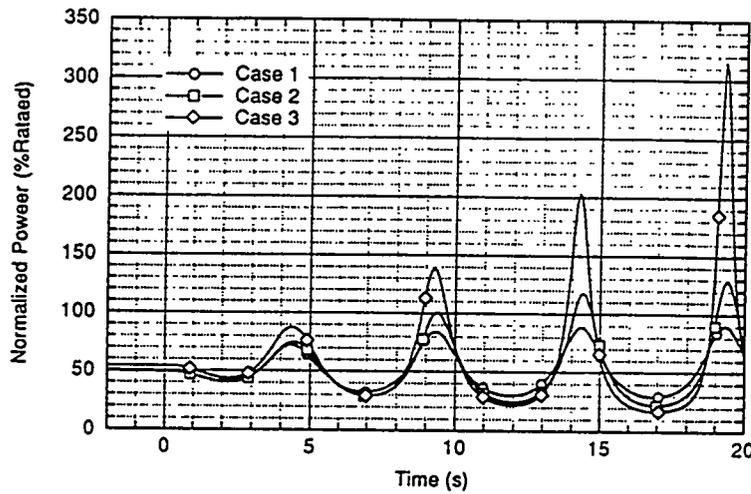


Fig.4 Transient of power in sensitivity calculations on the decay ratio.

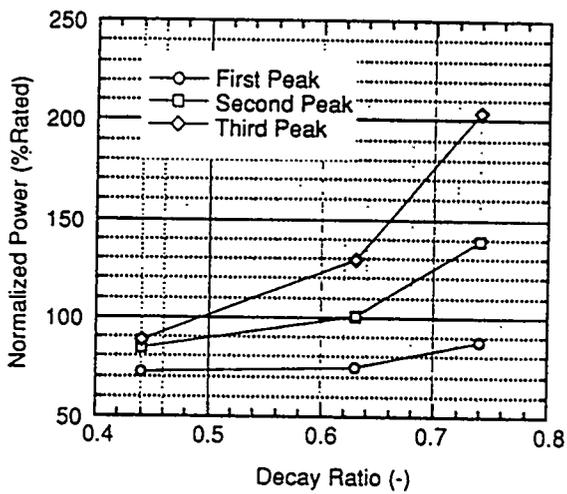


Fig.5 Peak power heights as a function of the decay ratio

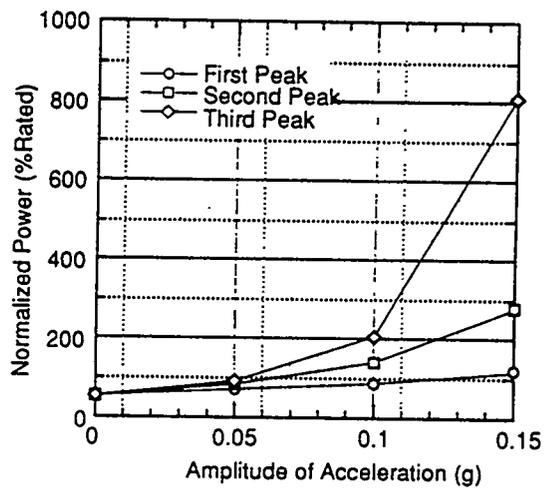


Fig.6 Peak power heights as a function of the amplitude of external acceleration

**Interface Requirements for Coupling a Containment Code
to
a Reactor System Thermal Hydraulic Codes**

by

Anthony J. Baratta

Pennsylvania State University

INTRODUCTION

To perform a complete analysis of a reactor transient, not only the primary system response but the containment response must also be accounted for. Such transients and accidents as a loss of coolant accident in both pressurized water and boiling water reactors and inadvertent operation of safety relief valves all challenge the containment and may influence flows because of containment feedback. More recently, the advanced reactor designs put forth by General Electric and Westinghouse in the US and by Framatome and Siemens in Europe rely on the containment to act as the ultimate heat sink.

Techniques used by analysts and engineers to analyze the interaction of the containment and the primary system were usually iterative in nature. Codes such as RELAP or RETRAN were used to analyze the primary system response and CONTAIN or CONTEMPT the containment response. The analysis was performed by first running the system code and representing the containment as a fixed pressure boundary condition. The flows were usually from the primary system to the containment initially and generally under choked conditions. Once the mass flows and timing are determined from the system codes, these conditions were input into the containment code. The resulting pressures and temperatures were then calculated and the containment performance analyzed.

The disadvantage of this approach becomes evident when one performs an analysis of a rapid depressurization or a long term accident sequence in which feedback from the containment can occur. For example, in a BWR main steam line break transient, the containment heats up and becomes a source of energy for the primary system. Codes such as MAPP and MELCORE have containment models built in, however, the thermal hydraulics are generally simple in nature and have difficulty modeling complex primary system phenomenon.

Recent advances in programming and computer technology are available to provide an alternative approach. The author and other researchers have developed linkage codes capable of transferring data between codes at each time step allowing discrete codes to be coupled together.

Several such approaches were developed and have seen limited application. In the 1980's the DATATRAN code developed by the Electric Power Research Institute was used to couple the RETRAN code to other analysis tools. However, its application was limited to certain operating systems and interest at that time in this capability was not present. The first significant effort to couple a containment code to a systems code was that of Bieniarz (Bieniarz 1991)). He used proprietary hardware and software to couple the CONTAIN and BWR SAR computer codes. While highly successful, the proprietary nature of the system limited its applicability to a few reactors.

More recently, efforts by the author and his associates as well as personnel at Siemens have identified alternative approaches that utilize conventional hardware. In the sections that follow, the work at Penn State and that at Siemens is described as well as the requirements for such code capability.

CODE REQUIREMENTS

The main purpose of coupling a system containment code to a systems code is to enable physical quantities such as pressure, temperature, mass and energy as well as trip information to be passed between the two codes. This passage of data must be done in such a way as to ensure the data is compatible with the needs of the two codes and in a temporally consistent manner. Mass and energy errors must be minimized as well. Finally, the process must be transparent to the user and be done with minimal changes to the two codes and with minimal impact on the execution times of the codes.

The systems and containment codes usually do not model the physical phenomenon in the same way. Often, the containment codes use a lump parameter approach and simplified mass and energy equations. The two types of codes frequently use different property tables and require the user ensure that data is referenced to the same zero points. In the case of CONTAIN and RELAP, the CONTAIN code uses enthalpy and liquid- and vapor-phase mass flow rates where the RELAP code uses total mass flow and void fraction and liquid- and vapor-phase internal energies.

To couple the information requires the generation of data in the appropriate form for each of the codes. Hence, a coupling scheme must have this feature.

Temporal coordination is also a critical concern. Generally, the equations solved in a containment code do not have significant high frequency components and therefore time step size is usually much larger than that used in systems codes. To coordinate the time steps requires either a detailed understanding of the transient response or an automatic method of time step coordination. Since user convenience is a strong requirement, the latter is the preferred approach.

In the next section, two different approaches are reviewed. The first developed at Penn State, the second by researchers at Siemens.

COUPLING METHODOLOGIES

To overcome some of the deficiencies of previous attempts to couple two or more codes together, Smith and Baratta (Smith 1995) employed the parallel virtual machine operating environment (PVM) (Geist 1991). The method developed by them uses PVM to coordinate and pass information between the severe accident analysis code SCDAP/RELAP (Allison 1989) and the containment analysis code CONTAIN (Murata 1989).

The PVM operating environment was developed by Oak Ridge National Laboratory to provide multi processing capabilities on a loosely coupled network of diverse computers. Written in C, PVM calls upon the UNIX message passing utility to send information in the form of messages between the processes coupled using PVM. In this particular case, the processes are the SCDAP/RELAP and CONTAIN codes. Both codes are written in FORTRAN. The process of coupling two such FORTRAN codes is however facilitated since there are FORTRAN to C interface routines provided with PVM. Also, the PVM software need not be run on two machines but instead can be run on one machine. Furthermore, the PVM operating system is designed to be almost machine independent enabling it to be used on a wide range of platforms.

The PVM interface routines may be divided into two distinct areas, process management and data transfer. The process management routines control the starting and controlling the processes. The data transfer routines place the data in data transfer routines and then send and receive the data. The data and process management routines are designed so that it is not necessary to know where the actual processes are running. The location is determined during the spawning process. This feature is attractive since the user does not need to determine in advance where the processes are to be run.

Figure 1 shows the original SCDAP/RELAP CONTAIN execution control program. In this case, the execution control process is enrolled (started) as srlcon on any UNIX machine and then the CONTAIN code is started on a specific machine, psunuke. The modified version of SCDAP/RELAP, selap, is then started on a third machine, Mongo.

The execution control program only sets up and initiates the programs which makeup the coupled codes. Actual communication sequencing is handled by the modified SCDAP/RELAP and CONTAIN codes. Modifications were made to each code to facilitate the extraction and passing of data and to receive and process the data from the other code.

In the case of SCDAP/RELAP, the subroutine TRAN was modified. This routine is the routine in RELAP that has access to any data required by CONTAIN. As mentioned earlier, supplemental coding was added to obtain the specific variables required by CONTAIN.

For data transfer from CONTAIN, the TSTATE in the SCDAP/RELAP code routine was modified. This routine is responsible for processing time dependent volume and junction data during code execution. Separate time dependent volumes were defined for each key region in the containment.

Because of the structure of the CONTAIN code, many more routines had to be modified to enable the communications. In addition, several new routines had to be created. Notwithstanding these changes, the effort did not involve changes to any of the models or correlations that might invalidate previous assessment studies. A key concern in codes used for licensing studies.

It should be mentioned that more recent work by Hayner (Hayner 1996) and Baratta has extended the original work by Smith and Baratta. Subsequent to the work by Smith, a need to couple corium and non-condensables as well as fission products was identified. Also, the problems with the original parameter passing scheme were found which caused large mass errors to occur.

Hayner modified the coupling to pass both integrated vapor- and liquid-mass as well as mass flows. He also followed the suggestion of Smith and passed the information at every SCDAP/RELAP time step to CONTAIN. Since RELAP generally uses much smaller time steps than CONTAIN, it was possible for the mass flow rates to change significantly during the much longer CONTAIN time step introducing large errors in the mass transfer. Tests to date show that using the SCDAP/RELAP time step for both codes results in no timing problems and reduces the mass errors to acceptable values.

Using the SCDAP/RELAP time step would seem wasteful of resources. Since the CONTAIN execution time is very fast compared to that of SCDAP/RELAP, the net change in total run time is very small.

Finally, it should be pointed out that the approach adopted here is an explicit method in that old time values of containment parameters are used by SCDAP/RELAP to calculate current time values of the primary system parameters. To date, the authors have not seen any problems with this approach.

The method has now been applied to an ATWS transient in a BWR 6 (Smith 1995) and to the analysis of a station blackout with pump seal failure in a PWR (Hayner 1996). Typical results are given for these two transients in Fig. 2 and 3 respectively.

Another approach used to couple two codes developed by Rothe (Rothe 1994) and used by Curca-Tivig and Kohler (Curca-Tivig 1994) to couple the RELAP5 and COCO codes for containment response analysis. The COCO code (Curca-Tivig 1994) is a containment analysis code used to predict the temperature and pressure in a containment during a large break LOCA.

The coupling is accomplished using the EUMOD (External User MODEL) interface code. As in the method developed by Smith and Baratta, the RELAP code is used to calculate the primary system response. Data is transferred to the containment code in the form of integrated and current break mass flow rates, integrated and current break enthalpy flow rates, enthalpy and mass flow rates of other injections into the containment, size of time step used last, and the containment pressure used in the last RELAP time step. Similar to the Penn State approach, RELAP time step is used to control the containment code COCO.

The authors point out that any variable in a RELAP minor edit may be transferred in this manner. Non-standard variables not in the RELAP minor edit may also be transferred as well but require special coding.

Figure 4 is a flow chart from Rothe. Unlike the PVM approach, the EUMOD interface acts as a subroutine in the RELAP code. Data is transferred via a call to the EUMOD interface and then to the coupled user code. This approach has a number of advantages and disadvantages. In the case of a large external user code, the machine that would be used to run the entire coupled package would likely need to be one with a large memory and disk storage. However, as Rothe points out, the implementation of the interface in RELAP required amazingly few changes to the RELAP code -- a total of three RELAP statements were modified and 3 new ones added.

The results of a LOCA analysis using RELAP5 coupled to COCO with EUMOD are shown in Fig. 5. Clearly the more accurate time dependent boundary condition imposed in this manner have an impact on the progression of the transient.

CONCLUSION

It is now possible to perform accurate coupled primary system containment analysis using best estimate thermal hydraulic codes such as RELAP or severe accident analysis tool such as SCDAP/RELAP coupled to containment codes. A variety of methods are available for this type of coupling. These include the use of conventional subroutine approach as used by Rothe and the parallel processing approach developed by Smith and Baratta.

These approaches enable the RELAP or SCDAP/RELAP codes to be coupled with minimal changes to containment codes such as CONTAIN. Software tools for the coupling are available that require no specialized hardware. These tools are not necessarily general enough to randomly couple any variable to any volumes, however. In both the PVM and EUMOD case, there is a clear need to understand the way in which the codes use the resulting information. Finally, independent time step control is unnecessary. Satisfactory coupling is obtained by using the RELAP time step for both codes.

References:

Allison, C. M. and E. C. Johnson, SCDAP/RELAP5/MOD2 Code Manual Volume 1: RELAP5 Code Structure, System Models and Solution Methods, Report NUREG/CR-5273-Vol 1 (EGG-2555-Vol 1), 1989.

Bieniarz, S., Susquehanna Steam Electric Station Individual Plant Evaluation Vol. 5, "Supplemental Source Term Calculations, December," 1991.

Curca-Tivig, F. and M. Köhler, "A code System for Coupled Analysis of Reactor Coolant system and Containment Thermalhydraulics," Proceedings of the International Conference on New Trends in Nuclear System Thermohydraulics, May 30th-June 2nd, 1994, Pisa Italy, Vol. II, 293, 1994.

Geist, G. A. and V. S. Sunderam, Network Based Concurrent Computing on the PVM System, ORNL/TM-11760, 1991.

Hayner, G. E., Improvements to the RELAP5/CONTAIN COUPLING, PhD Thesis, The Pennsylvania State University, 1996.

Murata, K. K., et. al., Manual for CONTAIN 1.1: Computer Code for Severe Nuclear Reactor Accident Containment Analysis, Report NUREG/CR-5026 (SAND87-2309), 1989.

Rothe, T., "Linking External User Models to RELAP5: A New Era of RELAP5 Applications," Proceedings of the International Conference on New Trends in Nuclear System Thermohydraulics, May 30th-June 2nd, 1994, Pisa Italy, Vol. I, 263, 1994.

Smith, K. A., A.J. Baratta, and G. E. Robinson, "Coupled RELAP5 and CONTAIN Accident Analysis Using PVM," Nucl. Safety, 36, 94 (1995).

```

program srlcon
c Host program to execute SCDAP/RELAP5/MOD3 V7af
c and CONTAIN 1.12 concurrently under the PVM system
integer info, mynum, inst
character*8 arch
character*12 nodename
c enroll host in PVM
call fenroll("srlcon\0", mynum)
if( mynum .lt. 0) then
  print *, 'failure in fenroll on host'
  stop
endif
c set ARCH to any available machine
arch = "RIOS0"
c Initiate contain node program on psunuke
c call finitiate("contain\0", arch, inst)
call finitiatem("contain\0", "psunuke\0", inst)
if( inst .lt. 0) then
  print *, 'failure to initiate'
  stop
endif
c Initiate relap node program on mongo
c call finitiate("selap\0", arch, inst)
call finitiatem("selap\0", "mongo\0", inst)
if( inst .lt. 0) then
  print *, 'failure to initiate'
  stop
endif
c leave PVM
call fleave()
stop
end

```

Figure 1. RELAP/CONTAIN execution control program.

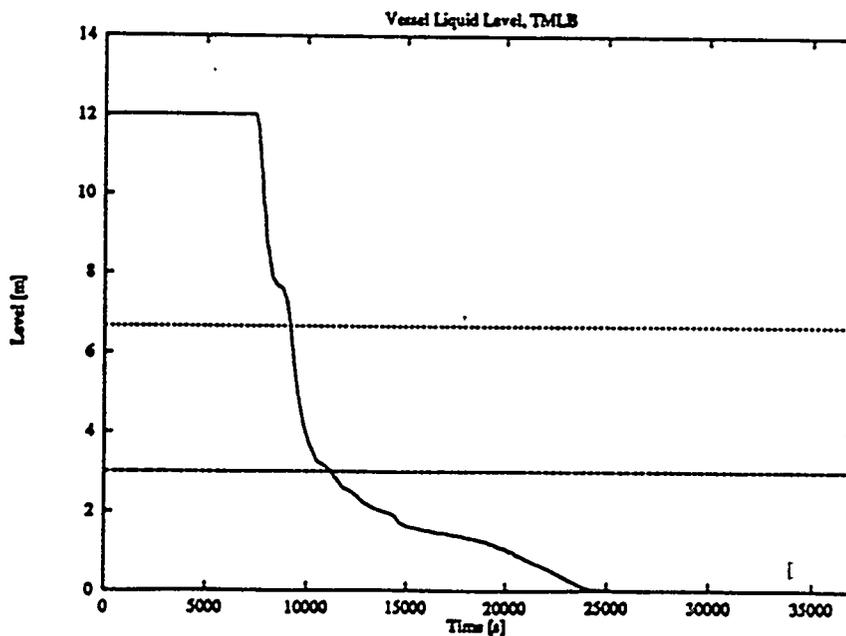


Figure 2. Vessel water level during TMLB' sequence station blackout (Hayner 1996).

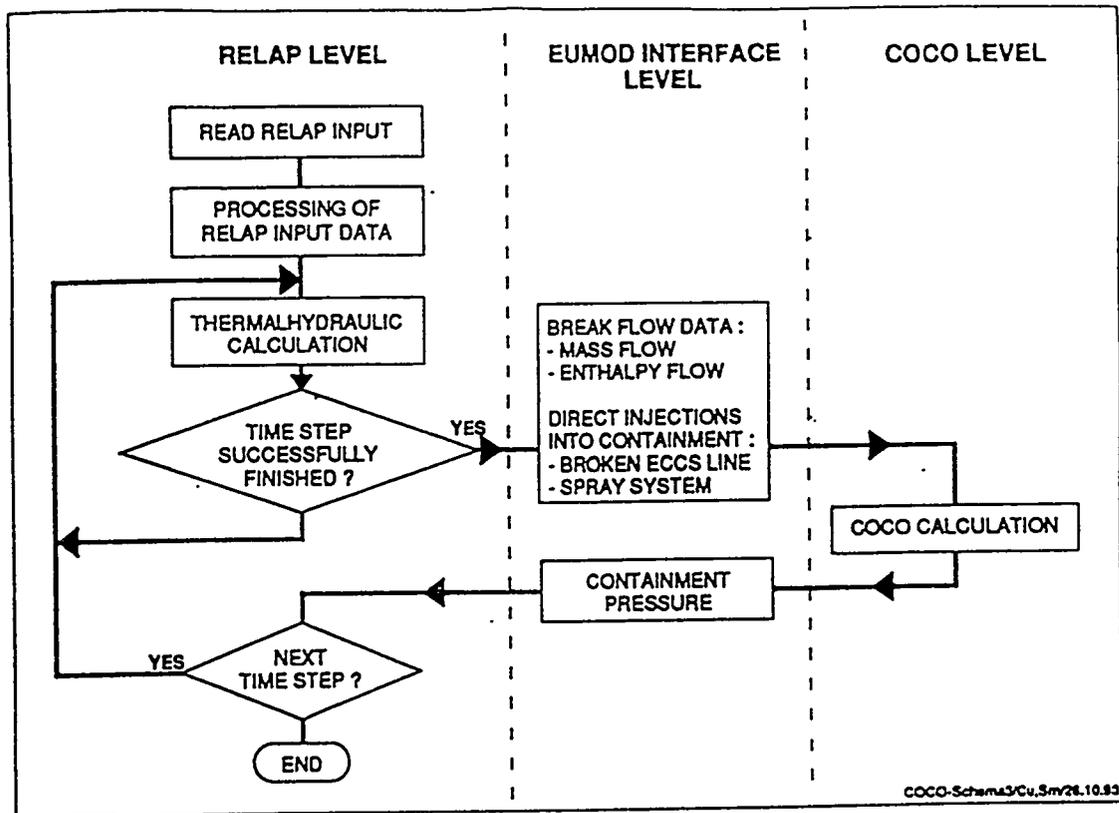


Figure 4. Data transfer between RELAP5 and COCO during coupled calculations

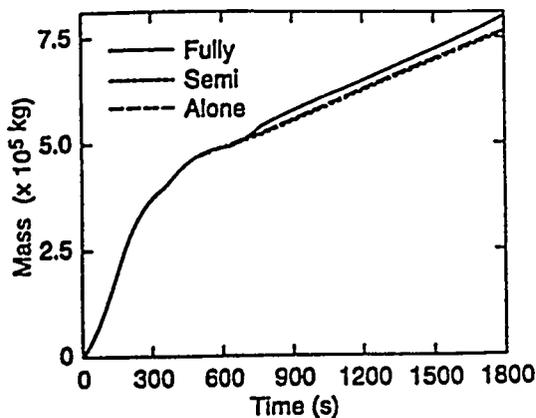


Figure 3. Integrated Safety Relief Valve mass discharged to containment for fully coupled (fully) and iterative (alone) cases for EWR ATWS depressurization transient (Smith 1995).

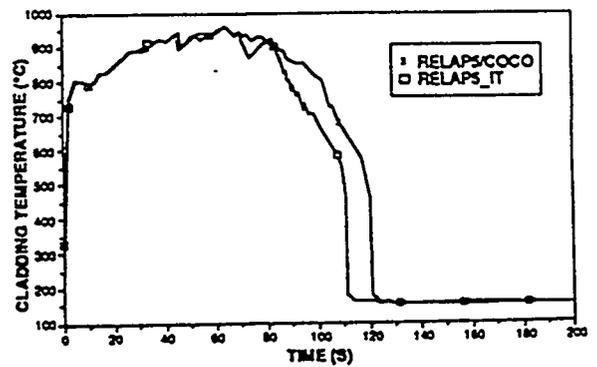


Figure 5. Test No. 1 - Comparison between iterative and coupled calculations. Fuel rod cladding temperature (Geist 1994).

THERMAL-HYDRAULIC INTERFACING CODE MODULES FOR CANDU REACTORS

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ABSTRACT

The approach for CANDU reactor safety analysis in Ontario Hydro Nuclear (OHN) and Atomic Energy of Canada Limited (AECL) is presented. Reflecting the unique characteristics of CANDU reactors, the procedure of coupling the thermal-hydraulics, reactor physics and fuel channel/element codes in the safety analysis is described. The experience generated in the Canadian nuclear industry may be useful to other types of reactors in the area of reactor safety analysis.

1. INTRODUCTION

A CANDU reactor is a pressure-tube, heavy-water-moderated, pressurized heavy-water-cooled reactor consisting of two figure-of-eight loops. The fuel channels consist of two concentric tubes (pressure tube and calandria tube) with the space between filled with an inert gas. The pressure tubes (390 in Pickering A, 480 in Bruce A, Bruce B and Darlington, 380 in Pickering B and CANDU-6 NGS) are horizontal and are rigidly jointed to end-fittings which are firmly supported by the end shields. The calandria tubes, which are roll expanded at both ends into the calandria side tube-sheets, separate the cold moderator in the calandria vessel from the hot pressure tubes. The pressure tubes are grouped so that there are four core passes, each containing a quarter of the core channels. The pressure tubes are connected by feeders to a common reactor header. There are one reactor inlet header (RIH) and one reactor outlet header (ROH) in each core pass. For example, each reactor header of Darlington NGS has 120 feeders. All reactor channels in the same core pass exhibit the same boundary conditions at the common reactor headers. By using natural uranium and heavy water, the CANDU reactor has relatively high fuel power rating, high flux and small excess reactivity (on-power refuelling). The reactivity constraint requires constant control in the reactor core. It has led to

the extensive use of automatic control in CANDU reactor design. As a result, the automatic controller actions play a key role in the CANDU operational and safety analyses.

In the Canadian approach to nuclear power safety (Reference 1), the owner of a nuclear power plant bears the basic responsibility for safety whereas the regulatory authority (the Atomic Energy Control Board (AECB) in Canada) sets the safety objectives and performance requirements and audits the owner's achievements. Therefore, the primary objective of reactor safety analysis is to determine whether the regulatory dose limits are exceeded for various events including the large loss of coolant accident (LOCA). In the reactor safety analysis, conservative assumptions are imposed in the models to insert the necessary safety margins in the analysis. These conservative assessments on the safety analysis require a review of all the modules used in the reactor system code. The axial and radial flux distributions, and the peaking factors and reactivity tables (functions of void, change in fuel temperature and shut-off rod position) are provided by the reactor physics codes. These values are assumed uniform in the core in the point kinetics model. The errors induced by these assumptions may not be important in the operational support and small LOCA analyses. However, they will affect the results for large LOCA analysis. In the analysis of a large LOCA, more attention is focused on the validation of these assumptions. In the Canadian nuclear industry, a comprehensive methodology for the CANDU safety analysis has been established. In this methodology, the conservative assumptions required by the regulatory authority (AECB), the analysis approach, and the computational tools required for a complete analysis of postulated loss of coolant accidents for CANDU reactors have been accounted for.

Considerable design effort and analysis have been devoted in Canada to ensure that the CANDU safety system mitigates the consequences of a large LOCA. The stagnated or critical break represents the most severe large break from the core heatup point of view. Considerable research has been conducted in this particular area in Canada. The main concern of a large LOCA is the amount of radioactive release to the environment. The regulatory dose limits should not be exceeded.

In this paper, the modules in the CANDU reactor system simulation and their interactions are first described. Then the interface among the thermal-hydraulics, the 3D reactor physics and the fuel channel codes in the CANDU safety analysis is presented. The approach for the code interfaces reflects the unique characteristics of CANDU reactors.

2. MODULES FOR CANDU REACTOR SYSTEM SIMULATION

To simulate the CANDU reactor system, the code requires modules dealing with reactor controllers, thermal-hydraulics, reactor physics, heat conduction and transfer, system components and other auxiliary or special models. The major functions of these modules and their interactions are briefly described. Figure 1 shows the interactions among various modules in a system code for CANDU reactors. A more detailed description of the functions of all modules simulating CANDU reactor systems can be found in Reference 2. Figure 2 shows the major interactions among the module codes used in the safety analysis. Except for safety reason, these interactions are not required in the operational support analysis.

CANDU Controllers Module

The main functions of the CANDU controllers are to deliver steam at acceptable pressure and to maintain a stable reactor power. During upset operations, they control the reactor in a safe mode of operation. The module simulates the following control systems: overall unit control, reactor regulating system, steam generator pressure and level controls, heat transport system pressure and inventory controls and safety systems.

The overall unit control is executed by three control programs: the unit power regulator, the steam generator pressure control and the demand power routine of the reactor regulating system. The reactor regulating system is an integrated system which directly controls the reactor power. It comprises the reactor power measurement, the reactivity control mechanisms (light water zone controllers, neutron-absorbing adjuster rods or mechanical control absorber rods), the demand power routines and the reactor power stepback and setback programs.

The steam generator pressure control system manipulates either the reactor power setpoint (normal mode of operation) or the turbine-governor reference setpoint (alternate mode of operation) to maintain the steam generator pressure at its setpoint. It also controls the opening of the atmosphere steam discharge and condenser steam dump valves to trim the steam generator pressure. The steam generator level control system is designed to control the levels in all steam generators by modulating the level control valves in the valve stations located in the feedwater lines. The heat transport pressure and inventory control system maintain the ROH pressure at its setpoint by modulating the pressurizer steam bleed valves and the pressurizer heaters. The heat transport system inventory is controlled by the pressurizer level controller. This system comprises a pressurizer, bleed condenser, bleed cooler, feed pumps, D2O storage tank and other control valves and over-pressure relief valves in the feed and bleed system.

The safety systems of CANDU reactors are totally independent of the control systems. They are triggered automatically when certain system parameters exceed pre-determined setpoint levels. The safety systems comprise two independent reactor shut-down systems (shut-off rods and soluble neutron-absorbing poison in the moderator), the emergency cooling injection (ECI) system, the steam generator controlled cool-down system and the steam generator emergency cooling system. In a large LOCA, the actions of the safety systems are the predominant factors that affect the outcome of all safety analysis, especially the availability of the ECI system.

Thermal-hydraulics Module

The thermal-hydraulic conditions at the following locations are the key parameters used in the reactor controllers: pressures at reactor outlet headers, pressurizer, bleed condenser, steam drums, condenser and steam chest; flow rates at reactor inlet feeders, steam main line, feedwater line and turbine governor valve; water levels in steam drum, pressurizer, deaerator, and bleed condenser; coolant temperatures at pressurizer and bleed condenser; coolant density and fuel temperature in the reactor core and reactor thermal power. The channel flow conditions are the key parameters for the fuel channel behaviour. The coolant density and temperature and the average fuel temperature in each reactor node are the parameters used in the reactor physics module.

The modelling of two-phase flow is the most difficult part in the reactor system codes. It constitutes the most profound differentiation between different codes. To improve the realism of safety prediction methods and to qualify the actual safety margins, a two-fluid model is usually adopted in the advanced thermal-hydraulics codes. In a large LOCA, the study of the effectiveness of the ECI system requires an accurate condensation model in the code. In degraded cooling conditions (e.g., in a large LOCA with a loss of ECI function), the amount of steam flow in the core becomes a dominant parameter in the safety analysis.

Reactor Physics Module

The reactor power measurement of the reactor regulating system in the reactor controllers is simulated by the reactor kinetics calculation. It can be simulated either by a point kinetics model (used in most reactor system codes) or by a three-dimensional space-time kinetics model (used in most reactor physics codes). In the kinetics model, the total reactivity change consists of the following components: fuel temperature, coolant temperature and density, moderator temperature, refuel process, bundle movement induced by a large LOCA, reactivity control mechanisms and shut-down systems. The reactivity control mechanisms consist of the following components: mechanical control rods, light water zone absorbers and adjuster rods.

Using the point kinetics model in a thermal-hydraulic code, the following assumptions are usually applied: (1) The light water zone controllers (14 in CANDU reactors) are simulated as one group with an average zone water level because flux tilt control is not simulated in the point kinetics model. (2) During an upset condition the power distribution is the same as that under normal operation condition. (3) The effect of dropping control rods or shut-off rods on the power distribution can be expressed as a function of the bulk reactor power.

The three-dimensional reactor physics codes not only provide the detailed information about the reactor core power and the reactivity control mechanisms, but also produce the axial and radial flux distributions and the associated

peaking factors for the reactor system codes when the point kinetics model is utilized. However, these codes are expensive to use for a large LOCA (about 30,000 mesh points, and up to 15 delayed neutron groups). Normally they are used to simulate short term transients (up to 60 seconds).

In a large LOCA, the power increase (about 3-5 times initial power for a typical CANDU reactor) due to coolant void and the effectiveness of the shut-off rods are the main concerns in the early phase of safety analysis. After the reactor is in a shut-down state, the simulation of decay power using a model similar to the point kinetics model is usually adequate. The importance of using the 3D kinetics model in the reactor system code becomes less compared with the two-fluid effects in thermal-hydraulics.

Heat Conduction and Heat Transfer Module

The heat conduction equations for fuel pins, pressure and calandria tubes, heat exchangers and piping wall are usually modelled in the reactor system codes. Solution techniques for these heat conduction equations are well established. Finite difference and lumped parameter methods are usually applied in the code to solve heat conduction equations.

Fuel in CANDU reactors consists of uranium dioxide pellets encased in zirconium alloy sheaths. The pellets and sheaths contain the fission products. In the simulation of a large LOCA transient for CANDU reactors, the following channel and fuel behaviour play an important part in the safety analysis: the thermal behaviour of fuel pins and pressure tube, the mechanical behaviour of pressure and calandria tubes, the fuel failure condition and the amount of fission product release. For the thermal-hydraulics in reactor channels, emphasis is usually placed on the effect of flow regimes. In stratified flow, different heat transfer coefficients are applied in each individual region. For the fuel pins in a channel, the power rating of each individual pin and the flow structure are the key parameters for the fuel pin temperature profile. Also, the sheath is strained outwards due to the thermal expansion and internal fission gas pressure. Oxygen, produced from the reaction between zircaloy and steam at high temperature, diffuses into the sheath and affect its physical properties. The metal-water reaction also generates the heat that diffused into the sheath. Failure of the sheath to contain the gaseous fission products may result from the combined effect of strain, temperature and change in physical properties due to metal-water reaction. The heatup assessment under degraded cooling becomes important as far as the channel integrity is concerned.

The amount of fission products released and the net energy deposition in the fuel are the parameters required for the containment and the radiological consequence codes. The heat load to the moderator is a parameter needed for the subcooling requirement in the moderator.

System Components Module

The following system components are modelled in the CANDU system codes: pumps, valves, pressurizer, bleed condenser, steam generators, turbine and accumulator. The engineering models are utilized in these components.

The pump model simulates a centrifugal pump under normal operating conditions (constant speed), run-down state or restart state. The brake state of a run-down pump is also included in the model. Pumps can be restarted from either the brake or idle state. The pump characteristic is normally supplied by the pump manufacturer only for the first quadrant operation at design speed. For a run-down or restart pump, data for the additional operating quadrants are required. Valves are a major component in power plants. The types of valves used in CANDU reactors include check valves, gate valves, globe valves, ball valves, butterfly valves, pressure relief valves and safety valves. The pressurizer and bleed condenser are the key components in the operational support and safety analyses of CANDU reactors. The boiler model includes the heat transport U-tube side, steam-water shell side, riser, steam drum and downcomer. The steam produced from all the steam generators is combined in a common steam header before going to the turbine. The relationship between the turbine load and the pressure differential across the turbine is represented by a linear function. The emergency coolant system, which is inactive but poised during normal operation, is activated automatically following the detection of a LOCA signal. The response of the ECI system can be divided

into short and long term phases. For CANDU stations, the short term phase consists of high pressure injection from the accumulator water tank. The accumulator and its associated butterfly valve are modelled in the system codes.

3. INTERFACE BETWEEN THERMAL-HYDRAULICS AND REACTOR PHYSICS CODES

An interface between thermal-hydraulics and reactor physics codes is normally used in cases with a large LOCA in the safety analysis. Before the interface, the modelling of a thermal-hydraulic circuit must be set up. It would be a very expensive model to include all the reactor channels in the thermal-hydraulic circuit of CANDU reactors. Normally, the averaged channel approach is adopted. For example, each reactor core pass can be simulated by one region (or zone) with averaged channels or several regions each having its own averaged channels. In the current Bruce safety analysis update of large LOCA at OHN, for example, ten regions in the broken core passes and two regions in the unbroken passes were modelled, each pass having five nodes axially within each region. Considerable effort and thought goes into selecting these regions, taking into account such physical parameters as the elevation and regional power of groups of channels. In the Wolsong 2 safety analysis at AECL, 7-10 regions for the critical core pass were modelled with 12 axial modes (one per fuel bundle). Since the approaches for code interface between thermal-hydraulics and reactor physics at OHN and AECL are not exactly the same, they are described separately. The main computational tools used in the safety analysis are described in the Appendix.

Interface Approach at OHN

The reactor system code TUF can be operated in two modes for the reactor core power calculation: self initiating or iteratively with 3D reactor physics codes. In the self initiating mode, the point kinetics model is used. In the iterative mode, a procedure to couple the thermal-hydraulics and reactor physics codes is applied. In the iterative procedure, the reactor physics code SMOKIN performs a three-dimensional neutron calculation using the results of coolant density and fuel temperature at each axial node of the various regions obtained from TUF. The regional power transients, as computed by SMOKIN, are then fed back to TUF to obtain a subsequent set of channel conditions for the reactor physics codes. The use of calculated regional power transients from SMOKIN replace the point kinetics calculations in the TUF code.

To illustrate the actual interaction between TUF and SMOKIN, the approach used in the Bruce station safety analysis for a large LOCA at OHN is described here. The TUF model groups the 480 channels into a number of thermal hydraulically similar regions maintaining such details as inner and outer flow zone boundaries and the elevation of channels corresponding to broken and unbroken passes in each region. Two notable conservative assumptions made in the simulation are: (1) an initial bottom-to-top flux tilt of 20 percent and (2) not crediting the three most effective shut-off rods when the shut-down system is activated. The tilted initial power distribution is defined by SMOKIN. This power distribution and the channel grouping definitions are used to produce the initial tilted powers in the TUF model. Figure 3 illustrates the channel groupings used for assessing the shut-down system 1 (SDS1) effectiveness in the presence of bottom-to-top flux tilts (Reference 3). The channel groups one to five represent the outer flow zone whereas the channel groups six to ten represent the inner flow zone. The calculation procedure is as follows:

- (1). First, the main conservative assumptions used in SMOKIN and TUF are established. These assumptions take into account the uncertainty in the parameters of the reactor kinetics model and the power measurement.
- (2). The self-initiating mode for reactor power (using the point kinetics model) in TUF is used to simulate this particular event up to 5 transient seconds. Reasonable reactivity tables for the fuel temperature and coolant void are estimated from the previous SMOKIN runs. Local power in each region and node is estimated by multiplying the core average power with some appropriate scaling (or peaking) factors. The reactivity control mechanisms in the reactor regulating system calculate the total reactivity including the action of shut-off rods. The averaged reactor power is calculated from the point kinetics model. This mode of simulation can provide a first degree of approximation for coolant density and fuel temperature in all the core regions.

(3). Using the thermal-hydraulics data from TUF, SMOKIN simulates the response (up to 5 seconds) of the shut-down systems and calculates the core reactivity which depends upon the distribution of flux and delayed neutron precursor population as a function of time. Then, SMOKIN supplies the power transients for all the core regions modelled in TUF.

(4). By-passing the point kinetics routine, TUF directly uses these region power transients as calculated by SMOKIN in modelling the response of the reactivity devices in the subsequent TUF simulation. TUF re-calculates the core coolant density and fuel temperature variations as function of time.

(5). Steps (3) and (4) are repeated until the process converges to a consistent set of thermal-hydraulic, reactivity and fuel power transients. This is achieved when the difference between consecutive SMOKIN results is less than 1 percent. The converged power transient in each region obtained from SMOKIN including the long term decay power is utilized in the TUF simulation. The SMOKIN results of detailed channel power distributions for all core channels including the hot channel power are transferred to the fuel channel codes CHAN, SMARTT, ELOCA and FACTAR codes for detail channel calculations (channel thermal/mechanical behaviour, amount of fission products release, channel integrity).

The TUF and SMOKIN iteration usually converges quickly after the first pass. This process of iteration, however, has to be carried out for each transient case. It results in a vast amount of data being transferred from TUF to SMOKIN and vice versa. Consideration is being given to the direct coupling of these two codes (TUF and SMOKIN) at OHN since it will not only simplify the calculation procedure but it will result in considerable saving in time when performing similar calculations for scoping analysis.

Interface Approach at AECL

The approach for the interface between the reactor system code (CATHENA) and the reactor physics code (CERBERUS) at AECL is similar to that described above, except that the coupling procedure is a one-time walkthrough of the transient (rather than several iterative passes through the transient). The approach used in the Wolsong 2 safety analysis is briefly described here. As mentioned before, the critical core pass of the broken loop in the reactor circuit is modelled by 7-10 regions with several channels each.

(1). The main conservative assumptions used in the reactor physics are established. For example, the nominal reactor power is assumed to be at 103% full power.

(2). The normal operational condition is calculated by CATHENA with a null transient run.

(3). The reactor circuit with a break is then simulated again by CATHENA up to a transient time, typically 0.05 second, by assuming a constant reactor power. The calculated coolant density and fuel temperature in each node of the core model are transferred to CERBERUS.

(4). The reactor power is calculated by CERBERUS from time zero to 0.05 second. The results at 0.05 second are fed back to CATHENA. Assuming a constant reactor power from 0.05 second to 0.1 second, CATHENA simulates the thermal-hydraulic conditions up to 0.1 second. The predicted coolant density and averaged fuel temperature in each node of the core model are transferred back to CERBERUS again.

(5). CERBERUS calculates the power transient for next transient interval and continues interacting with CATHENA up to the total transient time for the coupled calculation, i.e. typically 3-5 seconds at which time the neutronic power is smaller than the decay power.

(6). At that point, the coupling between the CERBERUS and CATHENA is terminated. The total reactor power for long term transient obtained from CERBERUS is used in the long term transient of CATHENA.

A huge amount of data is transferred back and forth between CATHENA and CERBERUS for a few seconds transient run. Similarly to the approach used in OHN, the reactor power transients for all channels are transferred to the fuel channel codes for detailed fuel channel analysis.

4. INTERFACE BETWEEN THERMAL-HYDRAULICS AND FUEL CHANNEL CODES

The interface between thermal-hydraulics and fuel channel codes is also applied to large LOCA cases. During the early fuel heatup in a large LOCA, a large temperature difference exists between the fuel centre-line and sheath. A detailed fuel pin model to predict the fuel temperature profile is needed. In the late fuel heatup period due to a degraded core cooling, this temperature difference becomes small and a detailed fuel pin model is not necessary. As a result, different fuel pin models have been applied in the fuel element and channel codes, driven by different considerations. For the fuel element codes, the main physical parameters are fuel thermal properties (functions of fuel burnup rate and fuel temperature), gap heat transfer coefficient (including fuel swelling effect), flux depression, sheath failure criterion and metal-water reaction. The mechanical analysis is performed to model the state of stress and strain in the fuel pin subjected to internal and external axial and radial loadings. The strain is normally made up of the following components: elastic, thermal, creep, plastic, fuel swelling and cracks. For the fuel channel codes, the following parameters are considered: criterion for pressure and calandria tubes contact, contact dynamics, bundle slumping criterion, metal-water reaction and flow re-distribution effect after bundle slumping. Not all of these detailed physical models are available in the reactor system codes. To provide a more realistic assessment on the reactor channels and to include the uncertainty of thermal-hydraulic results, the fuel element and channel codes to simulate different fuel channel behaviour are required in the CANDU safety analysis.

To use the characteristics of CANDU circuits, each individual reactor channel in each region can be simulated at the same time by using the same header conditions for the fuel channel codes. These boundary conditions at the reactor headers for each core pass are obtained from the reactor system code simulations. Therefore, the overall heat transfer rate between the fuel pins/pressure tubes and the coolant and the header conditions are the most important parameters in the thermal-hydraulic module.

The major functions of the fuel channel codes are: (1) to perform the thermal analyses of fuel pins in a bundle, pressure tube and calandria tube; (2) to simulate the mechanical behaviour of fuel/sheath and fuel bundle; (3) to calculate the amount of gaseous fission product in the core; (4) to assess the overall extent of pressure tube ballooning in the core; (5) to calculate the total heat load from the core to moderator; (6) to examine the integrity of the pressure boundary (channel integrity) for all postulated LOCA; and (7) to examine the availability of moderator subcooling.

Indirect Interface at OHN and AECL

The indirect interface between thermal-hydraulics codes and fuel channel codes was adopted in OHN and AECL for safety analyses of CANDU reactors. The header conditions and the channel flow rates from the thermal-hydraulics code and the channel power from the reactor physics codes are the main input parameters for the fuel channel codes. Based on those data, the spectrum of all possible channel conditions is assessed. There is an advantage to indirect interface between thermal-hydraulics and fuel channel codes. All channels in the severe core pass can be simulated by the fuel channel codes to provide a realistic estimate of the overall core behaviour. The condition at the averaged channel simulated in the thermal-hydraulics codes does not represent the conditions at the worst or hot channel. The conservative assumptions required in the thermal-hydraulic analysis may not be applicable to the detailed fuel channel analysis. For example, the heat loss from the coolant to the moderator induced by the pressure/calandria tubes contact is normally not credited in the thermal-hydraulic analysis for conservative reasons. However, it must be credited in the fuel channel codes since the contact due to pressure tube ballooning is an actual physical process for the fuel channel model. The assessments of channel integrity and the moderator subcooling requirement have to be based on the actual physical process such as the heat transfer path due to pressure tube ballooning.

The heatup assessment of the reactor core is the main task for the fuel channel codes in the large LOCA safety analysis. With a wide spectrum of local channel conditions possible in the core, the approach of using the worst channel flow transient is adopted. These conditions are then applied to a group of channels (usually on a core pass basis) to obtain a limit-consequence estimate of core heatup behaviour. The heatup assessment under degraded cooling becomes an assessment of complex thermal/mechanical interactions in a single channel, which is surrounded by cold moderator. A number of single channel assessments are used to obtain a bounding estimate of the core heatup behaviour. The end-point geometry of CANDU fuel can be defined for all possible approaches to the post-shutdown degraded core cooling state. The fuel remains confined within a distorted fuel channel which is cooled by the moderator. Analysis can be performed to demonstrate fuel channel integrity, as well as to estimate the maximum fuel temperature excursions in the core. Thus the unique feature of the CANDU is a well defined end point geometry of reactor channels.

Upon contact of pressure and calandria tubes as shown in Figure 4 for a typical CANDU fuel channel, there is a sudden release of heat from the pressure tube. The rate of release is affected by the magnitude of the contact pressure and temperature and by the mode of boiling heat transfer at the outer surface of the calandria tube (Reference 4). Analysis has to demonstrate that sufficient moderator subcooling remains following a large LOCA with coincident ECI system failure to prevent calandria tube dry-out following pressure tube ballooning. This then ensures the maintenance of fuel channel integrity.

Direct Interface at AECL

A new approach has been adopted at AECL for the interface between the thermal-hydraulics and the fuel channel codes (Reference 5). The direct linkage between CATHENA and ELOCA has been established. During the transient run, the information of thermal-hydraulic conditions (including the heat transfer coefficient) for each fuel pin are passed over to the ELOCA code to perform the fuel pin temperature calculations. Then the calculated fuel pin temperature profile is fed back to CATHENA to perform the pressure/calandria tubes temperature calculations. Two codes can be developed or run independently. This direct linkage removes the possible errors induced by indirect interface. Since the CATHENA code has the capability to simulate the same dynamic pressure tube ballooning process (Reference 6) as the CHAN code, the use of the fuel channel code CHAN is gradually being phased out in the current safety analysis, for example in the preliminary safety analysis of proposed CANDU-9 reactor.

5. FUTURE DIRECTIONS IN INTEGRATED SIMULATION OF CANDU REACTOR BEHAVIOUR

The methods described in this paper can sometimes involve iteration between codes in order to match boundary conditions, and in some cases, it would be desirable to proceed during a simulation with simultaneous solution of the various codes involved. A recent presentation (Reference 7) describes application to analysis of integrated experiments of the INTARES (or INTegrAted RESponse) software package under test at AECL. INTARES permits simultaneous solution of CATHENA (or potentially several copies of CATHENA for parallel channels), ELOCA and potentially reactor physics and fission product release and transport codes over a computer network (e.g. a LAN) or on a parallel computer. This technology is expected to pay dividends in safety analysis as we move towards "better" estimate calculations for postulated reactor accidents.

6. CONCLUDING REMARKS

The modules in the system simulation of CANDU reactors have been briefly described. The interface among thermal-hydraulics, reactor physics and fuel channel codes adopted in the large LOCA safety analysis has been presented. This approach is based on the unique characteristics of CANDU reactors and the required conservatism in the safety analysis.

APPENDIX: Main Computer codes used in CANDU safety analysis

Many computer codes at OHN and AECL have been utilized in various areas of CANDU safety analysis. For example, the Reactor Fuelling Simulation Programs (RFSP) at AECL and Ontario Hydro Nuclear (OHRFSP) are used in the static 3D calculations of neutron flux, power distribution and neutron balance in a CANDU reactor core. The codes PATRIC (at OHN) and PRESCON2 (at AECL) are used for containment response, FISSCON-II (at OHN) and SMART (at AECL) are used for radiological consequence calculation for a large LOCA safety analysis. In this appendix, only the dynamic codes used in the reactor physics, thermal-hydraulics and fuel channel modules and their functions are mentioned. Detailed physical models and associated numerical methods implemented in each code can be found either in the code manuals or in the papers presented in the literature.

Reactor System Codes

The TUF code (Reference 8), developed at OHN, is a two-fluid code which is currently being used as an analytical tool for operational support and licensing safety analyses for all CANDU reactors (total 19 units) at OHN. It is an upward reactor system code for SOPHT (Reference 9). TUF is a self-contained reactor system code. It can be used to simulate the LOCA cases without interface with other codes. More descriptions of the code characteristics can be found in an other paper presented at this workshop.

The CATHENA code (Reference 10), developed at AECL, is a two-fluid code which is currently being used as an analytical tool for licensing safety analysis for CANDU-6 and proposed CANDU-9 reactors at AECL. Similar to other reactor system codes, CATHENA requires an interface with a reactor physics code or a package of plant controllers to simulate the LOCA cases. Since this interface is a part of the process in CANDU safety analysis as described in this paper, the self-contained capability is not required in the safety analysis. More descriptions on the code characteristics can be found in Reference 10 or in an other paper presented at this workshop.

Reactor Physics Codes

The CERBERUS code (Reference 11), developed at AECL, is based on the improved Quasi-Static method to solve the 3D time dependent two-group neutron diffusion equations. The neutron flux is written in terms of a space-time dependent shape function and a space independent amplitude function. The resulting equations are similar in form to the time-dependent diffusion equations but contain, in addition to the delayed source terms, two sets of time derivatives: the time derivatives of the shape and the time derivatives of the amplitude. The equations are coupled with the amplitude equations which are similar in form to the point kinetics equations. CERBERUS requires a long computing time for a typical large LOCA case. This code has been verified against experiments.

The SMOKIN code (Reference 12), developed at OHN, is based on one energy group modal expansion technique coupled with a local flux effects correction technique (Reference 13). The 3D space-time distribution of neutron flux and delayed neutron precursors are expanded as a weighted series of fixed reactor harmonic modes. Applying the Galerkin weighted integration over the reactor core, a set of coupled differential equations are obtained from the modal amplitude weights. Local flux changes induced by the movement of reactivity devices are taken into account through the use of local flux effect functions. The reactor modes are pre-generated by the two-group neutron diffusion code MONIC assuming a nominal core configuration. The nominal configuration is based on the core with reactivity devices at their reference position. SMOKIN is used to cover the wide range of break sizes for LOCA analysis and trip parameter assessment at OHN in the short term (up to five seconds). SMOKIN has been validated against CERBERUS for LOCA transients and against experiments for operational transient in power reactors.

Fuel Channel/Element Codes

The ELESIM-II/MOD10 code (Reference 14) was developed at AECL and used at AECL and OHN. It is used to provide detailed axial-symmetric thermal/microstructural behaviour for a single fuel element during normal operation conditions. It provides a detailed, mechanistic assessment of the amount and location of fission gas within a fuel

element as a function of the power/burnup history. The details of fission gas distribution are then used to assess the gas pressure inside the fuel element.

The ELOCA.Mk4 code (Reference 15) was developed at AECL and used at AECL and OHN. It is used to provide detailed axial-symmetric thermal/mechanical behaviour during a transient for a single fuel element. It provides a mechanistic assessment of the high temperature deformation of the sheath and the effect of oxygen uptake by the sheath on this deformation behaviour. The effect of sheath deformation and pellet thermal expansion/contraction on fuel-to-sheath heat transfer is also modelled.

The HOTSPOT and SMARTT codes (Reference 16) were developed at OHN to provide a detailed (2D, radial and circumferential directions) transient, thermal response for the fuel elements in a symmetric segment of a bundle cross-section. The heat transfer mechanisms modelled are convection, conduction and radiation. It also models the thermal effects of the oxidation of the zircaloy sheath during a transient. HOTSPOT also provides a one-dimensional assessment of the thermal response of the pressure tube and calandria tube under elevated temperature conditions. The capability to simulate the mechanical behaviour of pressure and calandria tubes contact based on the strain model developed at AECL has been made in the SMARTT code which utilises the HOTSPOT channel thermal model. Currently the SMARTT code is being used in the safety analysis at OHN.

The CHAN-II/MOD7 code was developed at OHN based on the CHAN-II code at AECL (Reference 17). It is used to provide the transient thermal response of an entire fuel channel during a high temperature condition. The CHAN code series was developed to assess fuel channel behaviour during accident where cooling is severely degraded. It models the depletion of steam and consequent buildup of hydrogen along a channel due to the zircalloy and steam reaction at elevated sheath temperature. The code models the thermal effects of both pressure tube sagging and ballooning, and bundle slumping onto the pressure tube. The effects of flow redistribution in the channel as a result of these interactions are also accounted for.

The FACTAR code (Reference 18) was recently developed at OHN to unify and to upgrade the fuel channel and element codes (ELESIM and ELOCA code series). It is used to simulate the transient thermal and mechanical behaviour of 37-element or 28-element fuel bundles within a single CANDU fuel channel for any accident conditions that do not result in significant bundle deformation (i.e. extensive bundle slumping). The code has been verified against all fuel channel/bundle results simulated by HOTSPOT, CHAN and TUF codes. A detailed description on the code validation can be found in Reference 19.

The CATHENA code (Reference 10) includes a Generalized Heat Transfer Package (GENHTP), that is able to model heat transfer processes within a CANDU channel in detail. These processes are implicitly coupled to the two-fluid thermal-hydraulics. Conduction in the radial and circumferential directions can be calculated for individual fuel elements within a bundle, the pressure tube, and the calandria tube. The effects of thermal radiation, pressure-tube deformation, zirconium-steam reactor, steam starvation, and solid-surface contact (e.g., pressure tube to calandria tube) can all be modelled with the code. Thermal-hydraulic and channel heat transfer behaviour may be tightly coupled with fuel behaviour by using the CATHENA/ELOCA code suite (Reference 5).

REFERENCES

1. R.J. Atchison, F.C. Boyd and Z. Domaratzki, Canadian approach to nuclear power safety, Nuclear Safety, Vol. 24, No. 4, July-August 1983.
2. W.S. Liu, R.K. Leung and J.C. Luxat, Overview of TUF code for CANDU reactors, 5th International Conference on Numerical Methods in Nuclear Engineering, Montreal, Quebec, September 8-11, 1996.
3. M.Z. Farooqui and N.T. Le, Simulation of large break loss of coolant accident with TUF and SMOKIN computer codes, Fourth International Conference on Simulation Methods in Nuclear Engineering, Montreal, Quebec, Canada, June 2-4, 1993.

4. R.A. Brown, C. Blahnik and A.P. Muzumdar, Degraded cooling in a CANDU, 2nd International Topical Meeting on Nuclear Reactor Thermal-Hydraulics, Santa Barbara, California, USA, January 11-14, 1983.
5. L.N. Carlucci, J.R. Gauld, D.J. Richards, V.I. Arimescu, Coupling of subroutine version of ELOCA code for high-temperature fuel behaviour to CATHENA system thermalhydraulics code, 5th International Conference on Numerical Methods in Nuclear Engineering, Montreal, Quebec, September 8-11, 1996.
6. Q.M. Lei, D.B. Sanderson and R. Dutton, Modelling disassembled fuel bundles using CATHENA MOD-3.5a under LOCA/LOECC conditions, 16th Annual Conference of Canadian Nuclear Society, Saskatoon, Saskatchewan, Canada, June 4-7, 1995.
7. J.W. DeVaal et al., Parallel computing applied to the modelling of the complex interacting phenomena in severe fuel damage experiments, The ICHMT International Seminar on Heat Transfer in Severe Reactor Accidents, Cesme, Turkey, May 21-26, 1995.
8. W.S. Liu et al., TUF: A two-fluid code for thermal-hydraulics analysis, 10th Annual Conference of Canadian Nuclear Society, Ottawa, Ontario, Canada, June 4-7, 1989.
9. Y.F. Chang and J. Skears, SOPHT - A computer model for CANDU-PHWR heat transport networks and their control, Nucl. Sci. 35, pp. 591-602, Oct. 1977.
10. D.J. Richards, B.N. Hanna, N. Hobson and K.H. Ardron, CATHENA: A two-fluid code for CANDU LOCA analysis, 3rd International Topical Meeting on Reactor Thermal-Hydraulics, Newport, RI, 1985.
11. K.O. Ott and D.A. Meneley, Accuracy of the quasi-static treatment of spatial reactor kinetics, Nucl. Sci. Eng., 36, pp. 402-411, 1969.
12. M. Gold, SMOKIN - A family of codes for reactor space-time neutronics calculations based on modal kinetics - Theory Manual, Design and Development Division, Report No. 90133, Ontario Hydro, September 1990.
13. J.C. Luxat, The potential of a generalized modal analysis method in the design and analysis of CANDU-PHW reactor control and safety systems, Annual Conference of Canadian Nuclear Association, June, 1978.
14. J.M. Bunge and F.C. Iglesias, ELESIM-II(MOD10), AECL internal report CRNL-2011-1, 1982.
15. J.A. Walsworth and H.S. Sills, High temperature transient fuel performance modelling, ELOCA.Mk4, AECL internal report CRNL-2010-1, September 1984.
16. R.E. Paul, HOTSPOT: A computer code for predicting the fuel bundle temperature distribution history following a LOCA, GP-75-064, Ontario Hydro, 1975. K.E. Locke, SMARTT: A computer code to predict transient fuel and pressure tube temperature gradients under asymmetric coolant conditions, Nuclear Safety Department, Report No. 86007, March 1987, Ontario Hydro.
17. D.B. Reeves, O. Akalin and W. Kelly, CHAN-II(MOD7), A model for assessing channel thermal response under steam or two-phase cooling condition, Design and Development Division report No. 87088, Ontario Hydro, November 1987; V.Q. Tang et al., CHAN-II: A computer program predicting fuel channel thermal behaviour in a typical CANDU-PHW reactor core following a loss-of-coolant accident, AECL Report WNRE-489, Atomic Energy of Canada Limited, July 1981.
18. H.S. Sills, S.L. Wadsworth, L.J. Watt and P.J. Reid, FACTAR version 1: Fuel and channel temperature and response, Part 1: Model description and user manual, Reactor Safety and Operational Analysis Department, Report No. N-03553-940031, Ontario Hydro Nuclear, April 1994.
19. C.J. Westbye, A.C. Brito, J.C. Mackinnon, H.E. Sills and V.J. Langman, Development, verification and validation of the fuel channel behaviour computer code FACTAR, 16th Annual Conference of Canadian Nuclear Society, Saskatoon, Saskatchewan, Canada, June 4-7, 1995.

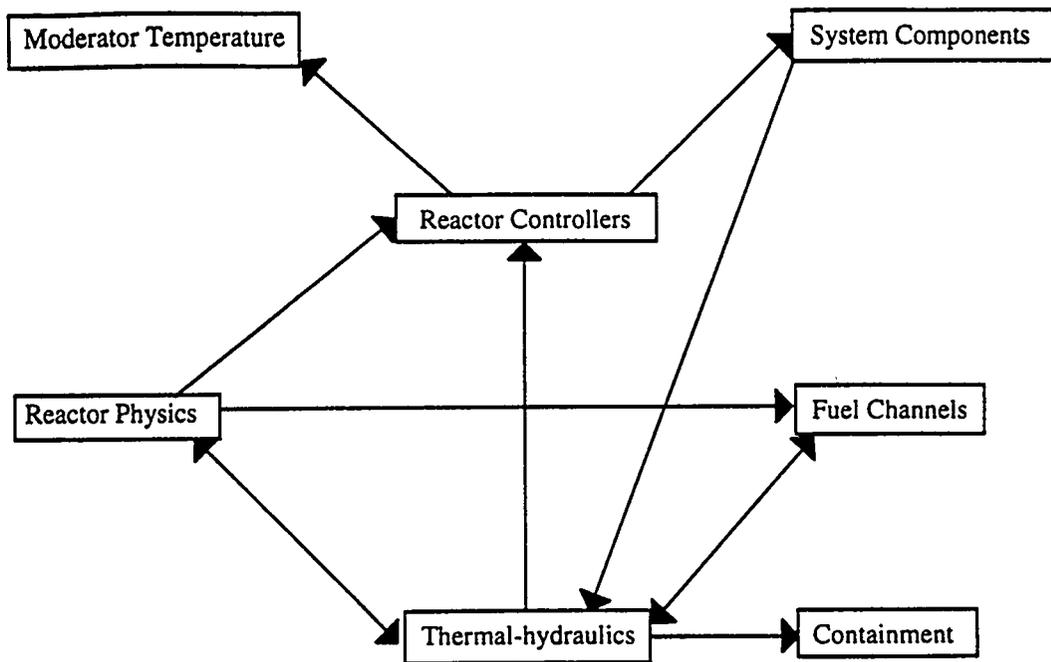


Figure 1: Interactions among various modules for CANDU reactors

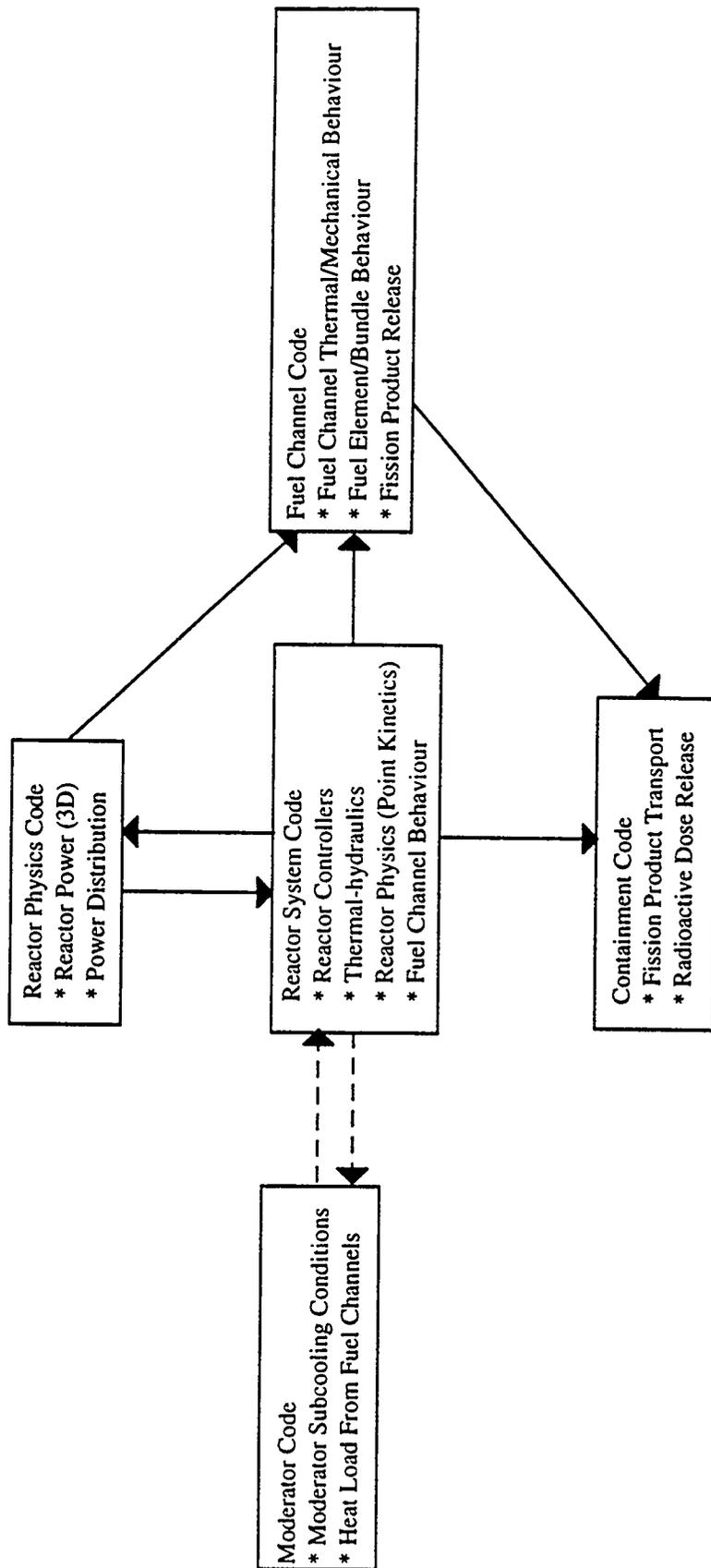


Figure 2: Inter-relationship of computer codes for CANDU safety analysis

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
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Figure 3. Channel grouping for modelling power distribution for Bruce A NGS

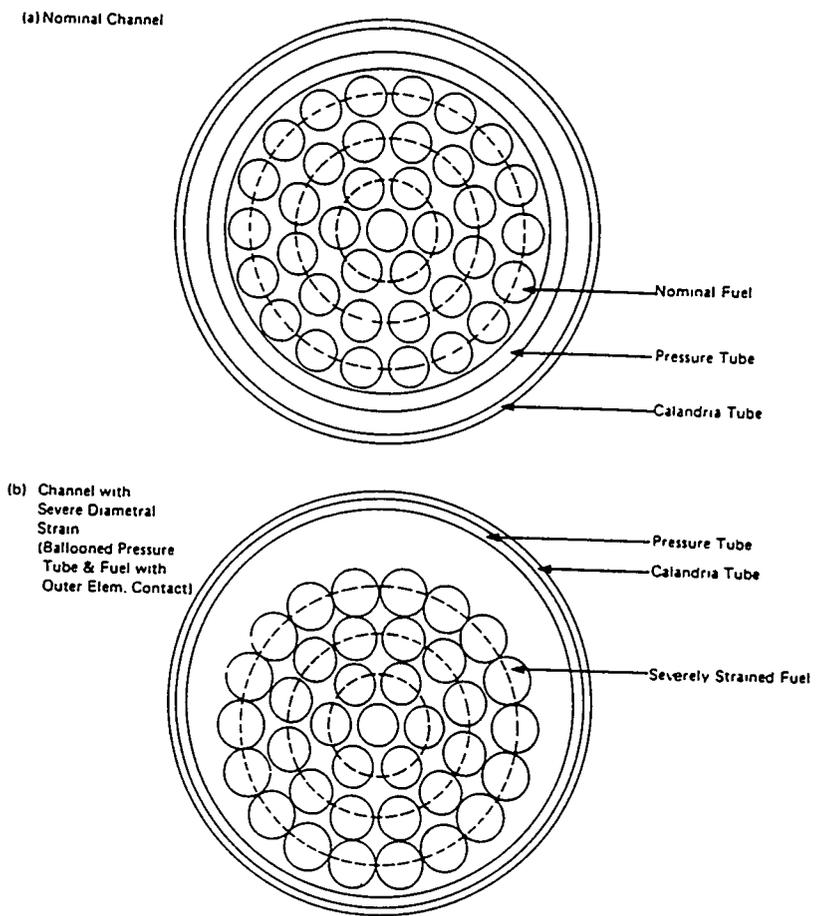


Figure 4. Cross section of a typical CANDU channel under normal and severe diametral strain conditions

**TECHNICAL SESSION 2: ADVANCES IN MODELING OF THERMAL-HYDRAULIC
PHENOMENA - ADDITIONAL EXPERIMENTAL NEEDS**

Co-Chair: Dr. Reocreux (France), Dr. Lillington (U.K.)

**OECD / CSNI WORKSHOP ON TRANSIENT
THERMALHYDRAULIC AND NEUTRONIC CODES
REQUIREMENTS**

Annapolis , Md, USA

5 th-8th November 1996

Hosted by

U. S. Nuclear Regulatory Commission

**Status of thermalhydraulic modelling and assessment :
Open issues**

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ABSTRACT

This paper presents the status of the physical modelling in present codes used for Nuclear Reactor Thermalhydraulics (TRAC, RELAP 5, CATHARE, ATHLET, ...) and attempts to list the unresolved or partially resolved issues. First, the capabilities and limitations of present codes are presented. They are mainly known from a synthesis of the assessment calculations performed for both separate effect tests and integral effect tests. It is also interesting to list all the assumptions and simplifications which were made in the establishment of the system of equations and of the constitutive relations. Many of the present limitations are associated to physical situations where these assumptions are not valid. Then, recommendations are proposed to extend the capabilities of these codes.

I INTRODUCTION

Best estimate thermal-hydraulic codes are irreplaceable tools for LWR safety analysis. They have already proven their capabilities to predict at least qualitatively and sometimes quantitatively many basic features of the accidental transients. In order to make the best use of such complex tools, a good knowledge of their limitations is necessary. Although important progress has been made up to now, some difficulties remain which have to be overcome. This paper presents the status of the physical modelling in present codes used for Nuclear Reactor Thermalhydraulics (TRAC, RELAP 5, CATHARE, ATHLET, ...) and attempts to list the unresolved or partially resolved issues. They are mainly known from a synthesis of the assessment calculations performed for both separate effect tests and integral effect tests. It is also interesting to list all the assumptions and simplifications which were made in the establishment of the system of equations and of the constitutive relations. Many of the present limitations are associated to physical situations where these assumptions are not valid. Then, recommendations for future developments are proposed to extend the capabilities of these codes.

The authors have a long experience in the development and assessment of the CATHARE code but a more limited knowledge of the other codes. Then the paper often refers to the CATHARE code and has to be considered as a point of view, although the authors tried to review all codes. It was observed that all these codes have many common features and rather similar capabilities.

2 RESULTS OF CODE VALIDATION

2.1 Validation on separate effect tests (SET)

The first step in code validation consists in calculating a wide range of SETs. As Separate Effect Tests have well known boundary conditions and a high density of instrumentation (measurement devices), they are the only way to determine the validity and the accuracy of each closure relationship. All basic physical processes and all closure terms have to be addressed. All flow geometries have to be investigated (pipe, rod bundle, annuli, bends, Tees,...) and, as far as possible, the test matrix should be able to qualify the scale effect. A OECD/NEA-CSNI SET test matrix was defined with an identification of all the basic phenomena to be addressed. The thermalhydraulic codes have generally a rather large SET test matrix but one must always clearly identify the code version which is used and which option of the code is used.

For example, for clarifying the validation process of the CATHARE code, code options on closure laws are not permitted and each package of closure laws (called Revision) must be qualified on an extensive test matrix. It is also recommended that the qualification calculations be used also for:

- giving the range of validity of closure relationship
- estimating the uncertainty on each closure relationship
- defining the best schematization for each component in relation to the physical situation
- defining the node size and time step required for a converged calculation

Thermalhydraulic code generally calculate rather well the SETs as they were first used for the development or the improvement of closure relationships.

2.2 Validation on integral effect tests (IET)

The second step in the assessment process consists in calculating IET to validate the general consistency of the closure laws and to point out the remaining shortcomings. Many IET are also well calculated. One can consider three main cases:

- All the important phenomena are well predicted with a good timing and a good accuracy.

- The most important phenomena are predicted. The timing and the accuracy are not perfect but it does not prevent from clear conclusions on safety issues.

- Some important phenomena are not predicted or are predicted with a very bad accuracy.

The first type of calculation is still exceptional but the second type becomes more and more frequent. Possible compensating errors, system effects, and a low density of instrumentation make it difficult to draw final conclusions on physical closure relationships from integral tests. However the analysis of code deficiencies in integral tests calculations is necessary to point out some problems such as:

- *Problems of schematization or nodalization*

The main source of problem is due to a bad choice of schematization. All the codes have several types of modules which have specific capabilities. The user must choose a schematization which may depend on the transient to calculate. For example, the classical schematization of a pressurizer with the CATHARE code uses a simple two node Volume module which is sufficient for all LOCA transients where the pressurizer is rapidly empty. But it is seen that for transients such as a Loss of Feedwater with Pressurizer Relief Valve opening, or a Multiple SGTR with pressurizer regulations, a more complex modelling is required. In order to reduce the User's Effect, code provide now a "User's Guidelines" document, which gives many recommendations for the nodalization.

- *Models used out of their domain of validity*

Some transients are not well predicted as the physical situation exceeds too much the range of validity of some closure relationships. For example the low pressure transients during mid loop operation with open manways are not very well predicted.

- *Physical process not modelled*

In some transients, physical mechanisms can be encountered which were not yet studied in analytical or separate effect tests and which are not modelled in the code. For example, when CCFL occurs in a zone with a complex geometry the corresponding flooding correlation must be established first from analytical tests before it is implemented in the code.

- *Transients highly sensitive*

It is observed that some transients are very sensitive to a certain physical process. In such cases, the accuracy of the models should be very good to obtain reliable predictions. In particular, transients with unstable behaviour are difficult to predict with a good accuracy. Instabilities may occur during strong direct contact condensation at ECC injections or at the beginning of a Reflooding when oscillations between core and downcomer take place.

Also, the loop seal clearing in some small break transients is an example of very sensitive process. The formation of a liquid slug in the intermediate legs of a reactor is a common feature of many small break LOCA transients. This occurs in particular after the rupture of the natural circulation when the reflux condenser mode starts. The primary circuit is divided in two parts separated by the liquid slugs in loop seals and in the vessel bottom. These two subsystems are practically uncoupled from the thermal point of view. They follow a thermal equilibrium defined by a saturation temperature resulting from all the energy exchanges. In the hot subsystem - core, hot legs, SG tubes - the temperature level is generally controlled by the secondary side except if a break in this part is able to discharge more vapour than the core produces. In the cold subsystem the energy balance generally depends on the presence of a cold leg break and of safety injections, both of them giving a trend to a temperature decrease. Most of the time a depression of the cold part is induced which shifts water from core to downcomer. This dangerous situation stops when the liquid level in the descending part of the intermediate leg reaches the horizontal part. The loop seal clearing occurs either simultaneously or at different times in the different loops. When the process is slow, it is very sensitive to small asymmetries between the loops. Once it happens in one loop, a stable state may be reached preventing from its occurrence in the other loops. Codes have many difficulties to predict these non symmetrical behaviour correctly.

3 CODE LIMITATIONS RELATED TO MODEL ASSUMPTIONS

Code limitations related to the system of equations

Advanced thermalhydraulic codes use the two-fluid model where mass momentum and energy balance equations are written for each phase. These equations can be derived from exact local instantaneous equations. The process includes several steps: space and/or time averaging, simplifications through physical assumptions, derivation of closure relationships. Models are restricted to zero order closure so that no more partial differential equations are derived.

The averaging process which restricts predictions to large scale phenomena allows to use a reasonably coarse meshing and makes the comparison with experiment easier. The time integration or averaging suppresses from calculated quantities fluctuations due to both the turbulent nature of the flows and the two-phase intermittency. The filtering of small scale phenomena allows to forget the complex structure of phase repartition and interface movements. The effects of small scale processes on macroscopic evolution are taken into account by closure relationships.

However the scale at which fluctuations can be filtered is not always evident. It is clear when the spectrum of fluctuations is cut into two separate zones, the range of small scale processes and the macroscopic range. Dispersed flows are generally in this favorable case. But there are also situations with a continuous spectrum and possible non linear interactions between the larger and smaller scale processes. Should for instance the intermittent nature of slug flows be filtered or described in the mean flow ? Filtering will not be a limitation if this intermittency does not interact with important physical processes like a wall dry out for example. A situation with large scale liquid plug movements in a pipe is a difficult case.

The domain of integration may also be troublesome when it puts together things which are too different. For example in an annular flow with droplet entrainment, there are two liquid fields which have very different velocities and very different types of interaction with the walls and the gas phase. Here, the phase averaging induces a limitation and a multi-field approach would be better.

Some codes use only one mixture momentum equation and model the slip between phases by the so called "drift flux" approach. This may be equivalent to the full 2-Fluid approach with two separate momentum equations when the slip between phases is an "equilibrium slip" (governed by an equilibrium between gravity and friction forces), but it is limited when inertial effects are relatively important in the phase slip. This occurs when interfacial friction forces are low in separated phase flow patterns, i.e. annular flows, stratified flows,...

Code limitations related to the simplifying assumptions

Some simplifying assumptions are necessary for writing the final system of equations. They must be kept in mind when interpreting assessment calculations as they can be source of mispredictions.

The current simplifying assumptions are:

- In 1-D models, the axial diffusion of heat and momentum by molecular diffusivity or by turbulence is neglected. Moreover, all the correlation coefficients due to space averaging are taken equal to 1 by simple lack of knowledge. The loss of information associated with this simplification can be partly restored by an appropriate modelling of the transverse momentum and heat fluxes. This is possible when the transverse profiles follow a similar or affine solution. But in cases where the profiles are rapidly changing, the simplification cannot be justified. Then the best accuracy can be expected in the description of established flows in long pipes without singularities whereas non established flows may be less accurately predicted.

- In 2-D or 3-D models only diffusion towards walls or interfaces is correlated. The internal turbulent diffusion inside each phase is not modelled or it is modelled by simple mixing length models. A more complete diffusion modelling is possible with some limitations. The meshing must be fine and the numerical scheme must not be too diffusive. Moreover, considering the state of the art in turbulence modelling in two phase flows, the present knowledge is limited to dispersed flows. For non-structured flows (churn flow) or for the intermediate void fraction range, no qualified turbulence modelling exists.

Code limitations related to closure relationships in a 1-D model

Closure relationships were extensively studied in the frame of the 1-D model. Many separate effect experiments have been analyzed to determine constitutive relationships concerning mass momentum and energy transfers between phases or between fluid and walls. The difficulties come from the large variety of situations to deal with: variety of geometrical configurations, variety of flow patterns, variety of heat transfer modes, large range of thermalhydraulic parameters.

Constitutive relationships are essentially algebraic expressions of the principal variables. In the CATHARE 1-D model, two differential terms are present in the interfacial momentum transfers : the added mass term associated with inertial effects has been derived for dispersed flows and another term proportional to the void fraction gradient plays an important role in stratified flows. Apart from these two terms, algebraic closure relationships are developed on the basis of steady and established flows (or quasi-steady and quasi-established flows). In unsteady or non established flows, it is implicitly assumed that this closure is still valid.

This assumption may be the source of some shortcomings, particularly if one considers the physical processes which have long relaxation times. Algebraic closure means that all the physical mechanisms involved have a relaxation time equal to zero. In 1-D models, all the

transverse profiles are considered as established even at the entrance of a pipe. It is then obvious that flows in pipes or ducts with a high length to diameter ratio are easier to describe correctly. But when the flow is perturbed locally the constitutive laws are no more valid.

Long relaxation times may also be present in flows without source of perturbation. Let us consider the simple case of the interfacial friction in the core. Several experiments were used for developing models but no very accurate correlation could be found. This can be attributed to some history effects which cannot be described by algebraic closure laws. In boiling or flashing flows, many small bubbles are created either at the wall or in the bulk. These bubbles coalesce and reach probably a maximum size controlled by their stability. The relaxation time which is associated to this coalescence is probably a function of the number of bubbles created per unit volume for flashing, or per unit heating rod surface. According to this, the spectrum of bubbles size at a given cross section of the core depends on what occurs upstream and not only on the local vapour superficial velocity and void fraction. Since the bubble drag force mainly depends on its diameter, it is not possible to derive an interfacial friction correlation using only local flow parameters, without regarding what occurred upstream. One more transport equation should be written to predict the dynamics of the interfacial area evolution. In present thermalhydraulic codes, where such a model is missing, some error may be found in the predictions, which probably depends on core power, power profile, boiling length, rate of depressurization...

Code limitations related to flow pattern maps

Every flow regime has its internal structure and its transfer mechanisms. So it seems natural to use a flow pattern map in a code and to develop correlations for mass momentum and energy transfers which depend on the flow pattern. Unfortunately, at present, there is not a universal map valid in the whole domain of simulation. Experiments with steam water at high pressure and in large diameter pipes are very expensive and observations very difficult. So the available flow pattern maps are not validated in this domain.

However, it is not absolutely necessary to determine all the transitions and to use specific correlation for each flow regime. In the CATHARE code, only the onset of droplet entrainment and the stratification criterion are explicitly written. These two transitions are important because they limit a separated flow and a more dispersed flow. Anyway, closure relationships can also be expressed directly as functions of the principal variables without reference to a particular flow pattern. So the absence of a unique and general flow pattern map in the codes is not a limitation by itself, but it reflects the limits of the physical knowledge in two phase flows.

Anyway, any flow pattern map uses algebraic transition criteria. A transition criterion is expressed as a limit value of a function of principal variables. This approach cannot take into account relaxation times necessary to change from one flow regime to another one. An example is the establishment of stratified or non stratified flows. The destratification by the Kelvin-Helmholtz instability takes a certain space and time since unstable waves have a finite growth rate. But stratification criteria used in codes assume instantaneous transition. On the other hand, starting from a bubbly mixture, stratification will occur in a horizontal pipe if the bubble rise velocity is large enough to dominate the mixing effects of the liquid turbulence. But this process of sedimentation requires a certain time which cannot be taken into account in a simple algebraic stratification criterion. A transport equation for a quantity representative of the rate of stratification could be necessary particularly for pipes with a small length to diameter ratio.

Code limitations related to the range of validity of correlations

Correlations used in the closure terms of the equations may be either empirical semi-empirical or phenomenological.

A purely empirical correlation is a best fit of experimental data where the quantity to model is expressed as any function of the principal variables. It can be very accurate within the domain of experimental investigation but the extrapolation beyond it is very dangerous. On the other hand, this method does not take any benefit from the knowledge which may exist in certain subdomains where good correlations are available.

Dimensional analysis allows in principle to determine the dimensionless numbers to use in the expression of the quantity to correlate. But in 2-phase conditions, the number of independent parameters is very high so that simplifying assumptions are necessary. When the controlling physical processes are well identified, one can keep only the few dimensionless parameters which play a role. In this case, the extrapolation beyond the investigated domain is less hazardous. Nevertheless there is no guarantee since the controlling processes can be different in an other range of parameters. For example, slug flow does not exist any more in large diameter pipes

The phenomenological or mechanistic approach consists in assuming a governing physical mechanism. The correlation is then derived theoretically without anything coming from experiments. An alternative is to keep some free parameters to adjust on experimental data. This semi-empirical approach was the most frequently used in the Cathare development. Even with this last precaution, the extrapolation beyond the qualified domain is not guaranteed. New effects, which are not present in the model, may become important in another range of parameters.

The experience shows that the 2-phase thermalhydraulics contains myriads of phenomena which make it difficult to generalize any theoretical breakthrough. Then none of the different methods used for deriving correlations can guarantee a good accuracy in extrapolation beyond the validation domain.

Code limitations related to closure relationships in 2-D or 3-D models

Closure relationships used in 3-D models are generally extrapolated from 1-D models. This may lead to important shortcomings as quantities averaged over the cross section of a duct have not the same meaning as local values. For example, the void fraction is an important indication for the determination of the flow pattern in a 1-D model, whereas it is not so in a 3-D model.

The main problem is associated with the lack of turbulent diffusion modelling in present 2-D or 3-D models implemented in system codes. These models should be used only when the turbulent diffusion effects are dominated by other effects.

A first example is the core, a very porous medium where the diffusion towards rod walls or interfaces is much higher than the large scale turbulent diffusion. Moreover, in low velocity two phase conditions, gravity effects are likely to produce the most important large scale mixing effects. The lack of diffusion terms is not very restrictive in this case.

The closure of multidimensional two phase flow models is still in its infancy. A tremendous lot of work is still required to reach the same quality as the 1-D models have, since there are much more physical processes to describe and more closure terms to correlate. So they must be used with caution only where and when 2-D or 3-D effects are important, and when the limitations of the multi-D model are not critical. As far as possible, the multi-D models must be validated with scale 1 data.

Code limitations related to complex geometries

The presence of geometrical singularities in a circuit, such as bends, flow area contraction or enlargement, is a difficulty for the two-phase flow models. At these locations, the flow is perturbed and closure relationships obtained in quasi-established flows are not justified. As the flow structure is affected, perturbations may concern all the physical processes such as momentum exchanges, heat and mass transfers. The turbulence is generally increased, giving enhanced heat and mass transfers as well as irreversible pressure drops. Unfortunately, these local effects are dependent on many geometrical parameters and no general modelling can be proposed. Each case should be studied separately. For example, when the CCFL occurs in a geometrical singularity, specific local closure laws were found necessary in the same way as singular pressure losses are modeled. Also, the local effect of the ECCS water jet on condensation has been modelled to take into account the enhanced heat transfer due to increased turbulence.

Code limitations related to the numerical scheme

Most of the codes use a first order finite difference scheme with a staggered mesh and the donor cell principle. The time discretization varies from the fully implicit discretization to the nearly implicit multi-step scheme. These methods are known for their robustness and their stability but they are rather diffusive. This may be a limitation when calculating propagation phenomena.

The Cathare code takes care of the hyperbolicity of the system in order to warrant stability even for very small time steps and meshes. Theoretically, all calculations should be converged in space and time. In practice, convergence tests are easily performed for simple analytical tests, and some recommendations are deduced for system tests or reactor calculations.

The problem of convergence in meshing is somewhat different for multidimensional models. As long as there is no turbulent diffusion in these models, convergence tests cannot reach the exact solution. So closure laws must be validated for a given meshing (corresponding to a given numerical diffusion) and possibly with scale 1 experiments.

4 THE LBLOCA

The large break LOCA in a PWR is still one of the most difficult transient to predict with a good accuracy. Many types of limitations listed here above are encountered particularly during the refill and reflood phase of the transient.

- The *refill phase* of a LBLOCA determines the amount of accumulator water not bypassed to the break which is available in the vessel at the beginning of the reflooding. The condensation rate during this phase controls also the liquid subcooling at the inlet of the core. An excess of bypass to the break will result in a reduced reflood rate as long as the downcomer mass inventory is not recovered by the low flowrate LHFI. An underestimated condensation gives a too high subcooling; the collapsed water level in the core is increased which is unfavourable as the water head difference between downcomer and core is reduced. On the other hand, the occurrence of an inverse annular flow pattern above the quench front will persist a longer time; during this phase the liquid carry over is very low which is favourable for the amount of steam which can be produced in the core. But as the liquid carry over is low, the heat transfers far downstream the quench front are not so efficient. Summarily a too high subcooling may give a very high QF velocity at the beginning of the reflooding but may not be so favourable for the peak clad temperature. Contrarily a too low subcooling may have the

inverse effects and will initiate earlier the boiling of water in the downcomer due to the RPV wall heat release, limiting the downcomer head. All these effects demonstrate that the whole reflooding transient prediction depends a lot on a reliable calculation of the refill phase. Present thermalhydraulic codes may have some difficulties to calculate correctly the condensation during the refill phase because of the very **unstable nature of the flow** observed in many experiments (UPTF, LOFT). The process of counter-current flow limitation occurs in the **complex geometry** of the top part of the downcomer with a significant effect of the condensation. A 2-D modelling of the downcomer is possible with CATHARE and TRAC codes. However, such models suffer from a lack of reliable modelling of **turbulent diffusion in 2-phase flows**. An extensive validation of the modelling on scale 1 UPTF data was required. Moreover, the rapidity of the downcomer and lower plenum refill controls the initial velocity of the water entering the core at the beginning of reflooding. Then, this initial velocity controls the amplitude of **oscillations between core and downcomer** during the reflooding.

The **steam binding effect during reflooding** represents the flow resistance between core and break. Let us consider the differential pressure between the upper plenum and the top of downcomer. The pressure loss is mainly due to wall friction in the SG tubes and in the pumps. There is also a pressure drop by acceleration in the steam generators due to drops evaporation and vapour superheating. It is equal to the gravity head difference between downcomer and core. It is limited by the value corresponding to a water level in the downcomer at the elevation of the cold legs. The steam flowing in the loops is mainly produced in the core and is the result of the heat release from the rods. A more or less important part of this steam is also produced out of the core by vaporization of the entrained liquid through wall heating in the upper plenum, hot legs or steam generators, or by vapour desuperheating. Then the system behaves approximately as if the core cooling rate was limited. The limitation is mainly related to the height of the downcomer which determines the maximum head available for reflooding the core.

The most favourable case is obtained when all the vapour flowing in the loops is created in the core and has participated to the rod cooling. The more liquid droplets are vaporizing in the steam generator, the less vapour can flow out of the core. Then it is very important to predict correctly the amount of water entrained to the steam generators. Some weaknesses of the codes may be suspected since the de-entrainment on the structures of the upper plenum is difficult to control. It was observed (ACHILLES test facility) that the droplet spectrum in the core was very wide and one can expect that the smallest drops follow the steam up to the SG when the largest ones are de-entrained in the upper plenum. Present system codes cannot predict such a partition as they generally describe what occurs for an average size drop. A **multi-field approach** could be able to better represent these phenomena by calculating separately liquid films along structures and either one population or two populations of droplets.

- **Oscillatory reflooding** was observed in system test facilities (LOFT, PKL, BETHSY) at least at the beginning of the transient. When water of the accumulator enters at the bottom of the core, the important vaporization in the core initiates flow oscillations between downcomer and core with a large amplitude (+ or - 1m/s in velocity). The correct prediction of the amplitude and the duration of this behaviour influences greatly the velocity of the whole reflooding phase. The maximum amplitude of the oscillations controls the quantity of coolant lost at the break and the average downcomer level which is a key parameter limiting the efficiency of the core cooling. At each cycle of the oscillations some water is entrained out of the core. This water will vaporize in the upper plenum by heat release from the hot structures or in the steam generator and will produce a very unfavourable steam binding. Moreover all this water is lost and reduces the downcomer level which is the driving force. The duration of this oscillatory phase is then a critical feature. Analysing the code predictions of such oscillatory

behaviour observed in reflooding tests, it is presumed that the interfacial friction downstream of the quench front controls the quantity of entrained water. The vaporization of this water downstream the quench front and outside of the core induces the flow reversal, exciting the oscillations. A fine mechanical description of the flow downstream of the quench front is then required with a modelling of the inverse annular flow which may take place during oscillations at the beginning of reflooding and of the droplet flow. The main difficulty in this modelling is related to the effects of the spacer grids which create strong local perturbation in a complex geometry. When there is a significant top-down quenching, the modelling of two liquid fields (droplet and films) as was done in COBRA, may be a better approach.

It must also be noticed that the numerical aspects have an influence in oscillatory reflooding. Numerical schemes which are diffusive may damp too much the oscillations; time and meshing convergence tests are necessary. On the other hand, many reflood codes use a fine meshing of the rods in the vicinity of the quench front with a more coarse hydraulic meshing. Some perturbations of the hydraulics are induced each time that the quench front progresses from an hydraulic mesh to the following. Attention must be paid to minimize these perturbations in order to avoid numerically induced oscillations.

The steam binding effects during an oscillatory reflooding is also a difficult problem. The damping of the oscillations is strongly dependent on the transit time for droplets created in the core to reach the hot steam generators. At each oscillation, during the phase of positive flow, droplets are entrained out of the core. If they vaporize immediately during the positive flow phase, the oscillation is damped. If they vaporize later during the phase of flow reversal, the oscillation is excited and the amplitude may be increased. Droplets with the smaller size have a velocity close to the steam velocity whereas the larger droplets have a lower velocity. Then a modelling of different populations of droplets may provide a better control of the oscillations.

5 SUMMARY OF MAIN CODE LIMITATIONS

The main limitations of present system codes are related to:

- Instable behaviour: condensation driven flow oscillations, oscillatory reflooding,...
- One phase with two or more separate fields: droplet + liquid films,...
- Non established flows: entrance effects,...
- Complex geometries: perturbations due to spacer grids, singularities, CCFL,...
- Algebraic closure relations without internal relaxation times: coalescence,...
- Algebraic transition criteria between flow regimes without internal relaxation times: stratification
- Closure relations used beyond the domain of validity: low pressure transients,...
- Flow pattern maps used beyond the domain of validity: high pressure, large diameter,...
- Small scale or large scale multi-D effects
- Transients very sensitive to a particular physical process: loop seal clearing,...

- Unsufficient physical modelling of multi-D modules: closure relations, turbulent diffusion,...
- Numerical scheme: numerical diffusion,...
- User Effect: bad choice of nodalization,...

6 RECOMMENDATIONS FOR FUTURE DEVELOPMENTS

6.1 Drift flux model, Two-fluid model or multi-field models

The **Drift Flux models** are still used in some code versions and have some advantages. Only one momentum equation is written for the two-phase mixture and the difference between the velocities of the two phases is calculated by an algebraic relation. The derivation of this algebraic relation from experimental data is rather simple and it is also possible to make it consistent with a flooding limit (see the ATHLET code). The drift velocity correlations may be dependent on the flow pattern and they generally assume that there is an equilibrium slip due to buoyancy, interfacial friction, wall friction forces,... The algebraic correlation may be understood as a simplified form of the cross momentum equation obtained by elimination of the pressure gradient term from the two phasic momentum equations. The differential terms of this equation (inertial terms, added mass terms) are neglected. The limitations of this approach are related to these assumptions. The physical situations where the differential terms play a role in the phase slip cannot be described with the same accuracy as with two momentum equations. This may occur when the phase coupling is weak, in separated flow patterns, annular flows, stratified flows, and also droplet flows. In these cases, the equilibrium slip is reached only after a certain relaxation time related to inertial effects.

The **two-fluid model**, with mass, momentum and energy equations written for each phase, is the most extensively used. It has shown its good capabilities to describe a wide range of phenomena. It is not much more accurate than the drift flux model for flow patterns with a high coupling between phases, but it has more capabilities for the other flow patterns. Its main limitations are:

- the closure relations being algebraic, some internal processes with relaxation times (coalescence, stratification, entrance effects,...) may not be described accurately enough
- when one phase is present in the form of two or more separate fields (liquid film + drops), the phase averaging may mask important processes.

The **multi-field models** have more capabilities for some flow patterns. A two-liquid field model has already been implemented in COBRA to model films along the structures and droplets during the reflood phase of a LBLOCA. These two liquid fields may coexist in the top part of the core when there is a significant top-down quenching and also in the upper plenum, where entrainment and de-entrainment phenomena occur. A generalization of this approach for all components of a system code can improve the code capabilities. Different multi-field models may be interesting:

- liquid film + droplet field for annular-mist flows
- stratified liquid field + droplet field in stratified-mist flows
- large droplet field + small droplet fields for some mist flows with a large spectrum of droplet sizes, for example during reflooding where large droplets may be de-entrained whereas

smaller droplets participate to heat transfers with superheated steam and are entrained by the steam

- small bubbles + larger bubbles

A more precise survey of each situation should be made to determine what kind of improvement can be expected by such models. The success of this approach depends on the solution of some problems:

- How many equations must be written for each field? (mass equation, mass + momentum equation, or mass + momentum + energy)

- What additional experimental information is necessary for developing and assessing the additional closure relations in such models ? Is this experimental information available with present measurement techniques?

- How to proceed when the flow pattern has not such a separation of the fields?

6.2 Needs for additional transport equations

It was mentioned that some small scale processes may have relaxation times which are not represented when using algebraic closure relations. Moreover, the flow pattern maps which are used in present system codes are also expressed by algebraic transition criteria and it does not take into account the time delay or the establishment length necessary to change from one flow regime to another one. Even in turbulent single phase flows, the same problem was encountered for modelling the turbulent diffusion. The first approach was to model the turbulent diffusion with an algebraic relation, the so-called "mixing-length" model. Then it was found that this simple approach was only limited to an established turbulence in simple geometries (boundary layer, jet,...). The next step was to derive transport equations to predict the dynamic evolution of the large turbulent scales responsible for the diffusion. This was achieved in the $k-\epsilon$ models. The modelling of two-phase flows in present system codes can be considered as the analogous to the "mixing-length" model for turbulent single phase flows. The next step would be to write additional transport equations to predict the evolution of the characteristic scales of the two-phase intermittency. A promising approach is to write a transport equation for the interfacial area concentration.

6.3 Needs for an improved 3-D modelling

6.3.1 Closure relations

Three-dimensional modules exist in some thermalhydraulic system codes such as TRAC, CATHARE or are in development. They are mainly used for PWR pressure vessel modelling in LOCA transients. They were extrapolated from previous 1-D, 2-Fluid models and are used with a rather coarse meshing (about 1000 nodes). Not a big effort has been paid yet to develop specific closure relationships. Simple extrapolations from 1-D closure relations, as used in CATHARE may not be adequate. When 1-D models use principal variables which represent area averaged quantities, local principal variables are used in 3-D correlations which have a different meaning. For example, the local void fraction may not be used as characteristic of the flow pattern and the interface structure. A local flow pattern map should be established using other characteristic local quantities such as the interfacial area concentration. A transport equation for this interfacial area concentration is even more necessary in 3-D calculations than in 1-D models. Then closure relations should be reformulated as functions of all the local variables.

6.3.2 Turbulent diffusion

The turbulence model is necessary for modelling momentum and heat transfers within each phase. The k- ϵ model was used successfully in some 2-phase scientific codes but only in the particular case of dispersed flows (droplet flows or bubbly flows). A general model of the turbulent viscosity valid in the full range of void fractions and for all flow patterns does not exist. In present 3-D modules used in system codes, the turbulent diffusion is either not modelled or modeled with very simple extrapolations of single-phase mixing length type models. It is not a very important shortcoming when 3-D models are used in very porous media such as the core of a reactor. The transfers with the structures and the interfacial transfers are probably much larger than the turbulent transfers. One must also keep in mind that the meshing is rather coarse in 3-D applications to the pressure vessel. Each mesh has several metallic structures in it. The numerical diffusion may also mask the physical diffusion. The situation would be different if 3-D models were used with a fine noding or in components without porosity. Progress in computer performance should allow in the future such finer modelling. This requires an important effort in turbulence modelling for all flow patterns.

6.3.3 DNS, LES, or turbulent viscosity model

In the frame of a long term development, the turbulence modelling in 2-phase 3-D codes will be an important challenge. The first approach consists in modelling a turbulent diffusivity either with algebraic relations (mixing length type) or with additional transport equations (k- ϵ model or Rij model). As mentioned above, such models exist in industrial codes for single-phase flows and for dispersed flows. They still have to be extended to all two-phase flow patterns.

The large eddy simulation (LES) is now currently used also in single-phase flows and for dispersed flows. Only the smaller scale turbulent structures are filtered and the larger are calculated. Such models have better capabilities than the turbulent viscosity approach. Extending this approach to all types of two-phase flows should be envisaged as a long term goal for reducing the empirism of the closure relations. This could also extend the understanding of the structure of two-phase flows and would reduce the needs of experimental data.

The direct numerical simulation (DNS) of Navier-Stokes equations is now within the range of some high performance computers for some flow configurations. It requires a very fine nodalization to calculate even the smallest turbulent structures. Applying this approach to two-phase flows is still difficult as the node size should also be smaller than the smallest bubble or drop. Interface tracking techniques are also necessary. Some attempts were made for a limited problem with one or a few bubbles in liquid. Extending this approach to the solution of industrial problems will not be possible in the near future. But it may be very useful as a "numerical experiment" to develop constitutive relations for the LES models or k- ϵ models. It may become a convenient tool for overcoming limitations of measurement techniques.

6.4 Needs of new experimental programs

New experimental programmes are required for extending the capabilities of present codes. They are necessary first to derive closure relations, and then for validation. They should include advanced measurement techniques to obtain a local information about all the physical quantities which are predicted.

For qualifying a multi-field model, it is necessary to be able to measure at least the flowrate of each field and preferably the mass transfers (entrainment, deposition,...).

For qualifying models with additional transport equations such as the interfacial area, information about the void distribution, the bubble or drop size, the interfacial area is required.

A local measurement of the velocities, temperatures, void fraction, interfacial area concentration, turbulent intensity and turbulent scales is a prerequisite for allowing a modelling of closure terms in the fine 3-D approach.

DIVIDING PHASES IN TWO-PHASE FLOW AND MODELING OF INTERFACIAL DRAG

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Abstract

Different models intended to describe one-dimensional two-phase flow are considered in this paper. The following models are introduced: conventional six-equation model, conventional model equipped with terms taking into account nonuniform transverse velocity distribution of the phases, several virtual mass models and a model in which the momentum equations have been derived by using the principle of Separation of the Flow According to Velocity (SFAV). The dynamics of the models have been tested by comparing their characteristic velocities to each other and against experimental data. The results show that the SFAV-model makes a hyperbolic system and predicts the propagation velocities of disturbances with the same order of accuracy as the best tested virtual mass models. Furthermore, the momentum interaction terms for the SFAV-model are considered. These consist of the wall friction terms and the interfacial friction term. We model wall friction with two independent terms describing the effect of each fluid on the wall separately. In the steady state, a relationship between the slip velocity and friction coefficients can be derived. Hence, the friction coefficients for the SFAV-model can be calculated from existing correlations, viz. from a drift-flux correlation and a wall friction correlation. The friction model was tested by searching steady-state distributions in a partial BWR fuel channel and comparing the relaxed values with the drift-flux correlation, which agreed very well with each other. In addition, response of the flow to a sine-wave disturbance in the water inlet flux was calculated as function of frequency. The results were compared to those obtained with the corresponding drift-flux model. The results of the models differed from each other already with frequency of order 5 Hz, while the time constant for the relaxation, obtained from steady-state distribution calculation, would have implied significant differences appear not until with frequency of order 50 Hz.

1 Introduction

In this paper, we consider the problems of deriving a one-dimensional two-phase flow model in which the total flow is divided into subfluids according to the phases. Also, we present a more general approach that retains the number of conservation equations but has substantially greater degree of freedom in describing various two-phase flow phenomena. More specifically, we have concentrated on the case in which the dividing logic of the flow is not based on mass, but rather on momentum. As a result, a six-equation two-fluid model applicable to gas-liquid flows in which the momentum conservation equations have been derived by using the principle of Separation of the Flow According to Velocity (SFAV), has been formed.

The following models for two-phase flow are considered in this study: conventional six-equation model, conventional model equipped with terms taking into account the nonuniform transverse

velocity distribution within the phases, different forms of virtual mass models (e.g. the forms used in the thermal hydraulic codes TRAC-PF1, RELAP5/MOD2 and CATHARE) and the SFAV-model.

The conventionally derived six-equation model for one-dimensional two-phase flow forms an elliptic PDE-system, viz. some characteristic velocities of the system are not real and the model is not stable against perturbations. This deficiency is commonly known and it has been tried to correct by introducing the concept of virtual mass. The physical meaning of the virtual mass is to describe the inertial interaction between the phases in a flow that involves temporal or spatial acceleration. Another way to modify the conventional model that we present in this paper, is to assume a suitable nonuniform transverse velocity distribution for the phases and to include the extra terms describing this effect into the existing derivative terms of the model.

The characteristic velocities of the models were compared with each other and against experimental data. These velocities can be associated with the propagation velocities of small disturbances. Characteristics referring to void fraction disturbance propagation and pressure wave propagation were studied.

The SFAV-model has been shown to be clearly hyperbolic over the whole range of void fraction from zero to unity, which means the introduction of the SFAV-formalism to the momentum equations has remarkable positive effect on the stability of the system [1].

The fact that only the momentum equations of the SFAV-model differ from the conventional six-equation model enables to use existing up-to-date correlations directly for all the source terms appearing in the mass and energy equations.

The separation of the flow into two subfluids always gives rise to the problem of describing the interfacial interaction between the fluids. In the conventional approach, in which the flow is separated into two phases, it has proved to be difficult to reliably describe the momentum transfer between the phases by using one-dimensional formalism. This is because of the complex nature of the interface and thus complex local distribution of the interaction force. In the SFAV-model, the interface between the subfluids is not such complex, because the interface does not need to follow the interfaces between the phases.

In this study, we consider also the means to obtain momentum interaction terms for the dynamic SFAV-model which produce the correct stationary state. These consist of the wall friction terms and the interfacial friction term. We model wall friction with two independent terms describing the effect of each fluid on the wall separately. The advantage is that more detailed effects like when major part of bubbles occupy the neighborhood of the channel wall in the low void fraction case, can be described. The approach requires friction coefficients for all three friction terms, which means wall friction coefficients for both of the subfluids and an interfacial friction coefficient.

In the steady state, a relationship between the slip velocity and the friction coefficients can be derived. Hence, a combination of drift-flux and total wall friction correlations can be converted into effective friction coefficients that can be applied for both transient and steady-state conditions. All three friction coefficients can be solved in one go by minimizing a suitably chosen and weighted error functional, which in the ideal case leads to the coefficients that agree with both of the chosen correlations.

The friction coefficients obtained by this means are far off simple because of possible contradictory nature of the correlations that are tried to be kept simultaneously valid. Thus, in numerical solving of the model equations, some smoothing of the friction coefficients may be necessary.

As an application of the derived friction coefficients, searching of a steady-state distribution of the model in a partial BWR fuel channel, resulting from different initial states and comparison to the drift-flux correlation was performed. Furthermore, response of the flow to a sine-wave disturbance in the water inlet flux was calculated as function of frequency. The results were compared to those obtained with the corresponding drift-flux model.

We begin by introducing the concept of characteristic velocities in Section 2. The different models considered in this study are considered in Sections 3 and 4. The construction of the SFAV-model is considered in more detail, especially the closure relations, in Section 4.3. Comparison of the characteristic velocities of the models with each other and further against experimental data is performed in Section 5. The searching of steady-state distributions of the SFAV-model and response to the sine-wave disturbance in water inlet flux are calculated in Section 6.

2 Characteristic velocities

All the two-phase flow models considered in this paper can be written in the primitive form of

$$\mathbf{A} \frac{\partial \vec{\phi}}{\partial t} + \mathbf{B} \frac{\partial \vec{\phi}}{\partial z} + \vec{C} = 0 \quad (1)$$

where $\vec{\phi}$ is a vector consisting of the unknown variables and \mathbf{A} and \mathbf{B} are $n \times n$ matrices where n is the number of equations in the model. The characteristics of the system, v_{char} , can be calculated from

$$\det(v_{char} \mathbf{A} - \mathbf{B}) = 0 \quad (2)$$

The characteristics of the complete six-equation model, consisting of mass, momentum and energy conservation equations for two subfluids, represent:

- $u \pm c$ in which u is order of the volumetric flux j and c is two-phase sonic velocity.
- the phase velocities v_g and v_l .
- two velocities order of magnitude of v_g and v_l which refer to void fraction disturbance propagation.

In the conventional form of the six-equation model, the conservation equations are derived over the domains occupied by the phases. Unfortunately, then the characteristics referring to void fraction disturbances become complex and the system is elliptic. This feature is clearly unphysical and prevents solving the system by any method that uses characteristic velocities and presupposes system hyperbolicity. From this basis, the need to derive supplementary terms, like virtual mass, into the model is reasoned.

3 Conventional six-equation model

In the conventional six-equation model for one-dimensional two-phase flow the flow domain is divided into two subflows according to the phases. After that the conservation equations for mass, momentum and energy are integrated over the cross-sectional area of each phase.

3.1 Basic form

The basic form of the conventional six-equation model for one-dimensional two-phase flow is

$$\begin{aligned} M_g &= 0 \\ M_l &= 0 \\ MO_g &= 0 \\ MO_l &= 0 \end{aligned} \quad (3)$$

$$E_g = 0$$

$$E_l = 0$$

where

$$\begin{aligned} M_n &= \frac{\partial}{\partial t} (A\alpha_n \rho_n) + \frac{\partial}{\partial z} (A\alpha_n \rho_n v_n) + S_{nn_2} - A\alpha_n S_n \\ MO_n &= \frac{\partial}{\partial t} (A\alpha_n \rho_n v_n) + \frac{\partial}{\partial z} (A\alpha_n \rho_n v_n^2) + F_n + A\alpha_n \frac{\partial p}{\partial z} + S_{mnn_2} - A\alpha_n S_{mz_n} \\ E_n &= \frac{\partial}{\partial t} (A\alpha_n \rho_n h_n) + \frac{\partial}{\partial z} (A\alpha_n \rho_n v_n h_n) - A\alpha_n \frac{\partial p}{\partial t} + Aq_{nn_2}''' - A\alpha_n q_n''' \end{aligned} \quad (4)$$

where $n = g, l$. The quantities appearing in the equations are statistically averaged, but for simplicity the averaging symbols are omitted here.

3.2 Model taking into account transverse distribution of the flow velocity

The averaging process in the derivation of the conventional six-equation model is equivalent with the assumption that the cross-sectional distributions of gas and liquid velocity and density are uniform. We questioned this assumption by introducing the terms into the conservation equations, Eqs. (4), that allow the transverse phasic velocity distribution to be nonuniform.

We assumed that the arranged transverse distribution of phasic velocity could be presented as piecewise linear function of generalized transverse coordinate θ (e.g. $\theta = (r/R)^2$ for a round pipe) as shown in Fig. 1. The parameter $\eta \in [0, 1]$ defines the steepness of the distribution in an unequivocal way.

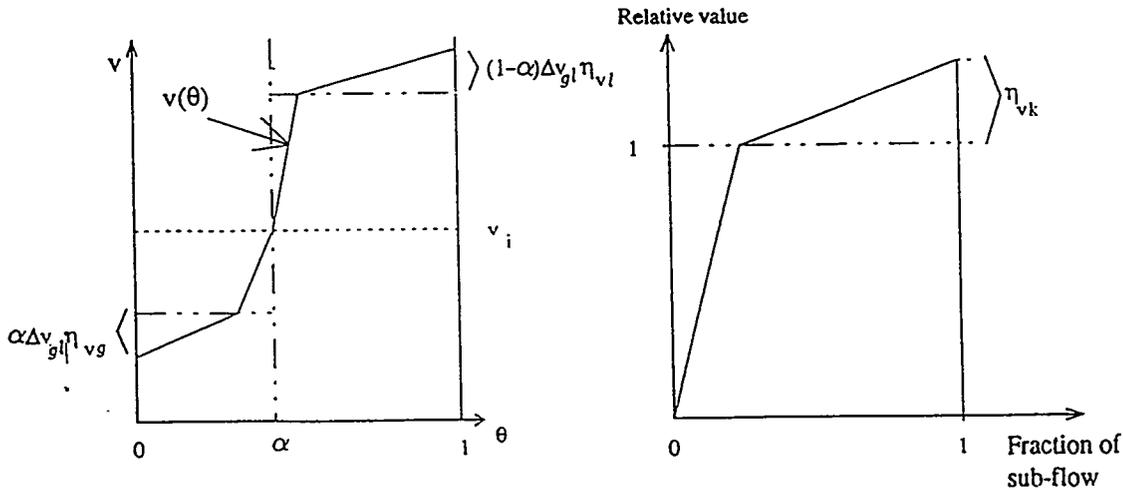


Figure 1: Assumed piecewise linear transverse distribution of flow velocity.

Introducing the transverse velocity distribution affects the momentum flux. Namely, then the average of the squared liquid flow velocity becomes

$$\begin{aligned} \langle v^2 \rangle_l &= \frac{1}{\Delta t \Delta z A_l} \int_t \int_z \int_{A_l} (\langle v \rangle_l + \delta v_l)^2 dA_l dz dt = \langle v \rangle_l^2 + \langle \delta v^2 \rangle_l \\ &= \langle v \rangle_l^2 + \frac{1}{3} \eta_{vl} (1 - \alpha)^2 (\langle v \rangle_g - \langle v \rangle_l)^2 \end{aligned} \quad (5)$$

where the term $\langle \delta v^2 \rangle_l$ is integrated from the function $D(\theta_l; \eta_{vl})$ (Fig. 1). This changes the equation $MO_l = 0$, in Eqs. (4), to the form

$$MO_l = \frac{\partial}{\partial t} [A(1-\alpha)\rho_l v_l] + \frac{\partial}{\partial z} \left\{ A(1-\alpha)\rho_l \left[v_l^2 + \frac{1}{3}\eta_{vl}(1-\alpha)^2(v_g - v_l)^2 \right] \right\} - S_{mgl} + F_l + A(1-\alpha)\frac{\partial p}{\partial z} - A(1-\alpha)S_{mz_l} \quad (6)$$

We assumed the nonuniform transverse velocity only for the liquid phase because the liquid momentum flux is substantially greater than gas momentum flux due to the fact that the phase density sets the scale (momentum flux = ρv^2). Thus, modifications into gas momentum flux probably would not be as significant as corresponding modifications into liquid momentum flux.

Taking into account the transverse distribution of the phase velocity is the only additional feature that can be straightforwardly included into the conventional model. Namely, any slip does not exist within a phase and turbulence within a phase cannot be easily modeled.

3.3 Model equipped with a virtual mass term

The virtual mass term is one of the terms in the interfacial momentum transfer term S_{mgl} (see Eqs. (4)). It represents the inertial interaction between the phases in a flow which involves temporal or spatial acceleration. In addition to its physical significance, the virtual mass term can have a large influence on the characteristic velocities and, that way, on numerical stability of the two-phase flow equations. Several different definitions of the virtual mass term have been proposed so far. Usually the suggested forms are not derived strictly from physical basis but mathematical fittings are needed in order to obtain a hyperbolic equation system over the whole range of flow parameters.

The forms for virtual mass term considered here are the objective form (invariant under changes of frame of reference) proposed by Drew and Lahey [2] (*Type I*) and a simplified form consisting only of the time derivatives [3] (*Type II*). *Type II* virtual mass is the most common form used with minor modifications in the thermal-hydraulic codes TRAC-PF1 [3] and RELAP5/MOD2 [4] and a version of the *Type I* virtual mass is used in the two-fluid thermal-hydraulic code CATHARE [5].

The virtual mass term can be expressed generally as [6]

$$M_{vm} = \alpha_d F_{vm} = \alpha_d \rho_c C_{vm} a_{vm} \quad (7)$$

where the subscripts d and c respectively refer to the dispersed and continuous phases, C_{vm} is the virtual mass coefficient and a_{vm} is the virtual mass acceleration.

The *Type I* virtual mass is an objective expression derived by Drew and Lahey [2] by considering the forces on a single sphere which was accelerated relative to an inviscid fluid undergoing a pure strain and rotation far from the sphere. In the one-dimensional formulation the virtual mass acceleration is given by

$$a_{vm} = \frac{D_d v_d}{Dt} - \frac{D_c v_c}{Dt} = \left(\frac{\partial v_d}{\partial t} + v_d \frac{\partial v_d}{\partial z} \right) - \left(\frac{\partial v_c}{\partial t} + v_c \frac{\partial v_c}{\partial z} \right) \quad (8)$$

For this form of virtual mass acceleration, the value of C_{vm} was determined empirically under the bubbly condition so as to obtain reasonable values for speeds of sound [7] as a function of the void fraction:

$$C_{vm} = 0.5(1 + 12\alpha^2), \quad \alpha < 0.2 \quad (9)$$

The form of virtual mass acceleration in Eq. (8) is used also in the CATHARE code. The coefficient $\alpha_d \rho_c$ (in Eq. (7)) is replaced by the following relation to obtain a smooth change of the

virtual mass term between $\alpha = 0$ and $\alpha = 1$:

$$\alpha_d \rho_c = \alpha(1 - \alpha)\rho = \alpha(1 - \alpha)[\alpha\rho_g + (1 - \alpha)\rho_l] \quad (10)$$

In addition to the virtual mass term, a differential term of the form

$$p_i \frac{\partial \alpha}{\partial z}, \text{ where} \\ p_i = \frac{\alpha(1-\alpha)\rho_g\rho_l}{\alpha\rho_l + (1-\alpha)\rho_g} (v_g - v_l)^2 \quad (11)$$

is included in the momentum equations in CATHARE. The expression for p_i is simply chosen to provide the hyperbolicity of the system [5]. In the calculations of Section 5, the value of C_{vm} equal to 1.36 was used because then the best agreement between the characteristic and experimental two-phase sonic velocity over the whole range of void fraction was achieved.

The *Type II* virtual mass is a simplified form of the virtual mass acceleration composed only of the time derivative terms in Eq. (8):

$$a_{vm} = \frac{\partial v_d}{\partial t} - \frac{\partial v_c}{\partial t} \quad (12)$$

The simplification is based on the fact that in reactor analyses the spatial acceleration terms are usually much smaller than the temporal acceleration terms since the reactor circuits can be considered to be mostly composed of pseudo one-dimensional components. This form is used in the codes TRAC-PF1 and RELAP5/MOD2 with the smoothing expression of Eq. (10). The value of C_{vm} is set equal to unity by considering the agreement between the characteristic and measurement-based sound velocity.

The effect of the different virtual mass types on the equation system was studied in Section 5 by comparing the characteristic velocities of the different models with each other and against experimental data.

4 Flow model based on Separation of two-phase Flow According to Velocity (SFAV)

4.1 Background

The phases are the most essential constituents of two-phase flow. In most flow conditions, mass and energy can be divided quite accurately according to the phases. However, due to the complex flow regimes of two-phase flow, the cross-section averaged velocities of the phases, $\langle v_g \rangle$ and $\langle v_l \rangle$, are not the best velocity variables to describe the total flow, if two separate variables for velocity is to be used. That is due to the fact that the momentum is not separable according to the phases even approximately. From this reasoning, the development work of a two-phase flow model based on Separation of Flow According to Velocity was started which we abbreviate as SFAV.

The principles of deriving an SFAV-based two-phase flow model and calculations considering the hyperbolicity condition of the model have been published in [1]. Reference [8] is about applying the ideas of SFAV to horizontal flow and predicting the low head flooding. Due to these older publications, the derivation of the model will not be repeated in detail here.

In derivation of the SFAV-model, the total flow is separated into two velocity fields and conservation equations are integrated over their domains. Formally, the cross-section of the flow channel is divided according to the velocity, into two subareas,

$$\begin{cases} \text{Flow 1} = \{\theta \in [0, \beta]\} \\ \text{Flow 2} = \{\theta \in [\beta, 1]\} \end{cases}, \quad 0 \leq \beta \leq 1 \quad (13)$$

where θ is a generalized cross-sectional coordinate, it can be e.g. $\theta = (r/R)^2$ for a round pipe.

The mass and momentum conservation equations of the flow model include the following kinds of averaged terms

$$\langle \rho v \rangle, \langle \rho v^2 \rangle \quad (14)$$

By dividing the variables ρ and v into average and fluctuating part, it can be written

$$\begin{aligned} \langle \rho v \rangle &= \frac{1}{\Delta t \Delta z A} \int_t \int_z \int_A \rho v dA dz dt = \frac{1}{\Delta t \Delta z A} \int_t \int_z \int_A (\langle \rho \rangle + \delta \rho) (\langle v \rangle + \delta v) dA dz dt \\ &= \langle \rho \rangle \langle v \rangle + \langle \delta \rho \delta v \rangle \end{aligned} \quad (15)$$

The same way

$$\langle \rho v^2 \rangle = \langle \rho \rangle \langle v \rangle^2 + 2 \langle v \rangle \langle \delta \rho \delta v \rangle + \langle \rho \delta v^2 \rangle \quad (16)$$

We denote

$$\begin{aligned} f_k &= \langle \delta \rho \delta v \rangle_k \\ g_k &= \langle \rho \delta v^2 \rangle_k \end{aligned} \quad (17)$$

where k refers to one of the subflows defined in Eq. (13). In [1], expressions for f_k and g_k have been derived based on physical reasoning and aiming for a hyperbolic system.

4.2 Conservation equations

The conservation equations forming the complete SFAV six-equation model are as follows (for convenience, the averages are not explicitly marked hereafter),

$$\begin{aligned} M_g &= 0 \\ M_l &= 0 \\ M O_1 + M O_2 &= 0 \\ D M O &= \frac{1}{\beta} (M O_1 - v_1 M_1) - \frac{1}{1-\beta} (M O_2 - v_2 M_2) = 0 \\ E_g &= 0 \\ E_l &= 0, \end{aligned} \quad (18)$$

where

$$\begin{aligned} M_k &= \frac{\partial}{\partial t} (A \beta_k \rho_k) + \frac{\partial}{\partial z} [A \beta_k (\rho_k v_k + f_k)] + S_{kk_2} - A \beta_k S_k, \quad k = 1, 2, \quad k_2 = 2, 1 \\ M O_k &= \frac{\partial}{\partial t} [A \beta_k (\rho_k v_k + f_k)] + \frac{\partial}{\partial z} [A \beta_k (\rho_k v_k^2 + 2 v_k f_k + g_k)] + F_k \\ &+ A \beta_k \frac{\partial p}{\partial z} + S_{mkk_2} - A \beta_k S_{mz_k}, \quad k = 1, 2, \quad k_2 = 2, 1 \end{aligned} \quad (19)$$

and M_g , M_l , E_g and E_l are the same as in the conventional model, viz. in Eqs. (4). Here k refers to k 'th SFAV-subflow, β_k is the volumetric fraction of the k 'th subflow, p is pressure, h is specific enthalpy and S_{gl} , S_g , S_l , S_{kk_2} , S_k , S_{mkk_2} , S_{mz_k} , F_k , q_g''' , q_l''' and q_{gl}''' are different sources of the system.

As the independent variables to be solved, e.g. volume fraction of 1st subflow, volumetric flux, velocity difference between the subflows, pressure and the specific enthalpies of the phases (β , j , v_r , p , h_g , h_l) can be chosen. However, nothing prevents from choosing the same phasic variables that are most commonly used in the conventional model, viz. void fraction, velocities of the phases, pressure and specific enthalpies of the phases.

4.3 Closure relations

Because of additional variables and definitions of the SFAV-model, special care have to be put on defining the closure laws which inevitably differ somewhat from the closure laws of the conventional two-phase flow model.

4.3.1 Densities and velocities of the subfluids

The enthalpies of the phases can be associated with the energy equations. Then the quantities β , v_1 , v_2 and p form a complete set of the unknown variables for four remaining equations. Therefore, the average densities of the SFAV-subflows, ρ_1 and ρ_2 , have to be expressed as functions of these variables. Formally one can write,

$$\rho_k = \alpha_k \rho_g + (1 - \alpha_k) \rho_l, \quad k = 1, 2$$

$$\sum_{k=1}^2 \beta_k \alpha_k = \alpha \quad (20)$$

where α_k are the void fractions of the subflows. Not much information exists supporting sensible choices for α_1 and α_2 . We are satisfied to give them β -dependent functions sufficiently amenable to fitting. The definition for α_k has to be in accordance with the induced mass term obtained from potential theory for dispersed flow by M. Ishii et. al. [9]. The simplest expressions to satisfy this condition when the total void fraction approaches zero or unity are of the form

$$\alpha_1 = 1 - a_{\alpha_1} (1 - \beta)^\mu$$

$$\alpha_2 = a_{\alpha_2} \beta^\mu \quad (21)$$

with $a_{\alpha_1} = a_{\alpha_2} = 1/3$. If a constant value for the exponent μ is to be used then $\mu = 1$ yields the best agreement between the measured sonic velocity and pressure wave characteristics of the model [1]. In addition, it produces a trivial connection between the void fraction and β , namely $\alpha = \beta$. Increasing the value of μ makes the model approach to the conventional model (corresponds to the limit $\mu \rightarrow \infty$).

The velocities of the phases are related with the velocities of the subflows as follows

$$\alpha v_g = \beta \alpha_1 v_1 + (1 - \beta) \alpha_2 v_2 - \beta \frac{f_1}{\Delta \rho_{lg}} - (1 - \beta) \frac{f_2}{\Delta \rho_{lg}}$$

$$(1 - \alpha) v_l = \beta (1 - \alpha_1) v_1 + (1 - \beta) (1 - \alpha_2) v_2 + \beta \frac{f_1}{\Delta \rho_{lg}} + (1 - \beta) \frac{f_2}{\Delta \rho_{lg}} \quad (22)$$

where $\Delta \rho_{lg}$ is the density difference between the phases. If the terms f_k are linear with respect to velocity, which can be assumed (see Sections 4.3.3-4.3.5) then the Eqs. (22) form a linear transformation between the velocity variables.

4.3.2 Source terms

The conservation equations of the SFAV-model, Eqs. (18), contain a number of source terms of which only those appearing in the momentum equations have to be modeled differently compared with the conventional model. Existing heat transfer, boiling, etc. correlations can be used directly in the mass and energy equations.

The source terms in the momentum equations that have to be modeled separately, are the wall friction terms for the subflows, F_k , and the term for momentum transfer between the subflows, S_{m12} . The formal expressions for the mass and momentum transfer terms, S_{12} and S_{m12} are

$$\langle S_{12} \rangle = P_\beta [(\rho v_y)_i + \langle \delta \rho \delta v_y \rangle_i] - \left[\rho_i \frac{\partial}{\partial t} (A\beta) + (\rho_i v_i + f_i) \frac{\partial}{\partial z} (A\beta) \right] \quad (23)$$

$$\langle S_{m12} \rangle = v_i \langle S_{12} \rangle + P_\beta \langle \delta v \delta(\rho v_y) \rangle_i - \left[f_i \frac{\partial}{\partial t} (A\beta) + (v_i f_i + g_i) \frac{\partial}{\partial z} (A\beta) \right] \quad (24)$$

where P_β is the perimeter of the 1st subflow in the cross-section, v_y is the transverse velocity and subscript i refers to the interface of the subflows. The transverse velocity v_y is uncertain at the interface in the present one-dimensional model, which is the main reason why the momentum difference equation $DMO = 0$ is written in the curious form of Eq. (18). Namely, by this means the term S_{12} can be made to vanish, when estimating the values at the interface by linear interpolation:

$$X_i = (1 - \beta)X_1 + \beta X_2, \quad X \in [\rho, v, f, g] \quad (25)$$

The term $P_\beta \langle \delta v \delta(\rho v_y) \rangle_i$ in Eq. (24) is the interfacial turbulent momentum transfer term which is modeled in the form analogous to the wall friction terms, viz.

$$\begin{aligned} P_\beta \langle \delta v \delta(\rho v_y) \rangle_i &= \frac{1}{2} \frac{A}{D_h} \xi_{12} \beta (1 - \beta) \Delta \rho_{21} v_r |v_r| \\ F_1 &= \frac{1}{2} \frac{A}{D_h} \xi_1 \beta \rho_1 v_1 |v_1| \\ F_2 &= \frac{1}{2} \frac{A}{D_h} \xi_2 (1 - \beta) \rho_2 v_2 |v_2| \end{aligned} \quad (26)$$

where ξ_{12} is the interfacial friction coefficient and ξ_1 and ξ_2 are the wall friction coefficients. The attempts to improve the accuracy of the friction terms for transient and developing flow conditions would lead to extra differential equations e.g. for the interfacial area [10]. Modeling the friction coefficients is discussed more in Section 4.3.7.

4.3.3 Effects of the temporally averaged transverse distributions of velocity and density

Measurements have confirmed that statistically averaged quantities of two-phase flow have certain transverse distributions. Since the partition into two fluids takes into account major effects in the transverse direction, additional accuracy can be achieved with very simple analytical expressions. Any nonuniform distribution with at least one degree of freedom assumed for subfluids yields a generalization to the traditional model. We use the same piecewise linear function $D(\zeta; \eta)$, introduced in Fig. 1, for all distributions inside the subfluid. It contains one parameter η . Varying η from zero to unity, makes $D(\zeta; \eta)$ change from uniform to linear. A continuous distribution for the entire flow, as presented in Fig. 1, results when we define

$$v(\theta) = \begin{cases} v_1 + (v_i - v_1)D(\theta_1; \eta_{v1}), & \text{for the 1st subfluid} \\ v_2 + (v_i - v_2)D(\theta_2; \eta_{v2}), & \text{for the 2nd subfluid} \end{cases} \quad (27)$$

with the scaled coordinates

$$\begin{aligned} \theta_1 &= \frac{\beta - \theta}{\beta} \\ \theta_2 &= \frac{\theta - \beta}{1 - \beta} \end{aligned} \quad (28)$$

The transverse distribution of density correlates strongly with the velocity and is modeled analogously to Eq. (27).

The nonuniform transverse distribution of velocity and density affect the fluctuation products f_k and g_k , defined in Eq. (17). The contributions to the terms due to the transverse distribution are denoted here as $f_k^{(td)}$ and $g_k^{(td)}$. They can be integrated from

$$\begin{aligned} f_k^{(td)} &= -\beta_k^2 v_r \Delta \rho_{21} \int_0^1 D(\theta_k; \eta_{\rho k}) D(\theta_k; \eta_{v k}) d\theta_k \\ g_k^{(td)} &= \left[\rho_k \int_0^1 D^2(\theta_k; \eta_{v k}) d\theta_k + (-1)^k \beta_k \Delta \rho_{21} \int_0^1 D(\theta_k; \eta_{\rho k}) D^2(\theta_k; \eta_{v k}) d\theta_k \right] \beta_k^2 v_r^2 \end{aligned} \quad (29)$$

The expressions within the integrals are composed of polynomials and thus they can be easily calculated in closed form.

4.3.4 Effects of fluctuations due to slip between the phases within a subfluid

The SFAV-approach allows to take into account the equilibrium slip between the phases within the subfluid as for example, the velocity difference between the liquid droplets and the gas core in the annular flow regime. In reality, the cross-sectional distributions of density consist of step functions. The slip can be modeled within the terms f_k and g_k by considering the average fluctuations of water and gas flow velocities within the subfluid. We define

$$\begin{aligned} \delta \rho_{kg} &= \rho_g - \rho_k = -(1 - \alpha_k) \Delta \rho_{lg} \\ \delta \rho_{kl} &= \rho_l - \rho_k = \alpha_k \Delta \rho_{lg} \\ \delta v_{kg} &= v_{kg} - v_k = (1 - \alpha_k) v_{kr} \\ \delta v_{kl} &= v_{kl} - v_k = -\alpha_k v_{kr} \end{aligned} \quad (30)$$

where $v_{kr} = v_{kg} - v_{kl}$ is the average velocity difference between the phases within the subfluid k . Thus the following expressions can be derived

$$\begin{aligned} f_k^{(slip)} &= \alpha_k (\delta \rho_{kg} \delta v_{kg}) + (1 - \alpha_k) (\delta \rho_{kl} \delta v_{kl}) = -\alpha_k (1 - \alpha_k) \Delta \rho_{lg} v_{kr} \\ g_k^{(slip)} &= \alpha_k (1 - \alpha_k) [(1 - \alpha_k) \rho_g + \alpha_k \rho_l] v_{kr}^2 \end{aligned} \quad (31)$$

To obtain restrictions for the new uncertain parameters v_{kr} , we assume

$$\begin{aligned} (v_1 - v_2)(v_i - v_{1l}) &\geq 0 \\ (v_1 - v_2)(v_{2g} - v_i) &\geq 0 \end{aligned} \quad (32)$$

By using these assumptions, the velocities v_{kr} can be scaled as follows

$$\begin{cases} v_{1r} = k_{v1r} \frac{\beta}{\alpha_1} v_r \\ v_{2r} = k_{v2r} \frac{1-\beta}{1-\alpha_2} v_r \end{cases}, \quad k_{vkr} \in [0, 1] \quad (33)$$

Hence Eqs. (31) can be written in the form

$$\begin{aligned} f_1^{(slip)} &= -k_{v1r} \beta (1 - \alpha_1) \Delta \rho_{lg} v_r \\ f_2^{(slip)} &= -k_{v2r} (1 - \beta) \alpha_2 \Delta \rho_{lg} v_r \\ g_1^{(slip)} &= k_{v1r}^2 \beta^2 \frac{1 - \alpha_1}{\alpha_1} [(1 - \alpha_1) \rho_g + \alpha_1 \rho_l] v_r^2 \\ g_2^{(slip)} &= k_{v2r}^2 (1 - \beta)^2 \frac{\alpha_2}{1 - \alpha_2} [(1 - \alpha_2) \rho_g + \alpha_2 \rho_l] v_r^2 \end{aligned} \quad (34)$$

4.3.5 Effects of fluctuations due to turbulence between the subfluids

The turbulent behavior between the SFAV-subfluids due to flow in the transverse direction can be taken into account also within the terms f_k and g_k defined in Eq. (17). When the turbulence is assumed to take place only between the subfluids, not within a subfluid, it is simpler to derive a turbulence model than it would be for one-phase flow. The velocity scale of turbulence is clearly v_r and the density scale is $\Delta\rho_{21}$. It is assumed that the flow in the transverse direction is caused by the cross-movement of a heavy part of the fluid which then pushes a lighter part downstream. Only the fluctuations that are close to the possible maximum of magnitude are of importance because only they are able to give significant contributions to the second-order terms f_k and g_k . The fluctuations that do not change the total volumetric flux cause the smallest damping along the channel. Therefore, it can be written

$$\begin{aligned} |\delta\rho_k| &\sim (1 - \beta_k)\Delta\rho_{21} \\ |\delta v_k| &\sim (1 - \beta_k)|v_r| \end{aligned} \quad (35)$$

Because only the turbulence between two subfluids is described and the fluctuations of small size suffer most damping, we assume that the local velocity fluctuations vanish when β is approaching zero or unity. Therefore, we set

$$|\delta v_k| \sim \beta(1 - \beta) \quad (36)$$

By combining and parameterizing the expressions above the following forms for f_k and g_k due to turbulence can be written

$$\begin{aligned} f_k^{(turb)} &= -\frac{\pi^2}{16} k_{l\rho} k_{tv} \beta_k (1 - \beta_k)^3 \Delta\rho_{21} v_r \\ g_k^{(turb)} &= \frac{16}{9} k_{tv}^2 \beta_k^2 (1 - \beta_k)^4 \rho_k v_r^2 \end{aligned} \quad (37)$$

where the parameters $k_{l\rho}$ and k_{tv} are scaled between zero and unity and the subscript $k = 1, 2$.

4.3.6 Suggested fittings for the SFAV-parameters

In the previous sections expressions were derived for the terms f_k and g_k , defined in Eqs. (17), describing the effects of the different sources of fluctuations. However, eight free parameters ($\eta_{\rho 1}, \eta_{\rho 2}, \eta_{v 1}, \eta_{v 2}, k_{v 1r}, k_{v 2r}, k_{l\rho}, k_{tv}$) appear in these expressions and have to be given specific values.

A general rule for the calculation of the parameter values as functions of the flow variables can be assumed to be nearly impossible to discover. Submodels for the parameters could be tried to derive according to up-to-date knowledge about two-phase flow small-scale phenomena, but that would probably raise the level of complexity of the model high enough to destroy its usability to any practical problem. The derivation of the expressions for the fluctuation terms involved some arbitrariness, and therefore their effect on the flow equations should not be of greatest significance. Due to this a natural choice was to try to fix the parameters in such a way that their values are close to the lowest possible values needed to maintain the well-posedness (the hyperbolic nature) of the flow equations.

We considered the qualitative effects of the parameters on the flow equations by performing sensitivity analyses over the void fraction - pressure region of $[0, 1] \times [0.1, 17.5]$ MPa. As the quantity to describe the nature of the flow equations we used the discriminant of the characteristic velocities referring to the void fraction disturbances, i.e. the discriminant of the characteristics that are complex in the conventional six-equation model. From the results it could clearly be seen that some expressions had negligible effect on the characteristic velocities. For simplicity these parameters

were omitted (by equalizing to zero), and thus the corresponding expressions were left out from the final expressions for f_k and g_k which are the sums of the expressions derived for separate effects in Sections 4.3.3–4.3.5. The summed expressions then become

$$\begin{aligned}
 f_1 &= - \left[k_{v1r} \beta (1 - \alpha_1) + \frac{\pi^2}{16} k_{t\rho} k_{tv} \beta (1 - \beta)^3 \Delta \alpha_{12} \right] \Delta \rho_{lg} v_r \\
 f_2 &= - \frac{\pi^2}{16} k_{t\rho} k_{tv} \beta^3 (1 - \beta) \Delta \rho_{21} v_r \\
 g_1 &= \left[k_{v1r}^2 \beta^2 \frac{1 - \alpha_1}{\alpha_1} ((1 - \alpha_1) \rho_g + \alpha_1 \rho_l) + \frac{16}{9} k_{tv}^2 \beta^2 (1 - \beta)^4 \rho_1 \right] v_r^2 \\
 g_2 &= \left[\frac{1}{3} \eta_{v2} \rho_2 (1 - \beta)^2 + \frac{16}{9} k_{tv}^2 \beta^4 (1 - \beta)^2 \rho_2 \right] v_r^2
 \end{aligned} \tag{38}$$

In order to maximize the realness of the characteristic velocities we searched, with respect to β , the volumetric fraction of the 1st SFAV-subfluid, the values for the parameters η_{v2} , k_{v1r} , $k_{t\rho}$ and k_{tv} that maximize the discriminant of the characteristics referring to the void disturbances. Because the assumed forms of f_k and g_k contain the velocities only as the factors of v_r and v_r^2 , the discriminant is proportional to v_r^2 and hence the velocity dependency does not affect the realness. Also, we found that the optimal value for the parameter k_{tv} depends on pressure. The following fitting describes this dependency approximately.

$$\begin{aligned}
 k_{tv}^{opt}(\beta, \Delta \rho_{lg}) &\approx 0.45 \left[\frac{429.4 \text{ kg/m}^3}{\Delta \rho_{lg}} \right]^6 \{ \cos [(2.6\beta^{0.8} - 0.3)\pi] - 1 \} + 1, \\
 \Delta \rho_{lg} &> 429.4 \text{ kg/m}^3 \quad (p < 17.5 \text{ MPa})
 \end{aligned} \tag{39}$$

We reduced the remaining four parameters to one parameter, k , the way which presupposes the changes in the fluctuations of the flow, or chaotic behavior, being equal in magnitude in all of the three fluctuation components.

$$\begin{aligned}
 \eta_{v2} &= k_{v1r} = k_{t\rho} = k \\
 k_{tv} &= k k_{tv}^{opt}(\beta, \Delta \rho_{lg}) \\
 k &\in [0, 1]
 \end{aligned} \tag{40}$$

The smallest value for k that maintains the model system hyperbolic was calculated and the results are presented in Fig. 2. Clearly, the permitted minimum value for k increases with increasing pressure, which can be interpreted that the chaotic nature of the flow tends to increase with more uniform density.

We derived a fitting for k that guarantees the hyperbolicity of the model and follows the information presented in Fig. 2.

$$\begin{aligned}
 k &\approx \frac{A}{\Delta \rho_{lg}} + B \\
 A &\approx 233.464 \text{ kg/m}^3, \quad B \approx 0.116, \\
 \Delta \rho_{lg} &> 430 \text{ kg/m}^3 \quad (p < 17.5 \text{ MPa})
 \end{aligned} \tag{41}$$

4.3.7 Formulation of friction terms

High quality experimental data on interfacial friction exists in the form of many void fraction correlations. These correlations behave generally well in versatile flow conditions. By utilizing the

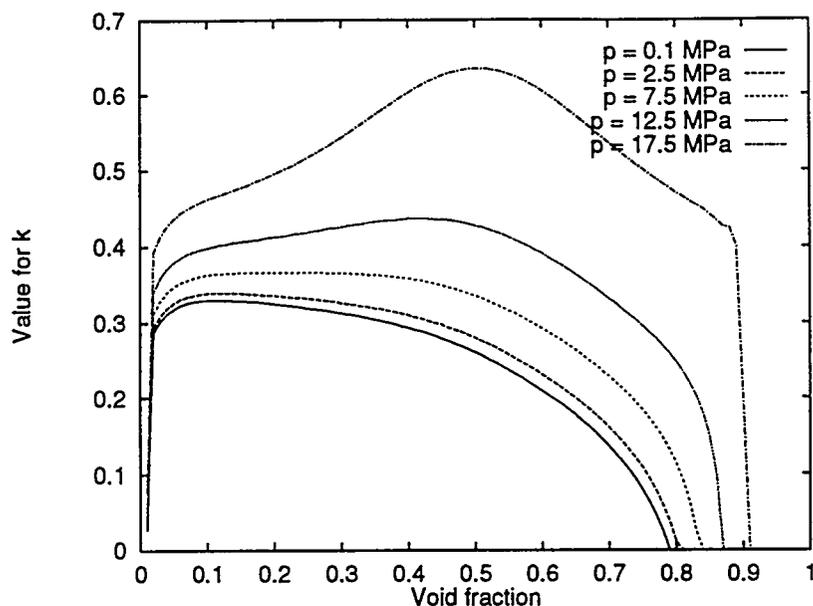


Figure 2: The smallest value for the parameter k as a function of void fraction and pressure that makes the model system hyperbolic.

relationship between void fraction and interfacial friction that exists for steady, fully developed flow conditions, the correlations can be converted into effective interfacial friction coefficients.

In our model, wall friction is modeled with two distinct terms corresponding to the wall friction caused by each subflow, instead of using one term for total wall friction. This approach has the potential to include more specific effects of two-phase flow into model, such as in the case of peaked void fraction distribution near the channel wall. Of course, to do this reliably requires values for two separate wall friction coefficients.

The wall friction coefficients could be approximated by equating the sum of the wall frictions caused by the subflows, Eq. (26) with a known correlation for total wall friction. Of course, this is a possible approach only in the flow conditions in which the chosen correlation is reliable (usually in cocurrent flow), and some other means like interpolation should be used elsewhere.

By these means the uncertainty in the friction model can be reduced to that present in the best available void fraction and wall friction data.

In principle, any available correlation for two-phase flow velocity coupling and wall friction can be used to convert into friction coefficients suitable for the SFAV-model. Our approach to calculate the friction coefficients has been formulated by maintaining the generality such that the correlations on which the calculation is based, can be easily changed. Thus the correlations used in this study serve as one example of many possible choices.

In this work we have used Chexal-Lellouche drift-flux correlation (EPRI) [11] to obtain steady-state information, Baroczy-Chisholm correlation for two-phase wall friction coefficient [12] and McAdams and Blasius relations for one-phase wall friction coefficient [13].

In the correlations for the wall friction coefficients used in this study, the total wall friction term is written in the form

$$F = \frac{1}{2} \frac{A}{D_h} \xi \phi^2 \frac{G|G|}{\rho_l} \quad (42)$$

where ξ is the one-phase wall friction coefficient, ϕ^2 is the two-phase wall friction coefficient and G is the mass flux.

We begin the derivation of equations for calculating the friction coefficients by applying the momentum equations for the subflows, MO_k , to steady, fully developed flow, in which the momentum flux terms will vanish. The same is done with the mass equations for the subflows, M_k , and the results are combined to eliminate the pressure gradient and thus the following momentum difference equation is formed.

$$\frac{F_1}{\beta} - \frac{F_2}{1-\beta} - v_i \frac{S_{12}}{\beta(1-\beta)} + \frac{S_{m12}}{\beta(1-\beta)} + A(S_{mz_2} - S_{mz_1}) = 0 \quad (43)$$

This is simply the momentum difference equation $DMO = 0$, in Eqs. (18), in steady-state condition. The approach is analogous to that used in the interfacial friction model for the PWR safety code RELAP/MOD3 [14].

Eq. (43) can be simplified in the form

$$DMO_{steady} = \xi_1 \rho_1 v_1 |v_1| - \xi_2 \rho_2 v_2 |v_2| + \xi_{12} \Delta \rho_{21} v_r |v_r| - 2D_h \Delta \rho_{21} g \cos \theta = 0 \quad (44)$$

where explicit forms for the friction and interaction terms have been inserted from Eq. (26).

Eq. (44) shows that, under steady state conditions, the interfacial friction force, the forces originating in the wall friction and the buoyancy forces must balance each other. Then the velocities of the subflows can be calculated from a drift-flux correlation by defining

$$\begin{aligned} v_1 &= C_0^{SFAV} j + V_{gj}^{SFAV} \\ v_2 &= \frac{1 - \beta C_0^{SFAV}}{1 - \beta} j - \frac{\beta}{1 - \beta} V_{gj}^{SFAV} \\ v_r = v_1 - v_2 &= \frac{C_0^{SFAV} - 1}{1 - \beta} j + \frac{1}{1 - \beta} V_{gj}^{SFAV} \end{aligned} \quad (45)$$

The relations between C_0^{SFAV} and V_{gj}^{SFAV} and the drift-flux parameters C_0 and V_{gj} are

$$\begin{aligned} C_0^{SFAV} &= 1 + k \frac{1 - \beta}{1 - \alpha} (C_0 - 1) \\ V_{gj}^{SFAV} &= k \frac{1 - \beta}{1 - \alpha} V_{gj} \\ k &= \frac{\alpha(1 - \alpha) \Delta \rho_{lg}}{\beta(1 - \beta) \Delta \rho_{21} - \left[\beta \left(\frac{L}{v_r} \right) + (1 - \beta) \left(\frac{L_2}{v_r} \right) \right]} \end{aligned} \quad (46)$$

Notice that f_1/v_r and f_2/v_r in the expression for k do not depend on velocity and thus the expression is in explicit form. Eqs. (45) and (46) can be used to eliminate the velocities from Eq. (44) which then leads to a relationship between the friction coefficients and drift-flux parameters.

The obtained equation contains terms with zero to second order explicit dependency on volumetric flux j . By assuming that each term class cancel to zero, three equations for the friction coefficients are obtained. In this procedure we assume that the coefficients do not depend on j , which is justified because the explicit velocity factors in the friction terms should carry most of the velocity dependency. In principle, the friction coefficients could be solved by this means using only the information given by the used drift-flux correlation. However, the assumption of the friction coefficients being totally independent on j may not be relevant in high velocities, where the equation $DMO_{steady} = 0$, Eq. (44), could be violated.

The available information about total wall friction is also utilized by equating the sum of wall friction terms for the subflows with the total wall friction term given by a chosen correlation, viz.

$$F_1 + F_2 = F \Leftrightarrow DF = \xi_1 \beta \rho_1 v_1 |v_1| + \xi_2 (1 - \beta) \rho_2 v_2 |v_2| - \xi \phi^2 \frac{G|G|}{\rho_l} = 0 \quad (47)$$

The mass flux G can be written in the form

$$G = \rho j - \left\{ \beta (1 - \beta) \Delta \rho_{21} - \left[\beta \left(\frac{f_1}{v_r} \right) + (1 - \beta) \left(\frac{f_2}{v_r} \right) \right] \right\} v_r \quad (48)$$

Terms F_1 and F_2 in Eq. (47) can also be written in terms of j and v_r , after which there appears only j^2 -, jv_r - and v_r^2 -dependent terms. By assuming that the wall friction coefficients are independent on velocity, each term class can be equated, which produces three equations for the two unknown wall friction coefficients, ξ_1 and ξ_2 . This assumption may not be globally justified because of probable violation of the original equation $F_1 + F_2 = F$, Eq. (47), in some conditions.

The following error functional that takes into account all the criteria described above is formed from which the friction coefficients can be solved by minimization

$$\begin{aligned} \mathcal{J} = \frac{1}{GRAV^2} \left[\frac{1}{3} w(j) \left(DMO_{steady}^2 |_{const} + \frac{DMO_{steady}^2 |_j}{j} + \frac{DMO_{steady}^2 |_{j^2}}{j^2} \right) \right. \\ \left. + (1 - w(j)) DMO_{steady}^2 \right] + \\ + \frac{1}{3} \frac{w(j)}{F_{norm}} \left(\frac{DF^2 |_{j^2}}{j^2} + \frac{DF^2 |_{jv_r}}{jv_r} + \frac{DF^2 |_{v_r^2}}{v_r^2} \right) + (1 - w(j)) \left(\frac{F_1 + F_2 - F}{F} \right)^2 \end{aligned} \quad (49)$$

where $GRAV = 2D_h \Delta \rho_{21} g \cos \theta$, $F_{norm} = \xi \phi^2 \rho^2 / \rho_l$, $|_x$ refers to explicitly x -dependent terms of the corresponding expression and DMO_{steady} and DF have been defined in Eqs. (44) and (47). The functional has been carefully normalized not to allow any solitary term dominate and thus to make a reliable general criterion for the friction coefficients. In addition, $w(j)$ is to weight Eqs. (44) and (47) more in high velocities and, correspondingly, the equations obtained by equating different term classes more in low velocities. For $w(j)$ we have used the form

$$w(j) = \exp \left[-\frac{1}{2} \left(\frac{j}{\sigma} \right)^2 \right] \quad (50)$$

where $\sigma = 1$ m/s. This means that in low velocities the friction coefficients are tried to keep as independent on velocity as possible while in higher velocities the velocity-dependency is let to be greater such that Eqs. (44) and (47) hold as well as possible.

If the total wall friction term is written in the form of Eq. (42) then the friction coefficients should be calculated by the minimization of \mathcal{J} only in high enough velocities (clearly cocurrent flow conditions) because elsewhere the bulk mass flux G is not a representative velocity variable. To obtain friction coefficients over the low-velocity region, interpolation can be used as the first guess. As a more elaborate way, information about counter-current flooding data could be taken into account.

Despite of the relative complex appearance of the functional \mathcal{J} , it is numerically simple to minimize, because of its quadratic form in the unknown friction coefficients ($\nabla \mathcal{J} = 0$ makes a linear system). Some extra numerical work is required for making sure that the solved friction coefficients are always nonnegative. Negative friction coefficients would be unphysical because they would mean that energy would be fed to the interface, instead of energy dissipation. However, they can appear

in some conditions because of possible contradictory information given by the chosen correlations. The problem is solved such that if the minimization of \mathcal{J} leads to the negative coefficients (one or more), then they are forced to be nonnegative by minimizing \mathcal{J} also in the boundaries of the feasible region, viz. $\xi_{12} = 0$, $\xi_1 = 0$ or $\xi_2 = 0$.

An example of the calculated friction coefficients is shown in Fig. 3 at pressure 7.0 MPa with the volumetric flux from 1 m/s to 10 m/s and over the whole range of void fraction.

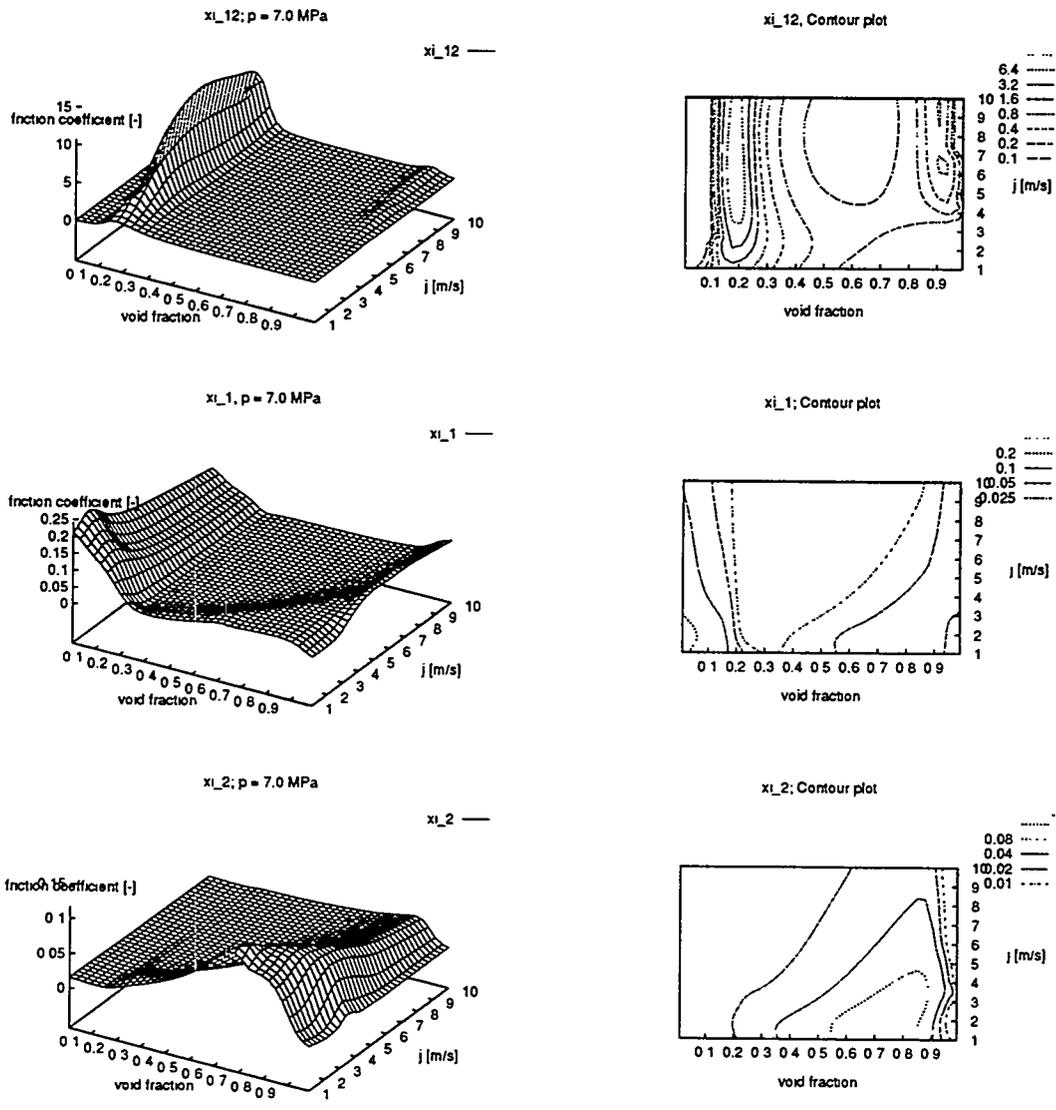


Figure 3: Examples of the calculated friction coefficients for the SFAV-model. :

5 Comparison of the characteristic velocities of the models

In this section, characteristic velocities of the models presented in Sections 3 and 4 are calculated and compared with each other and further to the experimental data.

5.1 Characteristics referring to the pressure disturbances

First, the characteristic velocity referring to the pressure wave speed, or two-phase sonic velocity, was considered. The characteristic velocity of the introduced models was compared with the measurement-based fitting for two-phase sonic velocity derived by Nguyen et. al. in [15].

In Fig. 4, the characteristic sonic velocity calculated from the conventional six-equation model (see Section 3.1) is plotted against the fitting of Nguyen at the pressure of 2.0 MPa. It can be seen that the characteristic velocity of the model is greatly erroneous. The conventional model in which the transverse velocity distribution has been taken into account (introduced in Section 3.2) produces virtually no changes in the sonic characteristics.

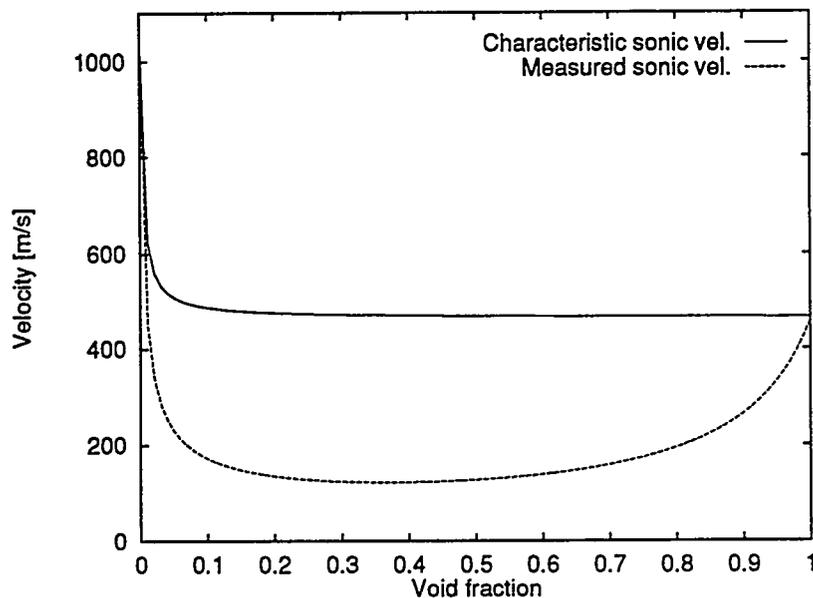


Figure 4: The characteristic sonic velocity calculated from the conventional six-equation model compared with the measurement-based two-phase sonic velocity at pressure of 2.0 MPa.

The effect of the different virtual mass types and of the SFAV-model on the sonic characteristics of the system is visualized by plotting the relative error in the characteristic sonic velocity compared with the measurement-based fitting mentioned above. The error was calculated over the void fraction - pressure region of $[0, 1] \times [0.1, 2.0]$ MPa and averaged over the pressure. Thus, average relative error in the sonic characteristics in the studied pressure region and as a function of void fraction was achieved. The following forms for the virtual mass were used:

- *VM Ia*: Eqs. (7), (8) and (9).
- *VM Ib*: Eqs. (7), (8), (10) and (11), used in the CATHARE code.
- *VM IIa*: Eqs. (7) and (12).

- *VM IIb*: Eqs. (7), (10) and (12), used in the codes TRAC-PF1 and RELAP5/MOD2.

The results are presented in Fig. 5. It can be seen that all the virtual mass forms studied here predict the two-phase sonic velocity very well, keeping in mind that the conventional model produced errors of several hundred percents. In addition, the sonic characteristics of the SFAV-model is in the same order of accordance with the measurement-based fitting as the virtual mass models.

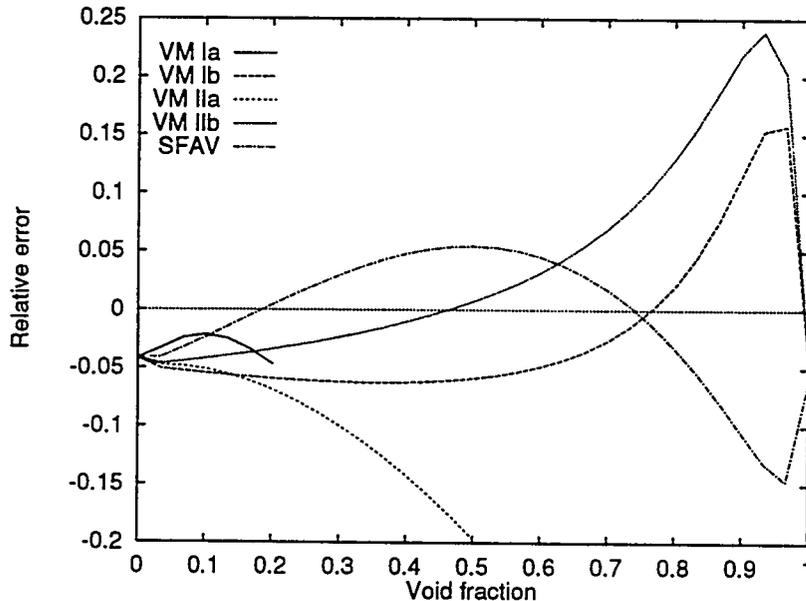


Figure 5: Relative error in the sonic characteristics of the studied virtual mass models and the SFAV-model averaged over the pressure region [0.1, 2.0] MPa.

5.2 Characteristics referring to the enthalpy disturbances

In the subsonic two-phase flow, enthalpy does not influence the other characteristics. The enthalpy disturbances propagate with the phase velocities and thus, two of the characteristic velocities should equal to v_g and v_l . This holds for all of the models considered in this study and therefore we do not consider these characteristics any further.

5.3 Characteristics referring to the void fraction disturbances

To study the validity of the characteristic velocities of the models further, the data of C. Pauchon and S. Banerjee on void disturbance propagation was used [16, 17]. We studied if the faster of the two characteristics void velocities could predict the experimental data. The data contained four series in which the liquid superficial velocity j_l is constant and the gas superficial velocity j_g is varying. The results are presented in Fig. 6.

The virtual masses *Type Ia* and *Ib* could not make the system hyperbolic in the conditions of the experiments. This is obviously because those forms of virtual masses were derived to get as good agreement as possible with the sonic characteristics only. It was surprising that the *Type Ib*, used in the CATHARE code with the term shown in Eq. (11) that was particularly derived in order to make the system hyperbolic, did not do that. However, as can be seen from Fig. 6, the real parts

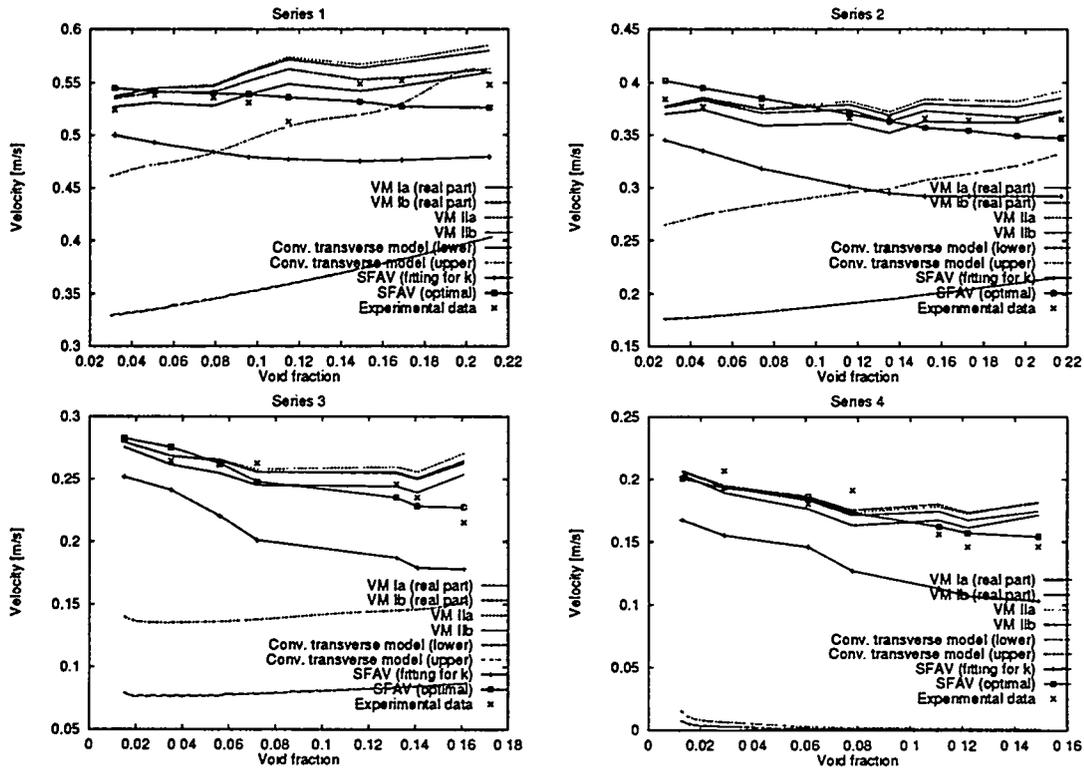


Figure 6: Calculated void fraction disturbance propagation velocities using the conventional model taking into account the transverse velocity distribution (Section 3.2), the different virtual mass models (Section 3.3) and the SFAV-model (Section 4). Comparison has been made with experimental data [16, 17]. The results of the conventional model with transverse velocity distribution describe the interval over which the characteristic velocity can be predicted. The results of the SFAV-model have been calculated with the suggested fitting for parameter k , presented in Eq. (41), and with the optimal constant value for k in each measurement series.

of the void characteristics are very well in accordance with the measurements in all of the series and with all the virtual mass types tested here.

The conventional model in which the transverse phase velocity distribution had been taken into account, formed a hyperbolic system in the used conditions. Of the two calculated values for the void propagation velocity the lower one is obtained by giving the parameter η_{vl} (see Eqs. (5) and (6)) such value that the two characteristic velocities, referring to void disturbance propagation, equal to each other and the higher value is correspondingly obtained with such value of η_{vl} that the lower characteristic velocity approaches to zero. Thus these two values represent the limits of the void propagation disturbance velocity that can be predicted with the model.

It can be clearly seen from the results that this model cannot predict the void propagation velocity well. Particularly, when the liquid superficial velocity j_l becomes smaller (it is smallest in 4th series) the error increases relatively much.

In the results, there are two different cases calculated with the SFAV-model. First, the suggested expressions for the SFAV-parameters meant for the pressure region of [0.1, 17.5] MPa (see Section 4.3.6), were used. The corresponding results are only fairly well in agreement with the experimental data. The measurements were performed at atmospheric pressure, which probably causes the main reason for this, i.e. the suggested fittings for the SFAV-parameters were derived with reference to higher pressure regions and the behavior near the borders of the validity-range is not predicted with the same level of accuracy.

Further results for the SFAV-model were achieved when the value for the SFAV-parameter k (see Eq. (40)) that gives the best agreement with each measurement series, was searched. This was to test if the degrees of freedom of the SFAV-model were enough to tune model to agree with the reality. This was easily done with systematically a bit greater value for k in each series than the value given by the fittings suggested in Section 4.3.6. In principle, very complicated correlations for the SFAV-parameters could be tried to derive that would hold in versatile flow conditions but the knowledge and experimental data about two-phase flow small-scale phenomena is currently not detailed enough to enable doing it in practice.

6 Comparison of SFAV and drift-flux model in steady-state and transient conditions

In this section, the results of calculated cases with the SFAV-model and corresponding drift-flux model are presented. The formulation of the cases was kept relatively simple in order to make it possible to observe fundamental phenomena the models predict, and thus not the ones caused by possible complicated source terms of the complete models, like e.g. the correlations for heat transfer.

The used geometry was a part of a BWR fuel channel between two spacers and no heating was assumed. This enabled omitting the energy equations from the calculation, which also resulted in simpler and faster numerics. The geometric dimensions used were from 9×9 rod bundle: $D_h = 4A/P_w = 0.01282$ m, $\Delta h_{spacer} = 0.568$ m.

The used partial differential equations in the SFAV-model were (see Eqs. (18) and (19))

$$\begin{aligned} M_g &= 0 \\ M_l &= 0 \\ DMO &= 0 \\ MO_1 + MO_2 &= 0 \end{aligned} \tag{51}$$

The corresponding drift-flux model was obtained simply by replacing the equation $DMO = 0$ with the drift-flux correlation.

The model system, Eq. (51), was solved with the CFDPLIM code, which has been shown to be capable of solving hyperbolic systems with great accuracy and without numerical diffusion [18, 19, 20, 21].

Two different cases were calculated: searching of a steady-state distribution of the system from different initial states and response of the SFAV and drift-flux model to a sine-wave disturbance in the water inlet flux with different frequencies.

6.1 Searching of steady-state distributions

As the first test case for the friction model, the steady-state distributions along the channel followed from different initial values for the velocity difference v_r , were calculated. The results were compared with the steady-state predicted by the drift-flux correlation.

The task was formulated with Eqs. (51) and with the initial and boundary conditions

$$\begin{aligned}
 u(0, z) &= u_0(z) \\
 \beta(t, 0) &= \beta_0 \\
 v_r(t, 0) &= v_{r0} \\
 j(t, 0) &= j_0 \\
 p(t, L) &= p_L
 \end{aligned}
 \tag{52}$$

where $u(t, z)$ is the vector of the unknown variables, $u(t, z) = (\beta \ v_r \ j \ p)^T$. The initial distribution was $u(0, z) = (0.4, v_{r0}, 4.0 \text{ m/s}, 7.0 \text{ MPa})^T$ and the boundary values corresponded to the initial values.

The steady state distribution was calculated with four different values for v_{r0} and the results are presented in Figs. 7 and 8. In the ideal case, the relaxed values for β (equal to the void fraction; see Eq. (21)) and v_r in the end of the channel, should equal to the values given by the drift-flux correlation.

From the results, spatial transients for β and v_r in the beginning of the channel can be noticed from which the relaxation length can be seen to be approximately 0.10 m. With the used value for j (4.0 m/s) this corresponds to time constant $\tau \approx 0.02$ s. The corresponding drift-flux model cannot predict any spatial transient. Hence, the scale of errors caused by the drift-flux model can be estimated by considering the size of the transient.

In Fig. 8, the relaxed values of v_r in the end of the channel are very well in agreement with the value given by the drift-flux correlation, which means that the minimization of the functional \mathcal{J} in Eq. (49) for the friction coefficients has been successful.

6.2 Frequency response of inlet water volumetric flux disturbance

To study the dynamic behavior of the SFAV-model, a sine-wave disturbance on the inlet water volumetric flux was introduced and the results were compared to those given by the corresponding drift-flux model. This kind of situation could happen in practice e.g. with feed-water pump partial damage or blockage in the fuel channel with such natural frequency that the cases studied here would apply.

The task was formulated with the same conservation equations as in the case of the steady-state distribution calculation, Eq. (26), and the initial and boundary conditions were

$$u(0, z) = u_0(z)$$

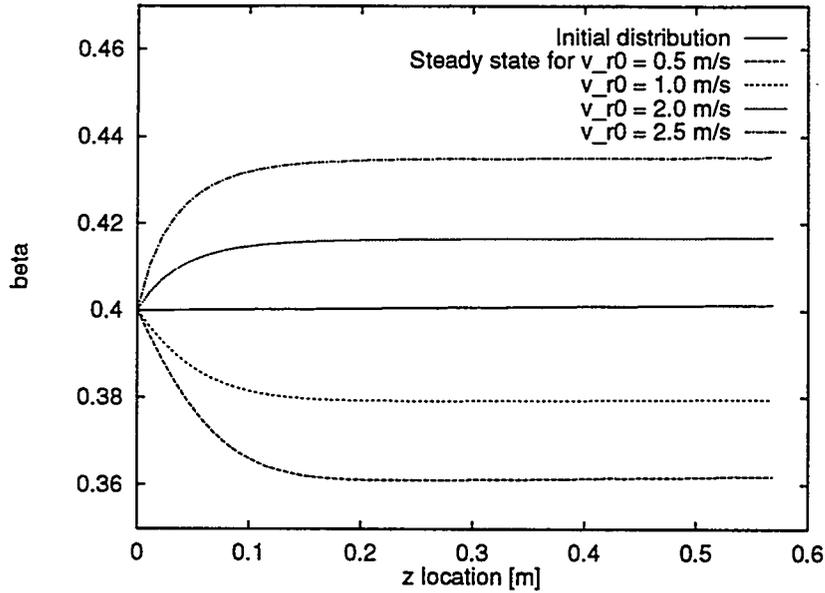


Figure 7: The initial distribution of β and calculated steady state distributions for different v_{r0} 's.

$$\begin{aligned}
 j_g(t, 0) &= j_{g0} \\
 v_r(t, 0) &= v_r^{drift-flux}(\alpha(t, 0), j(t, 0), p(t, 0)) \\
 j(t, 0) &= j_0 + \Delta j_0 \sin(2\pi ft) \\
 p(t, L) &= p_L
 \end{aligned} \tag{53}$$

where $j_0 = 4.0$ m/s, amplitude $\Delta j_0 = 0.1$ m/s, $\alpha(t, 0) = 0.4$, $v_r^{drift-flux}$ means the value given by the drift-flux correlation and the gas superficial velocity j_g is fixed via the relations $j_g = \alpha[j + (1 - \alpha)\Delta v_{gl}]$ and $v_r = k\Delta v_{gl}$, where the multiplier k is from Eq. (46). The initial distribution $u_0(z)$ was set according to corresponding steady-state distribution. The initial and boundary conditions were chosen such that the situation would be possible to construct and study also experimentally.

The calculation was performed with total of 5 different values for the inlet frequency f , namely 1 Hz, 5 Hz, 15 Hz, 25 Hz and 35 Hz. The results are shown in Figs. 9–13.

The results of the drift-flux model can be seen to differ from those of the SFAV-model already with 5 Hz frequency, while the time constant for the relaxation of β and v_r , $\tau \approx 0.02$ s (from Section 6.1), would have implied significant differences appear with frequencies as high as of order 50 Hz.

From the results of the SFAV-model, it can be noticed that voidage waves are formed that propagate through the whole channel with growing amplitude. The grow factor of the amplitude through the channel was found to depend on the frequency such that

$$C_{grow} \approx 1.00 + 0.10 (f/\text{Hz})^{1.50} \tag{54}$$

On the other hand, with the drift-flux model, the amplitude of the voidage waves stays constant which is a nice feature from the point of view of numerical solving of the system. However, the behavior is probably unphysical. Namely, shaking is used as a separation method for some kind

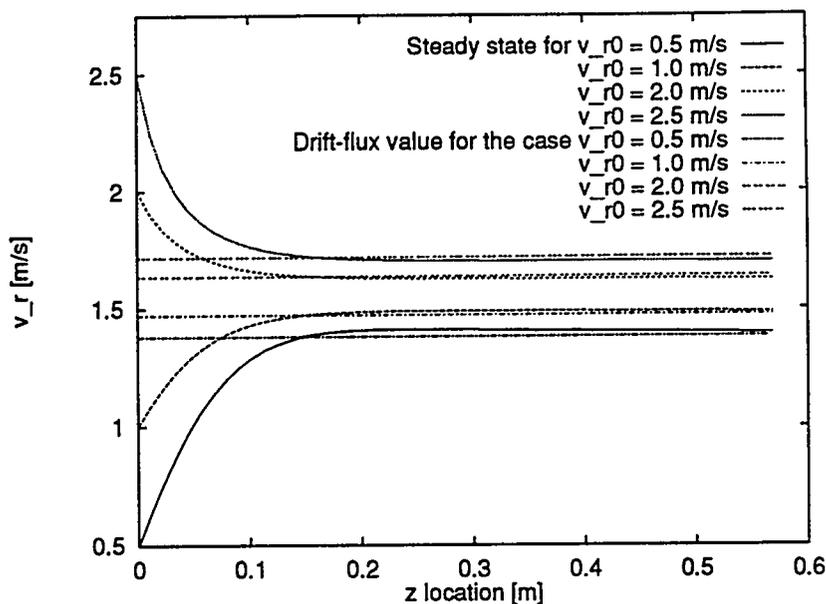


Figure 8: The calculated steady state distributions of v_r for different v_{r0} 's. The initial distributions were $v_r(0, z) = v_{r0}$ in each case.

of mixtures in chemical industry and the situations simulated here, especially the cases with high frequencies, correspond to one kind of shaking. In very high frequencies or in a long enough channel, the growing voidage waves would eventually end in totally separated slugs of liquid and gas if no change in geometrical or boundary conditions that would prevent the growing (like spacers) are faced.

Some of the distortions in the results were probably due to the disturbances that move with different velocities while some may have caused by the numerical scheme used. With growing frequency, the convergence was more difficult to achieve and thus the distortions due to the solution algorithm became unavoidably larger.

7 Conclusions

In this paper, the following forms of one-dimensional two-phase flow models have been considered: the conventional model in which the flow is separated into two subflows according to the phases, the conventional model equipped with terms taking into account nonuniform transverse velocity distribution within the phases, the conventional model equipped with different forms of virtual mass terms and the model in which the momentum equations are derived over two velocity fields, instead of the domains occupied by the phases. We abbreviated the last mentioned model as SFAV because the main idea in the model is Separation of the Flow According to Velocity.

Four different forms of virtual mass were studied, of which one is used in the thermal hydraulic code TRAC-PF1 and one in the codes RELAP5/MOD2 and CATHARE. Some of the virtual mass types have been derived in order to get a reasonable agreement between characteristic and measurement-based two-phase sonic velocity.

To test the dynamics of the models, the characteristic velocities of the models that can be

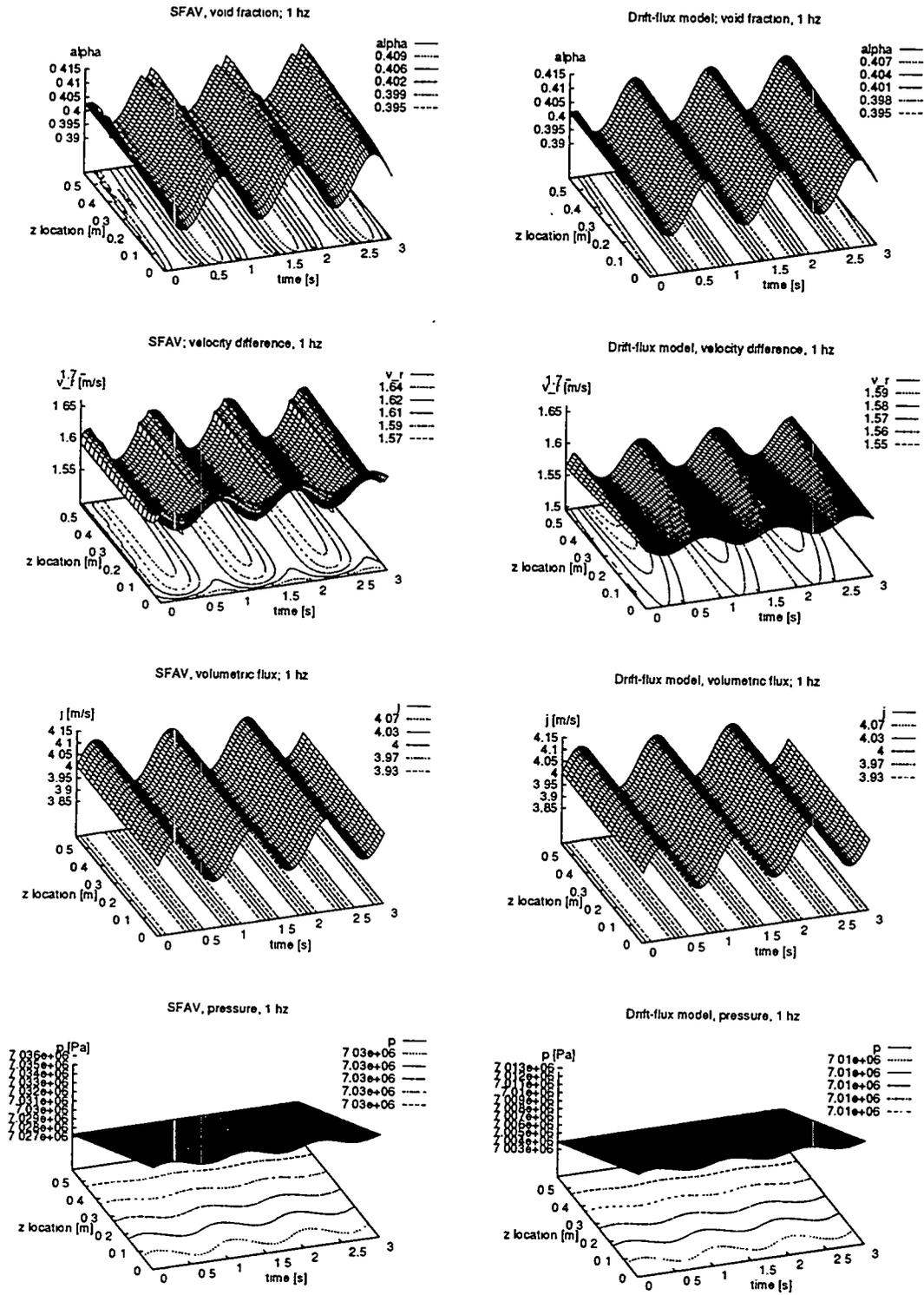


Figure 9: Response of the SFAV-model and the drift-flux model on the 1 Hz sine-wave disturbance in inlet water volumetric flux.

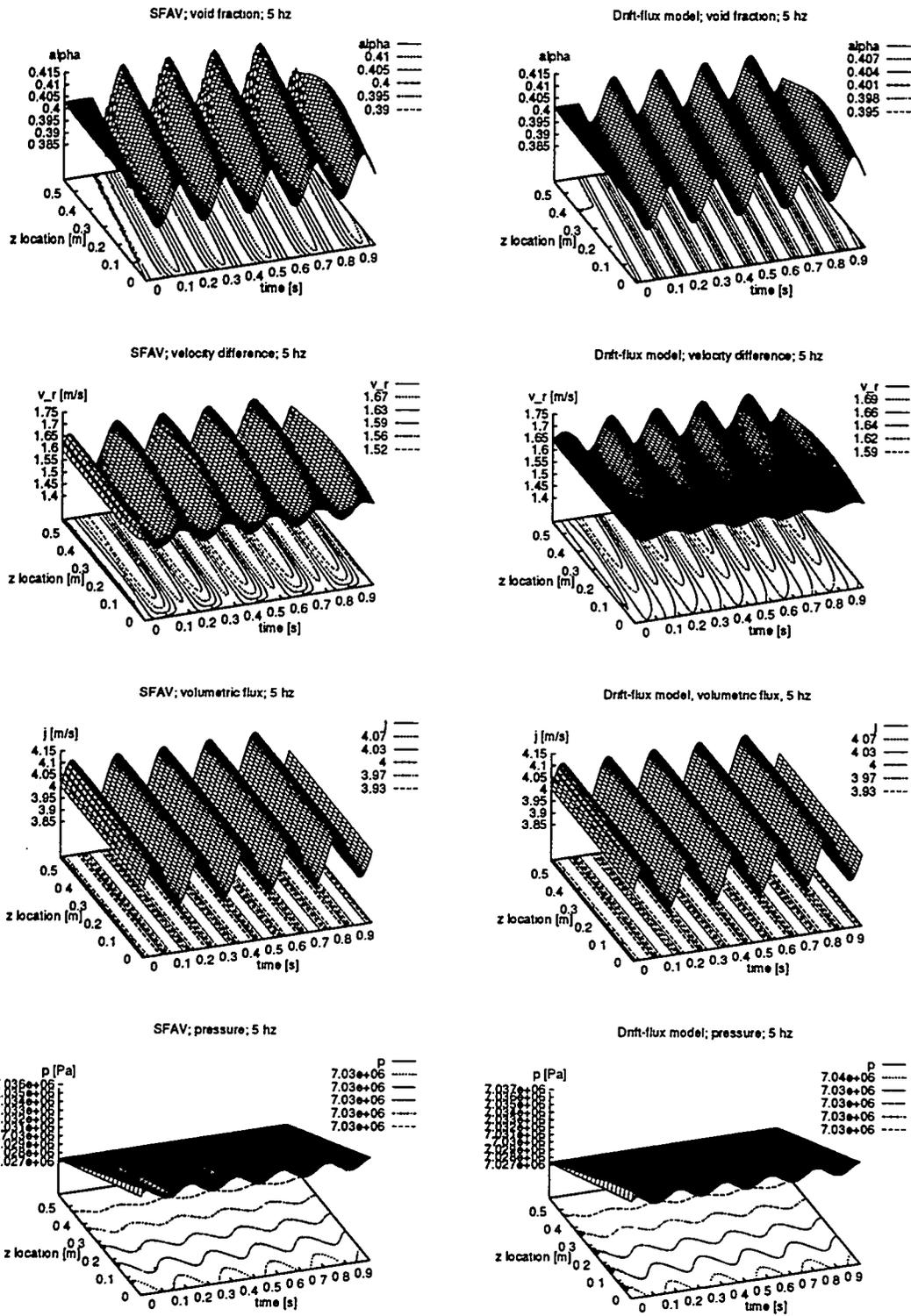


Figure 10: Response of the SFAV-model and the drift-flux model on the 5 Hz sine-wave disturbance in inlet water volumetric flux.

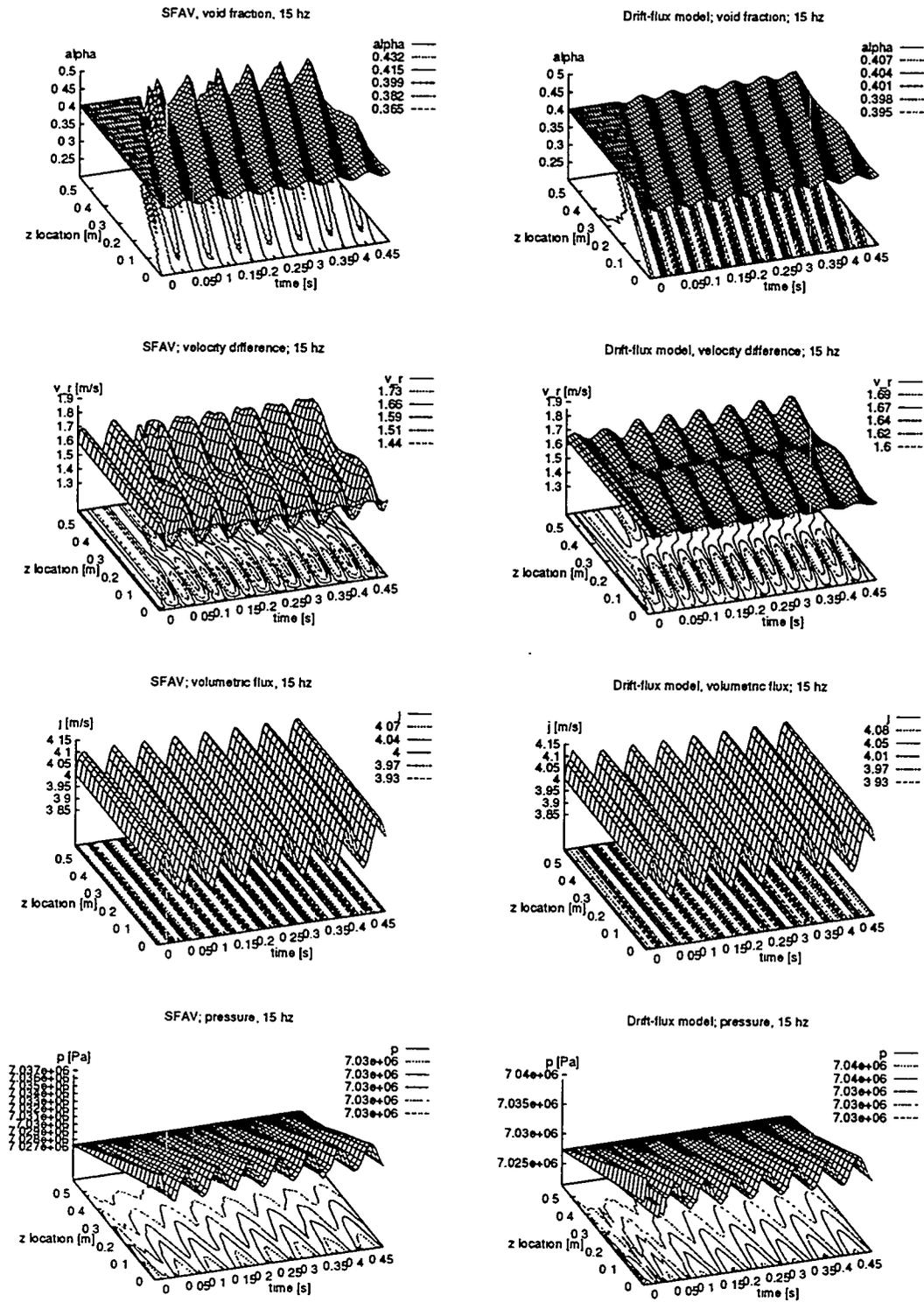


Figure 11: Response of the SFAV-model and the drift-flux model on the 15 Hz sine-wave disturbance in inlet water volumetric flux.

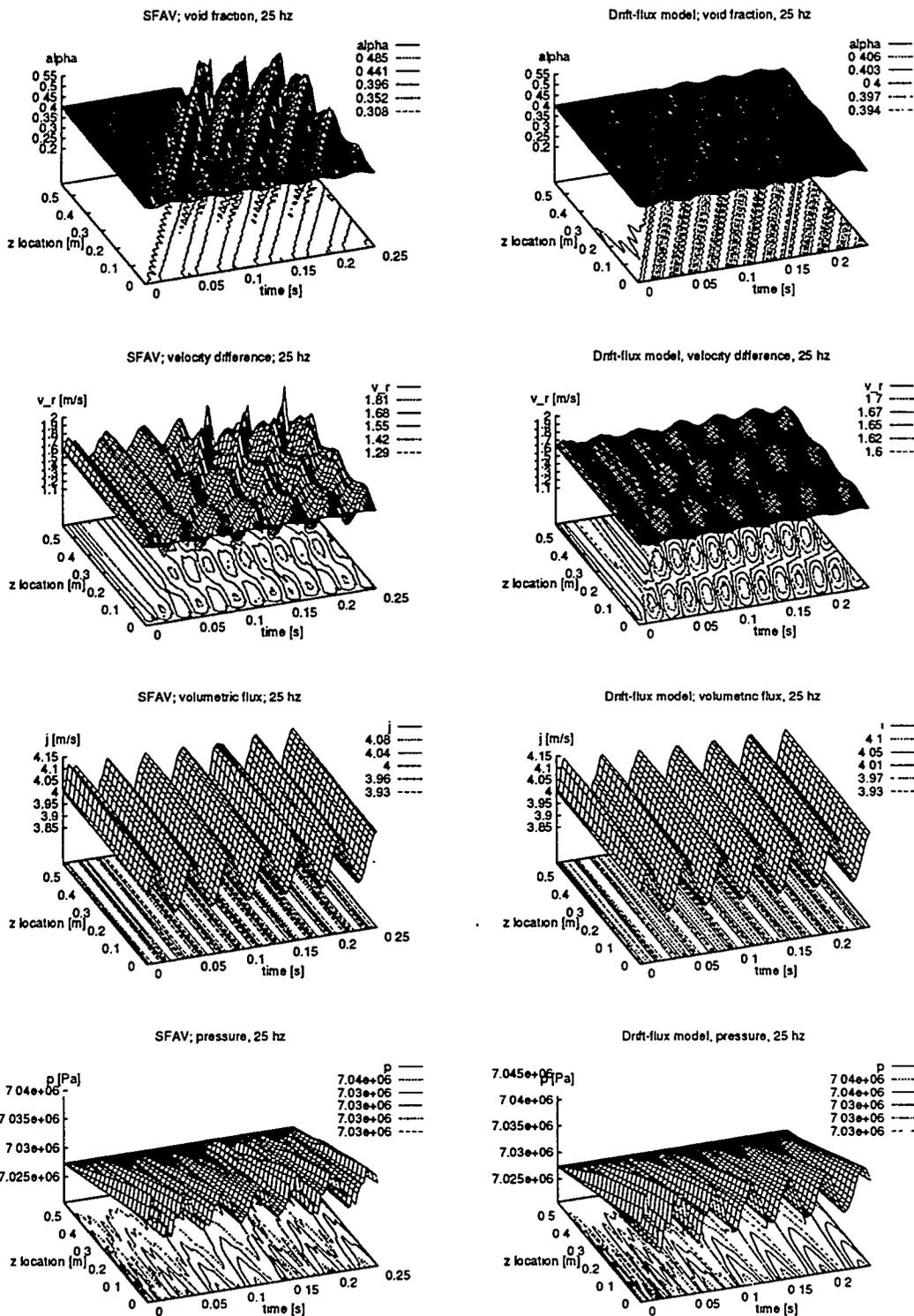


Figure 12: Response of the SFAV-model and the drift-flux model on the 25 Hz sine-wave disturbance in inlet water volumetric flux.

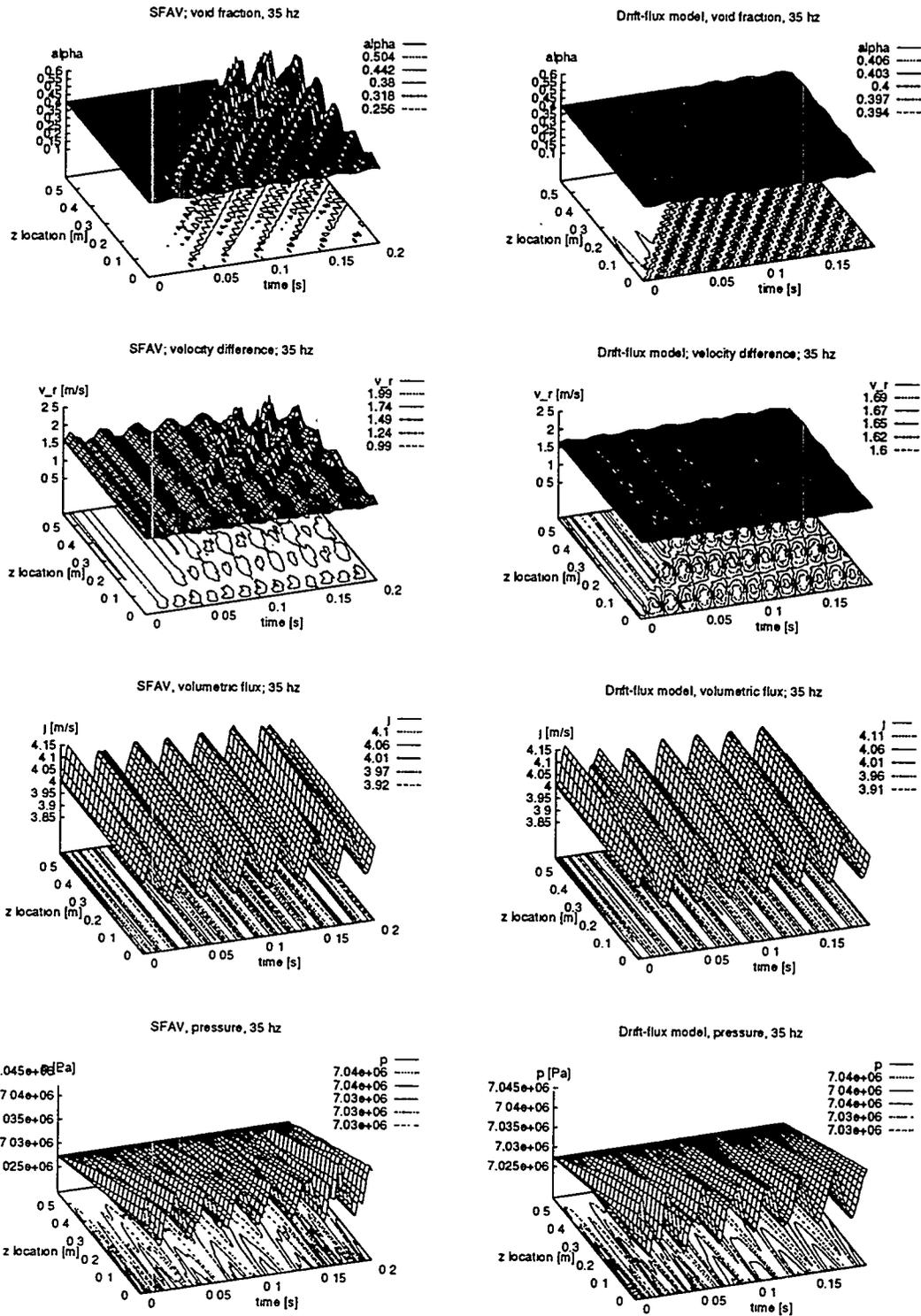


Figure 13: Response of the SFAV-model and the drift-flux model on the 35 Hz sine-wave disturbance in inlet water volumetric flux.

associated with the propagation velocities of small disturbances, were compared with each other and further against experimental data on void wave and pressure wave propagation speeds.

The void wave speed predicted by the conventional six-equation model is complex, which makes it impossible to solve the system by any advanced method that takes advantage of the characteristics. The conventional model in which the transverse velocity distribution information has been included, makes a substantial difference: the void wave characteristics are real but they still differ from experimental data too much to be used in practical applications. The virtual mass models predicted the void wave speed very well in accordance with the measurements, except that some virtual mass forms did not produce real void wave characteristics at all. Derivation of the virtual masses was directed mainly for bubbly flow regime and then extended over the whole range of void fraction by introducing new correction factors, which inevitably makes the process somewhat vague. The void wave speed predicted by the SFAV-model had the same order of agreement with the measurements as the best virtual mass models tested here. In addition, the characteristics referring to void wave propagation, are always real in the SFAV-model and thus the model makes a hyperbolic system.

The results obtained in comparing the measurement-based curve on two-phase flow sonic velocity with the pressure wave characteristics of the models were qualitatively much like in the comparison of void wave speeds, described above. Namely, the conventional model produced several hundreds of percents error at worst, the model with the transverse velocity distribution made no difference to that, the virtual mass models gave very good results and the SFAV-model gave even substantially better agreement.

In the SFAV-model, only the momentum equations differ from the conventional six-equation model, which enables to use existing correlations directly for all the source terms appearing in the mass and energy equations. The modeling of interfacial and wall friction unavoidably differs from the conventional approach. The friction is modeled with two independent terms for wall friction caused by each of two subflows and with one term for turbulent interfacial friction. The model is based on a set of existing correlations, namely for two-phase flow velocity coupling (drift-flux or slip correlations) and for wall friction factors. By utilizing the relationship between void fraction and interfacial friction that exists for fully developed flow conditions, the correlations are converted into effective friction coefficients.

The new friction model has been tested in the geometry of a BWR-fuel channel between two spacers with the following cases:

- Searching the steady-state distributions from different initial conditions and comparing the relaxed values of void fraction and the velocity difference between the subflows to the drift-flux correlation.
- Simulating the flow with a sine-wave disturbance in the water inlet flux with different frequencies and comparing the results to the drift-flux model.

In the steady-state distribution calculations, the relaxed values for void fraction and the velocity difference between the subflows agreed very well with the drift-flux correlation. The time constant for the relaxation was $\tau \approx 0.02$ s. For the frequencies used in the sine-wave disturbance calculation, $\tau f < 1$, and thus the derived model for the friction coefficients that was based on the steady-state conditions, should have been a valid approximation. According to the results of the SFAV-model, the voidage waves grow in amplitude and would eventually end, in unchanging geometric and boundary conditions, in total separation between liquid and gas, which should also be the case in reality. Namely, the situation corresponds to one kind of shaking which can be used as a separation method for suitable mixtures. However, with small frequencies of order 1 Hz, the grow factor through the channel was close to unity and increased from that with increasing frequency

such that the change was proportional to $(f/1\text{Hz})^{1.50}$. The cases were recalculated with the drift-flux model which predicted no growing of the voidage waves. In addition to the spatial transient in the beginning of the channel predicted by the SFAV-model, differences in the results between the models began to be seen with the frequencies of order 5 Hz. Thus noticeable differences appeared already with a decade smaller frequencies than the time constant estimated from the steady-state calculation would have implied.

Nomenclature

A	square matrix in Eq. (1)
A	cross-sectional area of the flow channel
a_{vm}	virtual mass acceleration
B	square matrix in Eq. (1)
\vec{C}	vector in Eq. (1)
c	two-phase sonic velocity
C_0	drift-flux distribution parameter
C_0^{SFAV}	drift-flux distribution parameter for SFAV-variables
C_{vm}	virtual mass coefficient
$D(\zeta; \eta)$	function describing transverse distribution of velocity or density
DF	wall friction difference equation, Eq. (47)
D_h	hydraulic diameter of the flow channel
DMO	momentum difference equation of the SFAV-model
DMO_{steady}	DMO -equation in steady state
E	energy conservation equation
F	frictional drag, $[\text{kgm/s} \times 1/\text{ms}]$
f	$\langle \delta \rho \delta v \rangle$; frequency
F_{norm}	$\xi \phi^2 \rho^2 / \rho_l$
F_{vm}	virtual mass force
G	mass flux, $[\text{kg}/(\text{m}^2 \text{ s})]$
g	$\langle \rho \delta v^2 \rangle$; acceleration of gravity
$GRAV$	$2D_h \Delta \rho_2 g \cos \theta$
h	specific enthalpy
\mathcal{J}	functional for friction coefficients to be minimized
j	volumetric flux, $j = \alpha v_g + (1 - \alpha)v_l = \beta v_1 + (1 - \beta)v_2$, $[\text{m/s}]$
j_g	gas superficial velocity, $j_g = \alpha v_g$
j_l	liquid superficial velocity, $j_l = (1 - \alpha)v_l$
k	parameter (Section 4.3.6); abbreviation for the multiplier in the relation $v_r = k \Delta v_{gl}$ (also in Eq. (46))
$k_{l\rho}$	parameter (Section 4.3.5)
k_{lv}	parameter (Section 4.3.5)
k_{v1r}	parameter (Section 4.3.4)
k_{v2r}	parameter (Section 4.3.4)
M	mass conservation equation
M_{vm}	virtual mass term
MO	momentum conservation equation
p	pressure

P_β	perimeter of the 1st SFAV-subflow in the cross-section
P_w	wetted perimeter
q'''	power into volume unit
q'''_{gl}	volumetric power transfer between the phases
\dot{S}	source term in the mass conservation equation, [kg/m ³ s]
S_{12}	mass transfer between the SFAV-subflows, [kg/ms]
S_{gl}	mass transfer between the phases, [kg/ms]
S_{m12}	momentum transfer between the SFAV-subflows, [kgm/s × 1/ms]
S_{mgl}	momentum transfer between the phases, [kgm/s × 1/ms]
S_{mz}	source term in the momentum conservation equation due to gravity, [N/m ³]
t	time
v	velocity
V_{gj}	drift-flux slip parameter
V_{gj}^{SFAV}	drift-flux slip parameter for the SFAV-variables
v_r	$v_1 - v_2$
$v_r^{drift-flux}$	v_r predicted by drift-flux correlation
$w(j)$	weighting factor in \mathcal{J}
z	space coordinate in the direction of the flow channel

Greek symbols

α	void fraction
β	fraction of the 1st SFAV-subflow of the flow domain
β_1	β
β_2	fraction of the 2nd SFAV-subflow of the flow domain (= 1 - β)
Δ	difference
$\Delta\rho_{21}$	$\rho_2 - \rho_1$
$\Delta\rho_{lg}$	$\rho_l - \rho_g$
Δv_{gl}	$v_g - v_l$
δ	fluctuation
η	parameter referring to steepness of transverse distribution of velocity or density
$\eta_{\rho 1}$	parameter (Section 4.3.3)
$\eta_{\rho 2}$	parameter (Section 4.3.3)
$\eta_{v 1}$	parameter (Section 4.3.3)
$\eta_{v 2}$	parameter (Section 4.3.3)
θ	generalized channel cross-sectional coordinate (for a round pipe e.g. $\theta = (r/R)^2$); angle between vertical direction and the flow channel
μ	exponent in Eq. (21)
ξ	one-phase wall friction coefficient
ξ_1	wall friction coefficient for the 1st SFAV-subflow
ξ_2	wall friction coefficient for the 2nd SFAV-subflow
ξ_{12}	interfacial friction coefficient
ρ	density; average density of total flow, $\rho = \alpha\rho_g + (1 - \alpha)\rho_l = \beta\rho_1 + (1 - \beta)\rho_2$
τ	time constant

ϕ	phase ;
	vector consisting of unknown variables in Eq. (1)
ϕ^2	two-phase wall friction coefficient

Subscripts

1	1st SFAV-subflow
2	2nd SFAV-subflow
21	difference between the SFAV-subflows
<i>c</i>	continuous phase
<i>char</i>	characteristic
<i>d</i>	dispersed phase
<i>g</i>	gas phase
<i>i</i>	interface
<i>k</i>	SFAV-subflow index; $k = 1, 2$
k_2	= 2, if $k = 1$ and vice versa
<i>l</i>	liquid phase
<i>lg</i>	difference between the phases
<i>r</i>	difference between SFAV-subflows
<i>v</i>	velocity
<i>vm</i>	virtual mass
<i>y</i>	transverse direction of the flow channel

Superscripts

(<i>slip</i>)	slip between the phases
(<i>td</i>)	transverse distribution
(<i>turb</i>)	turbulence

Symbols

$\langle \rangle$	statistical average
$X _x$	explicitly x -dependent terms of X

References

- [1] M. Rajamäki and T. Narumo. Six-equation SFAV model for two-phase flow with correct propagating velocities of disturbances. *Int. J. Numerical Heat Transfer, Part B*, **28**:415–436, 1995.
- [2] D. Drew and R.T. Lahey Jr. The virtual mass and lift force on a sphere in rotating and straining inviscid flow. *Int. J. Multiphase Flow*, **13**:113–121, 1987.
- [3] T. Watanabe, M. Hirano, F. Tanabe, and H. Kamo. The effect of the virtual mass force term on the numerical stability and efficiency of system calculations. *Nuclear Engineering and Design*, **120**:181–192, 1990.
- [4] V.H. Ransom and R.J. Wagner. RELAP5/MOD2 code manual volume I: Code structure, system models and solution method. EGG-SAAM-6377, 198.

- [5] D. Bestion. The physical closure laws in the CATHARE code. *Nuclear Engineering and Design*, 124:229-245, 1990.
- [6] D. Drew, L. Cheng, and R.T. Lahey Jr. The analysis of virtual mass effects in two-phase flow. *Int. J. Multiphase Flow*, 5:233-242, 1979.
- [7] A.E. Ruggles et. al. An investigation of the propagation of pressure perturbations in bubbly air/water flows. *J. Heat Transfer*, 110:494-499, 1988.
- [8] M. Saarinen. A dynamic model for horizontal two-phase flow predicting low head flooding. *Int. J. Numerical Heat Transfer, Part A*, 26:471-482, 1994.
- [9] M. Ishii and K. Mishima. Two-fluid model and hydrodynamic constitutive relations. *Nuclear Engineering and Design*, 82:107-126, 1984.
- [10] J.H. Stuhmiller, R.E. Ferguson, and S.S. Wang. Two-phase flow regime modelling. CONF-819307, 3rd specialists meeting on transient two-phase flow, March 1983.
- [11] B. Chexal and G. Lellouche. A full-range drift-flux correlation for vertical flows (revision 1). EPRI NP-3989-SR, September 1986.
- [12] D. Chisholm. Pressure gradients due to friction during the flow of evaporating two-phase mixtures in smooth tubes and channels. *Int. J. Heat Mass Transfer*, 16:347-358, 1976.
- [13] Neil E. Todreas and Mujid S. Kazimi. *Nuclear Systems I: Thermal Hydraulic Fundamentals*; Chapter 11. Hemisphere, 1990.
- [14] J.M. Putney. Development of a new bubbly-slug interfacial friction model for RELAP5. *Nuclear Engineering and Design*, 131:223-240, 1991.
- [15] D.L. Nguyen, E.R.F. Winter, and M. Greiner. Sonic velocity in two-phase systems. *Int. J. Multiphase Flow*, 7:311-320, 1981.
- [16] C. Pauchon and S. Banerjee. Interphase momentum interaction effects in the averaged multifield model, part I: void propagation in bubbly flows. *Int. J. Multiphase Flow*, 12:559-573, 1986.
- [17] C. Pauchon and S. Banerjee. Interphase momentum interaction effects in the averaged multifield model, part II: kinematic waves and interfacial drag in bubbly flows. *Int. J. Multiphase Flow*, 14:253-264, 1988.
- [18] M. Rajamäki and M. Saarinen. Accurate one-dimensional computation of frontal phenomena by PLIM. *Journal of Computational Physics*, 111(1):62-73, 1994.
- [19] M. Saarinen. Computation of horizontal two-phase flow by PLIM. In *Proceedings of Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications*, volume 1, pages 280-291. Karlsruhe, Germany, 1993.
- [20] M. Rajamäki and M. Saarinen. Numerical study of withdrawal and return of water following a volcanic eruption at sea. *Communications in Numerical Methods in Engineering*, 10(6):461-468, 1994.
- [21] M. Rajamäki. Elimination of numerical diffusion in one-phase and two-phase flows. *OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements*, Annapolis, USA, November 5-8 1996.

ADVANCES IN MODELLING OF CONDENSATION PHENOMENA

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ABSTRACT

The physical parameters in the modelling of condensation phenomena in the CANDU reactor system codes are discussed. The experimental programs used for thermal-hydraulic code validation in the Canadian nuclear industry are briefly described. The modelling of vapour generation and in particular condensation plays a key role in modelling of postulated reactor transients. The condensation models adopted in the current state-of-the-art two-fluid CANDU reactor thermal-hydraulic system codes (CATHENA and TUF) are described. As examples of the modelling challenges faced, the simulation of a cold water injection experiment by CATHENA and the simulation of a condensation induced water hammer experiment by TUF are described.

1. INTRODUCTION

The analysis of postulated loss of coolant accident (LOCA) conditions is an important aspect of safety analysis in pressurized water reactors (PWRs). A key reactor analysis component is the effectiveness of the emergency cooling injection (ECI in CANDU reactors) or emergency core cooling (ECC in PWR) system. The core of a CANDU reactor consists of a large number of horizontal fuel channels connected by individual feeder pipes to headers located above the core. The physical parameters governing ECI effectiveness analyses are: channel thermal-hydraulic conditions, convective heat transfer, condensation heat transfer, quench rewet characteristics, phase separation, countercurrent flows in feeder piping, and heat conduction from piping. A key consideration in an ECI effectiveness study in a CANDU is the distribution of the ECI flow between the headers. The ECI flow distribution is governed by the calculation of header pressures which is determined in large part by the condensation rates calculated in loop as a result of direct-contact between cold ECI water and the steam produced by quenching hot fuel and metal primary circuit piping. In addition, condensation induced water hammer is a key concern in the reactor design analysis. Condensation induced water hammer has caused piping ruptures in nuclear power plants, resulting in considerable operation loss.

It has been reported by some analysts that the condensation rate is overestimated in some two-fluid codes (References 1 and 2). A consequence of an overestimated condensation rate in the simulation of a large LOCA is the overestimation of ECI flows and therefore an underestimate of reactor core temperatures since the time period with degraded core cooling is limited. Conversely, a consequence of smaller condensation rates is lower ECI flows and therefore higher core temperatures. Therefore, the modelling of the condensation rate in reactor system codes is important in the analyses of ECI effectiveness.

In state-of-the-art two-fluid thermal-hydraulic codes, interfacial heat transfer and therefore vapour generation or condensation processes are determined through empirical correlations. These correlations have to cover the entire range of system pressures, temperatures and qualities over the entire range of flow regimes. Most two-fluid codes can predict voiding rates with reasonable accuracy. However, the accurate prediction of condensation is more difficult. Refinement in the modelling of condensation is an ongoing task in two-fluid thermal-hydraulic codes. The accurate prediction of condensation rates for the following conditions should be an important consideration in all two-fluid codes: steam generator tube side, bleed condenser and pressurizer, and cold water injection fronts. To validate the condensation model implemented in the reactor system codes, several experiments either involving integral tests or separate effect tests have been conducted in several countries, for example the integral experiment LOFT (Reference 3) in United States and the separated effect CCTF experiment in Japan (Reference 1). Integral tests can provide the overall system behaviour, however the individual effect of condensation on the system behaviour may not be easily distinguished. Separate effect tests can provide more direct information on the physical parameters governing condensation. An example of a separate effect test is the experiment of direct contact condensation of steam on slowly moving water described in Reference 4.

During the past two decades, three major Canadian experimental facilities have been used to study two-phase flow and condensation phenomena: the integral test RD-loops (RD-12, RD-14 and RD-14M) at Whiteshell Laboratories, AECL; the cold water injection test (CWIT) facility, at Stern Laboratories in Hamilton; and the condensation induced water hammer facility at Ontario Hydro Technologies (OHT). The RD-loops and CWIT experiments were jointly supported by AECL and CANDU Owners Group. The RD-loop facilities were constructed to study the key thermal-hydraulic phenomena occurring during LOCA events in CANDU reactors. They consisted of a primary heat transport loop, a pressurizer, a ECI accumulator and a secondary side system. A series of tests for LOCA with and without ECI system have been performed. The CWIT facility was constructed to simulate the cold water injection into a typical channel of CANDU reactors under LOCA conditions. The condensation induced water hammer facility at OHT was designed to examine the induced pressure pulses under various flow conditions and to define the threshold condition between the water hammer and no water hammer regions. A significant amount of condensation related data has been generated in these three facilities that can be used for the validation of CANDU reactor system codes, CATHENA (Reference 5) and TUF (Reference 6) that are briefly described below. Since the RD-loop experiments involve several phenomena and the effect of condensation on the system response can not be directly examined, experiments in this facility will not be discussed in this paper.

The CATHENA code (originally named as ATHENA, developed at AECL Whiteshell Laboratories) is a transient two-fluid code primarily to analyze postulated loss of coolant accident scenarios for CANDU reactors. CATHENA was developed from the RAMA two-fluid code with a different approach in the numerical scheme (a characteristic finite difference scheme with a non-staggered grid is used in RAMA whereas CATHENA uses a non-conservative finite difference scheme with a staggered grid). CATHENA contains modules dealing with thermal-hydraulics (two-fluid model), reactor physics (point kinetics or external coupling with reactor physics codes), heat conduction model (a general package for piping wall, heat exchanger tubes, pressure-calandria tubes and fuel pins), system components (pump, valve, boiler and general tank model which is used in pressurizer, bleed condenser and accumulator), and special models (discharge model, pressure tube strain model, metal-water reaction and level swell). Conservation equations for mass, energy and momentum are solved for each phase (liquid, vapour and non-condensable gas). A detailed channel model which is similar to those used in other fuel channel codes has been implemented in the code. Radial and circumferential conduction are calculated for individual pins within a bundle. The effects of thermal radiation, pressure-tube deformation, zirconium and steam reaction, pressure and calandria tubes contact, and the presence of non-condensable gas can all be modelled. A simple controllers package has been set up for general applications, which requires user's interface to set up the specific station control logic. A linkage between CATHENA and the plant controllers has been set up for the CANDU-6 at Point Lepreau. The reactivity changes due to mechanical control devices and shut-down systems are provided by the user's input data. The code uses a staggered-mesh, one-step semi-implicit, finite-difference scheme for the thermal-hydraulic equations.

The TUF code, developed at Ontario Hydro Nuclear, is made up of two separate programs: steady state and transient. In the steady state program, the equations dealing with thermal-hydraulic variables, nodal heat flux, heat exchanger

film resistance and valve position (or special link resistance) for a control system are solved. The set of simultaneous non-linear equations is solved by the Newton-Raphson iteration method. To match the steady state solutions with normal operating conditions, different control flags are used in the input data. These flags are used to define the degrees of freedom for the steady state simulation, particularly when the control systems are involved. TUF contains modules dealing with thermal-hydraulics (one-fluid, drift-flux and two-fluid), reactor physics (point kinetics or external coupling with other reactor physics codes), heat conduction (pipe wall, heat exchangers, pressure-calandria tubes and fuel pins), system components (pumps, valves, boilers, pressurizer, bleed condenser, turbine and accumulator), special models (discharge model, level swell, bundle movement, pressure tube strain model and metal-water reaction), and station controllers. The reactor control systems used in the code are station dependent. The reactor controllers simulate the following control systems: overall unit control, reactor regulating system, steam generator pressure and level controls, heat transport (HT) system pressure and inventory controls, bleed condenser pressure and level controls and safety systems.

The main purpose of this paper is to review the modelling of condensation phenomena in the Canadian nuclear industry. The physical parameters associated with the cold water injection are discussed. To illustrate the effect of condensation on the pressure transient, the condensation induced water hammer experiment is considered. Simulation of condensation induced water hammer is a challenging task for any thermal-hydraulics code because the prediction accuracy not only depends on the condensation model, but also on the numerical methods used in the code.

2. CONDENSATION MODELS IN CANDU REACTOR SYSTEM CODES

Overview of Physical Parameters for Condensation

Condensation is primarily controlled by the rate at which the latent heat is transported from the interface to the bulk liquid. Condensation appears essentially as a heat transport process, but one which differs from heat transport without phase change in that it is accompanied by the condensation induced bulk convection normal to the interface. Two conceptual approaches for modelling condensation have been proposed: the surface renewal theory and the turbulent diffusion approach. The surface renewal theory assumes that during the time period a typical eddy spends in contact with the interface, heat transfer by molecular diffusion into the subcooled eddy removes the latent heat. The turbulent diffusion approach typically uses the Reynolds averaged temperature equation with the Reynolds flux term approximated in terms of an effective turbulent diffusivity. In this latter approach, the condensation coefficient is mainly controlled by the turbulent intensity.

During the cold water injection process, both direct contact condensation of steam and two-phase mixing flow may be encountered. The first condition has been received considerable attention theoretically and through experiments. From the experimental results published in the literature, it is apparent that the condensation heat transfer coefficient may vary by several orders of magnitude from less than 1 kW/m²/C in stratified flow to about 2000 kW/m²/C obtained in the bubbly flow regime. Several experimental studies have examined local condensation rates in direct-contact stratified flow over the years. A number of empirical correlations for the condensation heat transfer coefficient have been developed based upon local parameters. In general, these correlations involve a power-law relationship in the liquid Reynolds and Prandtl numbers. From analyzing direct contact condensation data, it has been concluded that the heat transfer resistance lies only in a thin water layer very close to the interface. Also, the only parameter that significantly effects the heat transfer is the liquid mass flow rate. For the two-phase mixing process of injection water with steam several models have been proposed in the literature. For example, a multi-fluid model was suggested in Reference 7 and a physical mixing model in the vicinity of the injection location was suggested in Reference 8.

In a two-fluid code, the condensation is normally simulated at two locations, at the interface and at the wall surface. Condensation at the interface is modelled through heat transfer processes in all two-fluid codes. The difference between the averaged phase temperatures or specific enthalpies in a control volume and the respective saturation

values are the dependent variables controlling the model. Condensation on wall surfaces is simulated by two approaches in two-fluid codes. In the direct approach, the film condensation rate on wall surfaces is added to the overall condensation rate for the control volume. In the indirect approach, the wall condensation heat transfer is used to lower liquid-phase temperature that will eventually increase the condensation rate at the interface. There is a time delay in the indirect approach. In both approaches, condensation at the gas-liquid interface is the generally dominant process. Therefore, the interfacial area and the interfacial heat transfer coefficient are the primary physical parameters that control the overall condensation rate during a simulation. In some two-fluid codes, the interfacial heat transfer rate is assumed to be independent of the flow regimes. In most two-fluid codes, the interfacial area is determined through a flow regime map. As a result, discontinuities in the interfacial area and the accuracy of the flow regime map are a concern in all two-fluid codes. The flow regime based on the steady state regime maps may not be applicable to certain transient conditions. For example, the transient flow regime near an injection front is not included in most flow regime maps.

In this paper, the condensation models implemented in the CANDU reactor system codes CATHENA and TUF are briefly described. Since the condensation models implemented in the CATHENA and TUF codes are not the same either in formulation or in the correlations used, they are described separately. To illustrate the challenges faced, simulations of a CWIT experiment by CATHENA and a condensation induced water hammer test by TUF are presented.

Condensation Model in CATHENA

Two categories of two-phase flow regimes are adopted in CATHENA: mixed and separated. This categorization was adopted to provide smooth transitions between the flow regimes. The mixed flow category is characterized by high interfacial area and contains the disperse bubble, slug-churn and disperse droplet flow regimes. The separated flow category is characterized by low interfacial area and contains the horizontal stratified and vertical annular flow regimes. For horizontal pipes or channels, five flow regime transition criteria are used to determine the mixed-to-separated transition multiplier, w_s . The transition criteria are based on the liquid flux for transition to slug flow, Helmholtz instability at high relative velocities, transition to slug or the elongated bubble regime at low void fraction, countercurrent flooding for feeder piping and liquid droplet entrainment. Similarly, for vertical or inclined pipes the mixed-to-separated transition multiplier is determined from three transition criteria. The vertical pipe transition criteria are based on, the liquid volumetric flow for transition to slug flow, void fraction limits for transition to annular flow and liquid droplet entrainment.

The complete set of constitutive relations including interface heat transfer are calculated for all flow regimes during transitions. The value of each constitutive relation, ϕ_s , is then determined from the weighting relation,

$$\phi_s = w_s \phi_s + (1 - w_s) \phi_m \quad [1]$$

where ϕ_s and ϕ_m represent the values of the constitutive relation calculated for the separated and mixed flow categories. For the mixed flow category the value of the constitutive relation, ϕ_m , is determined from a weighted value of the correlations used for the disperse bubble, slug-churn and disperse droplet flow regimes. This weighting within the mixed flow category is determined by a flow regime map similar to that in Reference 9. For the separated flow category, the values are determined from correlations appropriate to the horizontal stratified or vertical annular flow regimes. A more complete description of the flow regime transition and constitutive relation weighting approach used in CATHENA can be found in Reference 5.

The interface mass transfer rate per unit volume, m_{gi} , is determined from an energy balance at the interface as

$$m_{gi} = -m_{fi} = \frac{q_{wi} - \sum_k \lambda_{ki} (h_k - h_k^{sat})}{h_g - h_f}, \quad k = g, f \quad [2]$$

where the subscripts g, f, i and w denote vapour, liquid, interface and wall respectively. The heat transfer rate from or to the wall resulting in vapour generation or condensation is denoted by q_w and h_k is the specific enthalpy for phase k with the superscript sat denoting the saturation value. The generalized heat transfer coefficient, λ_{ki} , can be defined as product of the interface area per unit volume and a interfacial heat transfer coefficient divided by the phase specific heat at constant pressure. Since the form of the generalized heat transfer coefficient is dependent on the flow regime and the phase state (subcooled or superheated) it will be described for each condition independently.

For the metastable states of superheated vapour or liquid, the following relations are applied for both mixed and separated flow categories: for liquid and vapour respectively

$$\lambda_{f1} = 2 \times 10^5 \alpha_g \alpha_f + 0.005 (h_f - h_f^{sat}) \quad [3]$$

$$\lambda_{g1} = 2 \times 10^4 \alpha_g \alpha_f + 0.005 (h_g^{sat} - h_g) \quad [4]$$

where α_k is the void fraction for phase k . These forms were assumed to ensure that the liquid does not become significantly superheated or the vapour does not become significantly subcooled. For these metastable conditions, the interface area per unit volume, phase specific heats and heat transfer coefficients are included in the numerical values of the coefficients chosen.

The correlations used for subcooled liquid and superheated vapour conditions were determined from a review of the two-phase flow literature. For the mixed flow category, separate correlations are used for the dispersed bubble, slug-churn and dispersed droplet flow regimes. For the dispersed flow regimes the form of the correlation used is,

$$\lambda_{ki} = \frac{A_i K_k}{C_{pk} d} (2 + 0.5 Re_{ki}^{0.5} Pr_k^{0.3}) \quad [5]$$

where K_k is the thermal conductivity for phase k , C_{pk} is the specific heat at constant pressure for phase k , d is the particle (bubble or droplet) diameter, Re is the Reynolds number based on the slip velocity and Pr is the Prandtl number. The interface area per unit volume for a disperse flow is given by,

$$A_i = \frac{6 \alpha_d}{d} \quad [6]$$

with α_d representing the void fraction of dispersed phase. For the slug-churn flow regime a weighted average interfacial area and heat transfer correlation, following the approach in Reference 10, of the dispersed correlation and correlations appropriate to a Taylor bubble interface geometry is used.

For the separated flow category, two sets of interfacial heat transfer correlations were adopted, one for the horizontal stratified flow regime and one for the vertical annular flow regime. Since the liquid-side interfacial heat transfer dominates the condensation process only the liquid-to-interface heat transfer will be outlined. For the annular flow regime the liquid-to-interface heat transfer coefficient is determined as maximum of the laminar or turbulent convection relations given by,

$$\lambda_{f1} = \text{MAX} \left(\frac{K_f A_i}{C_{pf} \delta}, 0.065 \frac{K_f A_i}{\mu_f C_{pf}} \sqrt{\rho_f Pr_f \tau_i} \right) \quad [7]$$

where ρ is the density, and δ and τ_i are the annular film thickness and the interfacial shear determined by,

$$\delta = 0.5 D_e (1 - \sqrt{\alpha_g}) \text{ and } \tau_i = 0.023 \rho_g v_g^2 \text{Re}_g^{-0.2} \quad [8]$$

and D_e is the pipe hydraulic diameter. The interfacial area per unit volume for the annular flow regime includes the effect of droplet entrainment through the approach taken in Reference 11. For the horizontal stratified flow regime the heat transfer correlation given in Reference 12,

$$\lambda_{f1} = \frac{K_f A_i}{D_e C p_f} (1 + 0.25 \text{Re}_f^{0.75} \text{Pr}_f) \quad [9]$$

was adopted with the interface area per unit volume determined from the liquid level in the pipe.

In addition to the flow regimes and interface heat transfer correlations described, a "piston" flow regime is used to modify the interface heat transfer, and therefore condensation rate, in a liquid injection front region. Within a liquid injection front the liquid-to-interface heat transfer coefficient is determined as a weighted average of the nominal value determined through the flow regime and a value determined by conduction at a liquid front spanning the pipe cross section. The modified liquid-to-interface heat transfer correlation is given by,

$$\lambda_{f1} = \lambda_f + W_p (\lambda_{f1}^* - \lambda_f) \text{ where } \lambda_f = \frac{K_f}{0.005 D_z C p_f} \quad [10]$$

D_z and λ_{f1}^* are the local finite-difference cell length and the generalized heat transfer coefficient determined for the mixed or separated flow categories. The "piston" regime weighting coefficient, W_p , is determined from the first and second spatial gradients in void fraction.

Condensation Model in TUF

The two-phase flow regime maps considered in TUF consist of bubbly, slug, annular, churn turbulent, mist, stratified, vertical separated and horizontal separated flows. The regime boundaries for the horizontal, vertical and other components are determined by the mixture mass flux and the void fraction, which are similar to those used in RELAP5 code (Reference 13).

The interfacial mass transfer rate F in a control volume V ($F=V m_{ij}$) is expressed by

$$F = \frac{-\sum_k q_{ki} + \sum_k q_{kw}}{h_{gs} - h_{fs}} \quad [11]$$

where q_{ki} is the interfacial heat transfer rate, q_{kw} is the wall heat transfer rate that result in a phase change, and h_{ks} is the saturated specific enthalpy for phase k . The interfacial heat transfer rate q_{ki} is expressed by

$$q_{ki} = V A_i H_{ki} (T_{ks} - T_k) \quad [12]$$

where T_k is the phase temperature and T_{ks} is the saturation temperature of phase k .

For the bubbly and mist flow regimes (or entrainment), the interfacial heat transfer coefficients are given by

$$H_{ki} = \max [H_{ki}(\text{conv}), H_{ki}(\text{cond})] \quad [13]$$

where the convective (conv) and conductive (cond) heat transfer coefficients are given by the following correlations:

$$H_{ki}(\text{conv}) = \frac{2 K_k}{d_p} [1 + 0.37 \text{Re}_k^{0.5} \text{Pr}_k^{0.33}] \quad [14]$$

$$H_{ki}(\text{cond}) = \frac{\text{Nu} K_k}{d_p} \quad [15]$$

where d_p is the averaged bubble or droplet diameter and Nu is the Nusselt number.

For the slug, annular and stratified flow regimes, the heat transfer coefficient is also expressed by Equation [11] with

$$H_{ki}(\text{conv}) = 0.023 \frac{K_k}{\delta_k} \text{Re}_k^{0.8} \text{Pr}_k^{0.4} \quad [16]$$

$$H_{ki}(\text{cond}) = \frac{\text{Nu} K_k}{\delta_k} \quad [17]$$

where δ_k is either the film thickness (for annular flow) or the other dimensional parameter depending on the flow regimes encountered. For the separated flows, the following correlation is used for the liquid phase:

$$H_{fi}(\text{conv}) = \text{St} \rho_f C_{pf} v_f \quad [18]$$

where St is so-called Stanton number and v_f is the liquid velocity.

Except for bubbly and mixed flows, either bubble or droplet entrainment caused by the interface movement is assumed in the flow regimes. The amount of entrainment depends on the system pressure, temperature and slip velocity. For several special components (for example steam drum, pressurizer or reactor channels), the level swelling model is used to determine the amount of bubble entrainment. The overall interfacial heat transfer rate q_{ki} is equal to the sum of three components:

$$\begin{aligned} q_{ki} = & q_{ki}(\text{distinct regime}) + q_{ki}(\text{entrained bubble}) \\ & + q_{ki}(\text{entrained droplet}) \end{aligned} \quad [19]$$

3. CATHENA SIMULATION OF COLD WATER INJECTION TEST

A schematic diagram of the Cold Water Injection Test (CWIT) at Stern Laboratories (Hamilton, Ont.) facility is shown in Figure 1. The test facility consisted of two 6-m long, horizontal, electrically heated channels at different elevations connected to inlet and outlet headers by inlet and outlet feeders. The experimental facility channels are approximately 10 and 5 m below the elevation of the inlet and outlet headers. Blowdown and injection systems were connected to the headers.

Figure 2 shows an isometric view of the CWIT heated channel, a cross-sectional view of the 37-element fuel element simulator (FES) and a cross-sectional view of an FES element. The heat channel assembly contained 37-element electrically heated fuel element simulators (FES) that maintained a CANDU typical radial power depression ratio (1.0/0.81/0.72/0.68) between the outer and inner heater pin rings. The 37-element FES consisted of two 3-m long pin arrays that were inserted from either end of the channel. Each 13-mm diameter rod in the FES was constructed of an Inconel alloy tube containing a coaxial Nichrome heating ribbon with a uniform spiral form resulting in uniform axial heating except for a 120 mm unheated region at the centre of heated channel where the FES bundles met. The remaining space in the FES element is packed with magnesium oxide power. The FES heater elements are capable of operating at up to 800°C.

Many test programs have been conducted in this experimental facility including feeder and channel refill, standing start, and flow stratification. The majority of the experiments were conducted to examine feeder and channel refill under a variety of facility configurations: single or double-injection, single or double-break, single or parallel channels over a range of channel powers, injection flow rates and facility preheat conditions. Only the single-break, double-injection feeder and channel refill experimental programs will be discussed in this paper. In these experiments, the test facility was preheated by circulating superheated steam until the desired conditions were established. The preset power was then applied to the FES elements and when any of the surface temperatures reached the desired temperature a quick acting valve was opened to initiate depressurization. When the system pressure dropped below the injection pressure subcooled liquid was injected into both headers. The experiment was terminated when the feeders and heated channel was completely refilled.

The key parameters in these feeder and channel refill experiments are: the condensation rate on the subcooled injection liquid, the subcooled vapour generation on the hot wall surfaces during the rewetting and refilling of the facility piping and the quench/rewet characteristics during the refilling of the channels. The balance between the condensation rate and the vapour generation rate by subcooled boiling controls the refilling rate since it determines the system pressure. The phase separation and quench rewet processes in the horizontal channels are important because they control the quenching behaviour in the heated FES bundles.

A number of CWIT experiments have been simulated by CATHENA. As an example, the simulation of the parallel channel experiment, CWIT-629, is described in this paper. For this experiment, the facility was preheated to a nominal temperature of 300°C (400°C for the FES elements), the injection liquid temperature was 30°C, the injection pressure was 3.0 MPa, and a FES power of 200 kW was maintained in each heated channel. The CATHENA idealization for the parallel channel, single-break double-injection experiment is shown in Figure 3. The idealization consisted of 239 thermalhydraulic nodes and contained 1490 wall heat transfer surfaces. The idealization for the feeders is shown separately for the upper and lower channels to simplify the diagram.

The simulation results for the parallel-channel, single-break double-injection experiment are shown in Figures 4 through 6. Figure 4 compares the simulated inlet header pressure and injection flow rate with the experimental data. Figure 5 compares the top channel FES temperatures (for the upper and lower pins in the 37-element bundle at the channel inlet and middle) with the experimental data. Similarly, Figure 6 compares the bottom channel FES temperatures (for the upper and lower pins) with the experimental data.

The CATHENA simulation generally captured the inlet header pressure behaviour for the entire transient and the correspondence between changes in the header pressure and the injection flow rate can be observed in Figure 4. The

more rapid depressurization rate predicted in the initial period of the transient was attributed to the flashing of an unknown amount of condensate that remained in the channels, feeders and headers after preheating the facility. The presence of the condensate can be inferred from Figure 6 by the decrease in the bottom FES temperatures just after the blowdown initiation. These results demonstrate that an acceptable balance in the simulation between condensation on the cold water injection front and subcooled vapour generation on the facility piping was maintained.

The simulated FES temperatures (for the top and bottom channels) demonstrate an acceptable degree of phase separation during channel refilling as indicated by a comparison of the time differences between the quenching of the upper and lower pins in the top and bottom channels in Figures 5 and 6 respectively. The overestimate of the time required to quench and rewet the upper FES pins was attributed to an underestimation of the film and transition regime boiling heat transfer rate.

4. TUF SIMULATION OF CONDENSATION INDUCED WATER HAMMER

Water hammer in nuclear power plants have been caused by voiding in a normally water-filled pipe line, by steam condensation in piping lines containing both steam and water, as well as by the classical cause of rapid valve action. As reported in Reference 14, over one hundred reported water hammer events occurred in U.S. nuclear power plants (both boiling and pressurized water reactors) between 1969 and 1981. The feedwater line rupture at the Indian Point No.2 plant in 1973 (Reference 15) was attributed to a condensation induced water hammer. This event along with other steam generator water hammer events spurred corrective design and operational actions in U.S. reactor plants. For CANDU reactor plants at Ontario Hydro Nuclear, a similar effort has been devoted to examine the possibility of condensation induced water hammer in the steam generator emergency cooling system.

During the past years, a series of tests for condensation induced water hammer has been conducted at Ontario Hydro Technologies (OHT). The main purpose of these tests was to examine the induced pressure pulses under various defined flow conditions and to define the threshold condition between the water hammer and no water hammer regions. The complexity of the tests was held to a minimum and the dominant physical parameters were accurately measured. Even though TUF was not designed to simulate the water hammer problems, TUF was chosen to simulate these tests since it was used in the simulation of the emergency cooling system of the steam generators. Therefore, these tests were used to examine the condensation model and the numerical method applied in the TUF code. The relevant physical parameter that controls the prediction is the steam condensation rate. A similar simulation of the two-phase water hammer phenomenon by the RELAP5/MOD3 code has been presented in Reference 16 for a lower pressure case. A criterion for the initiation of water hammer in horizontal pipe has been suggested by Bjorge and Griffith (Reference 17).

The setup for the tests consists of a vertical tank filled with subcooled water. The schematic diagram of the OHT apparatus is shown in Figure 7. The air supply system at the top of the tank is used to maintain a constant tank pressure during the transient. A horizontal pipe (length 5.5 m and diameter 0.0921 m or 4 inches) initially filled with subcooled water is connected from the bottom of the tank. A fast-acting ball valve is installed between this pipe and a closed-end vertical pipe (length 5 m with different diameters 5/8, 2 and 4 inches) initially filled with steam. The case with 4 inches diameter is presented here. Pressure transducers were mounted in the vertical pipe to record the pressure history of the experiment. A series of tests with different tank pressures (from 150 kPa to 650 kPa), water temperatures (from 20°C to 90°C) and steam temperatures (from 100°C to 150°C) were performed. The following results were observed: (1) the magnitudes of the induced pressure pulses are functions of the tank pressure, the water temperature and the steam temperature; (2) there is a threshold condition between the water hammer and no water hammer regions; and (3) a scatter of the test data with the same test conditions was observed. In the TUF simulations, the horizontal and vertical pipes are modelled by 15 and 20 nodes, respectively. The minimum and the maximum time steps used in the time-step control are 0.05 ms and 0.25 ms, respectively.

Two approaches have been tested for this particular problem in the TUF code. One uses the injection front model in the simulation, as described in Reference 18. This model is currently used in the production versions for general

applications. In this model, the averaged condensation rate over the steam filled pipe is used in the two-fluid model. The second approach is based on the physics observed from the OHT test data. Different models are used in three observed distinct regions: valve induced dispersion front, adiabatic region and fast condensation zone. The physics behind both approaches are the main subjects described here.

Injection Front Model

In this model, the valve opening is assumed to be in a condition that the injection front has a distinct interface before it collides with the pipe dead-end. Also, certain entrained bubbles and droplets caused by the movement of the interface are assumed to exist at the interface. The interfacial area per unit volume A_i consists of three components in the vertical piping: injection front, entrained bubbles, and entrained droplets

$$A_i = \frac{1}{L} + \frac{6 \Delta\alpha_b}{d_b} + \frac{6 \Delta\alpha_d}{d_d} \quad [20]$$

where L is the pipe length, d_b is the bubble diameter, d_d is the droplet diameter, $\Delta\alpha_b$ is the void fraction of the entrained bubbles in the liquid region, and $\Delta\alpha_d$ is the void fraction of the entrained droplets in the vapour region. The phase transfer rate is mainly controlled by the liquid phase. The amount of volume fraction for the bubble or droplet entrainment is about 1 percent in the model. As a result, the interfacial area is a constant value during the injection front propagation.

In this paper, two cases are reported: (1) the most severe case with a tank pressure 654 kPa, water temperature 23 °C and steam temperature 150°C (it caused damage at the closed end piping), and (2) tank pressure 551 kPa, water temperature 22°C and steam temperature 142°C. The predicted result of the pressure transient at the dead-end location for Case (1) is shown in Figure 8. The corresponding test data are plotted in Figure 9. The results for Case (2) are plotted in Figures 10 and 11, respectively. It shows that water hammer phenomenon is well predicted by this model. However, the magnitudes of pressure spikes at the dead-end location for Case (2) are over predicted. Also, the pressure transient before the first pressure spike does not reflect the transient behaviour observed in the tests since an average condensation rate was used over the steam filled pipe in this model.

Distinct Regions Model

In order to explain the reasons for data scatter in the OHT water hammer tests, the whole set of test data has been re-examined, especially in the pressure transients before the first pressure spike at the pipe dead-end. It has been found that three distinct regions in the pressure transient before the first pressure spike have been observed as shown in Figure 12 for Case 2: initial valve induced flow dispersion, slow condensation, and fast condensation regions. This phenomenon was not observed in Case (1) and also not reported in Reference 16. Nevertheless, a distinct region model was developed to simulate this phenomenon.

In this model, it is assumed that the valve opening results in a regime of liquid dispersion which is similar to that observed in the jet injection with a cloud of droplets, similar to the model suggested in Reference 7. In this region, a large condensation rate is obtained due to the large value of the interfacial area. After the supplied steam flow in the injection node (induced by condensation) forces the droplets to settle down to its water level, a perfect distinct interface (without entrainments) is assumed in the second region. The condensation rate is so low such that the steam compression process is close to the adiabatic condition. At the end of the compression process, an instability at the interface occurs which results in drastic changes in the flow regime and the condensation mode (from film condensation to drop-wise condensation). As a result, the condensation rate is so large such that the steam pressure drops significantly before the void collapses at the pipe dead-end.

This distinct regions model was hypothesized from the observation of the test results. There are several difficulties in implementing this model in the reactor system code. (1) Tracing of the jet position in the discrete grid is required. (2) Modelling of the interaction between the droplets with the steam flow during the injection front movement is required. (3) Formulation of a model for the interfacial instability criterion from the adiabatic region to the fast condensation region is required. (4) Determining if this particular model is applicable to other flow conditions, for example in the case of a horizontal pipe or higher tank pressures such as Case (1), is required.

In the development version of TUF, two criteria for the interface instability during the adiabatic compression have been proposed: the interfacial instability criterion based on the Kelvin-Helmholtz formulation and the compression effect acting on the water column. The first criterion is based on the slip velocity at the injection node (using liquid inlet and steam outlet flows) comparing with the Kelvin-Helmholtz instability criterion. The second criterion which was postulated from the analogy of the flow instability observed in a diffuser is described below. In this criterion, it is assumed that an interface instability occurs at the injection front when the following condition is satisfied:

$$-\frac{dv}{v} = C \quad [21]$$

where v is the injection front velocity and dv/dt is the rate of change in velocity. The constant value of C is an adjusted parameter to fit with experimental data. After this condition is satisfied, the adiabatic region is no longer valid. The film condensation mode is switched to the drop-wise condensation mode with a large interfacial heat transfer coefficient. Figure 13 shows the predicted pressure transient at the pipe dead-end for Case 2, where the initial pressure transient before the first pressure peak is well predicted. This simulation confirms the hypothesis of this model in the description of condensation induced water hammer.

5. DISCUSSION

The main objective of a thermal-hydraulics code is to predict the overall system response to postulated abnormal operating conditions. Although the emphasis is on the average behaviour, for example void fraction and flow rate, it is important that the models be mechanistically based to retain the predictive capability of the code.

The main challenges faced by thermal-hydraulics codes during the simulation of injection fronts such as those seen in either the CWIT injection test or the OHT water hammer test are the accurate propagation of the steep front while maintaining an accurate estimate of the condensation rate within the frontal region. The accurate propagation of the front is primarily a challenge to the numerical method while the estimation of condensation is primarily a challenge to the flow regime and interface area per unit volume calculation. Propagation of a steep front is difficult in a simulation since most thermal-hydraulic codes use first-order upwind donor-cell difference methods and the nodalization is often coarse. These methods tend to smear or diffuse the front over a number of nodes or cells. A steady-state based flow regime map interprets this smeared front as an extended region of vapour-liquid mixing producing an overestimation of the condensation rate. The TUF and CATHENA thermal-hydraulic codes have taken different approaches to resolving these difficulties each with its own limitations in the present implementation.

In the TUF code, the motion of the injection front is tracked. Within the frontal region the distinct regions model is applied to improve the estimate of condensation rates. The tracking procedure increases the computational complexity because potentially multiple injection fronts must be tracked in complex piping networks. This frontal tracking approach has proved adequate for vertical up-fill geometries and its application to other geometries is being assessed as other OHT experimental data become available. The other area being examined is the minimization of the frontal smearing by adjusting the numerical method around the front location. An example of this would be to use a higher-order upwind difference method just in the frontal region.

In CATHENA the present approach uses the calculated liquid fraction gradients to identify a front. In this way the computational complexity of frontal tracking is removed. The condensation rate within the front is reduced through a decrease in interfacial area per unit volume. This approach appears adequate for the fronts observed in feeder-channel network simulations and is being examined for application during two-phase water hammer simulations. To improve the code, the application of variable-order finite-difference methods such as flux-corrected transport to reduce the liquid front diffusion is being examined. Other work will examine the application of a transient flow-regime evolution model that calculates the interface area per unit volume which is the primary determinant of the condensation rate.

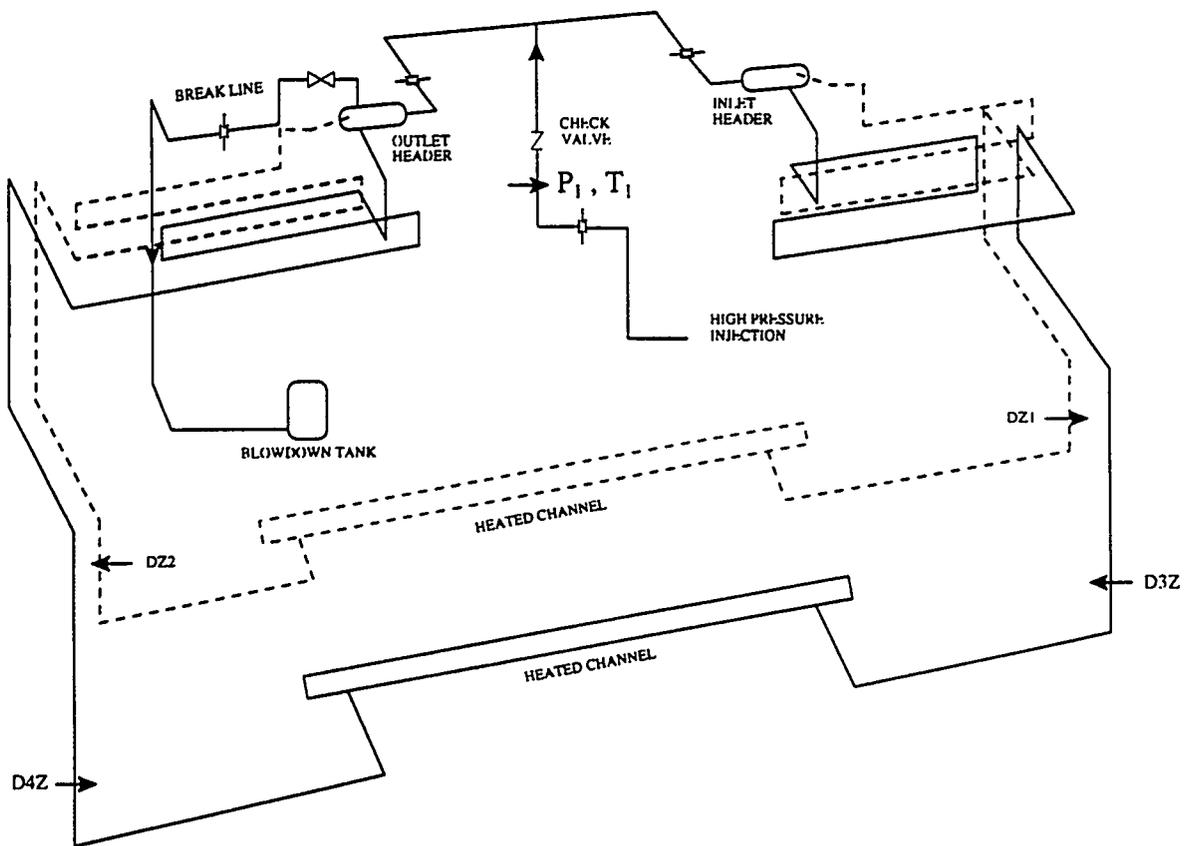
6. CONCLUDING REMARKS

The research work on the modelling of condensation phenomena in the Canadian nuclear industry has been reviewed. The physical parameters associated with cold water injection have been discussed. Continuous refinement in the physical parameters for the condensation rate remains a task for most two-fluid codes. The modelling in the vicinity of the injection front becomes crucial in the simulation of cold water injection, especially in the phenomenon of condensation induced water hammer.

REFERENCES

1. H. Asaka, Y. Murao and Y. Kukita, Assessment of TRAC-PF1 condensation heat transfer model for analysis of ECC water injection transients, *J. of Nuclear Science Technology*, 26, No. 11, 1045-1057, 1989.
2. B. Worth, C. Addabbo and H. Stadtke, Phase change phenomena and related modelling aspects in PWR safety analysis, European Two-phase Flow Group Meeting, Munchen, June 10-13, 1986.
3. D.L. Reeder, LOFT system and test description, EG&G Idaho, Inc. Report TREE-1208, NUREG/CR-0247, July 1978.
4. G.P. Celata, M. Cumo, G.E. Farello and G. Focardi, Direct contact condensation of steam on slowly moving water, *Nuclear Engineering and Design*, 96, 21-31, 1986.
5. D.J. Richards, B.N. Hanna, N. Hobson and K.H. Ardron, CATHENA: A two-fluid code for CANDU LOCA analysis, 3rd International Topical Meeting on Reactor Thermal-Hydraulics, Newport, RI, 1985.
6. W.S. Liu et al., TUF: A two-fluid code for thermal-hydraulics analysis, 10th Annual Conference of Canadian Nuclear Society, Ottawa, Ontario, Canada, June 4-7, 1989.
7. H. Akimoto, Analysis of direct contact condensation of flowing steam onto injected water with multifluid model of two-phase flow, *J. of Nuclear Science and Technology*, 20, 1006-1022, December 1983.
8. A. Janicot and D. Bestion, Condensation modelling for ECC injection, *Nuclear Engineering and Design*, 145, 37-45, 1993.
9. Y. Taitel, D. Bornea and A.E. Dukler, Modelling flow pattern transitions for steady upward gas-liquid flow in vertical tubes, *AIChE Journal*, 26, (3), 345-354, 1980.
10. M. Ishii, K. Mishima, I. Kataoka and G. Kocamustafaogullari, The importance of interfacial area in two-phase flow analysis, In Proceedings of the 9th U.S. Applied Mech. Conf., ASME, 1981.
11. N.K. Popov and U.S. Rohatgi, Effect of interfacial shear and entrainment models on flooding predictions, *AIChE Journal*, 33, (2), 274-281, 1983.
12. T.G. Theofanous, R.N. House and L.K. Brumfield, Turbulent mass transfer at free gas-liquid interfaces with application to open-channel, bubble and jet flows, *Int. J. Heat and Mass Transfer*, 4, 303-322, 1975.
13. V.H. Ransom, et al., RELAP5/MOD2 code manual Volume 1: Code structure, system models and solution methods, EGG-SAAM-6377, Idaho National Engineering Laboratory, April 1984.
14. A.W. Serkiz, An evaluation of water hammer in nuclear power plants, 2nd International Topical Meeting on Nuclear Reactor Thermal-Hydraulics, Santa Barbara, California, USA, January 11-14, 1983.

15. W.J. Cahill, Feedwater line incident report - Indian Point Unit No. 2, Consolidated Edison Co., AEC Docket No. 50-247, 1974.
16. W.S. Yeung, J. Wu, R.T. Fernandez and R.K. Sundaram, RELAP5/MOD3 Simulation of the Water Cannon Phenomenon, Nuclear Technology, 101, Feb. 1993
17. W. Bjorge and P. Griffith, Initiation of waterhammer in horizontal and nearly horizontal pipes containing steam and subcooled water, J. of Heat Transfer, Transaction of ASME, 106, November 1984.
18. W.S. Liu and R. Leung, TUF development status and applications, 15th Annual Conference of Canadian Nuclear Society, Montreal, Quebec, Canada, June 5-8, 1994.



— Bottom Channel Feeder System

- - - Top Channel Feeder System

Figure 1: CWIT Facility Schematic

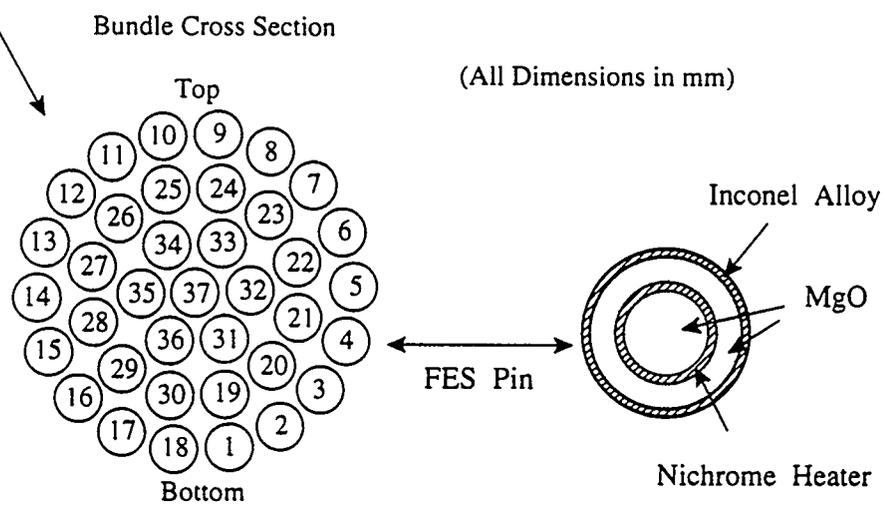
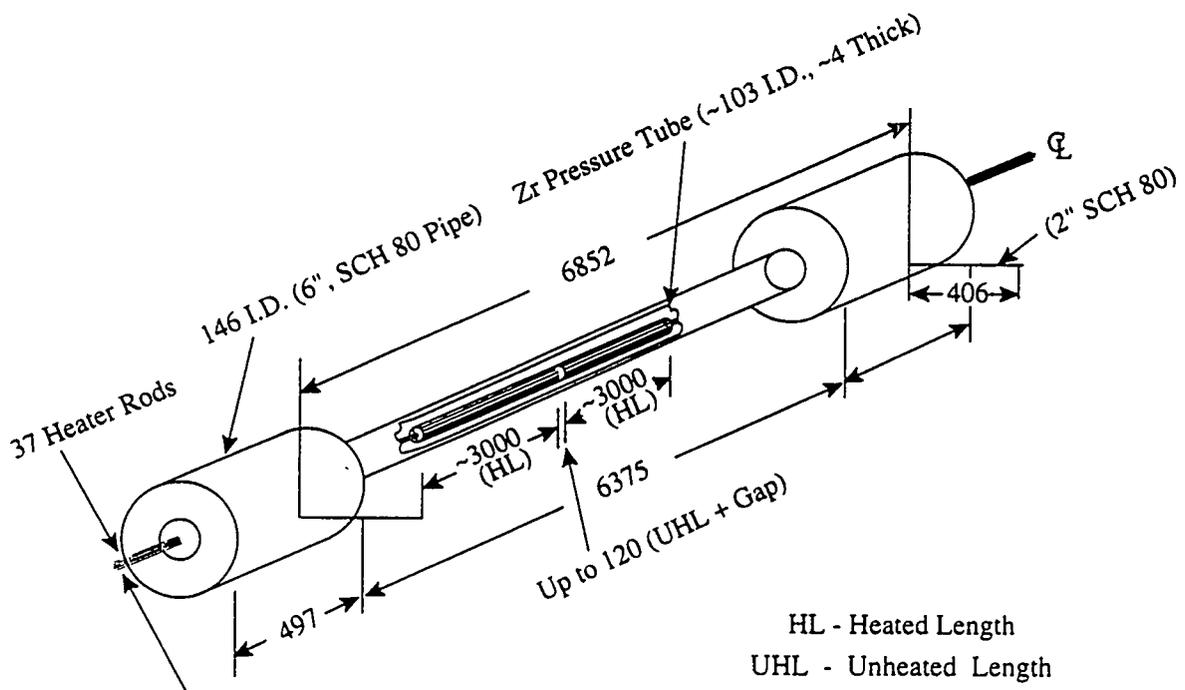
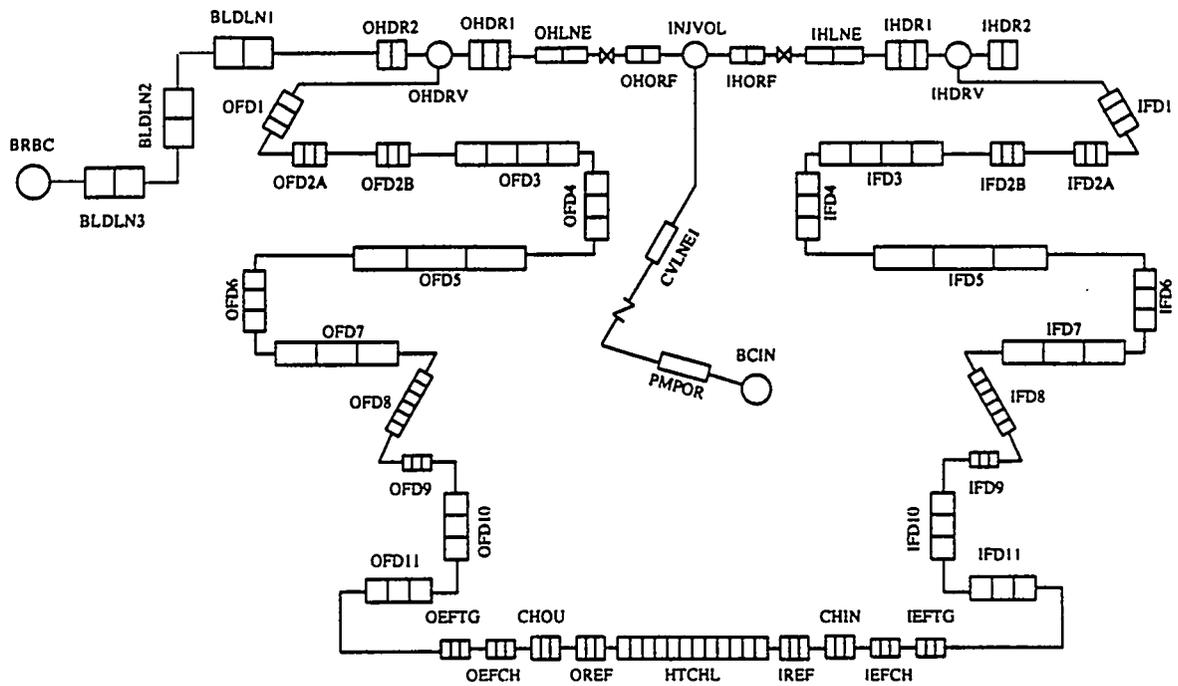
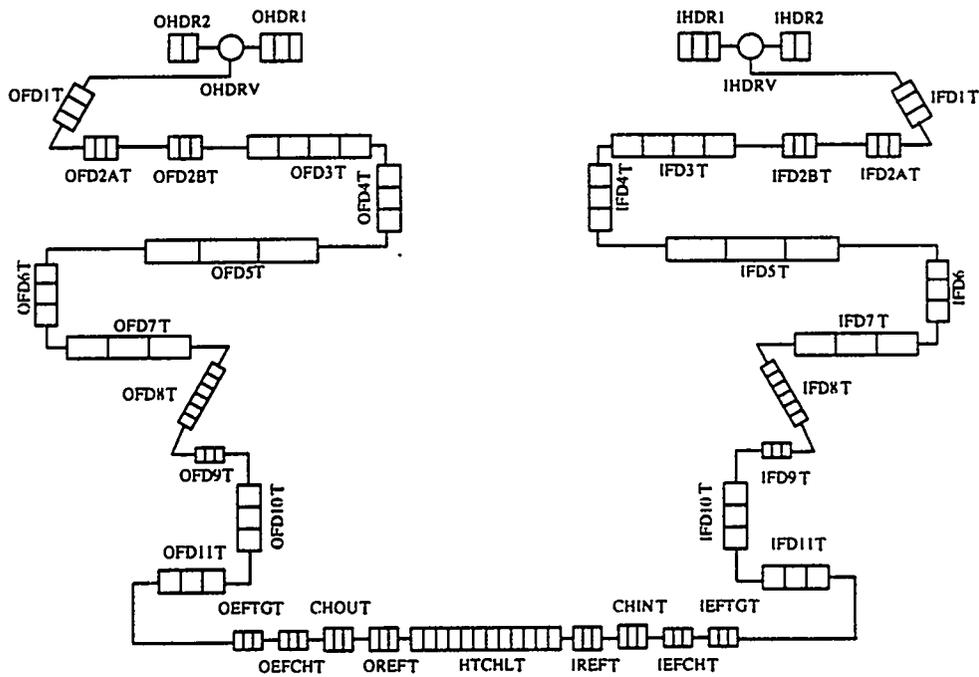


Figure 2: CWIT Heat Channel and FES Geometry



(a) Bottom Channel Idealization



(b) Top Channel Idealization

Figure 3: CATHENA Idealization for CWIT-629

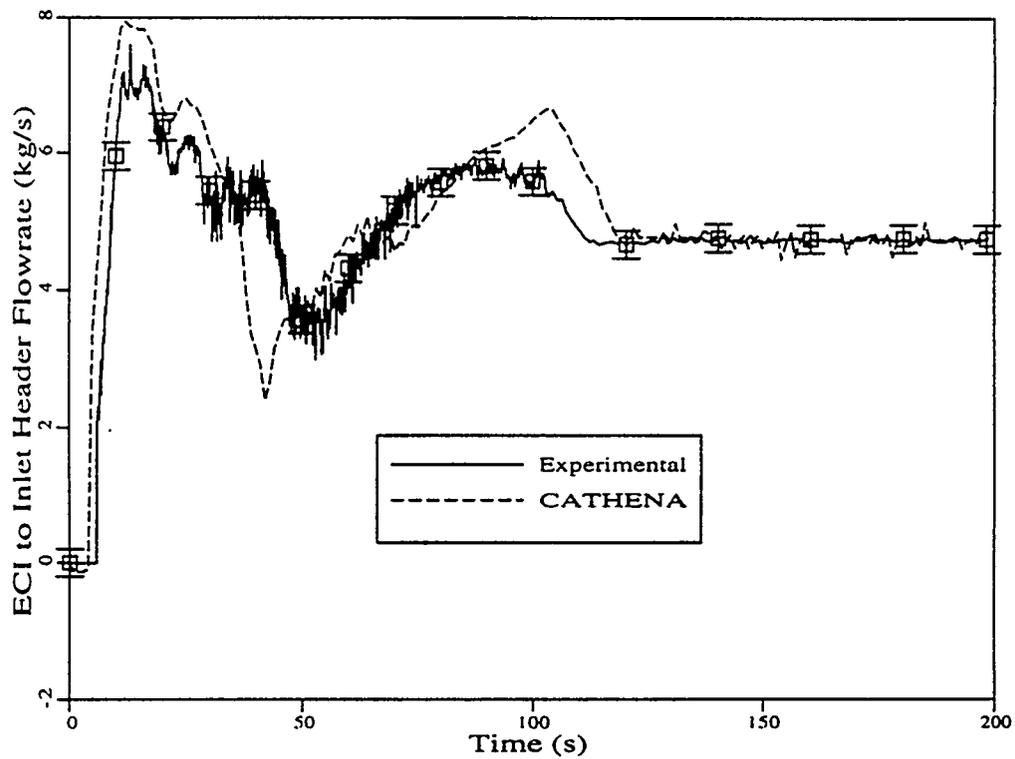
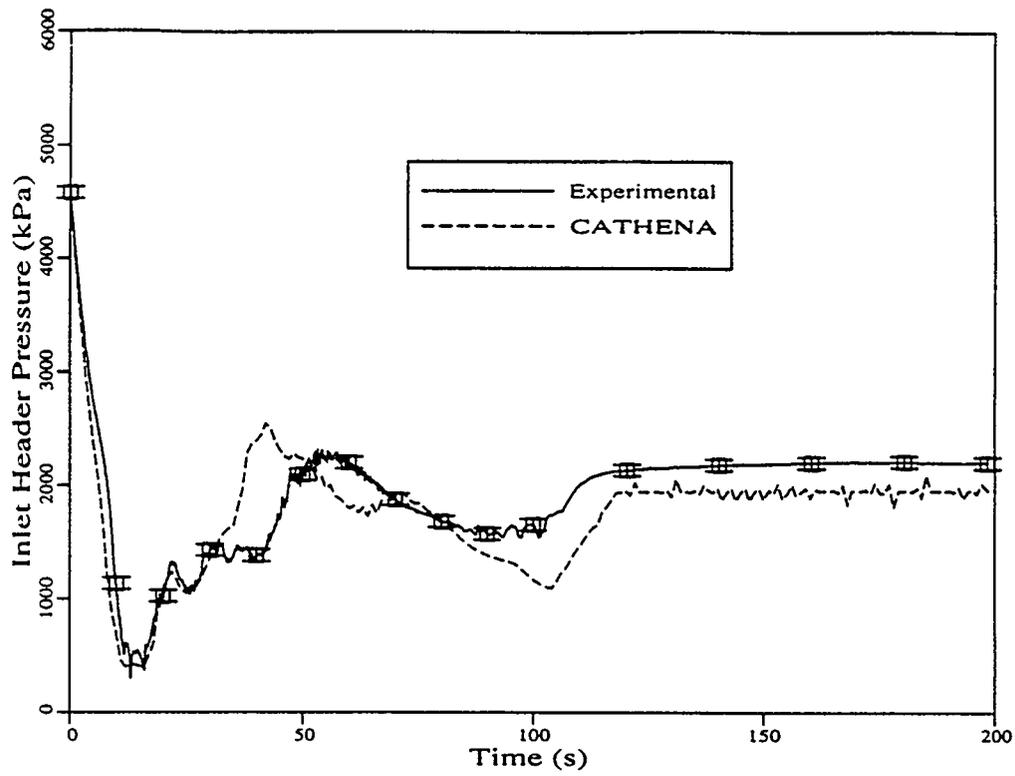


Figure 4: Inlet Header Pressure and ECI Injection Flow

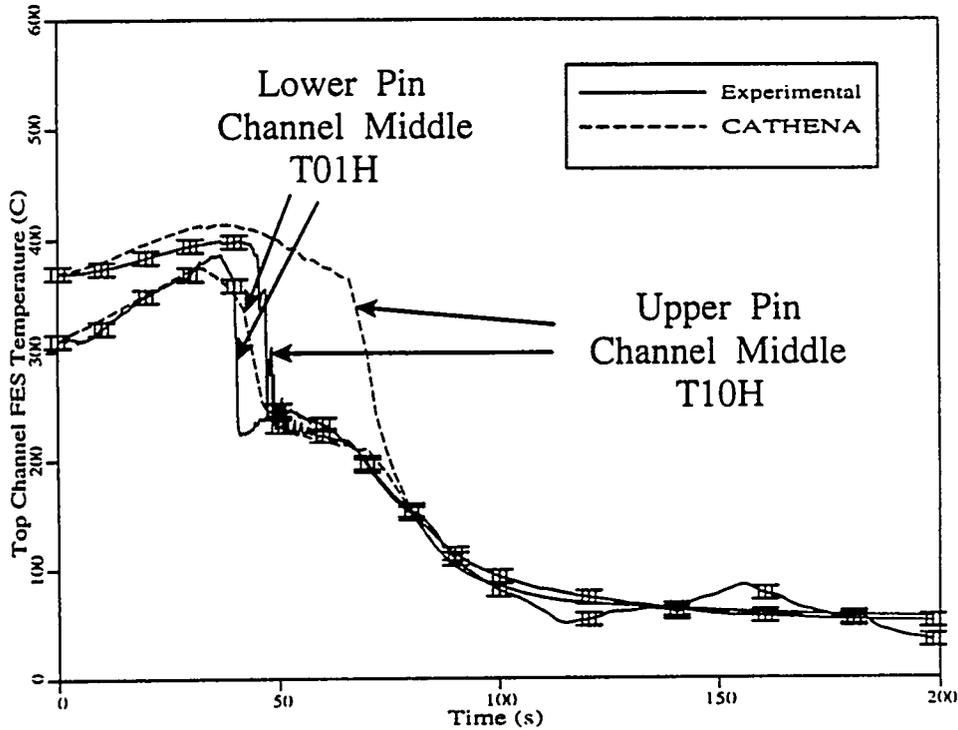
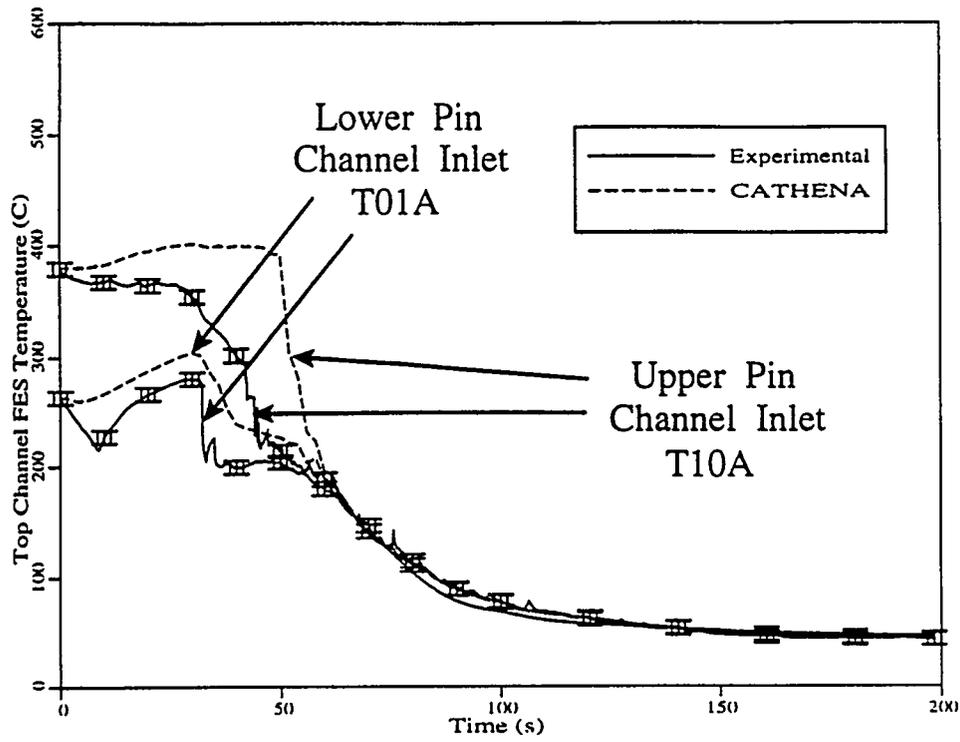


Figure 5: Top Channel FES Pin Temperatures

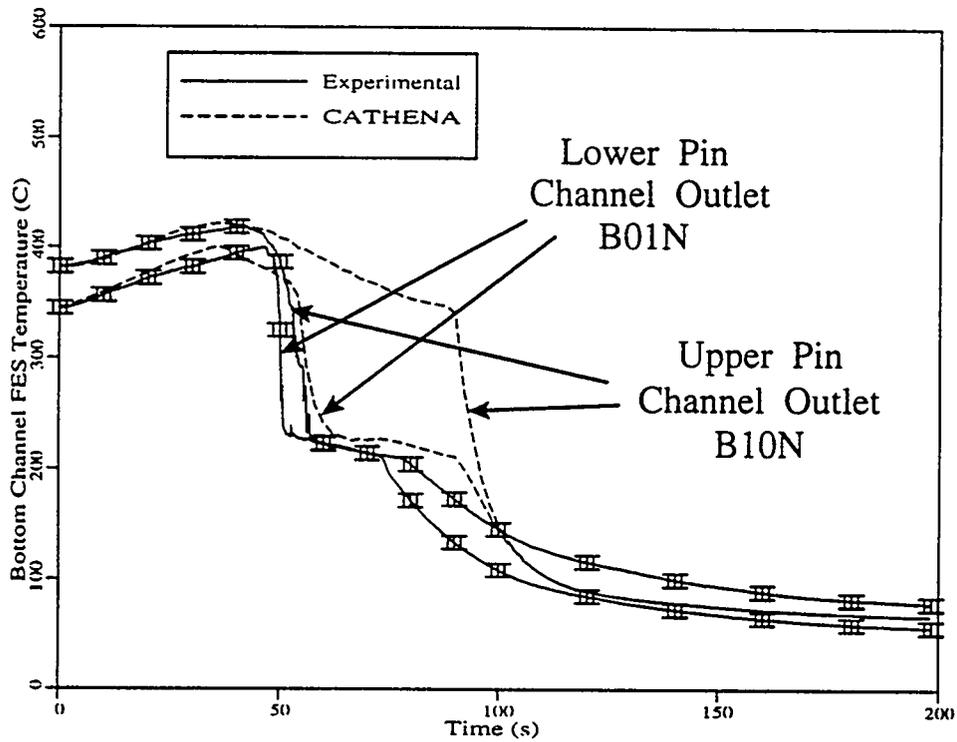
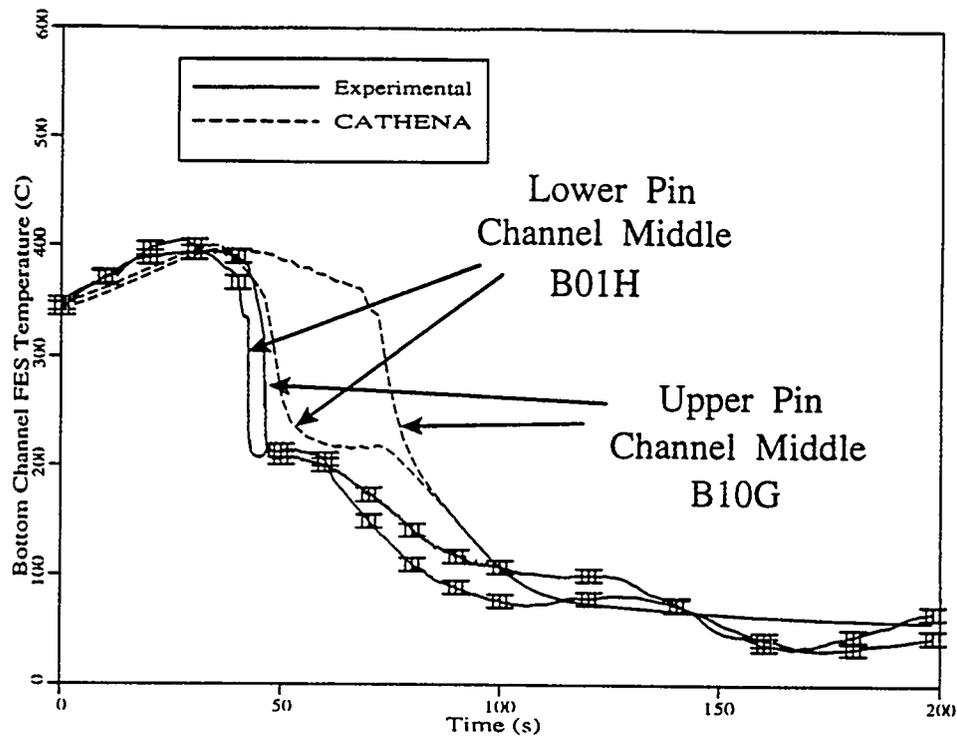


Figure 6: Bottom Channel FES Pin Temperatures

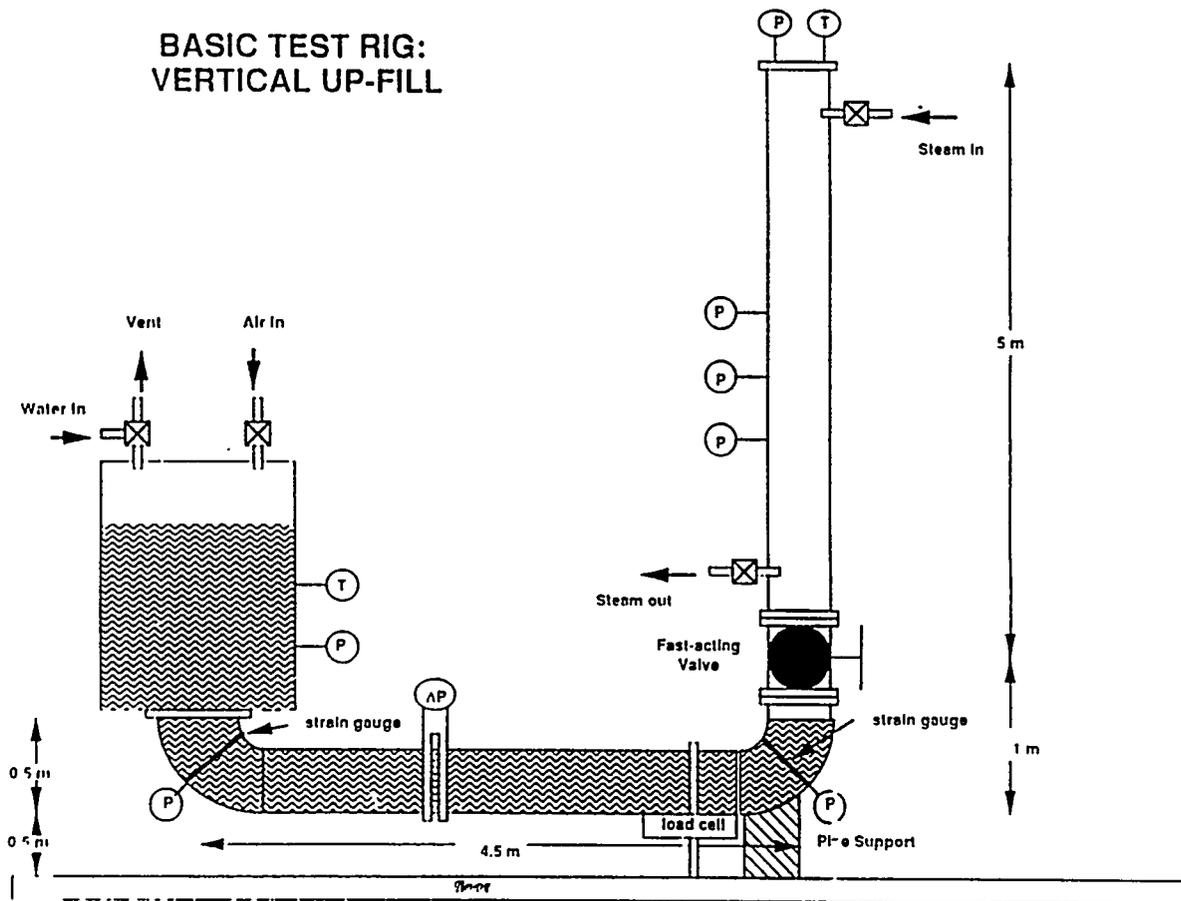


Figure 7. Water Hammer Facility Schematic at OHT

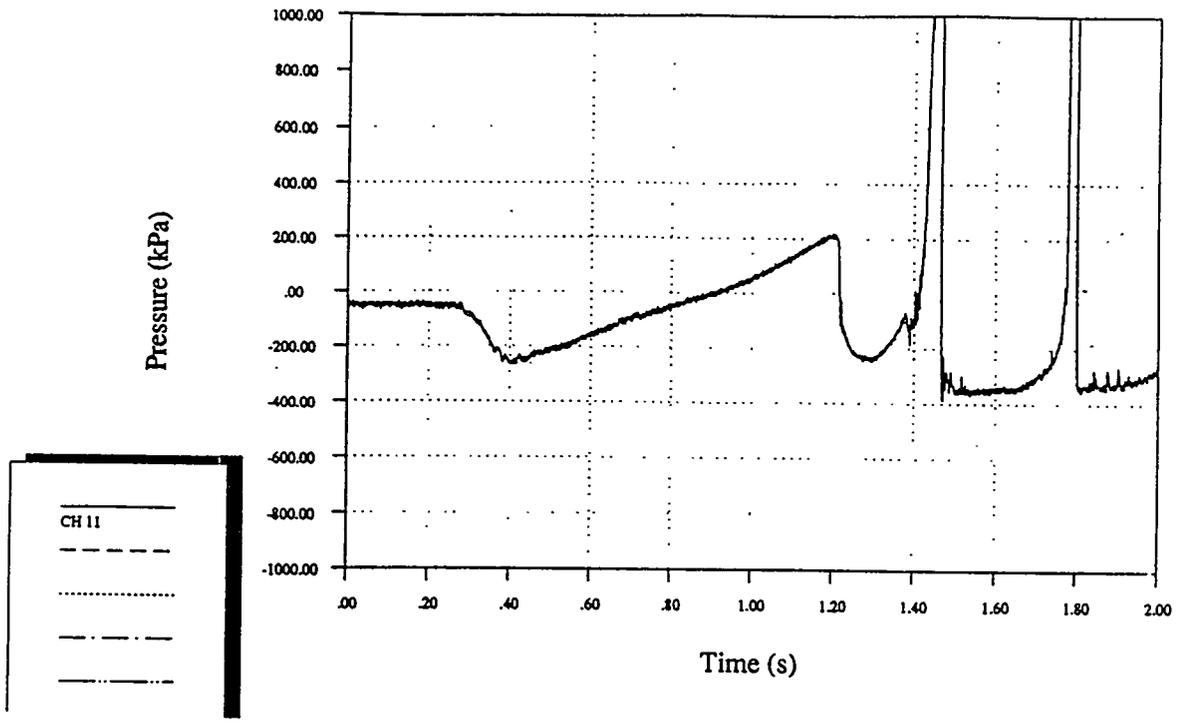


Figure 12. Experimental pressure transient at the dead-end location for Case (2) with tank pressure 551 kPa, water temperature 22 C and steam temperature 142 C.

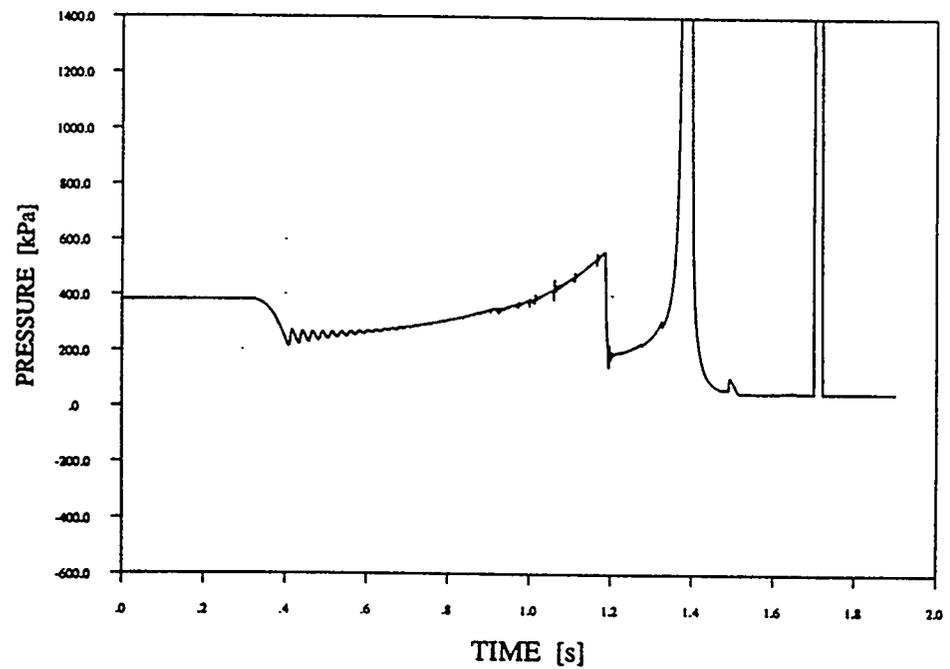


Figure 13. Predicted pressure transient at the dead-end location for Case (2) with tank pressure 551 kPa, water temperature 22 C and steam temperature 142 C.

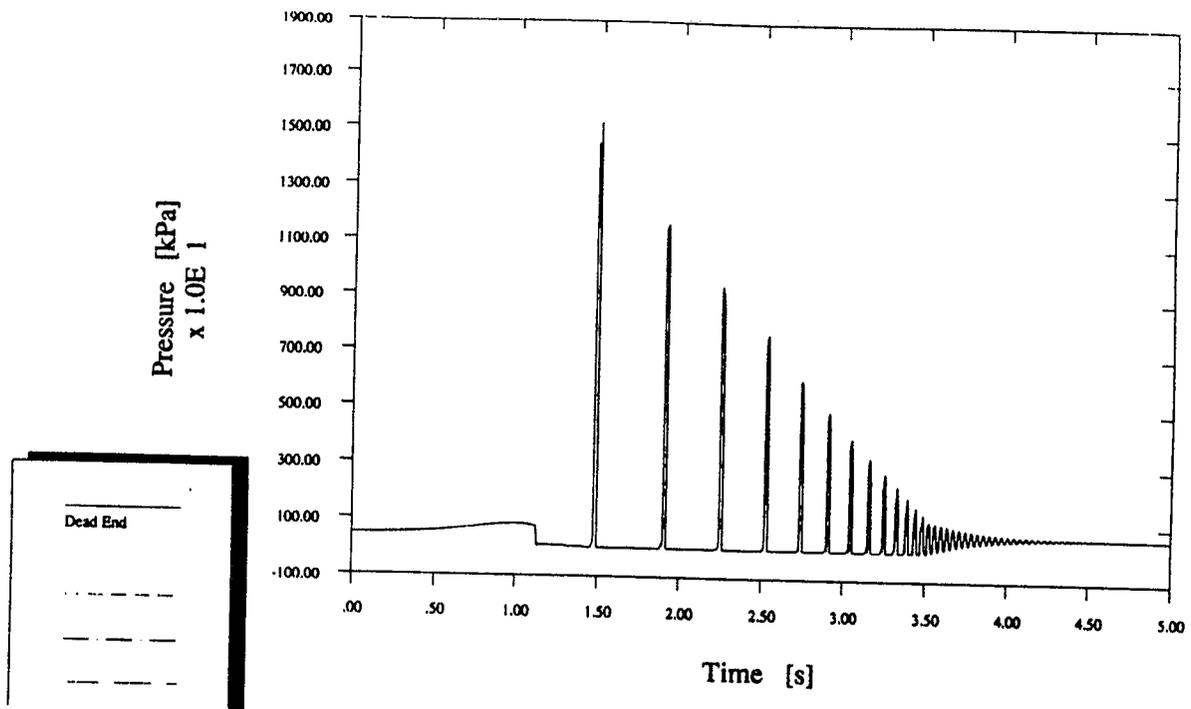


Figure 8. Predicted pressure transient at the dead-end location for Case (1) with tank pressure 654 kPa, water temperature 23 C and steam temperature 150 C.

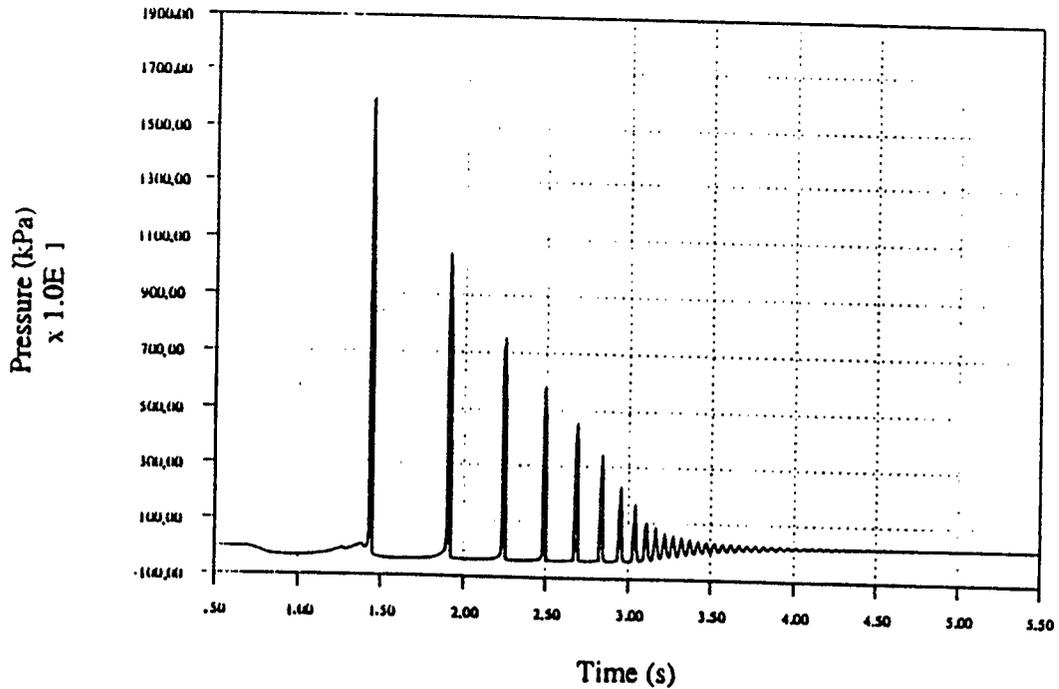


Figure 9. Experimental pressure transient at the dead-end location for Case (1) with tank pressure 654 kPa, water temperature 23 C and steam temperature 150 C.

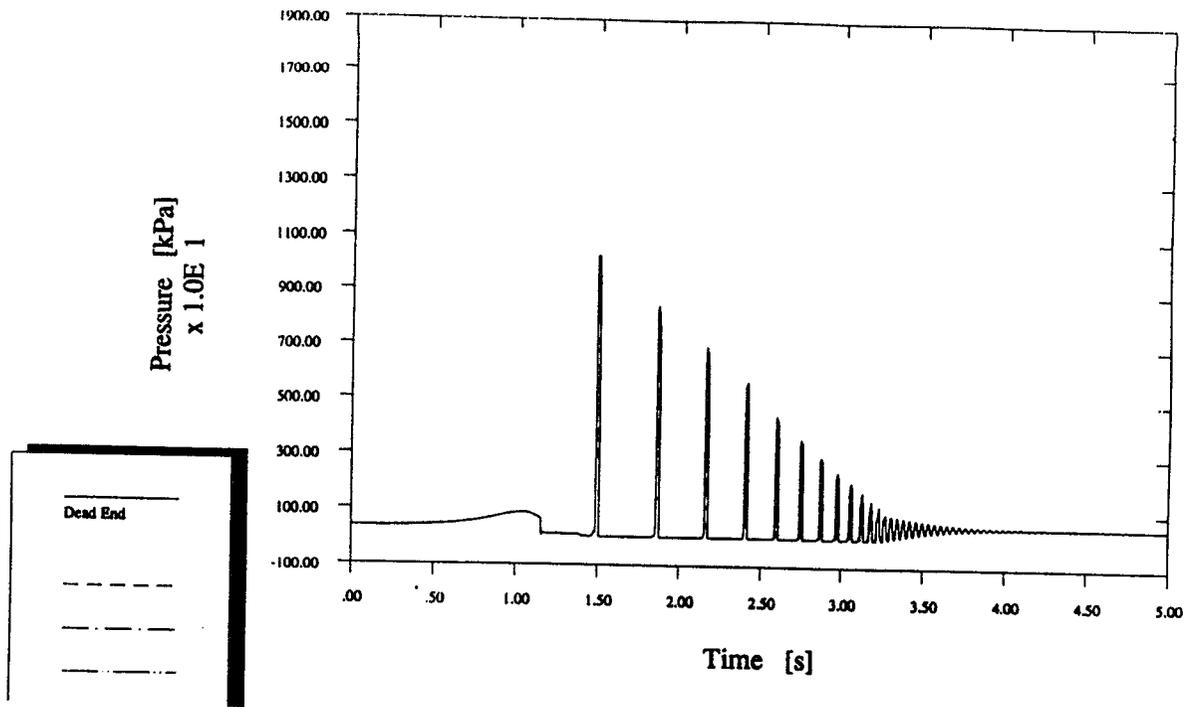


Figure 10. Predicted pressure transient at the dead-end location for Case (2) with tank pressure 551 kPa, water temperature 22 C and steam temperature 142 C.

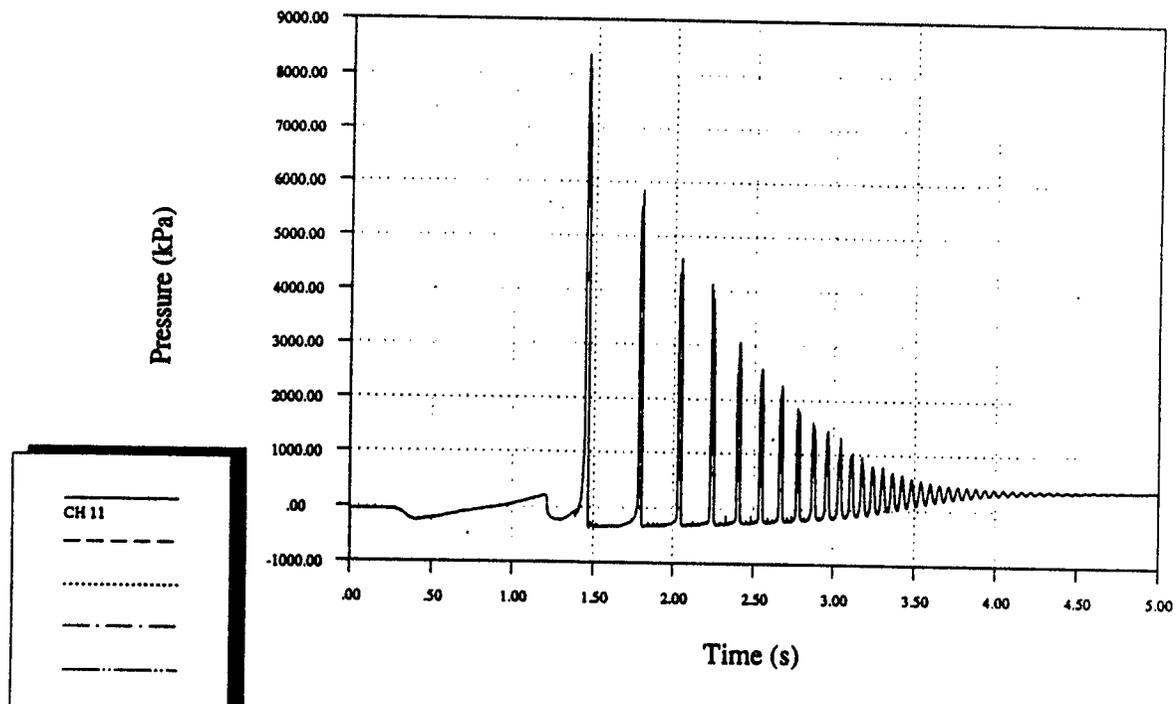


Figure 11. Experimental pressure transient at the dead-end location for Case (2) with tank pressure 551 kPa, water temperature 22 C and steam temperature 142 C.

Multidimensional Reactor Kinetics Modeling

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MULTIDIMENSIONAL REACTOR KINETICS MODELING

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Introduction

There is general agreement that for many light water reactor^a transient calculations, it is necessary to use a multidimensional neutron kinetics model coupled to a thermal-hydraulics model in order to obtain satisfactory results. These calculations are needed for a variety of applications for licensing safety analysis, probabilistic risk assessment (PRA), operational support, and training. The latter three applications have always required best-estimate models, but in the past, applications for licensing could be satisfied with relatively simple, but conservative, models. By using more sophisticated best-estimate models, the consequences of these calculations are better understood, and the potential for gaining relief from restrictive operating limits increases. Hence, for all of the aforementioned applications, it is important to have the ability to do best-estimate calculations with multidimensional neutron kinetics models coupled to sophisticated thermal-hydraulic models.

This need coincides with the fact that in recent years there has been considerable research and development in this field with modelers taking advantage of the increase in computing power that has become available. This progress has now led to coupling multidimensional neutron kinetics models to the nuclear steam supply system (NSSS) thermal-hydraulics. This is not new as modelers for training simulators have always had such a coupling. What is new is that the coupling can now be done with very sophisticated models, and the planning of this coupling and the requisite modeling can take advantage of the experience of many code developers in many countries. Indeed, the point of this paper is to present one approach for the neutron kinetics for future codes gleaned from the state-of-the-art.

Specifically, this paper reviews the status of multidimensional neutron kinetics modeling which could be used in conjunction with thermal-hydraulic models to do core dynamics calculations, either coupled to a complete NSSS representation or in isolation. Also discussed is the modeling which complements the neutron kinetics and completes the reactor dynamics package. The paper makes recommendations as to what should be the state-of-the-art for the next ten years. This includes some existing capability and some new modeling that is needed. The review is an update to a previous review of the status as of ten years ago.¹ It takes into account the capabilities and limitations of current codes and supplies references for the interested reader.

The paper is organized as follows. First, the basic multidimensional neutron kinetics model is discussed. This is the heart of a core dynamics capability, but ancillary models also need to be considered. These are treated in a following section. Next is found a section discussing the specific applications of these codes. In addition to demonstrating the need for multidimensional neutron kinetics, this section also shows how the applications determine other modeling that should be present. Another section summarizes state-of-the-art

^a This paper is meant to be applicable to boiling water reactors (BWRs) and to pressurized water reactors of both Western design (PWRs) and Russian design (VVERs).

codes which help provide the guidance needed for the next generation. The final section summarizes the main conclusions from this review.

The Basic Multidimensional Neutron Kinetics Model

The basic multidimensional neutron kinetics model that is currently the state-of-the-art and is expected to be applicable to LWR applications for the expected future is based on the 3-dimensional neutron diffusion equation for two neutron-energy groups and with six groups of delayed neutron precursors. Several solution methods are considered state-of-the-art although those that are expected to be most applicable in the future utilize a nodal method to handle the spatial dependence and direct integration to handle the temporal dependence. In the following, the basic equations are first considered and then the solution methods are discussed.

For LWRs, a 2-group diffusion theory approach has proven to be adequate for steady-state applications, and, for those transient applications where direct validation is possible, it also has been found to be adequate. One could argue that more energy groups might improve the rigor of the methodology, e.g., in events where voiding occurs quickly causing the energy spectrum to change rapidly. Similarly, a higher order approximation to the angular dependence of the neutron flux (i.e., a more rigorous approximation to the transport equation than diffusion theory) might improve the rigor, e.g., in boron dilution events when there is an abrupt change in neutron absorption across a wide region. However, since there is an interest in making the transient analysis compatible with steady-state core calculations, and since the research to provide direct evidence that these higher order methods give more accurate results has not yet been done, 2-group diffusion theory should continue to be the standard approach.

Six delayed neutron precursor groups are the standard for treating LWRs, and no change should be made in this area either. However, it should be noted that delayed neutron precursor parameters should be defined for each computational cell throughout the core. Although this is the practice in some state-of-the-art codes, some transient codes currently in use use global averages for the delayed neutron parameters.

The equations are to be solved in three dimensions using rectangular or hexagonal geometry. Multidimensional kinetics should be equated with 3-dimensional kinetics for the simple reason that there is no need to consider 1-dimensional or 2-dimensional models. The latter two approximations are only applicable for certain transients when there is separability between the axial and radial changes during a transient. Furthermore, both of these approximations require considerable analysis in order to obtain nuclear data that have been properly averaged over the remaining dimensions (e.g., over the radial plane when the axial direction is explicitly modeled). Their use also requires a mechanism for turning the simplified approach on and off during a calculation. This complicates the analysis and negates any simplification that might result from using a lower order spatial representation. Hence, it has become well-established that only 3-dimensional methods are of interest.

Note that this does not preclude the use of point kinetics models when the neutronic response of the core is not of primary importance, e.g., when the core is quickly shut down. A code which models the NSSS should have the ability to use point kinetics with parameters supplied by the user or calculated from the 3-dimensional neutronics model. The latter can easily be done under the assumption that the point kinetics parameters will only be used for small perturbations. When no kinetics is necessary, i.e., when the core is shut down, the decay heat model can utilize the calculated steady-state power distribution to obtain decay heat loads throughout the core.

The basic equations for neutron kinetics (3-dimensional diffusion theory in two groups) can be solved in many different ways. An excellent recent review of these methods exists,² and, hence, methods will not be discussed herein in any detail. It is sometimes convenient to separate the solution methods for the space dependence from those for the time dependence. For the space dependence, it is either nodal methods or coarse-mesh diffusion theory (CMDT) methods that are the most successful in terms of accuracy per unit of computation. Within these categories, it is perhaps transverse-integrated nodal methods that are the best. "These methods produce results that are comparable to those of fine-mesh finite difference calculations at a small fraction of the computational cost. The success of these methods is due to their ability to use large computational mesh boxes ... without sacrificing accuracy or limiting the type of information that may be obtained. The use of coarse computational mesh in space ... results in a dramatic decrease in the number of unknowns--and hence computer resources--while the high order spatial treatment within a node, coupled with the use of advanced homogenization procedures, maintains the accuracy at the level of the more expensive fine-mesh calculations. Dehomogenization methods have been developed which allow the determination of detailed intranodal flux and power distributions despite the coarseness of the mesh used for the nodal solution."² The Nodal Expansion Method (NEM) and the Analytic Nodal Method (ANM) are two nodal methods that have been applied successfully in current state-of-the-art codes.

Implicit in the use of nodal (or coarse-mesh) methods is that fuel assembly properties can be appropriately homogenized in order to use the large mesh of a nodal model. This is generally the case in spite of the fact that the homogenization is usually done by calculating an isolated assembly, i.e., without regard to the correct boundary conditions. However, with the introduction of assembly discontinuity factors, it is possible to enhance the accuracy.³ These factors are defined for each assembly (along with the cross sections) in order to account for some of the heterogeneity in the assembly. Although in the past they have been used for the radial direction, some consideration should be given to how they can be used in the axial direction to account for material discontinuities found in some reactor designs. The reverse process, dehomogenization, is also important because accuracy on a fuel-rod basis requires using a flux reconstruction algorithm. This will be discussed below.

The spatial solution method requires boundary conditions which are frequently at the boundary of the fueled region. At this boundary, complicated geometries and materials make it difficult to get accurate results. It is important that the boundary conditions (either at the edge of the fueled region or elsewhere) be sufficiently rigorous so that the accuracy of the method does not degrade at the boundary.

The time dependence can be treated with a direct or indirect approach. The best example of the latter is the improved quasistatic method (IQS). The IQS is based on a space-time factorization so that the spatial dependence can be solved using time steps much larger than used for the global power. Although this allows for flexibility in choosing time steps, the time steps are eventually determined by the rate at which the spatial shape is changing. Direct methods are indeed more direct and can be used in conjunction with time-step algorithms which improve the computational efficiency of the process. These algorithms allow for time steps to vary according to a set of criteria and may even allow for backstepping (the repeating of a calculational step) if necessary. In the same way that nodal methods have improved the efficiency of solving the spatial problem, new algorithms for solving sparse matrices have improved the efficiency of solving for the time dependence so that direct methods should now be the standard approach. Because of the stiffness of the neutron kinetics equations, implicit integration methods are generally used to advance the time.

Other Modeling Important to a Reactor Dynamics Capability

The neutron kinetics model is the heart of a core dynamics computer code, but there are many other components to consider when putting together a complete package. The additional models that are discussed below are for problem initialization, cross sections, and power generation. The thermal-hydraulics model is also important but is not the subject of this paper. However, thermal-hydraulic compatibility with the neutronics is discussed in the following section on applications.

It must be recognized that in order to do transient calculations, it is necessary to first have a steady state. The static form of the neutron kinetics equations is an eigenvalue problem, and the eigenvalue is equivalent to the multiplication factor for the steady-state core. A problem can be initialized in various ways. The parameters that determine the initial statepoint of the reactor are the power level, the control rod pattern, the boron concentration (for PWRs and VVERs), and inlet temperature, subcooling and flowrate. If these are all consistent, then one should obtain an eigenvalue of unity indicating that the reactor is just critical (steady state) at this statepoint. In practice, the eigenvalue is close to, but not equal to, unity. It is important that the code be able to search for either the power level, control bank position, boron concentration, or inlet condition to reach a particular eigenvalue (ideally unity) to represent a proper statepoint. This capability should be built into the steady state part of the calculation.

Another type of steady state that could be of interest is a fixed-source problem where the reactor is at shutdown conditions with an external (i.e., non-fission) source enabling the multiplication. A code with this steady-state capability would allow for much wider flexibility in treating different initial conditions for transient problems as well as in simulating startup operation.

In setting up initial conditions, it is necessary to include the effects of xenon and samarium. The distribution of these nuclides throughout the core can be calculated using the formulae for their equilibrium concentrations. However, it is a relatively straightforward addition to also include the appropriate fission product chains so that these distributions can be obtained for different slowly changing conditions (i.e., "xenon transients") in order to have additional flexibility in starting transients from different initial conditions. Other variations can also be included such as starting from maximum xenon or samarium.

Cross sections must depend on all the thermal-hydraulic feedback and control variables, i.e., fuel temperature, coolant temperature and density, boron concentration, and the presence of control rods. The fuel temperature should be an effective temperature based on the temperatures calculated by the fuel rod heat conduction model, e.g., a function of pellet average and centerline (or surface) temperatures. For BWRs, an effective coolant density and boron concentration can also be defined to account for voiding and boron in the bypass channel. This is connected to a need to have the bypass region represented in the thermal-hydraulic modeling in more detail than just as a single channel. This in turn is further complicated in new fuel designs by having not only the bypass region outside the fuel bundle channel but also a bypass region associated with special water channels within a fuel bundle.

The dependence of the cross sections on the above variables can be specified either through analytic functions (typically polynomials) or through a sophisticated table look-up. The cross section functions/tables must be specified for each mesh box along with the delayed neutron parameters and discontinuity factors for that mesh box. The spatial dependence of the cross section functions is due to changes in fuel assembly design and burnup throughout the core. Burnup dependence is usually through one or two independent variables: exposure (GWd/t), and a parameter that expresses the history of the bundle germane to spectral

effects. Exposure weighted void or coolant density history are the most common of the parameters in the latter category.

Implicit in the discussion of the cross section representation is the need for a methodology to calculate these quantities. Although that methodology is beyond the scope of this paper, it is necessary to emphasize that the neutron kinetics capability can only be used if this methodology exists.

The power generation model takes the fission rate, adds decay heat, and distributes the heat generation rate in fuel and coolant regions (and bypass regions for BWRs). The decay heat contribution may become important when starting a transient from low power or after shutdown of the fission power. Decay heat functions can be specified according to exposure throughout the core and used in conjunction with a steady-state power distribution when the neutron kinetics is not needed.

Applications of 3-Dimensional Neutron Kinetics

The specific types of transient calculations that require multidimensional neutron kinetics when analyzing PWRs and VVERs are listed in Table 1. These applications influence the modeling that should be present in a computer code beyond the basic multidimensional neutron kinetics. Although the emphasis in this paper is on reactor physics modeling, some applications also point to the need for special thermal-hydraulics modeling. For example, the first two transients in the list (steam line break and startup of cold loop) are calculated as part of a plant's safety analysis. In order to accurately represent the cooling of the core, it is important to know the inlet temperature distribution across the core. This may be available from a 3-dimensional thermal-hydraulic model for the vessel or from a special mixing model.

Table 1 PWR/VVER Transients for which Multidimensional Neutron Kinetics is Important

PWR/VVER Applications
Steam line break
Startup of cold loop
Rod ejection accident
Boron dilution events
Transients without scram
Instrumentation response

The third item in the list, the rod ejection accident, is the design-basis reactivity-initiated accident. The consequences of this accident as well as of most other accidents need to be evaluated in terms of fuel rod response rather than bundle-average response. For this event it is fuel rod enthalpy whereas for other events it may be DNBR (departure-from-nucleate-boiling ratio) or peak cladding temperature. This means that if a calculation is done with planar meshes that are the size of fuel assemblies (or even quarters of assemblies), modeling must be present to do the dehomogenization or flux reconstruction in order to obtain fuel rod response. This also implies that a multichannel thermal-hydraulic model may be necessary. The need for fuel rod information places a heavy burden on the overall calculation. Consideration needs to be given to

having only a certain segment of the core use flux reconstitution. It then becomes a challenge to understand what, if any, information from the microscopic (fuel rod) calculation should be fed back into the macroscopic (assembly average) calculation.

The fourth item in Table 1, boron dilution events, refers to any scenario that might be possible during shutdown, ascent to power, or full power operation. This requires the accurate modeling of boron transport through the system as well as the ability to represent a non-uniform distribution across the core inlet as was necessary for the cold water transients discussed above.

The fifth item, transients without scram, refers not only to the most limiting event, which is likely caused by a loss of feedwater at beginning of cycle, but also to a spectrum of events that might be important to analyze as part of a PRA. The last item in the table refers to the fact that for operational support (e.g., for determining setpoints) or training, it may be necessary to calculate transients for which it is important to note the response of incore and excore instrumentation. This requires that these instruments be modeled and that their connection to the reactor protection system and any control system also be modeled.

Large loss-of-coolant accidents are not listed in the table because the neutronic response is not usually of interest. However, the assumption is usually made that the forces during blowdown are sufficient to prevent the insertion of control rods. Therefore, it is of interest to see if the assumptions regarding the shutdown of the reactor due to voiding and injection of borated water are justified by doing the calculation with a neutron kinetics capability.

Table 2 shows the list of events for BWRs for which multidimensional neutron kinetics modeling is needed. Again, a review of these events sheds light on modeling that is needed and some of that modeling is the same as is needed for PWRs/VVERs.

Overpressurization events and inlet disturbances of both temperature and flowrate are analyzed as part of the licensing safety analysis. Some of the inlet perturbations (e.g., due to trip of one recirculation pump) should be specified as a function of position across the core inlet, and this requires either 3-dimensional modeling in the vessel or some multichannel model which will supply the appropriate core boundary conditions. These events along with the rod drop accident require knowing conditions in individual fuel rods, and, hence, as discussed above for PWRs/VVERs, dehomogenization or flux reconstruction is needed when using codes that use meshes the size of bundles.

Transients without scram must be analyzed with a boron transport model that models flow in individual channels including bypass channels. Because there are different boron injection points and because injection may proceed under low flow conditions there are considerable challenges for this modeling.

Table 2 BWR Transients for which Multidimensional Neutron Kinetics is Important

BWR Applications
Overpressurization events
Core inlet temperature disturbances
Core inlet flow disturbances
Rod drop accident
Transients without scram
Stability analysis
Instrumentation response

Current Computer Codes

It is instructive to look at the state-of-the-art in order to understand how much modeling capability that could be used for an advanced reactor analysis package already exists and how much might have to be developed. The focus here will be on codes in the U.S. although some of these codes are also used abroad.

One example of a code that is in the public domain that has many of the desirable features discussed above is NESTLE.⁴ The code uses the NEM approach and is applicable to both rectangular and hexagonal geometry. It does steady-state searches to solve the eigenvalue problem and has many other features that are desirable but peripheral to the discussion herein. Examples of these are the option of using four neutron energy groups, of using a finite difference method rather than the NEM, and the ability to calculate the adjoint (steady-state) problem (useful in deriving point kinetics parameters). NESTLE has been integrated into the system thermal-hydraulic codes RELAP5.⁵

There are several other similar codes that are in use in proprietary or special circumstances. There are also several codes that are currently in use which may not be considered state-of-the-art, but, nevertheless, they are used successfully for a range of applications and a study of their characteristics is informative and necessary for designing a new capability. These other codes are listed in Table 3 along with some special notes that identify unique features.

Table 3 Three-Dimensional Core Kinetics Codes Currently in Use

Code	Special Modeling Features	Comments
NESTLE ⁴	Two-group NEM	Has been coupled to NSSS thermal-hydraulic code (RELAP5)
SIMULATE-3K ⁶	Two-group NEM or semi-analytic nodal method	Has excore instrumentation models
ARROTTA ⁷	Two-group ANM	One version coupled to NSSS thermal-hydraulic code (RETRAN)
TRAC-PF1/NEM ⁸	Two-group NEM	Coupled to NSSS code TRAC-PF1 for PWR applications
SPNOVA ⁹	Two-group nodal method with approximation (G-matrix method) to speed up computation	For PWR applications
RAMONA ¹⁰	1½ energy groups, CMDT	Includes NSSS modeling for BWR
RAMONA ¹¹	Two-group ANM	New capability for PWR/BWRs
TRACG ¹²	One group, CMDT, IQS	Coupled to BWR NSSS code TRAC
DIF3D-K ¹³	Multigroup, direct or IQS, hex and rectangular geometry	
CONCERT ¹⁴	1½-group CMDT, IQS	Used for training simulators
REMARK ¹⁵	Two-group coarse mesh finite difference equations	Used for training simulators

Conclusions

The next generation of system thermal-hydraulic code should include a three-dimensional neutron kinetics capability based on the 2-group diffusion equation with six delayed neutron precursors represented. Existing nodal methods such as NEM and ANM along with the use of assembly discontinuity factors have already proven to be sufficiently accurate for many applications. New solution algorithms exist which allow for direct integrations of the equations in time. These are very important because in spite of improvements in computer hardware, the requirements for the next generation of codes puts a large burden on the computing capability. Current modeling does not automatically do the flux reconstitution that is needed to obtain limiting parameters for individual fuel rods. The additional ability to model fuel rods explicitly will be a challenge from the point of view of adding to the calculational time and resources needed. New methods to consider detail in some fraction of the core with feedback into the global calculation will need to be developed. Improved boundary conditions may also be necessary to improve the accuracy of the calculated power in assemblies with relatively low power.

The planning for a reactor dynamics capability requires consideration of modeling ancillary to the neutron kinetics such as for problem initialization, cross sections, and power generation. Initialization of the problem requires an ability to do both an eigenvalue or fixed source calculation with searches on the important reactor parameters which determine initial conditions. It is important that the code be able to handle not only full power conditions but also startup situations.

Cross sections in the next generation of codes should depend on more detailed thermal-hydraulic parameters than currently used. Effective fuel temperature should account for the pellet temperature distribution, not just the average temperature. Effective coolant density should account for nearby bypass regions as well as for the bypass regions within BWR fuel bundles. Data handling will become more complex to reflect the need to have different cross sections, assembly discontinuity factors, delayed neutron parameters, and decay heat parameters for each mesh box.

There are several requirements on the thermal-hydraulics imposed by the neutron kinetics modeling. One is the need to take into account bypass regions in more detail. Another is the need for subchannel thermal-hydraulics to be consistent with the need for flux reconstitution. For many transients the core response will depend on the distribution across the core inlet of flowrate, temperature, etc. This requires multidimensional thermal-hydraulic modeling in the reactor vessel.

References

1. D.J. Diamond and M. Todosow, Light Water Reactor Space-Dependent Core Dynamics Computer Programs, *Advances in Nuclear Science & Technology*, 18, pg 357, Plenum Press, 1986.
2. T.M. Sutton and B.N. Aviles, "Diffusion Theory Methods for Spatial Kinetics Calculations," *Prog. in Nuclear Energy*, 30, pg 119-182, January 1996.
3. K.S. Smith, "Assembly Homogenization Techniques for Light Water Reactor Analysis," *Prog. in Nuclear Energy*, 17, pg 303-335, 1986.
4. P.J. Turinsky, et al., "NESTLE: A Few-Group Neutron Diffusion Equation Solver Utilizing the Nodal Expansion Method for Eigenvalue, Adjoint, Fixed Source Steady State and Transient Problems," EGG-NRE-11406, Idaho National Engineering Laboratory, June 1994.
5. J.L. Judd, W.L. Weaver, T. Downar, and H.G. Joo, "A Three-Dimensional Nodal Neutron Kinetics Capability for RELAP5," Proceedings of the 1994 Topical Meeting on Advances in Reactor Physics, Knoxville, April 1994. J. Judd et al., "High Fidelity, Real Time Simulation with RELAP5/NESTLE," *Trans. Amer. Nucl. Soc.*, 75, November 1996.
6. J. Borkowski, J. Rhodes III, P. Esser, and K. Smith, "Three-Dimensional Transient Analysis Capability in SIMULATE-3," *Trans. Amer. Nucl. Soc.*, 71, November 1994. K. Tate, J.A. Borkowski, and S. Arai, "Verification of the SIMULATE-3 Kinetic Version Based on Transient Tests of Boiling Water Reactor," Proceedings of International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses, Portland, April 1995.
7. L. Eisenhart, et al., "ARROTTA-01 An Advanced Rapid Operational Transient Analysis Computer Code," EPRI NP-7375-CCM, Electric Power Research Institute, October 1991.

8. B.R. Bandini, "A Three-Dimensional Transient Neutronics Routine for the TRAC-PF1 Reactor Thermal Hydraulic Computer Code," PhD dissertation, Pennsylvania State University, May 1990.
9. Y.A. Chao and P. Huang, "Theory and Performance of the Fast-Running Multidimensional PWR Kinetics Code, SPNOVA-K," Proceedings of the 1988 International Reactor Physics Conference, Jackson Hole, September 1988.
10. W. Wulff, H.S. Cheng, D.J. Diamond, and M. Khatib-Rahbar, "A Description and Assessment of RAMONA-3B Mod.0 Cycle 4: A Computer Code with Three-Dimensional Neutron Kinetics for BWR System Transients," NUREG/CR-3664, Brookhaven National Laboratory, January 1984. U.S. Rohatgi et al., "RAMONA-4B: A Computer Code with Three-Dimensional Neutron Kinetics for BWR and SBWR System Transients," to be published, Brookhaven National Laboratory, 1996. "RAMONA-MB; A BWR System Analysis Code with Advanced 3-Dimensional Core Model," Siemens Power Corporation, to be published. A version is also in use at ABB Combustion Engineering.
11. S. Lindahl and D. Babala, "Transient Neutronics in RAMONA and POLCA Based on the Analytic Nodal Method," Proceedings of the International Conference on the Physics of Reactors, PHYSOR96, Mito, Ibaraki, Japan, September 1996.
12. J.G.M. Andersen, et al., "Licensing Topical Report - TRACG Model Description," NEDE-32176P, Rev. 1, General Electric Co., February 1996.
13. T.A. Taiwo and H.S. Khalil, "An Improved Quasistatic Option for the DIF3D Nodal Kinetics Code," Proceedings Topical Meeting on Advances in Reactor Physics, Charlston, March 1992.
14. G-H. Wang, E.K. Lin, D.J. Diamond, and G.W. Smith, "CONcERT - Core Neutronics Engineering in Real Time," Proceedings of the Simulation Multiconference on Simulators International VIII, New Orleans, 1991.
15. C. O. Tsaoi, "Real Time Simulation of Reactor Core Physics with REMARK and STK Core Models," Proceedings of the 1994 Simulation Multiconference, San Diego, April 1994.

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3D Neutronic Codes coupled with Thermal-Hydraulic System Codes
for PWR, BWR and VVER Reactors

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Abstract

This paper describes the objectives of code development for coupling 3D neutronics codes with thermal-hydraulic system codes. The present status of coupling ATHLET with three 3D neutronics codes for VVER- and LWR-reactors is presented. After describing the basic features of the 3D neutronic codes BIPR-8 from Kurchatov-Institute, DYN3D from Research Center Rossendorf and QUABOX/CUBBOX from GRS, first applications of coupled codes for different transient and accident scenarios are presented. The need of further investigations is discussed.

1 Introduction

The safety analysis of NPPs is based on analytical methods for different fields of plant behavior under accident conditions. System codes like ATHLET, CATHARE or RELAP have been developed for analysis of plant transients and loss of coolant accidents. 3D-neutronics codes solving neutron diffusion equations for static and dynamic conditions are available to analyze reactivity conditions and spatial power density distributions in reactor cores. In both fields of safety analysis very detailed physical models and efficient solution methods have been implemented. Nevertheless, there is a need for more

realistic modeling of accident conditions for transients with strong coupling between neutronics and thermo-fluid dynamics. This can be achieved only by coupling 3D neutronics codes to system codes. Work has been performed to couple the system code ATHLET to different 3D neutronics codes modeling VVER- and LWR-reactors with hexagonal and rectangular fuel assemblies respectively. The state of code development together with first examples of application will be presented. This paper is not intended as a general review, it is based on the specific considerations and experiences during planning, implementation and first applications of coupling 3D neutronics codes to ATHLET.

2 Current safety problems requiring realistic modeling by coupled codes

In the past the safety analysis has been performed mainly by applying system codes with point kinetics or 1D-neutronics for plant transient analysis and by applying 3D-neutronics codes for analyzing spatial effects on power density distribution and reactivity behaviour of the core. The uncertainties of feedback reactivity coefficients and local power density peaking using simplified neutronics models were considered by conservative assumptions. In the same manner uncertainties of the 3D neutronics core behaviour determined by the global plant behavior were considered by properly defined boundary conditions. Therefore, the interfacing problems between neutronics in the reactor core and the fluid dynamics in the primary circuit needed proper consideration by the analyst. This approach was mainly born by practical aspects separating nuclear analysis and fluid dynamic and systems analysis and, in addition, it was a consequence of the available computer capacity. The progress of reactor safety research identified several issues, where this approach reaches its limits, and in parallel the ongoing optimization of fuel cycle economics leads to reactor core conditions which can be approved only by eliminating uncertainties from the analytical methods. Generally, the coupling of 3D neutronics with thermo-fluid dynamic system codes can reduce uncertainties of analytical methods for such transients being determined by a strong cou-

pling between neutronics in the core and fluid dynamics in the primary circuit. Examples of such accident conditions are:

- The local boron dilution accident in PWR, which was identified as a potential reactivity initiated accident even in shutdown conditions when all RCCA's being inserted.
- The cooldown transients with strongly negative moderator temperature reactivity coefficient (MTC) in PWR. The occurrence of a recriticality during cooldown and its consequences have to be analyzed. Such high values of MTC result of increased high burnup fuel or of extended use of MOX-fuel.
- The results of ATWS analysis are strongly affected by feedback reactivity coefficients. The uncertainties in inherent feedback efficiency limiting power production and consequently pressure increase, can be strongly reduced by applying 3D neutronics models. The spatial effects are emphasized if partial failure of RCCA insertion is postulated.
- The BWR instability in plant conditions beyond the stability threshold.

An additional aspect will be:

- New reactor concepts are proposed, in which core cooling is based on natural circulation. Thus, driving forces of coolant flow are determined by the nuclear power generation in the core and the heat sink dependent on heat transfer from the primary to the secondary side.

The analysis of these plant conditions of NPP with available analytical methods needs many assumptions and approximations related to the interface between 3D neutronics and system behavior. The only way to minimize these uncertainties and to avoid unnecessary limiting conditions for plant operation will be the development and application of coupled codes.

3 Description of 3D neutronics models coupled with system code ATHLET

The work of coupling the system code ATHLET, developed by GRS, with 3D neutronics models has been performed within various cooperations. Since problems discussed are not only relevant for PWRs and BWRs, but also for Russian VVERs, the work resulted in coupling following 3D neutronics codes:

- BIPR-8 for VVER reactor types with hexagonal fuel assemblies developed by Kurchatov-Institute,
- DYN3D for VVER reactor types developed by Research Center Rossendorf (RCR),
- QUABOX/CUBBOX for LWR reactor types with rectangular fuel assemblies. This code is also applied for analysis of RBMK reactors after some adaptations.

These 3D neutronics codes have been coupled with the system code ATHLET. The considerations of implementation of this coupling are presented in a companion paper of this workshop /LAB 96/. The main feature is that the coupling was implemented by defining for ATHLET a general interface to nuclear models. The approach is based on coupling of the 3D neutronics models to the system code which models completely the termalhydraulics in the primary circuit including the core region.

The codes being coupled can be characterized as follows:

ATHLET

ATHLET /AUH 95/ is a modular system code like CATHARE and RELAP describing all phenomena involved in the operation of light water reactors. It provides models for thermofluidynamics, heat transfer and heat conduction, neutron kinetics and control simulation modules. A detailed description is given in the contribution /TES 96/ to this workshop.

BIPR8KN

The three-dimensional reactor kinetics code BIPR8KN /LIZ 92/ is a branch of the stationary code BIPR8 including reactivity control, feedback effects, fuel burnup and re-

loading. The series of BIPR codes is one of the main part of the code package for VVER's design and operational neutronics calculations. Relations to other neutronics codes (including processing of nuclear data libraries) and examples of validation can be seen from /NOV 89/. The main idea of stationary neutron balance equation of BIPR8 is based on the representation of the two groups diffusion equation solution in each hexagonal node (one fuel assembly in plane and part of assembly axially) by the superposition of asymptotic and transient modes. The set of trial functions used for the asymptotic mode of solution for homogeneous nodes consists of cos and sin in axial direction and multiplications of corresponding orders of cos and Bessel functions for radial-azimuthal direction. Taking into account the short action of transient mode relative node size the approximation of two semispaces and exp trial function is used for this mode. To satisfy neutron flux and current continuity conditions for all boundaries of adjoined nodes the weighting factors for all trial functions have to be determined. To determine the weighting factors the values of some functionals of trial functions in addition to traditional average neutron cross sections are used in neutron balance equation of BIPR8. This functionals are defined only by the nodes properties and can be obtained together with average nodes neutron cross sections (analytically or numerically). For kinetics calculation the term of flux derivative on time was implemented into initial diffusion equations and part of delayed neutrons source was separated from full source. Six groups of delayed neutrons are taken into account in delayed neutrons source. The same set of trial functions is used in BIPR8KN for description of inner assembly neutron flux structure as for stationary case. During transient calculation the time step size is defined before each step by the common estimation of current process speed and properties change from the condition that expected maximum of local power change to be not greater then the required value.

The BIPR8KN code consists only of the 3D neutronics model, no thermohydraulic model was implemented to describe the coolant flow in the core region. Verification of BIPR8KN was made on analytical and numerical benchmarks (including three 3D AER benchmarks /AER/ and on RRC KI V1000 full scale critical facility kinetics experimental data /LIZ 92/.

DYN3D

The three-dimensional reactor core model DYN3D /GRU 93, GRU 96/ has been developed in the Research Center Rossendorf (RCR) to improve the simulation of reactivity initiated accidents (RIA), where space-dependent effects in the reactor core are relevant. The version DYN3D/H1.1 of the code deals with hexagonal fuel element geometry. Recently, a version for rectangular geometry has been developed and is under testing /GRU 95b/.

The neutron flux distribution is calculated in DYN3D/H1.1 using a nodal expansion method for hexagonal geometry. The neutron diffusion equations are solved for two energy groups. Steady state and transient behavior can be calculated. An option of the code allows the determination of burn up distribution after a given reactor operation history during the fuel cycle which can be used as initial condition for transient analyses. The steady state neutron balance equations are solved by applying an iterative procedure including inner and outer iteration cycles. In the outer iteration cycle a fission source iteration with Chebyshev acceleration is carried out. The time-dependent equations are solved using an implicit difference scheme with exponential transformation technique.

The code comprises a model of the thermohydraulics of the core, a fuel rod model describing the thermo-mechanical behavior of fuel and cladding and a heat transfer regime map ranging from one- phase liquid flow to superheated steam. A special model for the mixing of coolant from different primary loops in the lower plenum of VVER-440 type reactors is also included. The code allows the estimation of safety relevant parameters like critical heat flux ratio, maximum temperatures or cladding oxide layer thickness due to metal-water reaction in the high temperature region.

The modeling of thermohydraulics is based on four balance equations for mass, energy and momentum of the two-phase mixture and mass balance of the vapor phase. Thus, the dynamic modeling of thermal non-equilibrium between the phases (subcooled boiling) is possible. The set of equations for thermohydraulics is numerically treated by an iterative coupling of the individual balance equations, which are solved by applying different implicit schemes. The time step sizes for neutron kinetics and thermohydraulics are controlled independently in such a way, that the changes of

relevant parameters during each time step are limited. Between neutron kinetics and thermohydraulics iterations are accomplished until a given accuracy is reached.

The code has been validated on

- steady-state 2D and 3D and kinetic Benchmarks,
- kinetic experiments at the zero power reactor LR-0,
- comparisons of calculated results for critical boron acid concentration, reactivity worth of control rod groups and reactivity coefficients with measurement data from NPP.
- the thermo-hydraulic single effect tests and experiments on fuel rod behavior under RIA conditions at pulsed reactors.

QUABOX/CUBBOX

The 3D neutronics code solves two group neutron diffusion equations for static and time-dependent problems /LAN 77, LAN 77a/. It uses a coarse mesh method based on a polynomial approximation of spatial neutron flux distributions, achieving high accuracy for a nodalization corresponding to fuel assembly size in radial plane and an axial mesh size of 20 to 30 cm. The static solution is obtained by solving an asymptotic time-dependent problem with adaptation of criticality conditions by k_{eff} -search or adjustment of boron concentration.

The time-dependent neutron diffusion equations are solved with up to six groups of delayed neutron precursors by a direct solution using a matrix decomposition scheme, which allows to solve a series of one-dimensional implicit equations. The time-integration method is stable without limitation of maximum time-step size by numerical stability. A frequency transformation method is implemented using values of mean frequencies for prompt neutron groups and delayed neutron precursors. An option is available to calculate those frequencies by solving averaged point-kinetics equations.

The homogenized two-group cross-section data and the dependency on feedback parameters are described in a very flexible manner by interpolating from polynomial expansions or from functions tables.

The full 3D reactor core model QUABOX/CUBBOX-HYCA consists of this 3D neutronics model and a parallel coolant channel model describing coolant flow in the channel by a 1D solution of conservation equations of mass, energy and momentum for single and two-phase flows including a drift-flux correlation, and describing the average fuel rod by solving radial heat conduction equations.

The code has been validated by

- static and transient nuclear benchmark problems /FIN 93/
- extended code comparisons for different reactor types
- comparison with data from nuclear measurements during startup or operation e.g. critical boron concentration, reactivity worth of control rods, reactivity equivalents, power density distributions.

4 Results of calculations with coupled codes

In the present stage of code development calculations are performed mainly for defined test problems. The BIPR8 application includes comparisons with real plant data. The objective of results presented is mainly the demonstration of successful solution of typical problems from the intended field of applications.

BIPR8

A solution of ATHLET coupled with 3D neutronics code BIPR8 is presented for a transient of a single pump coastdown (1 out of 4) in a VVER-1000, Plant transient data exist from a startup experiment in NPP Balakovo 1, which have been used for comparison.

The event sequence is the following:

- The initial power is 95% of nominal power N_{nom} . At the beginning of the transient the pump in loop 1 is switched off.
- Three seconds after pump switching off the reactor power limitation device (ROM) started to reduce reactor power up to 71% N_{nom} by the insertion of control rod

group. Later, the second ROM action reduced reactor power up to 62% N_{nom} by inserting the same control rod group. Afterwards, the reactor power controller keeps the reactor power constant.

- According to the signal „ROM actuation“ the turbine control system started to reduce turbine power, while keeping the main steam-line nominal pressure constant.
- The actuation of control systems kept values of primary side pressure, pressurizer water level, water level in the steam generator within their operational ranges.

The calculation was performed by using a two-loop representation of the plant. The reactor core was modelled in 30 degree symmetry with 19 thermal-fluid channels and an additional reflector channel.

The Figs 1 and 2 show main plant parameters for this transient including comparisons with experimental results for reactor neutron power, relative speed of the pump switched off, primary and secondary side pressure and inlet and outlet temperatures for all four loops.

DYN3D

For a first test of the coupling ATHLET-DYN3D transient calculations for a simplified VVER-440 data set were compared with pure ATHLET calculations using point kinetics. In the simplified VVER-440 plant model used for this test calculations, the primary circuit is represented by a 5-fold loop and a 1-fold loop with steam generators and separate downcomers, the lower and the upper plenum of the reactor and the pressurizer connected to the 5-fold loop by the surge line. The secondary circuit is represented only by the secondary sides of the steam generators with inlet and outlet mass flow rates controlled by the water level and the pressure values in the steam generators. The core model has a 30 degree symmetry. This 30 degree sector of the core comprises 37 fuel elements and 37 corresponding coolant channels.

One of the test cases was the hypothetical ejection of the control rod group K6 from the initial position $z = 125$ cm within 0.1 s at full power without scram. This case does not represent a realistic accident scenario, but is a very demanding task for testing the code. The test case was chosen so that space-dependent neutron kinetic effects are

not very relevant so that the results of internal coupling, external coupling and point kinetics can be compared.

The tuning of steady state was done in the instationary calculations from 0 to 500 s. After that, the control group was ejected. The high reactivity insertion leads to a strong power pulse which was nearly compensated by fuel temperature Doppler feedback (see Fig. 3). The magnitude of the power peak is about 46 for point kinetics, 31 for the internal coupling and 26 for the external coupling. The high power level causes an increase of pressure in the primary circuit leading to repeated opening of pressurizer safety valves (see Fig. 4). At about 30 s after the ejection boiling of coolant occurs in the core. The asymptotical power level after the transient was stabilized at about 170% of the nominal power. Additionally, a comparative calculation with variations of the number of coolant channels in the core was carried out for the ejection of K6.

QUABOX/CUBBOX

A test problem was defined using a one-loop presentation of a PWR with a quarter core model. The core loading and the nuclear data were taken from the 3D LWR reactor core transient benchmark. The ATWS transient total loss of heatsink was calculated for this plant model. Typical results of main plant parameters are shown in Fig. 5 and 6.

5 Discussion of experiences and need of further investigations

It is practice to apply 3D reactor core models comprising 3D neutronics and multidimensional fluid dynamics either based on a parallel coolant channel model or a sub-channel model for safety analysis of reactor core transients. Referring to the current safety issues as discussed in chapter 2, the main objective of code development was to couple 3D neutronic codes to the thermal-hydraulic system code ATHLET. The 3D neutronics models have not been adapted by simplifications, they were coupled including all features of static design and core transient calculations. Not much experience is available up to now for the application of these coupled codes. The presented exam-

ples show the capability of these codes. But following questions need further investigations:

- Will it be possible by the available numerical methods to solve efficiently problems with hundreds of thermal-hydraulic channels?
Additional optimization of the numerical methods and their algorithms may be necessary. The effect of multiprocessor computers must be evaluated.
- How successful will be the grouping of thermal-hydraulic channels into regions describing the feedback effects on nuclear power generation?
This should be investigated by studies using different nodalization schemes.
- What is the effect of different fluiddynamic models on the power density distribution and its changes?
The system code ATHLET provides various fluiddynamic models, e.g. 5-equation model with drift-flux, 6-equation model, variants with integrated momentum equation. The effect of these fluidmodels on the transient behaviour should be investigated.
- What accident conditions need a multi-dimensional flow model of the downcomer and core region?
At least for boron dilution transients and for subcooling transients the mixing along the flow path through the downcomer must be modelled. The availability of such refined models will be an essential contribution to more realistic analyses.
- How accurate must be modelled the cross-flow between bundles in core geometries like in PWR and VVER-1000?
In design codes it is practice to apply for the core subchannel codes to determine thermal-hydraulic margins. The effect for accident conditions should be analyzed, e.g. by code comparisons because prototype implementations of such models are available /BOE 92, KNO 94/.

All these questions have to be evaluated by further studies in order to answer the question: how accurate the fluiddynamic modelling must be?

As the next step it is necessary to perform a thorough validation of available codes. This validation should be based on evaluation of plant data obtained during startup experiments or by specific transient events. Because plant data will not allow very extreme fluiddynamic conditions, this effort should be accompanied by benchmark activities for realistic accident conditions.

6 Summary

This paper has discussed the accident conditions which should be analyzed by 3D neutronics codes coupled to system codes. The main objective is to perform more realistic analyses for transients with strong coupling between neutronics in the core and thermo-fluiddynamic in the primary circuit. Therefore, the system code ATHLET developed and applied in GRS for plant transient and accident analysis has been coupled with different 3D neutronics codes for modeling VVER and LWR conditions. The examples have demonstrated first applications of these coupled codes. In the next years it is planned to perform extended validation of these coupled codes by analysis of plant transient data. Also necessary will be code comparisons for benchmark problems from the field of design basis accidents.

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7 References

- /AER/ Proceedings of AER Symposiums, 1992, 1993, 1994, 1995
- /ATH 95/ G. Lerchl, H. Austregesilo
ATHLET User's Manual
GRS-P-1/ Vol. 1, October 1995

- /BOE 92/ R. Böer, R. Böhm, H. Finneemann, R. Müller
The Coupled Neutronics and Thermal-Hydraulics System PANBOX 2 for
PWR Safety Analysis, Kerntechnik, 57, 1, 49 (1992)
- /FIN 93/ H. Finneemann, H. Bauer, A. Galati, R. Martinelli
Results of LWR Core Transient Benchmarks, Mathematical Methods and
Super Computing in Nuclear Applications
Karlsruhe, 19.-23. April 1993
- /FOM 93/ P. Fomitchenko, M. Lizorkin, L. Gilvanov, H. Austregesilo, S. Langenbuch
Coupling of the thermal-hydraulic system code ATHLET and 3D-neutronics
model BIPR8
Report of RRC KI and GRS, 1993
- /FOM 94/ P. Fomitchenko, M. Lizorkin, L. Gilvanov, M. Podshibiakin, I. Schekin, S.
Langenbuch, K.D. Schmidt
Verifikation of the coupling of the thermal-hydraulic system code ATHLET
and the 3D-neutronics model BIPR8
Report of RRC KI, OKB Hydropress and GRS, 1994
- /GRU 93/ U. Grundmann, U. Rohde
DYN3D/M2 - a Code for the Calculation of Reactivity Transients in Cores
with Hexagonal Geometry
Report FZR 93-01, Rossendorf, January 1993
- /GRU 95a/ U. Grundmann, U. Rohde, S. Mittag, D. Lucas
Weiterentwicklung und Verifikation eines dreidimensionalen Kernmodells
für Reaktoren vom Typ WWER und seine Ankopplung an den Störfallcode
ATHLET
Report FZR-84, Rossendorf, April 1995
- /GRU 95b/ U. Grundmann
The code DYN3DR for Steady-state and Transient Analyses of Light Water
Reactor Cores with Cartesian Geometry,
Report FZR-114, Rossendorf, November 1995
- /GRU 95c/ U. Grundmann, D. Lucas, U. Rohde
Coupling of the Thermohydraulic Code ATHLET with the Neutron Kinetic
Core Model DYN3D
Int. Conf. on Mathematics and Computations, Reactor Physics and Envi-
ronmental Analyses, Portland, Oregon, Proc. Vol. 1, p. 257, April 30 - May
4, 1995
- /GRU 96/ U. Grundmann, U. Rohde
DYN3D - a 3-dimensional Core Model for Steady State and Transient
Analysis of Thermal Reactors,
Int. Conf. on Physics of Reactors, Mito (Japan), Sept. 16-20, 1996 (to be
published)

- /KNO 94/ A. Knoll, R. Müller
Coupling RELAP 5 and PANBOX 2: A Three-Dimensional Space-Time Kinetics Application with RELAP 5
New Trends in Nuclear System Thermohydraulics, Pisa, 30th May - 2nd June 1994
- /LAN 77/ S. Langenbuch, W. Maurer, W. Werner
Coarse-Mesh Flux-Expansion Method for the Analysis of Space-Time Effects in Large Light Water Reactor Cores
Nuclear Science and Engineering 63, pp 437-456, 1977
- /LAN 77a/ S. Langenbuch, W. Maurer, W. Werner
High-Order Schemes for Neutron Kinetics Calculation based on a Local Polynomial Approximation
Nuclear Science and Engineering 64, pp 508-516, 1977
- /LAN 96/ S. Langenbuch et al.
Interface Requirements to Couple Thermal-Hydraulic Codes to 3D Neutronic Codes
Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Nov. 5-8, 1996
- /LIZ 92/ M.P. Lizorkin, V.N. Semenov, V.S. Ionov, V.I. Lebedev
Time dependent spatial neutron kinetic algorithm for BIPR8 and its verification
Proceedings of the 2nd Symposium of AER (Atomic Energy Research) for Investigating Neutron Physics and Thermohydraulics Problems of Reactor Safety, Paks, Hungary, September 21-26, 1992, Budapest: KFKI, 1992, pp 389-408
- /NOV 82/ A.N. Novikov
Generalized approximation of differential operators of one group equations
Proceedings of the 11th Symposium of TIC (Temporary International Collective for joint research into physics of VVER-type reactors) Bulgaria, Varna, 1982 (in Russian)
- /NOV 89/ A.N. Novikov, V.V. Pshenin, M.P. Lizorkin, V.V. Saprykin, V.D. Sidorenko, A.A. Suslov
Problems of VVER in-core fuel management
Proceedings of the meeting on in-core fuel management, Vienna, December 4-7, 1989, IAEA-TECDOC-567, 1990, pp 325-335,
- /TES 96/ V. Teschendorff, H. Austregesilo, G. Lerchl
Methodology, Status and Plans for Development and Assessment of the Code ATHLET
Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Nov. 5-8, 1996

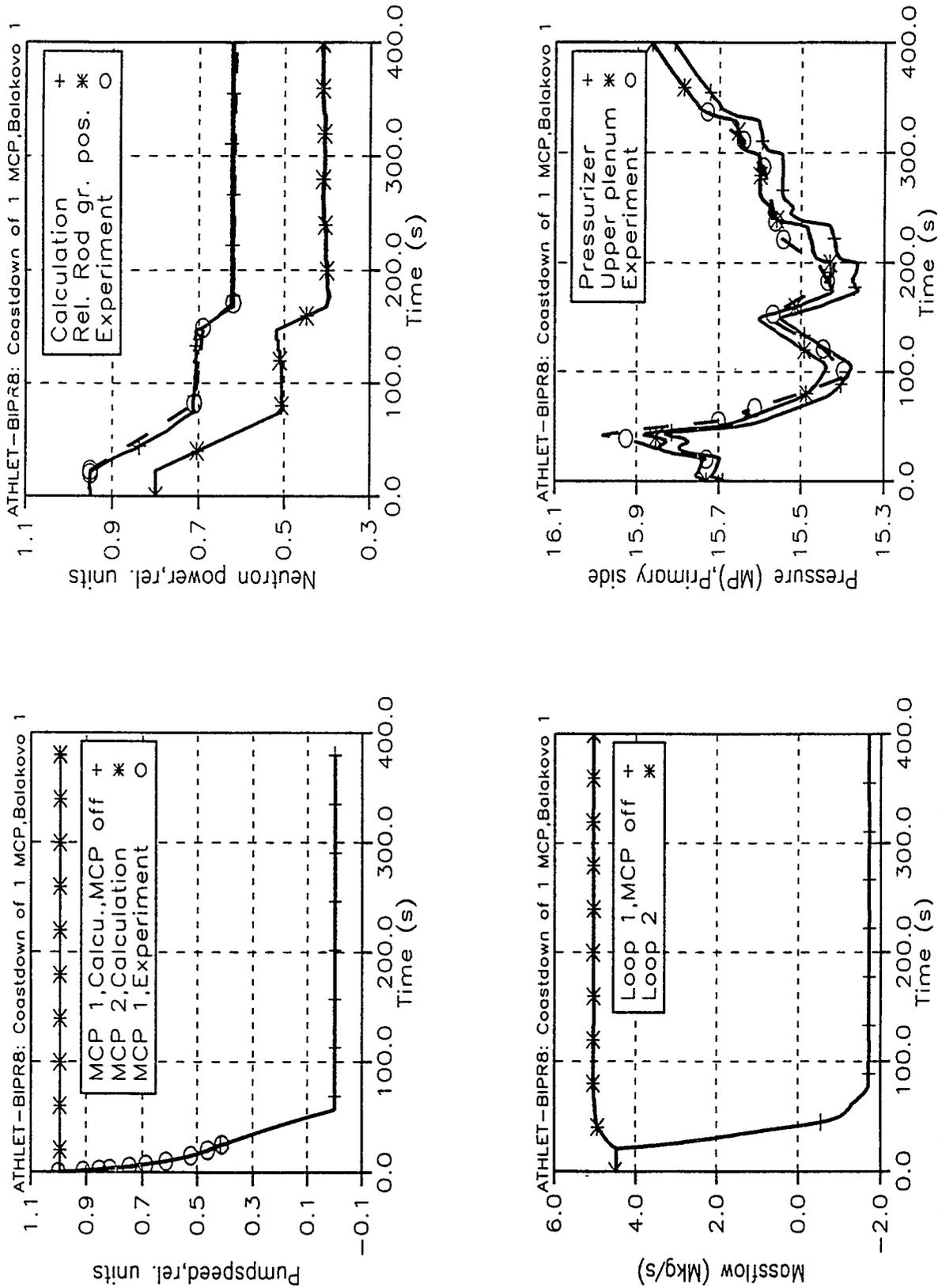


Fig. 1: Calculation of coupled code ATHLET-BIPR8 for a single pump coastdown transient (1 out of 4) for a VVER-1000. Results of main plant parameters including comparison to experimental data.

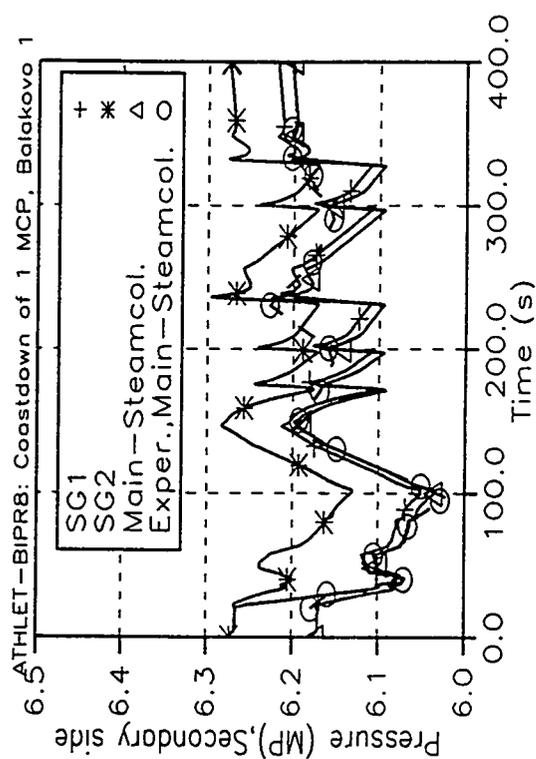
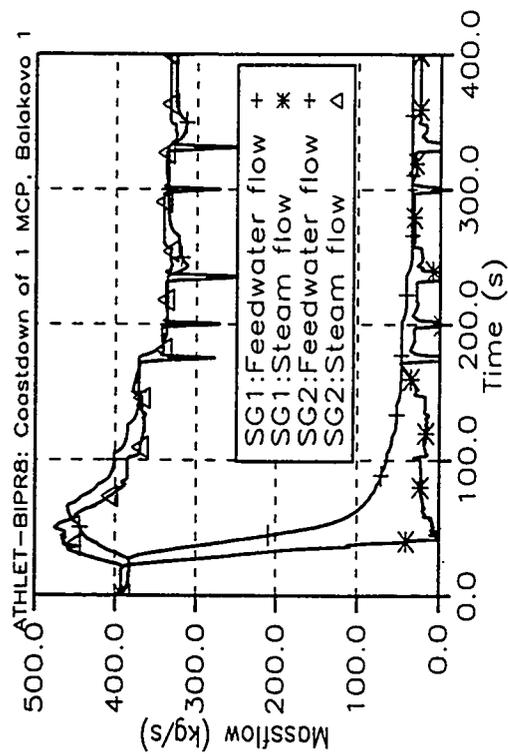
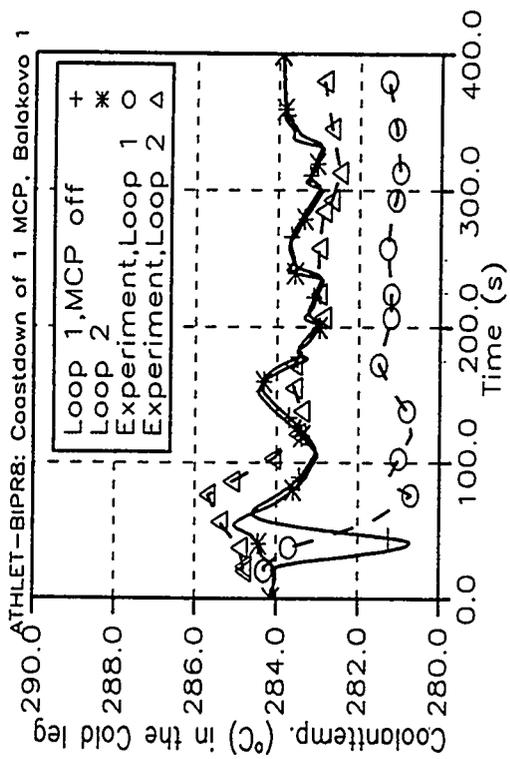
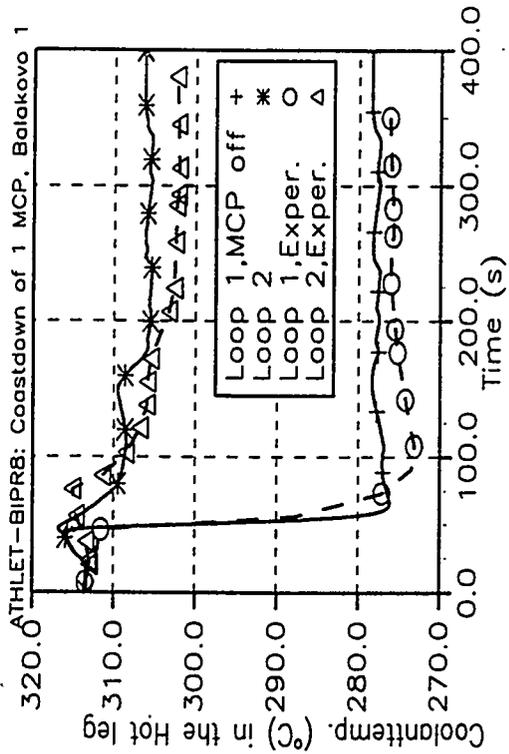


Fig. 2: Calculation of coupled code ATHLET-BIPRB for a single pump coastdown transient (1 out of 4) for a VVER-1000. Results of main plant parameters including comparison to experimental data.

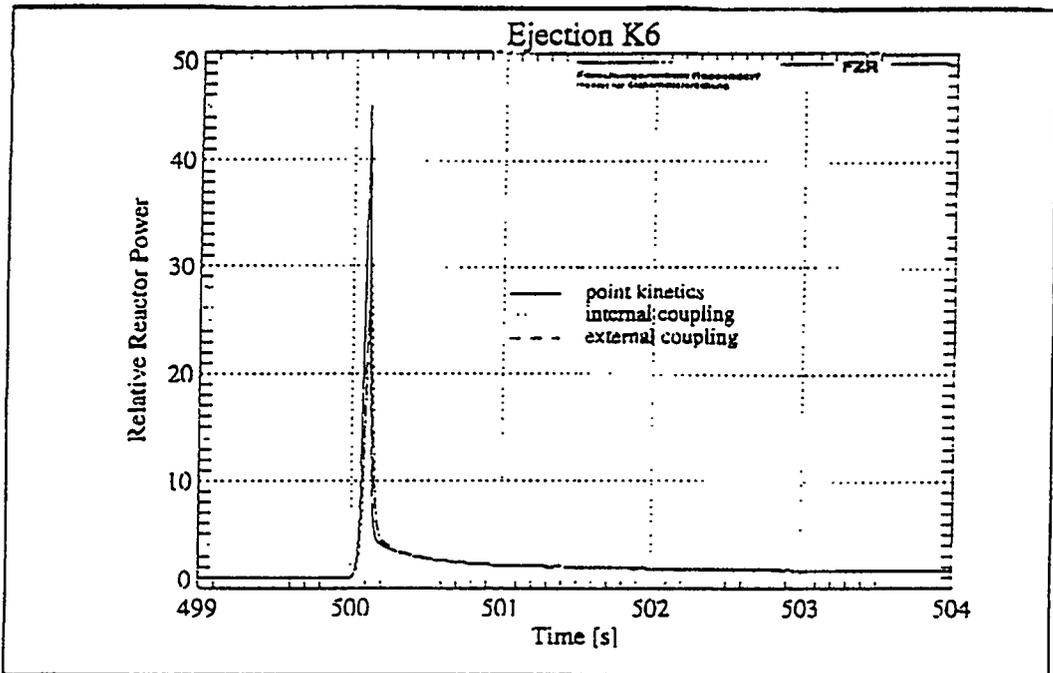


Fig. 3: Reactor power relative to nominal for ejection of control group K6 - ATHLET calculation with point kinetics and coupled with DYN3D

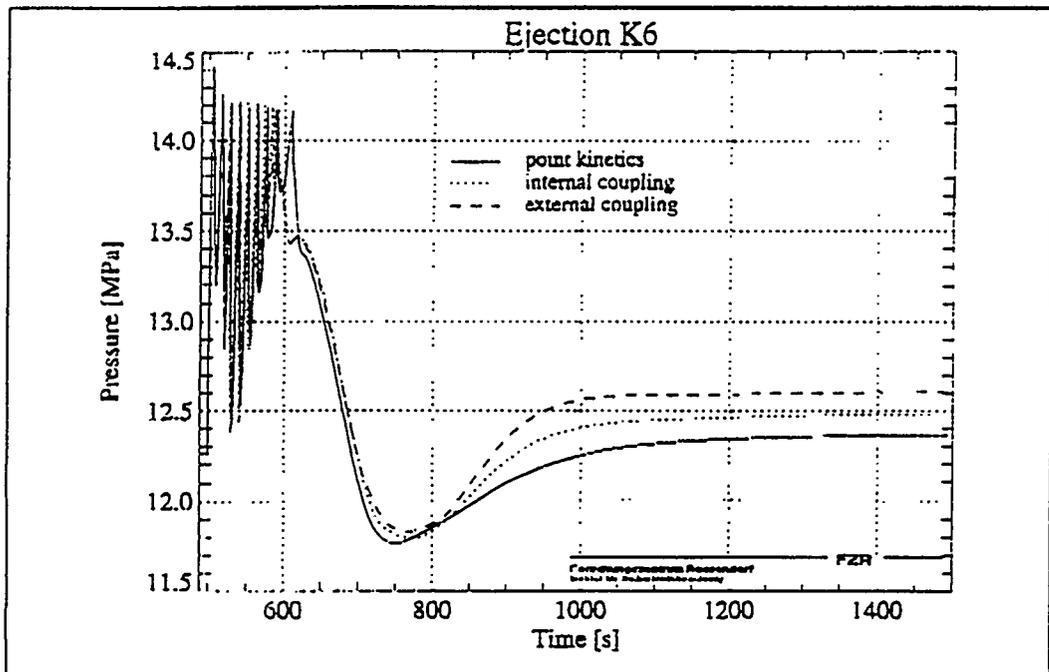


Fig. 4: Primary circuit pressure for ejection of control group K6 - ATHLET calculation with point kinetics and coupled with DYN3D

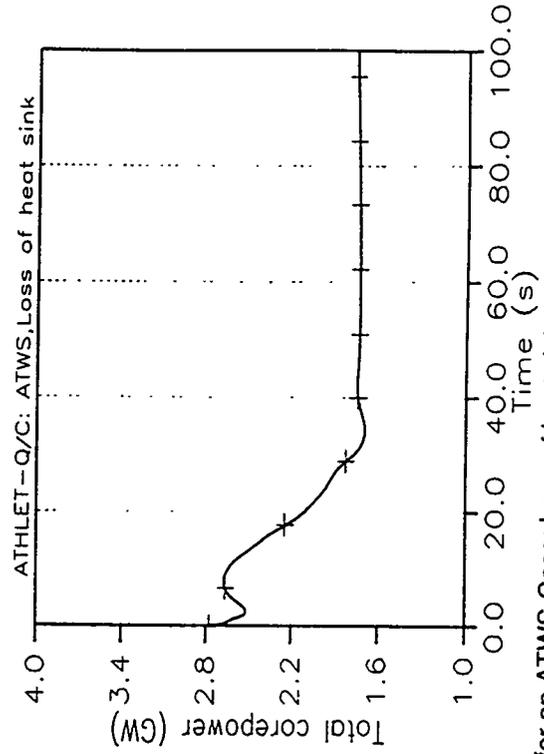
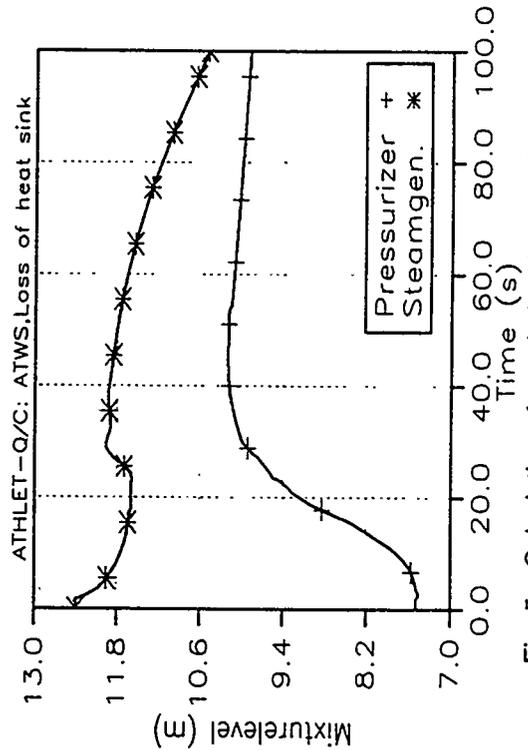
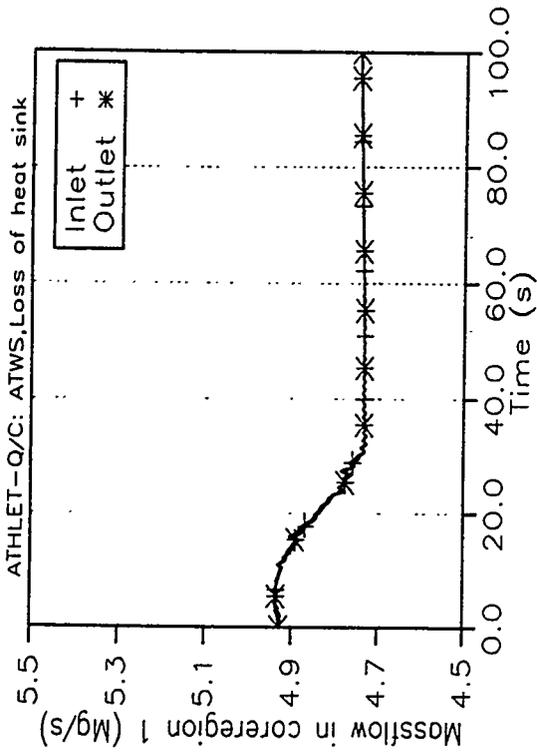
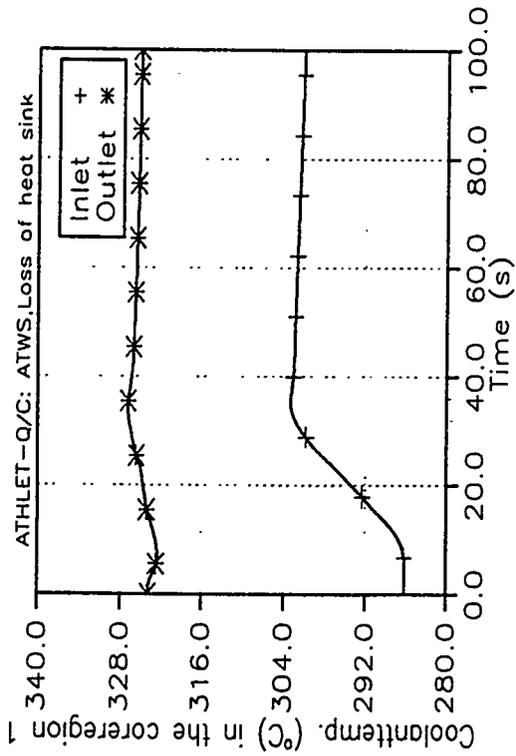


Fig. 5: Calculation of coupled code ATHLET-QUABOX/CUBBOX for an ATWS-Case: Loss of heat sink. Results of main plant parameters for a PWR model.

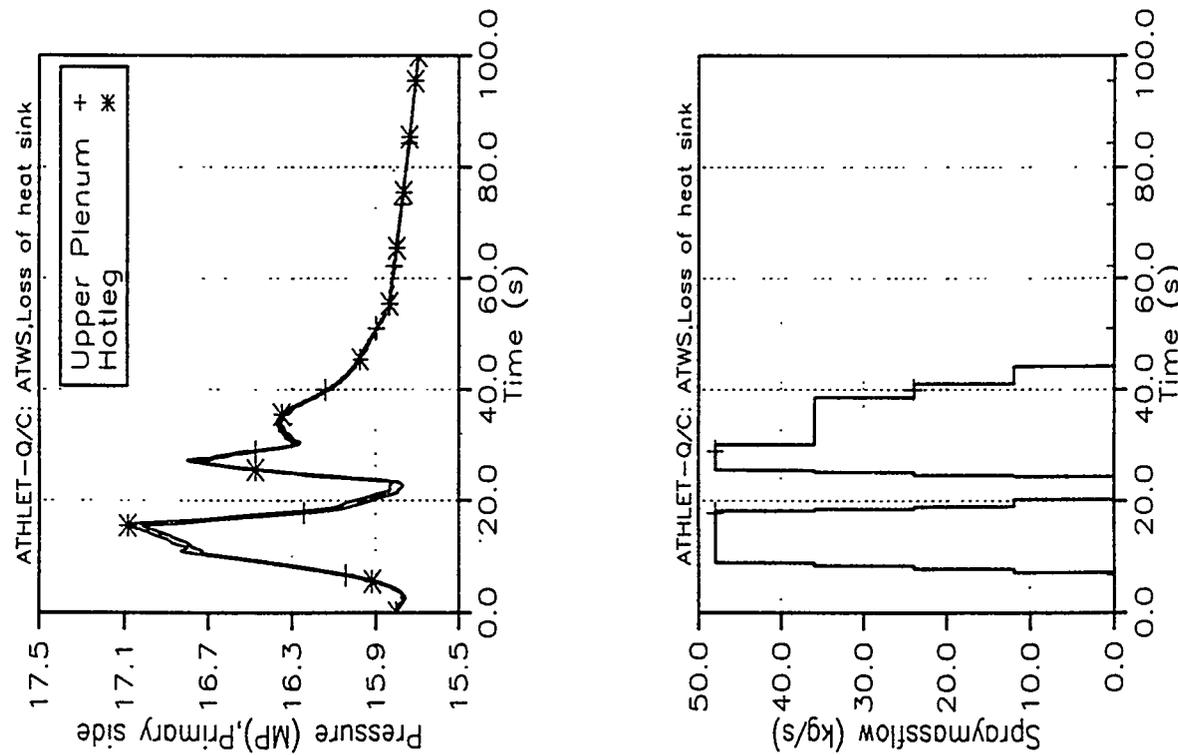
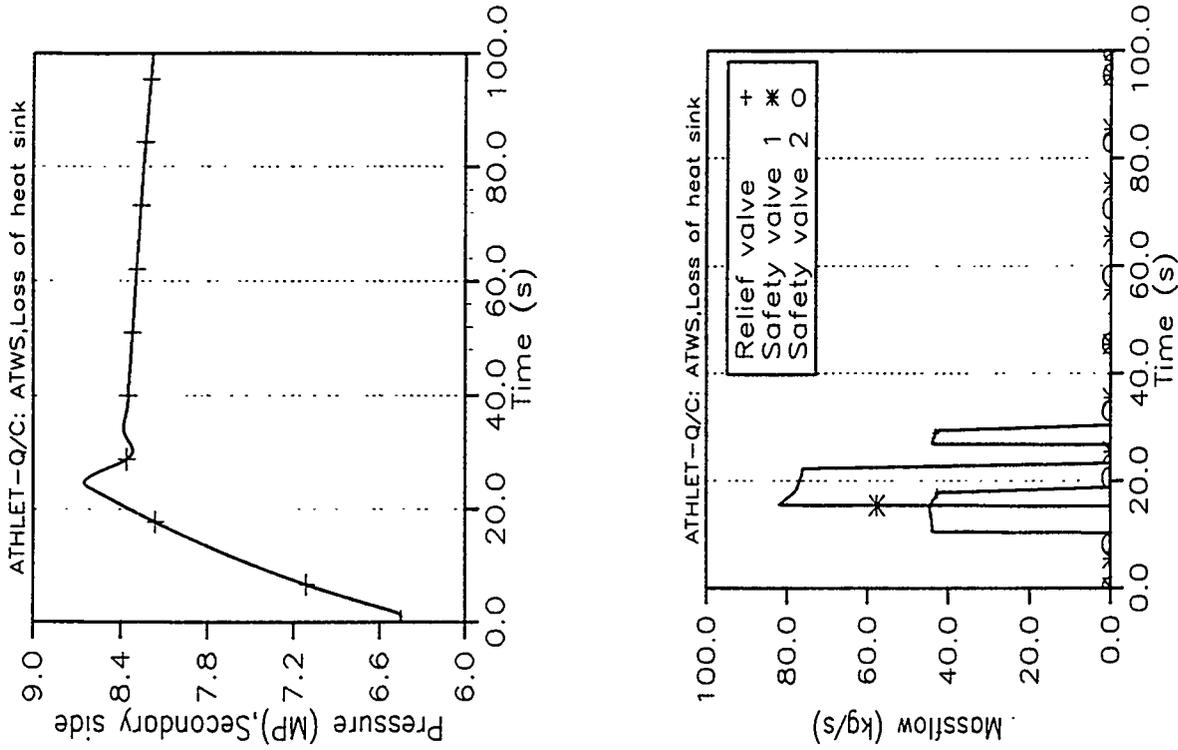


Fig. 6: Calculation of coupled code ATHLET-QUABOX/CUBBOX for an ATWS-Case: Loss of heat sink. Results of main plant parameters for a PWR model.

Perspectives on Multifield Models

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Abstract

Multifield models for prediction of nuclear reactor thermalhydraulics are reviewed from the viewpoint of their structure and requirements for closure relationships. Their strengths and weaknesses are illustrated with examples, indicating that they are effective in predicting separated and distributed flow regimes, but have problems for flows with large oscillations. Needs for multifield models are also discussed in the context of reactor operations and accident simulations. The highest priorities for future developments appear to relate to closure relationships for three-dimensional multifield models with emphasis on those needed for calculations of phase separation and entrainment/de-entrainment in complex geometries.

1. INTRODUCTION

Two-phase flows occur in a variety of nuclear reactor processes, ranging from normal operation to transients and accident conditions. For certain accidents that go beyond the design basis, more than two phases may arise—e.g. in fuel-coolant mixtures—and the modelling problem becomes increasingly complicated. Be that as it may, current approaches to predicting such flows are based primarily on the so-called "multifield model." This approach began its application to nuclear problems in the 1970s and was first extensively discussed, in this context, at the 1976 OECD/CSNI Specialists Meeting on Transient Two-Phase Flow (see Banerjee and Weaver (1976)). Since that time the model has formed the basis for computer codes such as COBRA-TF, TRAC, RELAP5, CATHARE, CATHENA, etc. for the nuclear industry, and versions are also incorporated in commercial computational fluid dynamics codes such as PHOENICS, FLUENT AND CFX (formerly FLOW3D).

To clarify what is meant by a field, consider Figure 1, which shows two flow regimes, *viz.* annular flow and slug flow. A field may then be thought of as a clearly identifiable portion of a flow regime, e.g., in annular flow, the fields might be the liquid film, the droplets and the gas or vapor core. Such "three-field" models are now routinely used in computer codes, applied to both nuclear problems and to oil-gas transportation in pipelines.

For more complex flow regimes such as slug flow, it may be necessary to describe the regime with four fields, e.g., one for the large gas bubbles, the second for the liquid film surrounding the bubbles, the third for the dispersed gas bubbles in the wake and the fourth for the liquid slug. This level of sophistication may eventually be needed to capture the behavior of some intermittent flows, but has not yet been applied.

Selection of the fields depends on the modeller, but should generally be that portion of a flow where the mean velocity is relatively uniform. To make this more concrete, consider annular flow. If all the liquid is lumped together into a field, then we have droplets which travel at a much higher velocity than the liquid film leading to a very nonuniform profile for the liquid field. This gives strong distribution effects in the momentum flux (and other nonlinear terms in the field conservation equations). A better selection would be to consider a mixture of the droplets and the vapor core as a field, if one must confine consideration to only two fields. In choosing fields, or assigning portions of the flow to a field, one usually tries to remove distribution effects so far as possible, as suggested in the previous discussion for annular flow.

While this illustrates the basis for the multifield approach, it should not be taken too literally in the sense that the fields are not chosen specifically on the basis of the flow regimes obtained, i.e., present models do not change between two, three or four fields depending on the local flow regime. Rather the maximum number of fields incorporated in a model characterizes the level of flexibility that is available for modelling different flow regimes. For example, the three-field model could be thought of as a liquid field that moves at a different velocity from the vapor field, a second liquid field that travels at a velocity much closer to that of the vapor field, and the vapor field itself. This would allow not only annular flow to be modelled, but also stratified flow where droplets may be dispersed in the vapor phase, and inverted annular flow where droplets may also be carried by the vapor phase in contact with the hot wall. While it might be stretching the model a bit, it might also be possible, within such a structure, to characterize horizontal slug flow where liquid slugs run at nearly the vapor velocity over a much slower stratified liquid layer.

In any case, multifield modelling then proceeds by averaging the local instantaneous conservation equations for mass, momentum and energy over each field. Averaging may be done in time, space, over an ensemble, or in some combination of these. Details may be found in the early work of Vernier and Delhaye (1968), Ishii (1975), Yadigaroglu and Lahey (1976), Delhaye and Achard (1976), Panton (1978), Agee, et al (1978), Banerjee and Chan (1980) and Drew (1983), amongst others. While averaging makes the mathematical solution of the problem tractable, information regarding local gradients between fields is lost and has to be resupplied in the form of semi-empirical closure relationships, also called "constitutive" equations. These are typically relations for interfield forces, interfield heat transfer, and interfield area. In addition, for multicomponent problems, interfield mass transfer relationships are needed. To a large

measure, the ability of a multifield model to predict two-phase flows depends on the quality of such closure relationships.

At this point it is worth noting that most formulations for the nuclear industry are based on the so-called Eulerian-Eulerian, interpenetrating-continua, approach, and the closure relationships are phrased in this context. On the other hand, for problems involving sprays and combustion, an approach based on treating the continuous phase in an Eulerian framework, and the dispersed phase with a Boltzmann-like probability distribution formulation has been common for some time (see Williams (1959)). Because the dispersed phase is characterized by a distribution function that gives the particle-number density in physical space, velocity space, and particle radius intervals, the formulation is actually like a multifield model, but with a large number of fields. It can be shown that if the equation for the distribution function is multiplied by particle mass and then integrated over the velocities and particle radii, then the mass conservation equation arising in the interpenetrating-continua model arises. Similarly, if the distribution function equation is multiplied by particle momentum and again integrated over velocities and radii, then the momentum conservation equation arises. The advantages of this type of formulation are that the distribution function equation is effectively one for the interfacial area evolution. It remains to be seen whether such an approach can, with some modification, be extended to flow regimes other than the dispersed.

Having said this, it is worth reviewing, briefly, the interpenetrating continua and Boltzmann-type formulations in Section 2. Section 3 will then discuss some examples illustrating strengths and weaknesses of the multifield approach to set the context for Section 4 which will consider phenomena that require a multifield approach, and are of interest for nuclear problems. This discussion will also cover some problems of normal operation, but focus on nuclear safety.

Before getting into details, it is noted that early approaches to two-phase flow modelling relied on treating the flow like a variable density mixture. While such "mixture models" may capture the dynamics of closely coupled flows such as bubbly and churn turbulent, in vertical passages, it is difficult to extend them to loosely coupled flow regimes—particularly when the individual dynamics of each phase is important in a transient. As we will see, multifield models do well for separated flows, and droplet flows—both important for many nuclear problems, explaining the present dominant role of such approaches.

2. MULTIFIELD MODELS: A BRIEF REVIEW

2.1 Interpenetrating Continua Formulation

We turn now to dealing with the conservation equations in the interpenetrating continua framework. While many different approaches are used, they result, essentially, in the same form of the equations. Here we follow the approach of Banerjee & Chan (1980) because it is straightforward, and results in closure relationships whose physical significance is clear.

We choose to volume average first followed by ensemble averaging. The operations are commutative and could be reversed. Double averaging is desirable to ensure continuity of first derivatives, which might otherwise be discontinuous, e.g. for certain flow regions where field interfaces move in a deterministic manner in time or are stationary, when ensemble averaging, by itself leads to discontinuities. Note that volume averaging alone would lead to a sort of filtering over the subgrid scales—which could then be interpreted in the same way as for single-phase large eddy simulations. This approach has not been applied to multiphase flows, however, as yet.

Consider the elementary volume shown in Figure 2. We have shown it as intersecting a solid boundary for generality, but it could as well be a volume interior to the fluid.

The notation is as follows:

a_i	- interfacial area in volume V , m^2
a_{kw}	- area intersected at wall by field k in volume V , m^2
$V_k(\vec{x}, t)$	- volume of field k in volume V , m^3
\vec{n}_k	- outward directed normal from field k on a_i
\vec{n}_{kw}	- outward directed normal at wall from field k on a_{kw}
\vec{v}_i	- velocity of the interface, m/s
\vec{v}_k	- velocity of field k , m/s
ρ_k	- density of field k , kg/m^3
p_k	- pressure of field k , Pa
\vec{x}	- spatial coordinate

The subscript k denotes field k , and in this general formulation there are only some topological restrictions on the field quantities.

The local instantaneous conservation equation for each field is

$$\frac{\partial \rho_k \psi_k}{\partial t} + \nabla \cdot (\vec{v}_k \rho_k \psi_k) = -\nabla \cdot \vec{J}_k + \rho_k \phi_k \quad (1)$$

where ψ_k - conserved quantity

\vec{J}_k - the efflux term

ϕ_k - the body source term

The various conservation equations are recovered by substituting appropriate values of ψ_k , \vec{J}_k and ϕ_k in (1).

To volume average we need to use Gauss' theorem and Leibnitz's rule which are

Leibnitz rule

$$\int_{V_k(\vec{x}, t)} \frac{\partial f_k}{\partial t} dV = \frac{\partial}{\partial t} \int_{V_k(\vec{x}, t)} f_k dV - \int_{a_i} f_k \vec{v}_i \cdot \vec{n}_k dS \quad (2)$$

Gauss' theorem

$$\int_{V_k(\vec{x}, t)} \nabla \cdot \vec{a}_k dV = \nabla \cdot \left[\int_{V_k(\vec{x}, t)} \vec{a}_k dV \right] + \int_{a_i} \vec{a}_k \cdot \vec{n}_k dS + \int_{a_{kw}} \vec{a}_k \cdot \vec{n}_{kw} dS \quad (3)$$

Defining

$$\langle f_k \rangle = \frac{1}{V_k} \int_{V_k} f_k dV \quad (4)$$

and the volume fraction of field k as

$$\epsilon_k = \frac{V_k}{V} \quad , \quad (5)$$

we have

$$\begin{aligned} & \frac{\partial \epsilon_k \langle \rho_k \psi_k \rangle}{\partial t} + \nabla \cdot \epsilon_k \langle \rho_k \vec{v}_k \psi_k \rangle + \nabla \cdot \epsilon_k \langle \vec{J}_k \rangle \\ & = \epsilon_k \langle \rho_k \phi_k \rangle - \frac{1}{V} \int_{a_i} \vec{n}_k \cdot [(\vec{v}_k - \vec{v}_i) \rho_k \psi_k + \vec{J}_k] dS - \frac{1}{V} \int_{a_{kw}} \vec{n}_{kw} \cdot \vec{J}_k dS \quad , \quad (6) \end{aligned}$$

assuming also that $\vec{v}_k = 0$ at the wall, i.e., no blowing or suction (though these effects can be incorporated without difficulty).

Equation (6) has been left in volume-averaged form at present, but to proceed we would need to have subgrid scale models. Clearly the integrals on the right-hand side of (6) involve interfield transfers of the conserved quantity ψ_k (the integral over a_i) and at the wall (the integral over a_{kw}). Resolution below the size of the averaging volume V cannot

be obtained, though V can be made infinitesimally small. To obtain closure relationships independent of the averaging volume, averages taken over the volume must be equivalent to those over planes through its middle (Nigmatulin (1979)), i.e., the volume must be large enough to contain a large number of representative structures. This is possible for dispersed flows, but more difficult when the structures are large, like slugs or waves. This is similar to large eddy simulations, then, of turbulent flows—the slugs and waves would be at supergrid scales, i.e., would be resolved in the simulation. The closure relationships must depend on the size of the various dimensions of the averaging volume, i.e., on the grid scale—again like subgrid scale models for turbulence.

Ensemble-averaging by itself leads to exactly the same form of the equations except that the integrals are replaced by summations over large numbers of identical experiments. The instantaneous volume fraction of phase k is replaced by the fraction of the ensemble of experiments for which phase k appears, at a point, at a given time from initiation of the experiments. The interfacial area integrals turn into summations involving interfacial velocities in the directions of the normals, \vec{n}_k (see Ishii (1975) for details).

It is also possible to ensemble-average (6) in which case the closure relationships become independent of the averaging volume V , which can be shrunk down to infinitesimal volumes. Such double averages have been considered in detail by Delhaye and Achard (1976). To derive the individual conservation equations we can make the substitutions for ψ_k , \vec{J}_k , and ϕ_k shown in Table 1 below.

Table 1. Forms of the Conserved Quantities

Conservation Law	ψ_k	J_k	ϕ_k
Mass	1	0	0
Momentum	\vec{v}_k	$p_k \bar{I} - \bar{\tau}_k$	\vec{g}_k
Energy	$i_k + \frac{v_k^2}{2}$	$\vec{q}_k + \vec{v}_k \cdot (p_k \bar{I} - \bar{\tau}_k)$	$\vec{g}_k \cdot \vec{v}_k$

Here i - internal energy
 \vec{q} - heat flux vector field
 \vec{g} - gravitational acceleration vector
 $\vec{\tau}$ - shear stress tensor
 \bar{I} - identity tensor

The double-averaged equations are presented below, with the volume averaging signs shown, but the ensemble-averaging signs left out. Henceforth we will understand that all arguments within derivatives or integrals are ensemble-averaged. The *mass* conservation equation is then

$$\frac{\partial \epsilon_k}{\partial t} \langle \rho_k \rangle + \nabla \cdot \epsilon_k \langle \rho_k \vec{v}_k \rangle = - \frac{1}{V} \int_{a_i} \rho_k \vec{n}_k \cdot (\vec{v}_k - \vec{v}_i) dS \quad (7)$$

The integral on the right hand side of (7) gives the mass transfer rate *out* of field k over the interfacial area a_i in volume V , i.e., it is the "outward" mass transfer rate per unit volume of fluid.

Similarly the momentum conservation equation can be written

$$\begin{aligned} & \frac{\partial \epsilon_k}{\partial t} \langle \rho_k \vec{v}_k \rangle + \nabla \cdot \epsilon_k \langle \rho_k \vec{v}_k \vec{v}_k \rangle + \epsilon_k \nabla \langle p_k \rangle + \epsilon_k \nabla \langle \vec{\tau}_k \rangle \\ & = \epsilon_k \langle \rho_k \vec{g}_k \rangle - \frac{1}{V} \int_{a_i} \rho_k \vec{n}_k \cdot (\vec{v}_k - \vec{v}_i) \vec{v}_k dS \\ & + \frac{1}{V} \int_{a_i+a_{kw}} \vec{n}_k \cdot (\Delta \vec{\tau}'_{ki}) dS - \frac{1}{V} \int_{a_i+a_{kw}} (\Delta p'_{ki}) \vec{n}_k dS \end{aligned} \quad (8)$$

In (8), the stress and pressure integrals that arise over the interfacial area have been manipulated to clarify the physical significance of the terms.

The interfacial pressure at any point on a_i in V has been expressed as

$$p_{ki} = \langle p_k \rangle + \Delta p'_{ki} \quad (9)$$

where $\langle p_k \rangle$ - double-averaged pressure in phase k ,

$$\Delta p'_{ki} = p_{ki} - \langle p_k \rangle \quad (10)$$

with p_{ki} being the local pressure on the interface. Similarly

$$\Delta \bar{\tau}_{ki} = \bar{\tau}_{ki} - \langle \bar{\tau}_{ki} \rangle \quad (11)$$

Thus Δp_{ki} is simply the difference between the pressure at the interface and the average in the phase at the point under consideration. That this difference can be non-zero is evident by considering the pressure at the surface of a bubble or drop, moving through a continuous fluid. Because of the curvature of the interface the continuous phase accelerates in a layer around the object, giving a pressure lower than the average. The term involving Δp_{ki} gives "form drag," "added mass" and "lift" effects. Similar considerations can be applied to the shear stress term.

A conservation equation can also be written for total energy and, if necessary, for conservation of various species if several are involved (as in mass transfer, and chemical reaction problems).

These relationships are supplemented by the jump conditions for the sum of the interfacial closures required, i.e.,

$$\sum_k \Gamma_k = \sum_k \frac{1}{V} \int_{a_i} \rho_k \bar{n}_k \cdot (\vec{v}_k - \vec{v}_i) dS = 0 \quad (12)$$

$$\sum_k \vec{M}_k = \sum_k \frac{1}{V} \int_{a_i} \bar{n}_k \cdot [\rho_k (\vec{v}_k - \vec{v}_i) \vec{v}_k + p_{ki} \bar{I} - \bar{\tau}_{ki}] dS = 0 \quad (13)$$

in the absence of surface tension effects.

$$\begin{aligned} \sum_k E_k = \sum_k \frac{1}{V} \int_{a_i} \bar{n}_k \cdot [\rho_k (\vec{v}_k - \vec{v}_i) \left(i_k + \frac{v_k^2}{2} \right) \\ + (p_{ki} \bar{I} - \bar{\tau}_{ki}) \cdot \vec{v}_k + \vec{q}_k] dS = 0 \end{aligned} \quad (14)$$

again in the absence of surface tension effects. In (13) the interfacial pressure, p_{ki} , and shear stress tensor, $\bar{\tau}_{ki}$, are retained. These are the so-called "Kotchine conditions"—see Ishii (1975). Conditions (12) to (14) lead to the interfacial interaction terms canceling out when the individual phase equations are added to derive "mixture" equations.

The left hand sides of (7) and (8), the averaged mass and momentum equations, involve quantities like $\langle \rho_k \vec{v}_k \rangle$ and $\langle \rho_k \vec{v}_k \vec{v}_k \rangle$ which are averages of products of local instantaneous dependent variables. The relationship between quantities like these and the products of averages are unknown. In addition, the right hand sides, involving integrals of the type $\frac{1}{V} \int_{a_i} f_k dS$, are also unknown. The right hand side integrals clearly involve interfield transfer of heat, mass and momentum.

To reduce the averages of products to products of averages, one needs to define fluctuating quantities. If we define $\langle \vec{u}_k \rangle = \frac{\langle \rho_k \vec{v}_k \rangle}{\langle \rho_k \rangle}$ —a sort of Favre averaging (similar to that done in turbulence), and the fluctuating velocity $\vec{u}' = \vec{v}_k - \langle \vec{u}_k \rangle$, (recalling that \vec{v}_k is the local instantaneous velocity), then (7) and (8) become

$$\frac{\partial \epsilon_k \langle \rho_k \rangle}{\partial t} + \nabla \cdot \epsilon_k \langle \rho_k \rangle \langle \vec{u}_k \rangle = -\Gamma_k \quad (15)$$

and

$$\begin{aligned} \frac{\partial \epsilon_k \langle \rho_k \rangle \langle \vec{u}_k \rangle}{\partial t} + \nabla \cdot \epsilon_k \langle \rho_k \rangle \langle \vec{u}_k \rangle^2 + \nabla \cdot \epsilon_k \langle \rho_k \rangle \\ + \nabla \cdot \epsilon_k [\langle \vec{\tau}_k \rangle - \langle \rho_k \vec{u}'_k \vec{u}'_k \rangle] = -\vec{M}_k + \text{wall terms} \end{aligned} \quad (16)$$

where the RHS of (16) has been left in the form of (13), i.e., involving p_{ki} and $\vec{\tau}_{ki}$ rather than Δp_{ki} and $\Delta \vec{\tau}_{ki}$ as was done in (8). (This is why the ϵ_k is contained within the derivatives in the 3rd and 4th terms of the LHS). Note that the term $\rho_k \vec{u}'_k \vec{u}'_k$ arises. This is equivalent to the usual Reynolds stress tensor for single-phase turbulence problems. By examining the form of \vec{M}_k given in (13), it is evident that correlation terms exist also between fluctuations in local interfacial mass transfer (given by $\vec{n}_k \cdot (\vec{v}_k - \vec{v}_i) \rho_k$) and interfacial phase velocity \vec{v}_k . Therefore in addition to closure relationships for the terms of the type Γ_k , \vec{M}_k and ϵ_k , we also need closure relationships for the turbulent momentum fluxes (Reynolds stresses) and scalar fluxes.

This is the interpenetrating continua formulation in an Eulerian framework. It is widely used with three or two fields, and with various simplifications. We will briefly discuss requirements for closure later.

2.2 Boltzmann-type Formulations for Discrete Phase Fields

Consider an approach similar to that of Williams (1959) in which the quantity

$$f_j(r, \vec{x}, \vec{v}_d, t) dr d\vec{x} d\vec{v}_d$$

is the probable number of discrete phase "particles" of composition j with radius between r and $r + dr$, located about \vec{x} and $\vec{x} + d\vec{x}$, and with velocities between \vec{v}_d and $\vec{v}_d + d\vec{v}_d$.

If

$$\vec{F}_j \triangleq \frac{d\vec{v}_d}{dt} |_j \quad \text{and} \quad R_j \triangleq \frac{dr}{dt} |_j \quad (17)$$

are the acceleration and growth rate, respectively, of a "particle" in the dispersed phase, then

$$\begin{aligned} \frac{\partial f_j}{\partial t} = & - \frac{\partial}{\partial r} (R_j f_j) - \nabla_x \cdot (\vec{v}_d f_j) - \nabla_{\vec{v}_d} \cdot (\vec{F}_j f_j) \\ & + Q_j + \sigma_j \quad \text{for } j = 1, \dots, M \end{aligned} \quad (18)$$

The subscript d denotes the dispersed phase and c the continuous phase. The derivatives, ∇_x and $\nabla_{\vec{v}_d}$ are with regard to the spatial and particle velocity coordinates respectively. Q_j is the source term giving the rate of dispersed phase formation and destruction, whereas σ_j represents the increase in f_j due to collisions which may change the size and velocity of the colliding particles. The quantity $-\nabla_x \cdot (\vec{v}_d f_j)$ represents the convergence of particles of composition j into the spatial volume element $d\vec{x}$, and $-\nabla_{\vec{v}_d} \cdot (\vec{F}_j f_j)$ the acceleration into the velocity range $d\vec{v}_d$. If we multiply by the surface area of "particles" of radius r_j , and integrate over all species, radii and velocity, then we obtain an equation for interfacial area transport. Therefore, (18) may be regarded as a multifield version of the interfacial area transport equation.

The acceleration of the particles is derived simply by summing the forces acting on them. Thus (17) can be written, for example, as gravitational force

$$\vec{F}_G = + \vec{g} (\rho_d - \rho_c)/\rho_d$$

drag

$$\vec{F}_D = + \frac{3}{8} \frac{\rho_c}{\rho_d} \frac{C_D}{r} |\vec{v}_c - \vec{v}_d| (\vec{v}_c - \vec{v}_d)$$

added mass

(19)

$$\vec{F}_A = - \frac{\rho_c}{\rho_d} C_A \left[\frac{d}{dt} (\vec{v}_d) - \frac{D}{Dt} \vec{v}_c \right]$$

hydrostatic

$$\vec{F}_p = - \frac{\nabla p_c}{\rho_d}$$

to which lift, Basset forces etc. may be added, as required. $\frac{d}{dt}$ is the total derivative taken, moving with the particle, whereas $\frac{D}{Dt}$ is taken moving with the fluid. In principle, (17) and (19), if \vec{v}_c is the instantaneous continuous phase velocity, can account for the effect of turbulent fluctuations in the continuous phase, which we will consider later. Therefore, if the continuous phase motion is known, then the dispersed phase particles can be moved using (17), and relations of the type (19). If the variation of R_j (say due to mass transfer) and Q_j and σ_j are known, then f_j can be calculated from (18).

For the continuous phase, we have

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \vec{v}_c) = - \sum_{j=1}^M \iint \rho_{dij} 4\pi r^2 R_j f_j dr dv_d \quad (20)$$

where

$$\rho = \rho_c \left[1 - \sum_{j=1}^M \iint \frac{4}{3} \pi r^3 f_j dr d\vec{v}_d \right] \quad (21)$$

assuming spherical discrete phase "particles." Shape factors may be included to allow consideration of nonspherical shapes. This corresponds to (7) with the right hand sides of (20) and (7) being equivalent (and the integral on the right-hand side of (21) being ϵ_d , the volume fraction of the dispersed phase).

The momentum equation is

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \vec{v}_c \vec{v}_c) + \frac{\rho}{\rho_c} \nabla_x \cdot (p \vec{I} - \vec{\tau}) =$$

$$\begin{aligned}
& - \sum_{j=1}^M \iint \rho_{dij} \frac{4}{3} \pi r^3 \vec{F}_j \, dr \, d\vec{v}_d \\
& - \sum_{j=1}^M \iint \rho_{dij} 4\pi r^2 R_j(\vec{v}_d - \vec{v}_c) f_j \, dr \, d\vec{v}_d
\end{aligned} \tag{22}$$

which is equivalent to (8) with the first term on the RHS of (22) being due to all the forces exerted on the dispersed phase by the continuous phase and the second term being the average momentum per unit volume, added to the continuous phase, due to evaporation of the dispersed phase.

Species conservation equations for each component in the continuous phase can be written in a form similar to (21), and the energy equation also has essentially the same form as for the interpenetrating continua formulation.

Up to this point the differences with the interpenetrating media equations are negligible. However, introduction of the distribution function readily leads to an equation for the evolution of interfacial area, and allows explicit consideration of size distributions in the discrete phase. Furthermore, the various forces acting on the discrete phase are made clear in the momentum equation, i.e., the physical significance of each term is clear—which is more than can be said for the interpenetrating continua formulation. The Boltzmann equation can easily be extended to nonspherical particles by allowing two or more parameters to characterize the shape. This could result in an interfacial area parallel to the flow direction at a point, and one normal to the flow direction. Having said this, one still has the requirements for the Reynolds stress closures that arise in the interpenetrating continua form. Even if such closures are phrased in terms of a turbulence model, difficulties arise with how to model the dispersion of the discrete phase due to turbulent fluctuations in the continuous phase (see, for example, Berlimont et al (1990)).

2.3. Requirements for Closure Relationships

Interfield Closures

From the previous discussion on the interpenetrating continua model it is clear that we require relationships for Γ_k , M_k and E_k for the mass, momentum and energy conservation equations, respectively. In specifying these, the jump conditions given in (12), (13) and (14) must be satisfied.

The first thing to note is that, for vaporization and condensation processes, if we neglect kinetic energy and viscous work terms at the interface, then from (14)

$$\Gamma_k = \frac{\sum \frac{1}{V} \int_{a_i} \vec{n}_k \cdot \vec{q}_k dS}{h_{fg}}$$

$$= \frac{\text{net heat transport to interface}}{\text{latent heat of vaporization}} \quad (23)$$

Thus if we know the heat flux on each side of the interface, then the mass flux due to vaporization or condensation can be estimated. This mass flux will be out of the liquid phase if the liquid side heat flux to the interface exceeds the vapor side heat flux, i.e., there will be vaporization. The reverse is true for condensation.

In most vapor-liquid systems, it can be shown quite easily that it is the liquid-side interfacial heat flux that dominates the process, and to a first approximation,

$$\Gamma_f \cong \frac{\frac{1}{V} \int_{a_i} \vec{n}_f \cdot \vec{q}_f dS}{h_{fg}} \cong \frac{\beta_{if} \hat{a}_i (T_f - T_i)}{h_{fg}} \quad (24)$$

- where β_{if} - heat transfer coefficient at interface on liquid side
 \hat{a}_i - specific interfacial area, i.e. per unit volume of the mixture
 T_f - bulk liquid temperature
 T_i - interfacial temperature

The heat transfer coefficient may be modelled using surface renewal theory and is dependent on the interfacial shear stress or the far-field turbulent Reynolds number if the shear stress is below a critical value (see Banerjee (1990)).

Similar ideas can be used for multicomponent systems where mass transfer coefficients on the liquid side may dominate. For heat transfer in single-component, vapor-liquid systems, the temperature T_i is taken to be that in equilibrium with the pressure at the interface p_i . Sometimes, but not always, the interfacial pressure is taken to be the same as the average pressure on the liquid side—otherwise some relationship between the interfacial and average phase pressure must be specified.

We see therefore that if the scalar transport coefficients are known on the liquid side, Γ_k and E_k can be estimated provided we also know \hat{a}_i . (For some cases, an "overall" transfer coefficient may be needed e.g., for mass transfer in liquid-liquid systems or for some special cases of gas-liquid systems—though the liquid side still tends to dominate in the latter systems).

For the momentum closures, M_k , we need to know

- drag coefficients for those portions of the interface in dispersed form,
- friction coefficients for those portions of the interface in continuous form,
- added mass coefficients for the dispersed portion.

In the interpenetrating continua formulation, some portion of the interfacial area at a point may be due to a continuous interface between fields, e.g., a wavy liquid film, and some portion due to discrete pockets, e.g., droplets. A central difficulty in multifield modelling lies in how to separate these contributions.

Figure 3 illustrates the problem for a wavy stratified flow using a volume close to the vapor-liquid interface.

The requirements with regard to the interfacial closure relationships are summarized below in Table 2.

Table 2. Requirements for Interfacial Closure Relationships

Conservation Equation	Interfacial Closures Required		Wall Closures Required	
	Mass Γ_k	Dispersed specific interfacial area, \hat{a}_{id} Continuous specific area, \hat{a}_{ic}	Scalar transfer coefficient, β_{ik} (for dispersed and continuous interfaces)	Area of wall intersected by phase k \hat{a}_{kw}
Momentum M_k	"	Drag coefficient, C_{id} ; Friction coefficient, f_i ; Added mass coeff., C_A	"	Wall friction or drag coefficient f_{wk}
Energy E_k	"	Scalar transfer coefficient, β_{ik}	"	Scalar transfer coefficient, β_{wk}

As mentioned earlier, the most uncertain parts of the closure relationships relate to the specific interfacial areas. The vast majority of processes involving multiphase systems in the process and power industry result in interfacial configurations that are difficult to

characterize, let alone predict. The division into "dispersed" and "continuous" at a point is rather artificial. Detailed forms for the scalar transfer coefficients, drag coefficients, friction factors and added mass coefficients must also be specified. These are usually based on single-phase relationships.

Reynolds-Stress Closures

Returning to (16) we see that in addition to the interfacial closure relationships of the type discussed above we also need relationships for terms of the type $\langle \rho_k \dot{u}_k \dot{u}_k \rangle$ where \dot{u}_k is the difference between the local instantaneous velocity and the phase average (mass-weighted) velocity. Similar correlation terms arise in the energy equation between fluctuating scalar quantities and velocities. While the problem is familiar in single-phase flows, it is more complex for multiphase flows because there are two contributions to these fluctuations, viz

- that due to turbulent fluctuations in phase k
- that due to fluctuations in distribution of phase k in the averaging volume.

In the case of single-phase fluid the averaging volume can be made very small so that the "subgrid" structure of the turbulence, perhaps, approaches universality (except near boundaries or regions of high mean shear). If this approach is taken in multiphase flows, the fluctuations due to distribution of phase k in the averaging volume increase, indicating that there are two important length scales in the problem. The first is characteristic of the phase distribution (interfacial configuration), and the second characteristic of the turbulence in the phase. This means that a formulation of the Reynolds stress like terms as a product of mean velocity gradients and eddy diffusivities is difficult. Little progress has been made, except for dispersed flow where versions of k-ε models have been tried.

A kinetic energy equation may be derived for each phase by taking the dot product of the momentum equation (16) with the phase average velocity (leaving aside the wall terms for the moment), to give

$$\begin{aligned} & \frac{\partial \epsilon_k \langle \rho_k \rangle \langle \frac{u_k}{2} \rangle^2}{\partial t} + \nabla \cdot (\epsilon_k \langle \rho_k \rangle \langle \frac{u_k}{2} \rangle^2 \langle \vec{u}_k \rangle) + \langle \vec{u}_k \rangle \cdot \nabla \epsilon_k \langle \rho_k \rangle \\ & + \langle \vec{u}_k \rangle \cdot \nabla \cdot \epsilon_k [\langle \vec{\tau}_k \rangle - \langle \rho_k \dot{u}_k \dot{u}_k \rangle] = - \langle \vec{u}_k \rangle \cdot \vec{M}_k + \langle \frac{u_k}{2} \rangle^2 \Gamma_k \end{aligned} \quad (25)$$

One can, of course, obtain the fluctuation kinetic energy equation by subtracting (25) from the local instantaneous kinetic energy equation. However, it is unnecessary to do this

to understand the main point of interest that arises. If (25) is summed over the phases then a mixture kinetic energy equation is obtained (just as mixture mass, momentum and energy conservation equations may be obtained). In the mixture mass, momentum and energy conservation equations, the *interfacial* interactions (i.e., all the integrals over a_i) cancel due to the jump conditions (12), (13) and (14). It is immediately evident by summing (25) that the mixture kinetic energy equation has a "source term" on the RHS (leaving aside the wall terms) due to the interfacial interactions (since $\vec{M}_1 = -\vec{M}_2$ and $\Gamma_1 = -\Gamma_2$)

$$\text{Kinetic Energy Source} = -[\langle \vec{u}_1 \rangle - \langle \vec{u}_2 \rangle] \cdot \vec{M}_1 + \left[\langle \frac{u_1^2}{2} \rangle - \langle \frac{u_2^2}{2} \rangle \right] \Gamma_1 \quad (26)$$

Even in the absence of mass transfer (when $\Gamma_1 = -\Gamma_2 = 0$) we have the kinetic energy source $[\langle \vec{u}_1 \rangle - \langle \vec{u}_2 \rangle] \cdot \vec{M}_1$. The term $[\langle \vec{u}_1 \rangle - \langle \vec{u}_2 \rangle] \cdot \vec{M}_1$ is always negative, since \vec{M}_1 is the *outward* flux of momentum per unit volume from phase 1. This follows because when $\langle \vec{u}_1 \rangle > \langle \vec{u}_2 \rangle$, \vec{M}_1 is positive and when $\langle \vec{u}_1 \rangle < \langle \vec{u}_2 \rangle$, \vec{M}_1 is negative. The consequence of this is that when (25) is *subtracted* from the local instantaneous equation for kinetic energy, then the *fluctuation* kinetic energy always has the source term *positive*, i.e.,

$$\text{Fluctuation k. e. source} = [\langle \vec{u}_1 \rangle - \langle \vec{u}_2 \rangle] \cdot \vec{M}_1 - \left[\langle \frac{u_1^2}{2} \rangle - \langle \frac{u_2^2}{2} \rangle \right] \Gamma_1$$

The first term is always positive, whereas the sign of the second term depends on the direction of mass transfer. If the mass transfer effect is neglected, the mixture fluctuation kinetic energy equation always has a positive energy source due to the relative motion between the phases.

In the absence of mass transfer (and surface tension effects) one can therefore immediately write down the fluctuation kinetic energy equation for each phase assigning some fraction of the source $[\langle \vec{u}_1 \rangle - \langle \vec{u}_2 \rangle] \cdot \vec{M}_1$ to each phase. The total amount to be assigned is known but the fraction to be assigned to each phase is unknown. Only in the case that the fluctuation kinetic energy of one dominates, can the mixture fluctuation kinetic energy approximate that of one of the phases. This situation is perhaps obtained for bubbly flows since the bubbles have low mass. In any case, the qualitative concept that arises from these considerations is that one might attempt to write a fluctuation kinetic energy

equation for each phase, but there will be a source term, even for the mixture equation, due to relative motion between the phases.

If one takes the process a step further, then a transport equation for the dissipation rate may also be derived, but here the interfacial interaction terms are difficult to interpret. Furthermore, one must question the reason for following such a procedure. Apparently, it is to derive an eddy diffusivity based on kinetic energy and a length scale (the fundamental hypothesis behind all this is from Prandtl). The process is usually taken one step further and a connection made between the fluctuating velocity, the length scale and the dissipation rate, resulting ultimately in an eddy diffusivity related to fluctuation kinetic energy and the turbulent dissipation rate. While this procedure is perhaps understandable for some single-phase flows, there is less to recommend it for multiphase flows. As pointed out previously, the physics of the problem suggests that there are at least two very different length scales that affect the Reynolds stress-like terms in multiphase flows—one related to the turbulence in the phase, the other to the length characteristic of the interfacial configuration.

We are therefore left with a problem as to how the Reynolds stress-like terms might be approached for multiphase flow. That the modification of turbulence can be profound due to such effects has been demonstrated by many authors, in that turbulence modification in the continuous phase has been seen even with small quantities of a dispersed phase present. The reasons are subtle and won't be detailed here.

3. THE MULTIFIELD MODEL: STRENGTHS AND WEAKNESSES

We will discuss briefly here the ability of the multifield model to predict the behavior of various two-phase flow regimes. As might be expected, the model does best when the phases are relatively uncoupled, i.e., separated flow regimes like annular, inverted annular and stratified. Closely coupled flows such as bubbly and mist may also be predicted, but quite complex formulations for the coupling, through added mass and pressure gradient terms are necessary (see Pauchon and Banerjee (1986), Drew *et al* (1979), Lahey *et al* (1980)). The model does most poorly for intermittent flows as discussed later.

To summarize, the structure of the multifield model is well developed, but the closure relationships—particularly for three-dimensional problems—are still a long way from being satisfactory. In the three-dimensional form, such multifield models may be integrated in current CFD (computational fluid dynamic) codes such as FLUENT, CFX and PHOENICS. Such codes already incorporate forms of the Euler-Lagrangian formulation with a simplified Boltzmann-type equation. However, these can only be

applied to dispersed flows. For other flow regimes the interpenetrating continua approach is used, but the problem with three-dimensional closure relationships then becomes acute, and problems also develop with the convergence of the CFD solvers. These areas, then, are those in which research must be focused. The model structure can be examined, though, for cases where closure relationships are unimportant or well-established.

3.1 Separated Flows

As mentioned, the model is best examined in situations where the closure relationships are relatively unimportant. To this end, we discuss two nontrivial applications to elucidate the strengths of the model. Consider an incompressible stratified flow in the flow situation shown in Figure 4, i.e., a horizontal channel. Here ϵ is the volume fraction of the lighter phase averaged over a thin cross-sectional volume slice and the lighter phase is otherwise identified by the subscript 1. If viscous effects are modelled by algebraic terms involving friction factors as is conventional in single-phase flow and we assume no heat or mass transfer and equal field pressures, then the characteristics for the quasi-linear set of conservation equations are wholly real only if (in the one-dimensional approximation which is sufficient for this case)

$$-\epsilon(1-\epsilon)\rho_1\rho_2(u_1-u_2)^2 \geq 0. \quad (27)$$

We have assumed $\langle u_k^2 \rangle = \langle u_k \rangle^2 = u_k^2$. This relationship cannot be satisfied for two-phase flow, so the characteristics are always complex and high frequency instabilities may be expected (as discussed by Drew (1983), Ramshaw and Trapp (1978) and Banerjee and Chan (1980)). The equal field-pressure model therefore cannot predict stratified flows. In the actual physical situation, the pressures are not equal. The form of the momentum equation can then be derived by writing

$$p_{ki} = \langle p_k \rangle + \Delta p_{ki} + \Delta p'_{ki} \quad (28)$$

where

$$\Delta p_{ki} = \langle p_{ki} \rangle - \langle p_k \rangle$$

and

$$\Delta p'_{ki} = p_{ki} - \langle p_{ki} \rangle$$

Since $\langle p_k \rangle$ and $\langle p_{ki} \rangle$ are constant in the averaging volume, therefore the term

$$\frac{1}{V} \int_{a_i} p_k \vec{n}_k \cdot \vec{n}_z dS = [\langle p_k \rangle + \Delta p_{ki}] \frac{\partial \epsilon_k}{\partial z} + \frac{1}{V} \int_{a_i} \Delta p_{ki} \vec{n}_k \cdot \vec{n}_z dS \quad (29)$$

The linear momentum equation then becomes

$$\begin{aligned} & \frac{\partial \epsilon_k \langle \rho_k u_k \rangle}{\partial t} + \frac{\partial \epsilon_k}{\partial z} \langle \rho_k u_k^2 \rangle + \epsilon_k \frac{\partial \langle p_k \rangle}{\partial z} - \Delta p_{ki} \frac{\partial \epsilon_k}{\partial z} \\ & = - \frac{1}{V} \int_{a_i} [m_k u_k + \vec{n}_z \cdot \vec{n}_k \Delta p_{ki} - \vec{n}_k \cdot (\vec{n}_z \cdot \vec{\tau}_k)] dS + \frac{1}{V} \int_{a_i} \vec{n}_z \cdot (\vec{n}_k \cdot \vec{\tau}_k) dS. \end{aligned} \quad (30)$$

To proceed we now require expressions for Δp_{ki} and $\Delta p_{ki}'$ for the stratified flow situation in Figure 4, the pressure difference between phases may be expressed in the static approximation as

$$p_i - p_1 = \Delta p_{1i} = \rho_1 g \epsilon H / 2 \quad (31)$$

$$p_i - p_2 = \Delta p_{2i} = -\rho_2 g (1 - \epsilon) H / 2 \quad (32)$$

At the level of this approximation, $\Delta p_{ki}'$ vanishes. Therefore the right hand side of the momentum equation now contains additional terms that are derivatives of ϵ .

The condition for real characteristics is then

$$(\rho_2 - \rho_1) g H \left[\frac{\epsilon}{\rho_1} + \frac{1 + \epsilon}{\rho_2} \right] \geq (u_1 - u_2)^2 \quad (33)$$

This is the stability criterion for long waves. If the inequality is not satisfied, then interfacial instabilities will grow, because the restoring forces due to gravity will not be sufficient to balance the sucking action at the wave crest due to Bernoulli's effect. The criterion in (33) signals a transition to slug flow, and this more carefully phrased, multifield model then captures real physical effects.

We will now consider another example of a separated flow to illustrate the capability of the model to predict complex phenomena. Inverted annular flows similar to the schematic in Figure 5 often occur during reflood and rewetting of vertical tubes. The wall may be thought of as being very hot and a film of vapor is generated that prevents the liquid from wetting the wall. The vapor-liquid interface is wavy and this enhances heat transfer compared to condensation through a uniform laminar vapor film. To model such a situation, the pressure difference between the phases due to surface tension must be incorporated into the momentum equations. The momentum equation for the liquid then becomes (dropping the averaging signs)

$$\rho_2 \epsilon_2 \frac{\partial u_2}{\partial t} + \rho_2 u_2 \epsilon_2 \frac{\partial u_2}{\partial z} + \epsilon_2 \frac{\partial p_1}{\partial z} - \frac{\sigma}{2R\sqrt{\epsilon_2}} \frac{\partial \epsilon_2}{\partial z} - \frac{\sigma R \sqrt{\epsilon_2}}{2} \frac{\partial^3 \epsilon_2}{\partial z^3}$$

= algebraic terms that do not affect phase speed. (34)

Note that the reference pressure is p_1 , i.e., the pressure in the vapor, σ is the surface tension, R is the tube radius and we have assumed distribution coefficients ~ 1.0 .

If a linear stability analysis is performed for the conservation equations assuming the phases are incompressible, we find the phase speed is real if

$$(u_1 - u_2) \leq \left[\frac{k^2 \sigma R}{2\sqrt{\epsilon_2}} - \frac{\sigma}{2R\epsilon_2^{3/2}} \left(\frac{\epsilon_1}{\rho_1} + \frac{\epsilon_2}{\rho_2} \right) \right]^{1/2} \quad (35)$$

where k is the wave number.

Interfacial mass transfer has only a weak effect on this criterion. In particular the short wavelengths (large k) are stable even at very high velocity differences between phases.

The length of the most unstable waves can be found by seeking the maximum growth factor. Kawaji and Banerjee (1985) show that this wavelength is given by

$$\lambda = \frac{2\pi \epsilon_2^{1/4} (\sigma R)^{1/2}}{\left[\frac{\epsilon_2 \rho_2 \rho_1 (u_1 - u_2)^2}{\epsilon_1 \rho_2 + \epsilon_2 \rho_1} + \frac{\sigma}{2R\sqrt{\epsilon_2}} \right]^{1/2}} \quad (36)$$

As shown in Figure 6, this result compares well with the experimental data of De Jarlais (1983).

We will not discuss dispersed flows here, except to note that if the pressure forces between fields are correctly phrased, then good predictions are again possible for phenomena such as propagation of void waves (see Pauchon and Banerjee (1986)).

3.2 Limitations of the Model

The preceding discussion illustrates that the multifield model can predict a variety of phenomena. The cases were selected such that the results were rather independent of the closure relationships. The model works well for both separated and distributed flows provided the pressure interactions between fields are developed with care.

We turn now to the closure relationships required for forces at the wall and between fields due to viscous effects, i.e., the terms containing $\bar{\tau}$ and the part of the $\Delta p'_{ki}$ term affected by viscosity—called form drag in Bird et al (1960). For the multifield model, these terms are written by analogy with single-phase flow, so the forces are expressed as:

$$\text{total drag (form + friction)} = -\frac{1}{8} \rho_c \hat{a}_i C_D |\langle u_c \rangle - \langle u_d \rangle| (\langle u_c \rangle - \langle u_d \rangle)$$

for submerged objects;

$$\text{frictional drag} = -\frac{1}{2} \rho_c \hat{a}_i f |\langle u_c \rangle - \langle u_d \rangle| (\langle u_c \rangle - \langle u_d \rangle)$$

for separated flows;

$$\text{wall drag} = -\frac{1}{2} \rho_c \hat{a}_{kw} f |\langle u_c \rangle| \langle u_c \rangle \quad (37)$$

where \hat{a}_i and \hat{a}_{kw} are the interfield and wall areas per unit volume, C_D is a drag coefficient, f is friction factor, and subscripts c and d denote continuous and dispersed phases, respectively. The absolute value signs are used to take flow reversal into account so that the force points in the right direction.

For each flow regime, expressions have been developed for the unknowns in (37) (see, for example, Ransom, et al (1984) and the TRAC-PD2 manual (1982)).

A difficulty arises however when flows are oscillatory. Consider a flow and wall shear stress history shown schematically in Figure 7. Here the time-averaged flow vanishes. However, the time-averaged wall shear stress does not because it is proportional

to the square of the velocity. Thus expressions like (37) do not predict wall (or interfacial shear stress) in such situations.

To illustrate this, some data on reflux condensation is presented. The physical situation for refluxing near the flooding point is shown in Figure 8. Vapor flow is introduced at the bottom of a vertical pipe, e.g., at the entrance to steam generator tubes in a PWR, flows upwards, and condenses. The liquid, on the average runs down countercurrent to the vapor flow. This situation is of importance in assessing small break accidents in PWRs (pressurized water reactors). Here, steam may be formed in the reactor core in certain phases of the oscillating flow to the steam generators where it condenses, and the condensate runs back countercurrent to the steam flow. However, if the steam flow is slightly above the flooding value, the steam generators do not drain completely on the riser side and liquid is held up, as shown in the figure. The liquid head exerts back pressure on the core and causes the liquid level to drop. In certain cases, portions of the core may be uncovered.

It is therefore important to predict the liquid inventory distribution in the system, and particularly on the riser side of the steam generators. This is impossible to do on the basis of shear stress correlations of the form in (33).

To demonstrate this, data on liquid and vapor velocities and void fraction is plotted in Figure 9. The average liquid flow is downward and the average vapor flow is upward as shown in the figure. A single-phase region exists above the condensing two-phase region, i.e., above the point a goes to zero.

The average wall shear stress is plotted in Figure 10 together with the quantity $\langle u_2 \rangle / \langle u_1 \rangle$. It is evident the average wall shear stress goes through a change in sign. The average wall shear stress if modelled by an expression of the type in (37) would indicate that the flow at the bottom of the condenser is upward and downward at the top. This is at variance with the measurements. The same result is found in all the experiments we have done in this regime (see Banerjee and Nguyen (1987)).

The reasons for this curious behavior in wall shear stress may be explained qualitatively as follows. Consider the flow to be oscillatory with large waves traveling upwards at velocities close to that of the vapor and relatively slow downflow in the liquid film between waves. The shear stress under the waves is high because of the high velocity upflow, whereas the wall shear stress in the draining film is low. However, as the vapor condenses, its velocity is reduced and the wave velocity is also reduced. As a consequence, the shear stress at some point goes to zero because the component due to upflow in the waves is exactly balanced by downflow in the film. Below this point, the wave velocity is high enough to give a negative shear stress, whereas above this point,

shear stress is positive. The data can be explained more quantitatively if observed values of wave frequency and velocity are used together with appropriate velocity gradients at the wall in the wave and draining film regions.

The question, however, is to determine whether the multifield model can be modified to incorporate such phenomena. The correlations required for wall and interfacial shear stress in the slug/churn would clearly have to be quite different from (33).

A methodology to deal with problems of this nature has not yet been developed. One possibility is to divide the liquid flow into two fields—a wave or slug field and a film field. The momentum interactions in these fields with the gas/vapor and the wall would be quite different. At present, there appears to be no information about the division of liquid between these fields which can be obtained from the model. Information on disturbance length, amplitude and frequency is needed to proceed further, and it appears this has to be supplied to the model on the basis of experiments, and perhaps, analysis.

In summary, then, the multifield model successfully captures many subtle phenomena in two-phase flows where oscillations are small compared to the mean flow. However, in regimes where the oscillations are large, the model is more difficult to apply. The difficulty arises when the closure relationships are nonlinear in the fluctuating variables.

4. THE NEED FOR MULTIFIELD MODELS

The need for multifield models may be divided, for nuclear problems into, two broad categories, viz. arising from

- normal operations
- transients and accident conditions

Each of these will now be considered in turn.

4.1 Normal Operations

All nuclear power plants boil water to generate steam that drives turbine-generators. For pressurized light, heavy water, and liquid metal systems, the steam generation occurs on the secondary side—though some recent pressurized heavy water reactors do allow low-quality, steam-water core outlet flows. Boiling water reactors, of course, generate steam on the primary side to drive the turbine(s). Whether steam is generated on the primary or the secondary side, two-phase flows do occur and modelling needs arise associated with circulation, steam separation, condensation and erosion. The modelling issues are perhaps more crucial for boiling water (direct cycle) systems, since the primary circuit is involved. Modelling of two-phase flows is also necessary to establish the limits of normal operation

due to critical heat flux. While such limits have usually been established on the basis of large-scale experiments and quite empirical models, recent approaches apply multifield modelling models.

Table 3 lists some of the two-phase phenomena that must be modelled for various nuclear systems and identifies those that require a multifield approach for reliable predictions. The need for such models is most apparent in predictions of

- critical heat flux
- steam separator performance (including quality distribution at the separator inlets)
- droplet-induced erosion.

Table 3 Normal Operations: Modelling Requirements

Component	Phenomenon(a)	Key Issues	Model Level Required
Core (BWRs mainly)	Parallel Channel Stability	<ul style="list-style-type: none"> •Void Distribution (boiling length) •Pressure Losses 	<ul style="list-style-type: none"> •Mixture Models (1D) "
Fuel	Critical Heat Flux	<ul style="list-style-type: none"> •Entrainment/Deposition •Subchannel Mixing •Spacer Effects •Core Void Distribution 	<ul style="list-style-type: none"> •Multifield Models (1D) •1D Multifield, Parallel Channel •3D Multifield •1D Multifield, Parallel Channel
Steam Separators	•Rotating Two-Phase Flows	<ul style="list-style-type: none"> •Deposition/Centrifugal Effects •Re-entrainment •Bubbly Carryunder •Inlet Quality Distribution to Separator (Void Distribution) 	<ul style="list-style-type: none"> •3D Multifield •3D Multifield •3D Multifield •3D Multifield
Steam Generators (PWR's)	•Two-Phase Nat. Circulation	<ul style="list-style-type: none"> •Shell-Side Void Distribution (radial and axial) •Particulate Deposition 	•3D Mixture Models
Condensers LP Stage (Turbine)	•Droplet-Induced Erosion	<ul style="list-style-type: none"> •Droplet Motion •Droplet Impact —Erosion Relationship 	•3D Multifield Models

While multifield models have been applied in all these areas, there are still problems in obtaining reliable predictions. For critical heat flux predictions, the effects of spacers (and other appendages) on entrainment and liquid-film disruption are difficult to calculate. Three-dimensional computational fluid dynamic (CFD) solvers, integrated with a multifield model, are likely to be necessary for regions around appendages, but it is not clear whether even these will succeed for such a complex problem. On the other hand, predictions of steam separator performance based on the multifield approach (two-dimensional axisymmetric) have been successful. Yokobori et al (1996) report on a study of the separator shown in Figure 11. Table 4 shows the results of air-water tests compared with predictions, and Table 5 shows comparisons with steam-water tests. In both cases, the agreement between data and the calculations is good—remarkable since Yokobori et al. use very simple formulations for the closure relationships.

Table 4 Comparison of Analysis Result with Test Data (Air-Water Test)

	Test	Analysis
Discharge flow fraction	0.96	0.992
Carry over	0.04	0.008

Table 5 Comparison of Analysis Result with Test Data (Steam-Water Test)

	Test	Analysis
Primary discharge flow fraction	0.84	0.79
Carry over from 1st stage	0.16	0.21

So far as phase distributions at BWR separator inlets is concerned, Tinoco and Hemström (1990) have presented multifield calculations with a modified version of PHOENICS. While there is no direct validation of the results, which are shown in Figure 12, they are consistent with observations of separator performance in the plant. The model used includes the separators, through their pressure drop-mass flow/quality characteristics (based on experiments. Note how the relatively uniform steam-water mass flow

distribution at the core outlet leads to a distribution with multiple peaks in the water mass flow distribution at the separator inlets. This occurs because the steam is able to turn more readily and the steam flow gets disproportionately diverted toward the center of the separator array. The opposite happens to the water. The peaks occur due to the water being drawn toward the separator inlets on the periphery. Such phenomena cause significant degradation in overall steam separation.

Turning now to erosion problems, most modern CFD codes (FLUENT, PHOENICS, CFX) can handle a dispersed phase using the Euler-Lagrangian formulation—which is "equivalent" to the multifield approach as discussed previously. Such codes can handle very complex geometries including rotating components, tube arrays, etc. Jal and Tinoco (1993) have presented a three-dimensional CFD study of droplet erosion in nuclear condensers and shown comparisons with observations. From these investigations, they were able to indicate how their erosion problem could be reduced.

From the preceding discussion, it is clear that multidimensional multifield models coupled with CFD solvers, have been used for a variety of normal operations problems. In this area, their use will surely increase as the financial incentive to improve performance and reduce maintenance, of nuclear plants is large. Furthermore, plant operators can take advantage of rapid increases in computing power, in sophistication of grid generators, and in robustness of CFD solvers. However, these advances must be accompanied by corresponding advances in our understanding of the closure relationships that are needed—an area in which much less development is occurring.

4.2 Transients and Accident Conditions

Multifield models are often needed for abnormal events, in nuclear systems, that result in relatively low velocity, two-phase flows. The flow regimes in horizontally-oriented pipes tend to become stratified or slug, with levels between liquid-rich and vapor-rich phases appearing in vessels. In vertically-oriented flow passages, regimes with the liquid films on the wall and vapor cores may appear, when the walls are cool. For walls above the rewetting temperature, e.g., hot fuel cladding before refilling of the core, regimes with vapor at the wall and a liquid core (inverted annular flow) may occur. While flows in the vertical components still have closer coupling between the phases than flows in horizontal components, and may therefore be described by "drift-flux-type" mixture models, still a uniform approach for the whole system necessitates use of a multifield-type model. It is worth noting, however, that mixed approaches are also in use with drift-flux

mixture models for the vertically-oriented flows, and multifield for the horizontally-oriented.

With careful phrasing of the coupling terms and if necessary, introduction of some distribution terms, multifield models can, however, encompass mixture models. It is for this reason that multifield models are often used for calculations of abnormal conditions, even for systems where the flows are primarily vertical, e.g., BWRs.

To illustrate the need for multifield models, use is now made of PIRTs (Phenomena Identification and Ranking Tables) to pick out important phenomena in various phases of certain accidents like LBLOCA and SBLOCA. Only the highly ranked phenomena (ranked for their potential impact on key system responses, such as clad temperature and reactor-vessel coolant inventory) are discussed here for brevity. Some of these do not require multifield models for their portrayal, whereas others do.

Table 6 summarizes the highly ranked phenomena, various parts of the system, for various stages of a LBLOCA in a PWR. Also indicated in the table are those phenomena for which multifield models are needed and why. Most of these involve separated flows like inverted-annular, film condensation and/or phase separation. Such phenomena are difficult to capture in mixture models.

**Table 6 PWR-LBLOCA Highest Ranked Phenomena:
Need for Multifield Modelling**

Phenomenon	Blowdown	Refill	Reflood	Multifield Model?	Why?
•Fuel Rod Stored Energy	x	-	-	No	
•Core Reflood Heat Transfer			x	Yes	Inverted ann. flow and carry-over
•3-D Flow Entrainment/De-entrainment			x	Yes	Phase separation
•Upper Plenum Entrainment//De-entrainment			x	Yes	Phase separation
•Hot Leg Entrainment//De-entrainment			x	Yes	Phase separation
•Steam Generator Steam binding			x	Yes	Phase separation and vaporization
•Pump 2-Phase Performance	x			No	
•Cold Leg/Acc Condensation		x		Yes	Film formation, stratification/unequal phase temperatures
Noncondensable Gas			x	Yes	Phase separation
•Downcomer Condensation		x		Yes	Unequal phase temperature
•Break Critical Flow	x			Perhaps	Could use empirical correlation
•Loop Oscillations			x	Perhaps	Could probably be done with mixture model with level tracking

Table 7 summarizes the highest ranked phenomena for SBLOCAs in the AP600 to illustrate what happens for PWR plants with passive safety features. The SBLOCA is divided into two stages—the first (Stage 1) starting with rapid depressurization and emptying of the pressurizer and ending with ADS4 discharge, followed by refilling of the system to the hot leg level through the IRWST flow. The second stage has to do with long term cooling and includes, in its early phases, draindown of the IRWST and filling of the sump, till spilling occurs. This is followed by a quasi-steady state in which the decay heat is transmitted to the containment walls by steam, generated in the core, and discharged primarily through the ADS4 valves. The steam is condensed by water film cooling of the outer containment shell.

From the table, it is clear that most of the highest ranked phenomena may be modelled with mixture or single-phase formulations. The exceptions relate to phase separation at tees, such as PBL-CL junctions or ADS4 junctions. These may three-dimensional multifield approaches because of the complexity of the phenomena. While not shown explicitly, the ADS4 tee separation is also important in determining mass and energy discharge. Finally, predictions of two-phase level and associated problems like entrainment/de-entrainment may yield one-dimensional multifield approaches.

**Table 7 PWR-LBLOCA Highest Ranked Phenomena:
Need for Multifield Modelling**

Phenomenon (alphabetical order)	Stage 1	Stage 2	Multifield Model?	Why?
•Accumulator: Flow	x	—	No	
•ADS: Energy Release	x	x	Perhaps	Empirical discharge model pos.
^{g)} •ADS: Mass Flow	x	x	Perhaps	Empirical discharge model pos.
•Break: Mass Flow	x	—	Perhaps	Empirical discharge model pos.
•Cold Leg: PBL Phase Sep	x	—	Yes	Phase separation
•Core: Flashing	x	—	Perhaps	Empirical corr. poss.
Flow Resistance	x	—	No	
Subcooling Margin	x	—	No	
Two-Phase Level	x	x	Perhaps	Mixture model possible
•CMT: Flow Resistance	x	—	No	
•Downcomer/LP: Level	—	x	Perhaps	Mixture model possible
•Fuel Rods: Decay Heat	x	x	No	
•Hot Leg: Tee Phase Sep.	x	—	Yes	Phase separation
•IRWST: Flow Resistance	x	x	No	
Pool Level	—	x	No	
Thermal Stratif.	—	x	No	3D CFD single-phase poss.
•Pressurizer: Level	x	—	No	
•Sump: Fluid Temp.	—	x	No	
•Upper Plenum: 2-phase Level	—	x	Yes	Phase separation

For the long term cooling stage, phase separation in tees—particularly related to the ADS4 line—may be an important issue and it may be possible to treat in the three-dimensional multifield framework.

5. SUMMARY

As indicated in the previous discussion, multifield models already play an important role in simulations of reactor normal operation and accident behavior. While one-dimensional models have had the greatest use to date, multidimensional models are becoming of increasing importance—particularly for calculation of phase separation and de-entrainment. The requirements for closure relationships are more stringent for three-dimensional models, and this is the area where research must be focused in the next few years. Note that the greatest uncertainties in the closure relationships arise because of

interfacial area evolution. Therefore, modelling of, and data on, interfacial area evolution in two-phase flows is the most important task. The evolution may be based on Boltzmann-type formulations (e.g., (18)) integrated over "particle" velocities and radii—at least a good starting point.

References

- Agee, L. J., Banerjee, S., Duffey, R. B., and Hughes, E. D., 1978, "Some Aspects of Two Fluid Models and Their Numerical Solutions" *Second OECD Specialists Meeting on Transient Two Phase Flow 1*, 27-58.
- Banerjee, S., 1985, "Closure Relationships and Constitutive Equations," Lecture presented at Two-Phase Flow Short Course, ETH-Zurich, March.
- S. Banerjee, 1990 "Turbulence Structure and Transport Mechanisms at Interfaces" Keynote Lecture, 9th Int. Heat Transfer Conf, Hemisphere Press, NY, pp. 395-418.
- Banerjee, S., and Chan, A. M. C., 1980, "Separated Flow Model I. Analysis of the Averaged and Local Instantaneous Formulations" *Int. Journal of Multiphase Flow 6*, 1-24.
- S. Banerjee and Q. Nguyen, 1987 "Reflux Condensation" in *Multiphase Science and Technology*, Vol. 3, ed. by G.F. Hewitt, J.M. Delhaye and N. Zuber, Hemisphere Publishing Corp., 360-367.
- S. Banerjee and K.R. Weaver, "Transient Two-Phase Flow" *Proc. of First OECD/NEA Specialist Meeting on Transient Two-Phase Flow*, Hemisphere Press, 1978.
- Berlemont, A., Desjonqueres, P. and Gouesbet, G. 1990, "Particle Lagrangian Simulation in Turbulent Flows," *Int. J. Multiphase Flow 16*, 19.
- Bird, R. B., Stewart, W. E. and Lightfoot, E. J., 1960, *Transport Phenomena* J. Wiley, N.Y.
- Boure, J. A., 1975, "On a Unified Presentation of the Non-Equilibrium Two-Phase Flow Models in Non-Equilibrium Two-Phase Flows," (Ed. R. T. Lahey, Jr., and G. B. Wallis), ASME Symposium Volume, ASME New York.
- De Jarlais, G., 1983, "An Experimental Study of Inverted Annular Flow Hydrodynamics Utilizing an Adiabatic Simulation" NUREG/CR-3339.
- Delhaye, J. M., and Achard, J. L., 1976, "On the Averaging Operators Introduced in Two-Phase Flow Modeling," *Proc. CSNI Specialists Meeting in Transient Two-Phase Flow*, Toronto, August 3-4, 1976 (Ed. S. Banerjee and K. R. Weaver).
- Drew, D. A., Cheng, L., Lahey, R. T., Jr., 1979, "Analysis of Virtual Mass Effects in Two Phase Flow," *Int. J. Multiphase Flow 5*, 233-242.
- Drew, D. A., 1983, "Mathematical Modelling of Two Phase Flow," *Ann. Rev. Fluid Mech. 15*, 261-291.

- Ishii, M., 1975, *Thermo-Fluid Dynamic Theory of Two Phase Flow*, Byrolles, Paris.
- Jal, E.N. and Tinoco, H., 1993, "Mathematical Modelling of Industrial Power Condensers with an Application to Droplet Erosion," in *Eng. Applications of CFD, Proc. IMech E*, 1993-95 IMechE Publications, London pp. 93-108.
- Kawaji, M., and Banerjee, S., 1987, "Application of a Two-Field Model to Reflooding of a Hot Vertical Tube I. Model Structure and Interfacial Phenomena," *J. Heat Transfer* **109**, 204-211.
- Lahey, R. T., Jr., Cheng, L., Drew, D., Flaherty, J., 1980, "The Effect of Virtual Mass on the Numerical Stability of Accelerating Two Phase Flow," *Int. J. Multiphase Flow* **6**, 281-294.
- Nigmatulin, R. I., 1979, "Spatial Averaging in the Mechanics of Heterogeneous and Dispersed Systems," *Int. J. Multiphase Flow* **5**, 353-385.
- Panton, R. J., 1978, "Flow Properties for the Continuum Viewpoint of a Non-Equilibrium Gas Particle Mixture," *Int. J. Fl. Mech.* **31**, 273-303.
- Pauchon, C., and Banerjee, S., 1986, "Interphase Momentum Effects in the Averaged Multifield Model: I. Void Propagation in Bubbly Flows," *Int. J. Multiphase Flow* **12**, 559-573.
- Ramshaw, J.D., and Trapp, J.A., 1978, "Characteristics, Stability, and Short Wavelength Phenomena in Two-Phase Flow Equation Systems," *Nuc. Sci. and Engineering* **66**, pp. 93-102.
- Ransom, V.H., et al., 1984, "RELAP5/MOD2 Code Manual Vol. I, Code Structure, System Models and Solution Methods," EGG-SAAM-6377.
- Tinoco, H. and Hemström, B., 1990 "Numerical Modelling of Two-Phase Flow in the Upper Plenum of a BWR by a Three-Dimensional, Two-Fluid Model" In *Eng. Turbulence Modelling and Experiments* ed. W Rodi and E. N. Gamé, Elsevier, London, pp. 927-936.
- TRAC-PD2, 1981, "An Advanced Best Estimate Computer Program for PWR Loss of Coolant Accident Analysis," Los Alamos National Lab. Rept. LA-8709-MS (NUREG/CR-2054).
- Vernier, P., and Delhaye, J. M., 1968, "General Two Phase Flow Equation Applied to the Thermo-hydrodynamics of Boiling Water Nuclear Reactors," *Energie Primaire* **4**, (1-2).
- Williams, F. A., 1959. "Spray Combustion Theory" *Combustion and Flame*, **3**, 215.
- Yadigaroglu, G., and Lahey, R. T., 1976, "On the Various Forms of the Conservation Equations in Two Phase Flow," *Int. J. of Multiphase Flow* **2**, pp. 477-494.
- Yokobori, S., Akiba, M., Terasaka, H., Kudo, Y., Koh, F., and Saito, T., 1996, "Investigation of Two-Phase Flow Characteristics in the BWR Separator," ICONE-4 Vol. 1 Part A pp. 131-140, ASME-JSME Int. Conf.

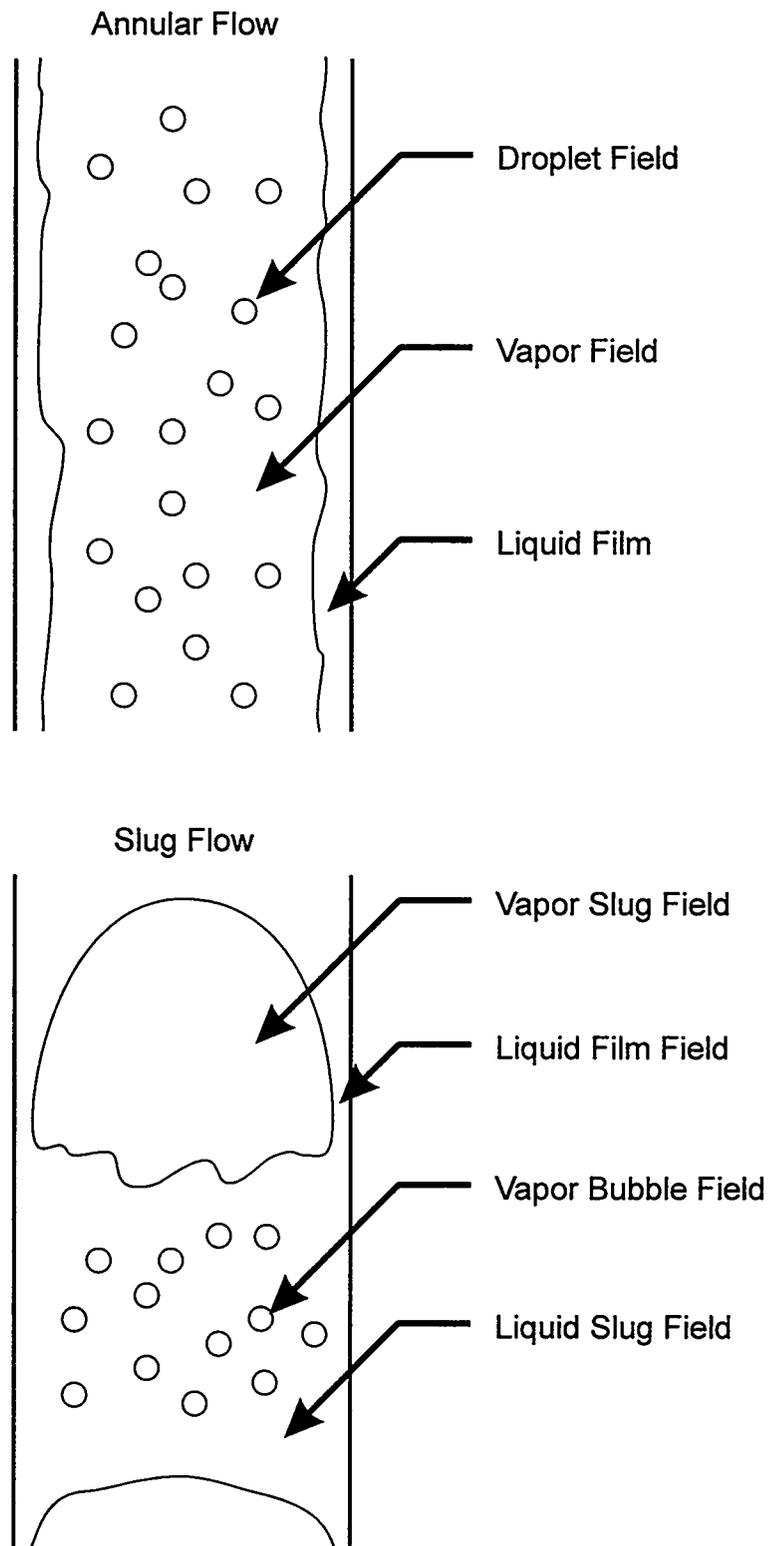
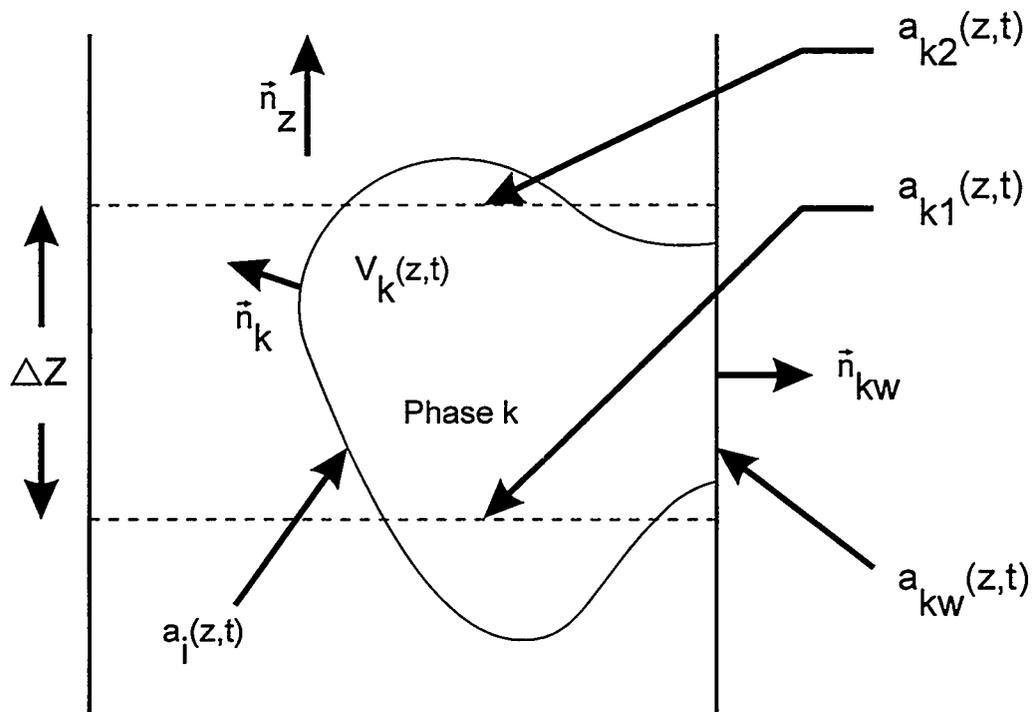


Figure 1: Illustration of Fields



(1)

PASTE EQUATIONS HERE

(2)

Figure 2: Schematic defining various interfacial and planer quantities.

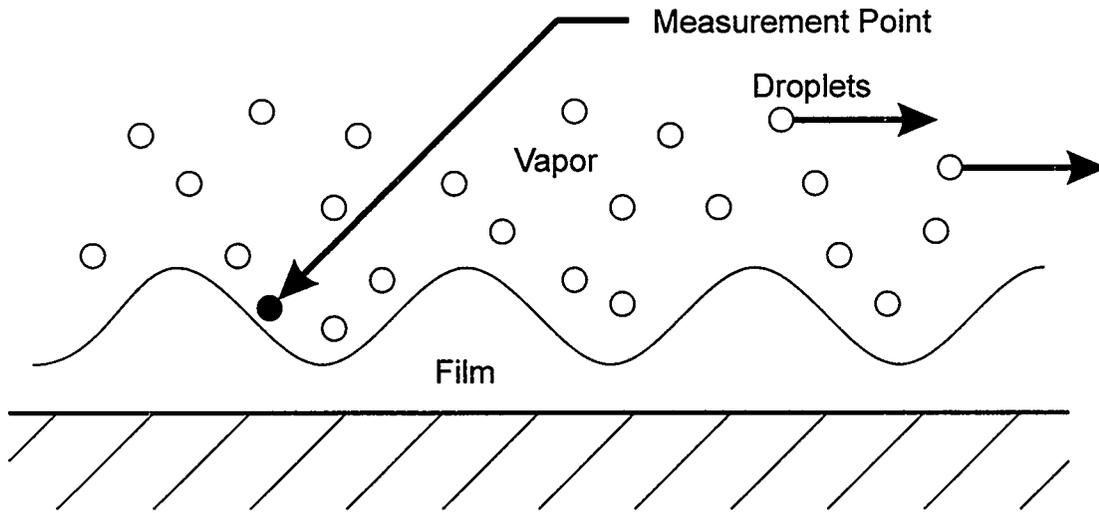


Figure 3: The measurement point sees both waves (continuous interface) and drops (dispersed phase) for some fraction of the time. This is typical of the problem involved in assigning interfacial areas and transport mechanisms.

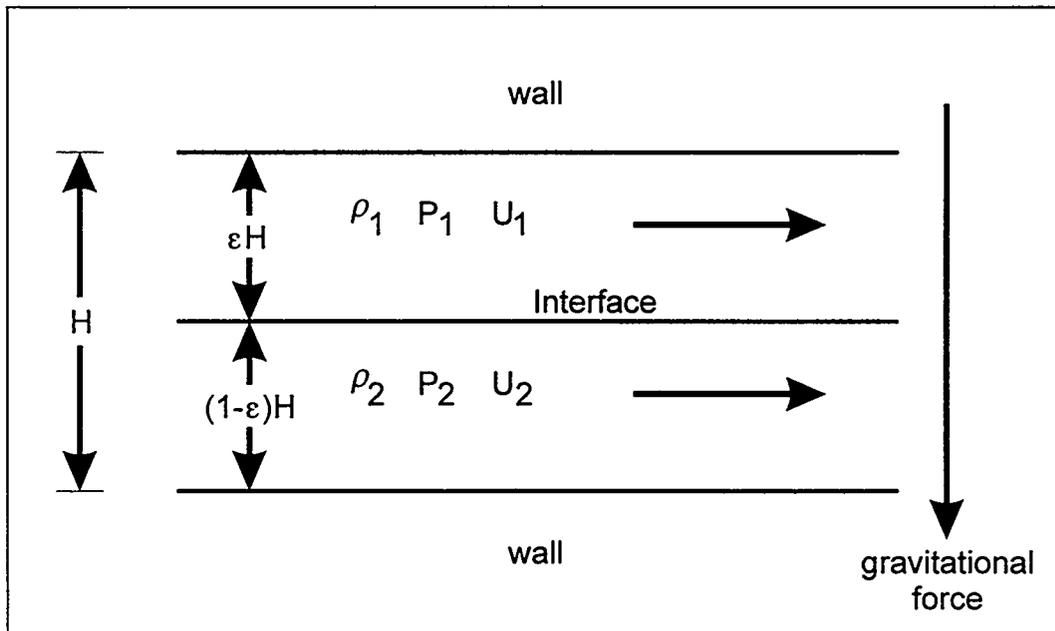


Figure 4: Schematic of stratified two-phase flow field defining the symbols.

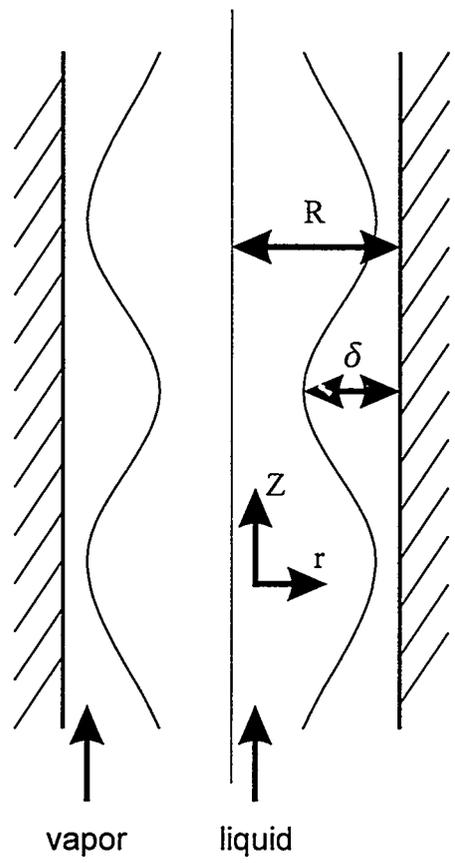


Figure 5: Schematic of inverted annular flow.

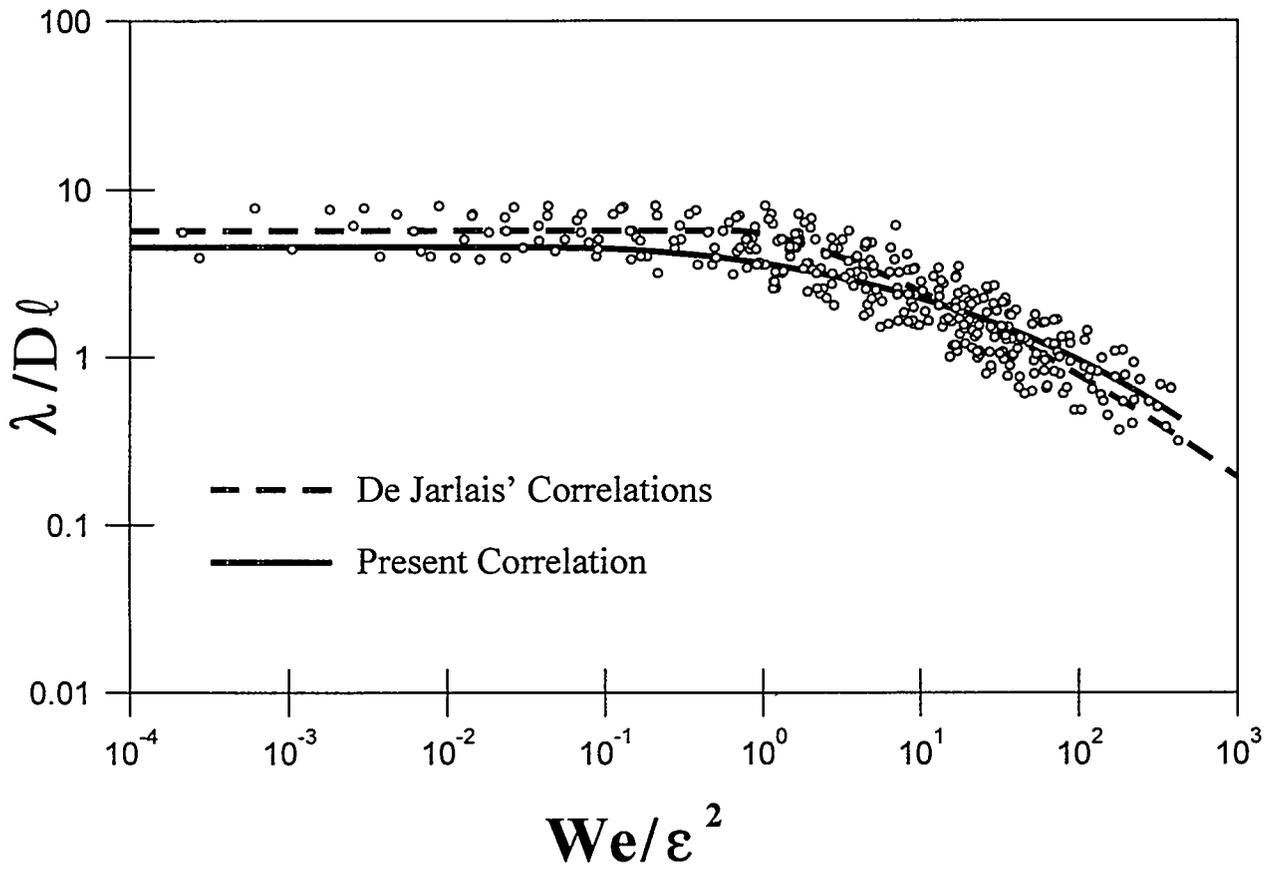


Figure 6: Comparison of predictions with De Jarlais' data.

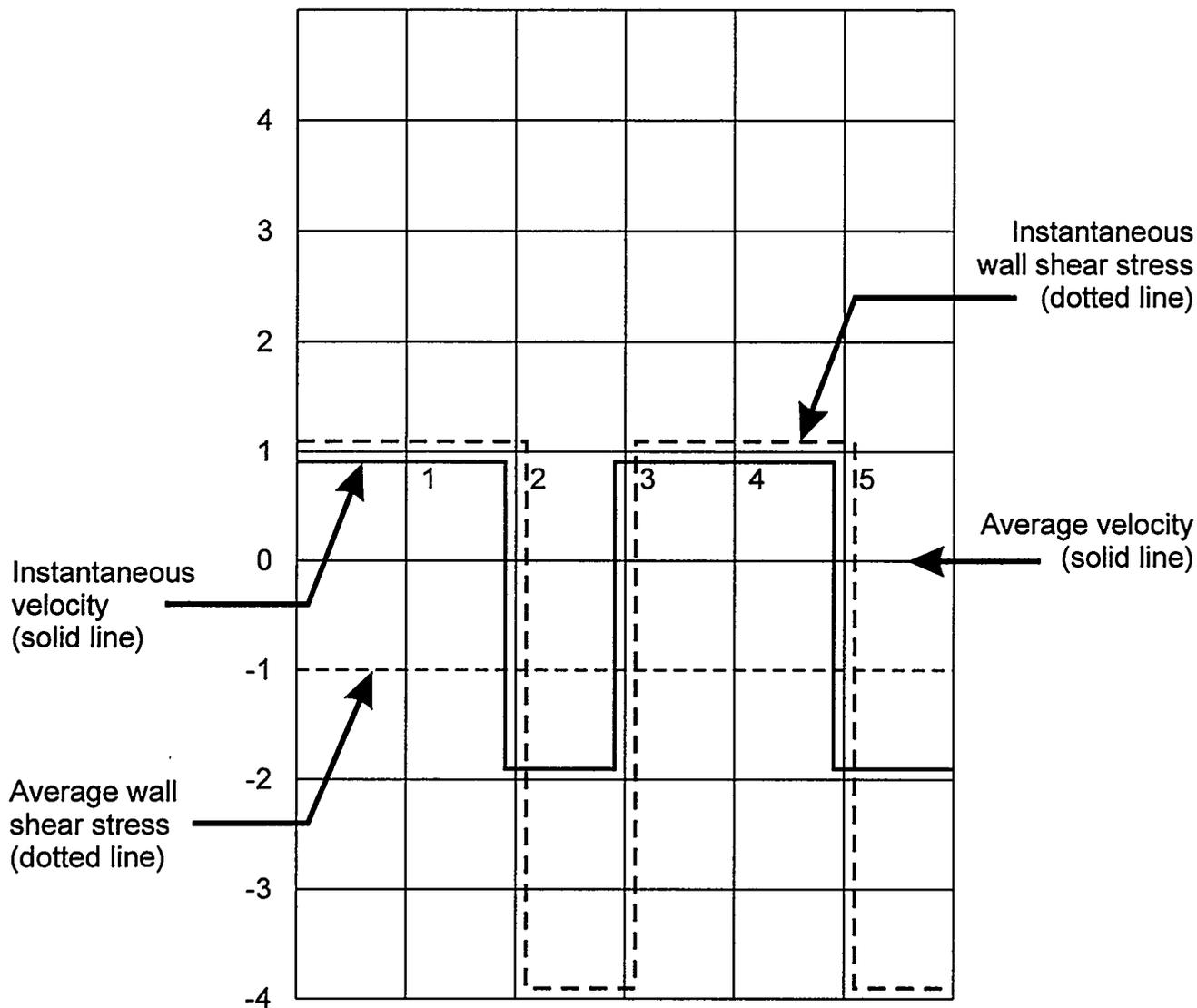


Figure 7: Schematic showing a postulated instantaneous velocity field with mean velocity = 0, and instantaneous and average wall shear stress. The wall shear stress is assumed to vary as the square of the velocity.

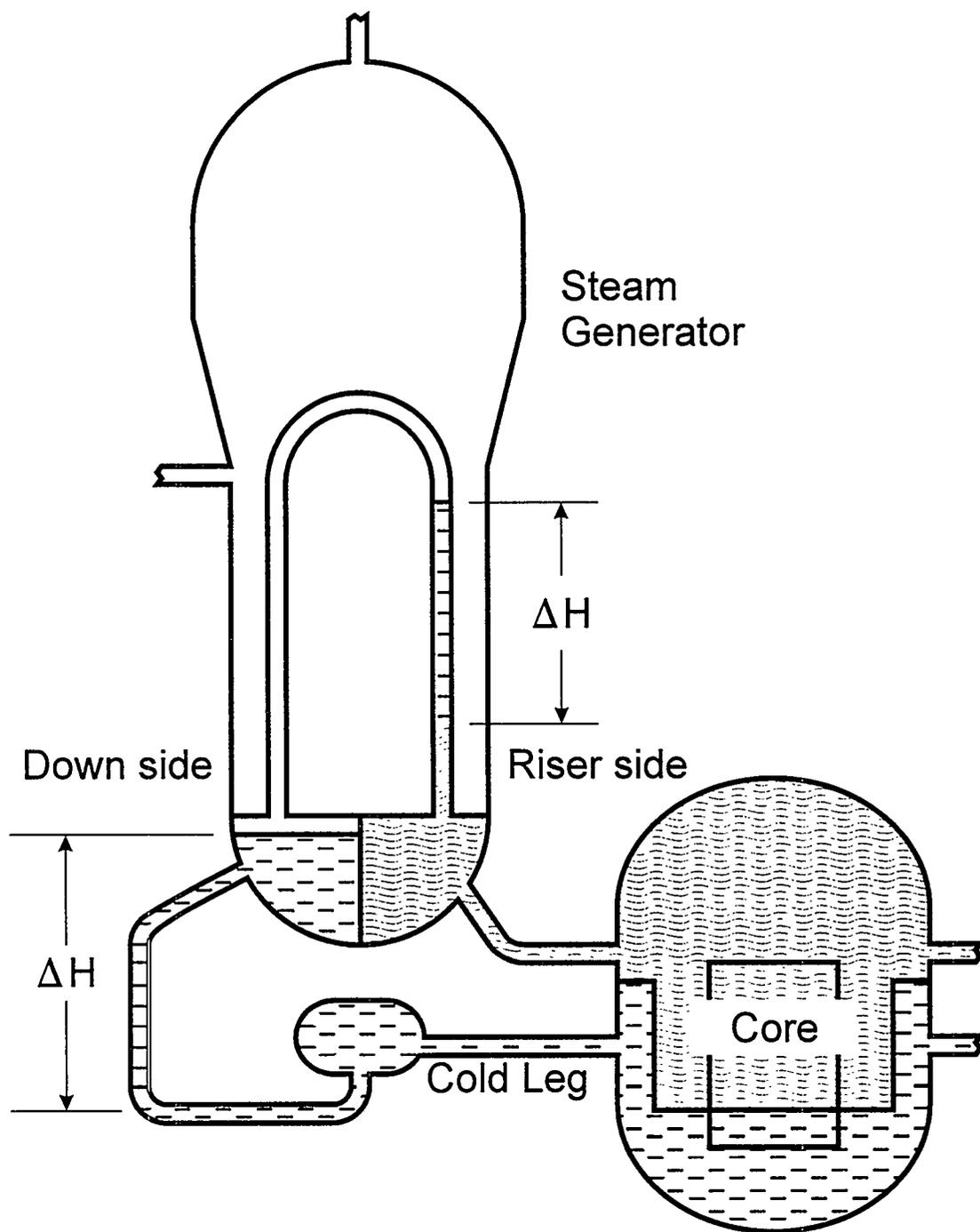


Figure 8a: Small break accident scenario with steam generation rate leading to flooding during reflux condensation.

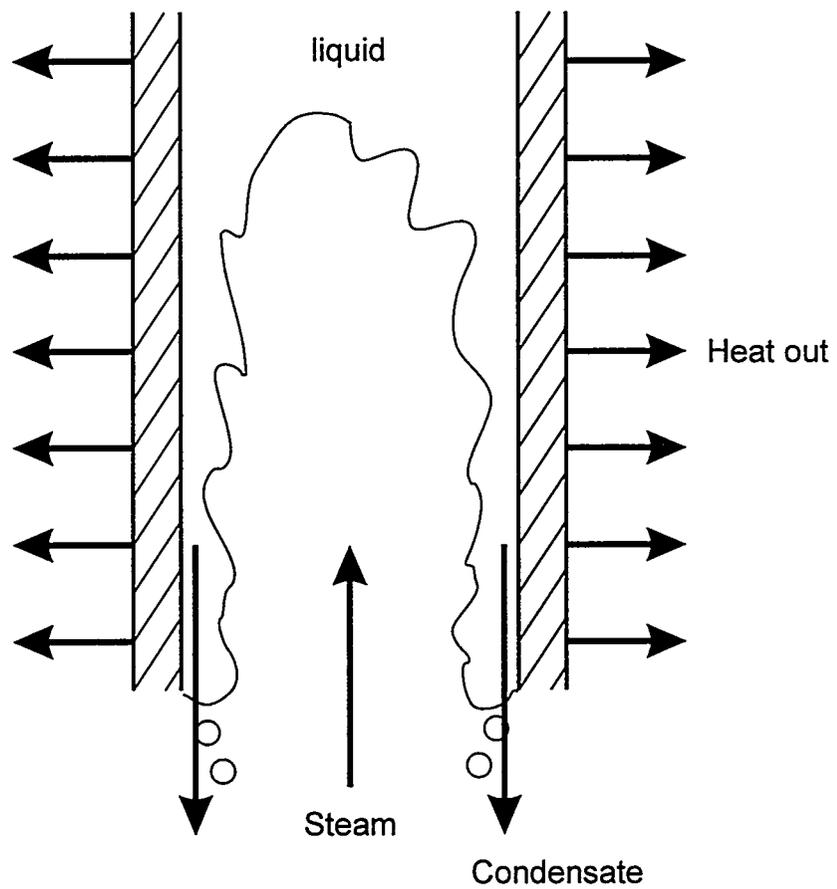


Figure 8b: Detail of countercurrent film condensation in SG tubes.

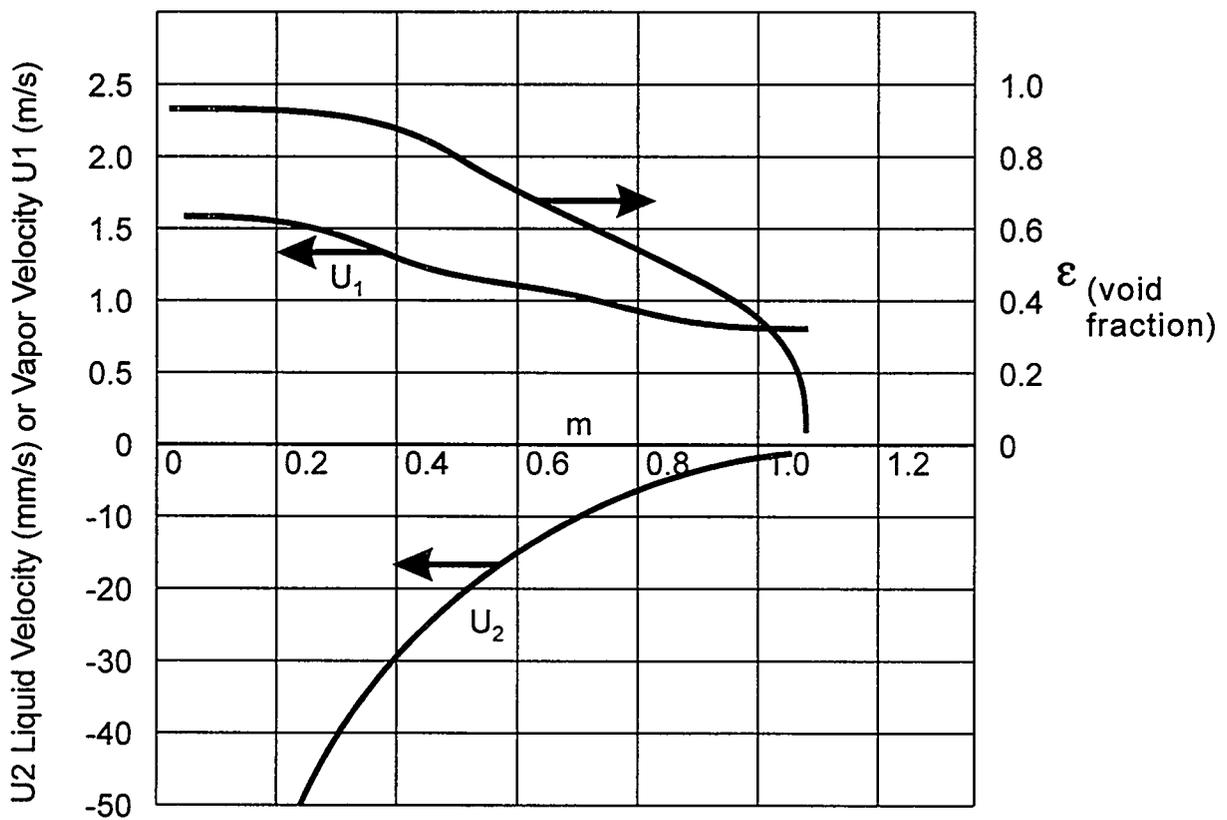


Figure 9: Data on liquid and vapor velocities and void fraction during reflux condensation near flooding point. The abscissa is distance from inlet of the tube shown schematically in Figure 8b.

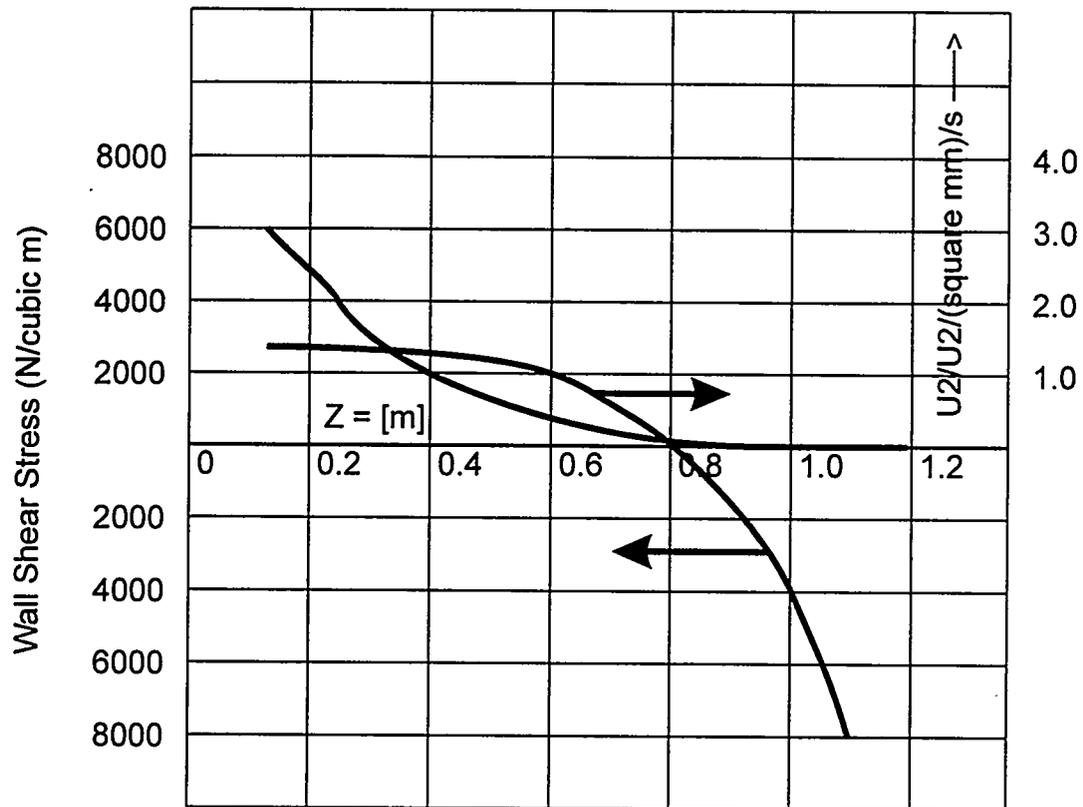


Figure 10: Data on wall shear stress and liquid velocity during reflux condensation showing that the wall shear stress is *not* proportional to the square of the mean velocity. In fact it points in the wrong direction for $z < 0.8$ m.

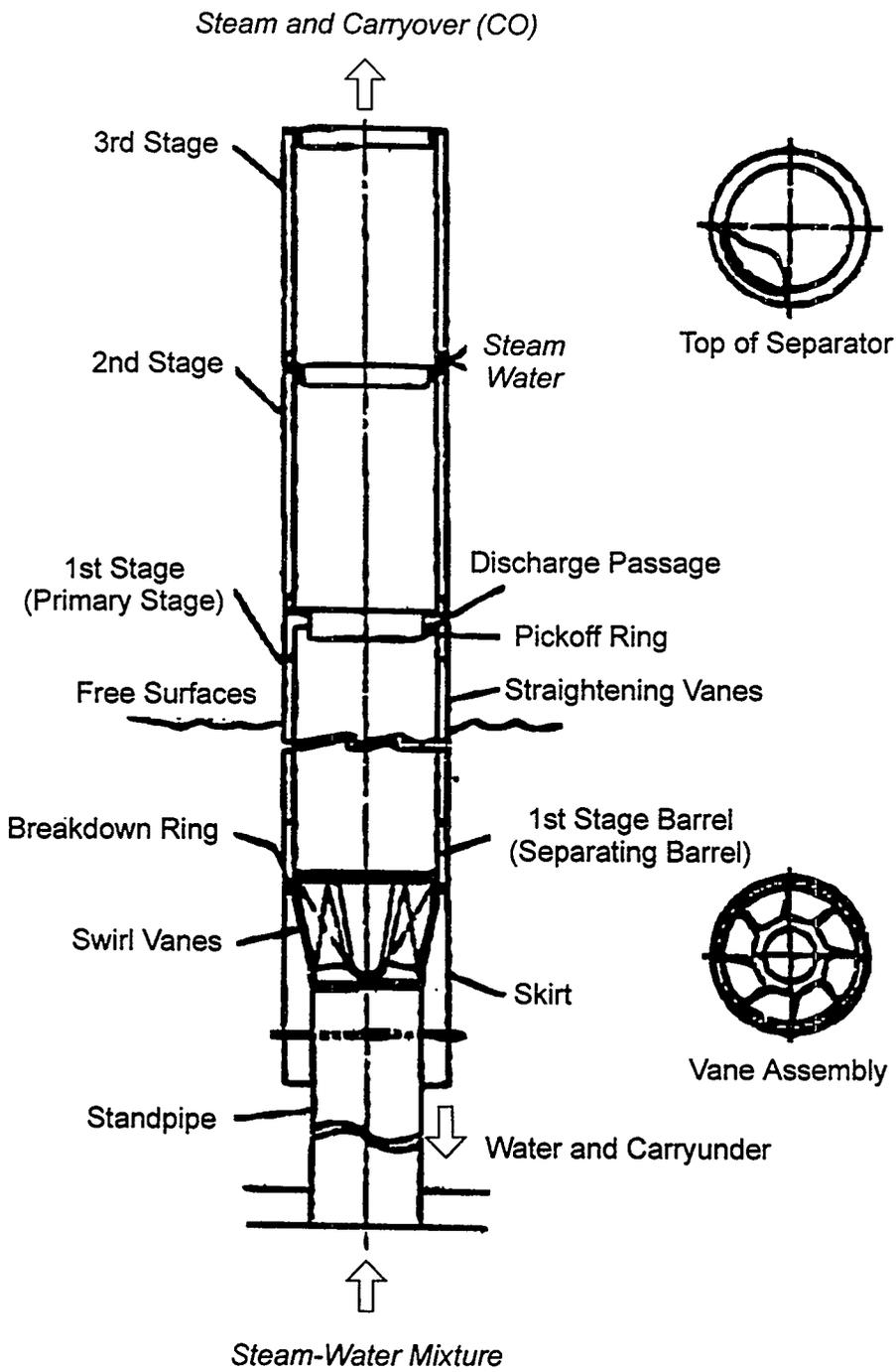


Figure 11: AS-2B BWR steam separator

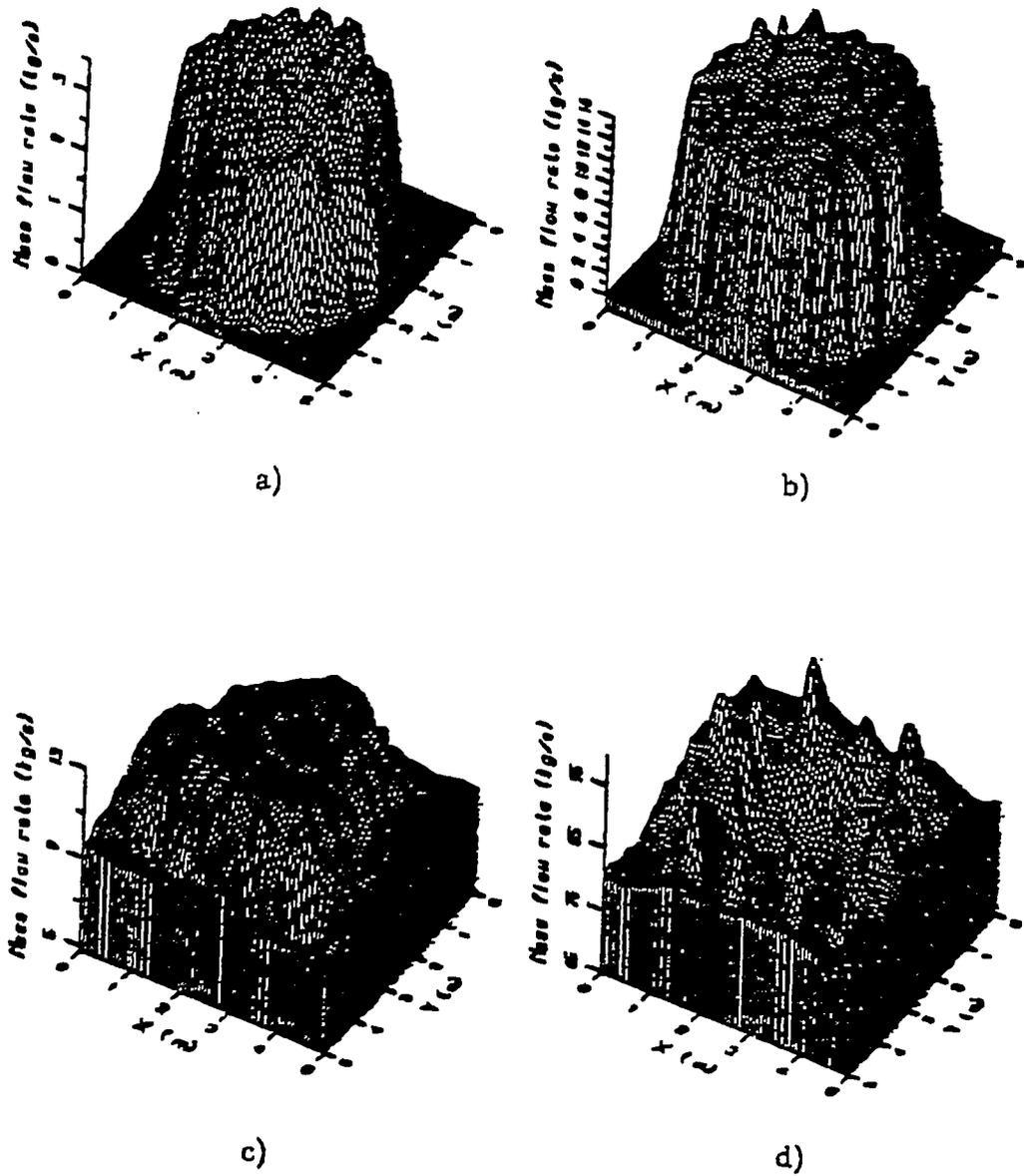


Figure 12: a) Steam mass flow rate into the upper plenum; b) Water mass flow rate into the upper plenum (kg/s); c) Steam mass flow rate at the separator inlets (kg/s); d) Water mass flow rate at the separator inlets (kg/s).

TECHNICAL SESSION 3: NUMERICAL METHODS IN MULTI-PHASE FLOWS

Co-Chair: Dr. Teschendorff (Germany), Dr. Luxat (Canada)

PROBLEMS WITH NUMERICAL TECHNIQUES: APPLICATION TO MID-LOOP OPERATION TRANSIENTS

W M Bryce #
J N Lillington
Winfrith Technology Centre
May 1996

Safety and Performance Services Department
Power Systems Consultancy Division
AEA Technology plc

Now at 30 Bosworth Way, Long Eaton, Nottingham, NG10 1EA

SUMMARY

There has been an increasing need to consider accidents at shutdown which have been shown in some PSAs to provide a significant contribution to overall risk. In the UK experience has been gained at three levels:

- Assessment of codes against experiments;
- Plant studies specifically for Sizewell B;
- Detailed review of modelling to support the plant studies for Sizewell B.

The work has largely been carried out using various versions of RELAP5 and SCDAP/RELAP5. The paper details some of the problems that have needed to be addressed. It is believed by the authors that these kinds of problems are probably generic to most of the present generation system thermal-hydraulic codes for the conditions present in mid-loop transients. Thus as far as possible these problems and solutions are proposed in generic terms.

The areas addressed include: condensables at low pressure, poor time step calculation detection, water packing, inadequate physical modelling, numerical heat transfer and mass errors.

In general single code modifications have been proposed to solve the problems. These have been very much concerned with means of improving existing models rather than by formulating a completely new approach. They have been produced after a particular problem has arisen. Thus, and this has been borne out in practice, the danger is that when new transients are attempted, new problems arise which then also require patching.

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1 INTRODUCTION

There has been an increasing need to consider accidents at shutdown which have been shown in some PSAs to provide a significant contribution to overall risk. In the UK experience has been gained at three levels:

- Assessment of codes against experiments simulating accidents at shutdown;
- Plant studies to support Sizewell B;
- Detailed review of modelling in the codes.

The codes used have been RELAP5/MOD2 and MOD3 and also SCDAP/RELAP5/MOD2.5 and MOD3.

Calculations have been carried out for the BETHSY 6.9 series of shutdown transients using versions of RELAP5/MOD3.1, 3.1.2 and 3.2. This series includes experiments at low pressure and temperature both with and without the presence of non-condensables, with and without loss of inventory etc. The experiments have posed challenges to successive versions of the code, particularly when non-condensables are present. Calculations have also been carried out to assess RELAP5/MOD3 against an Achilles low pressure boil-down test. This posed a challenge to the code in so far as boil-off tends to be overpredicted, thought to be associated with the difficulties in modelling interphase drag. Problems were encountered with low velocity choking and oscillatory behaviour. The improvements in the MOD3 predictions (over MOD2) which resulted in less mass error were at the expense of reduced stability when subsequently analysing a Sizewell mid-loop loss of RHR scenario.

Plant calculations have been carried out using both SCDAP/RELAP5 and RELAP5 for Sizewell B loss of RHR studies. The initial work was carried out using SCDAP/RELAP5. The objective was originally to study the effects of prolonged core uncover in the progression of meltdown. In practice considerable attention had to be paid to the early phase thermal hydraulic modelling and this led to a detailed study at the code modelling level to determine the underlying reasons behind poor code performance.

The background to the work was as follows. Nuclear Electric had identified a need for further Sizewell B severe accident plant calculations for the plant at shutdown. Preliminary attempts were made [1] to use SCDAP/RELAP5/MOD2.5 Version 3f [2,3] to analyse a shutdown accident sequence with the reactor drained for mid-loop operation. These calculations met with limited success because of difficulties apparently associated with the presence of air in the primary circuit. Typically, the code time step size reduced to the minimum and the code stopped executing giving extensive debug prints. The immediate problem could sometimes be avoided by reducing the maximum time step a few seconds before the failure point. However, similar problems often appeared again and again later in the transient. This paper details some of the problems that needed to be addressed and for which solutions were proposed that are thought to be of a generic nature and therefore may apply to other system thermal-hydraulic codes.

It should be noted however that the specific problems identified and improvements made only directly apply to SCDAP/RELAP5/MOD2.5 version 3F (ie containing a version of RELAP5/MOD2.5). Relevant parts of these changes, enhanced where necessary, formed the

basis for a similar improvement programme for the newer SCDAP/RELAP5/MOD3. Documentation was sent to INEL/USNRC which described the details together with annotated source changes. Since however the purpose of this paper is not aimed at describing improvements to RELAP5 or SCDAP per se, the best approach here is to include these changes for illustration purposes to bring out some possibly generic problems, remembering that they were only intended for SCDAP/RELAP5 version 3F and that a newer set was produced for SCDAP/RELAP5/MOD3 and given to INEL/USNRC.

This paper describes how these problems were investigated. In some cases, simple code modifications could be proposed to avoid the problems. These modifications enabled the calculation to proceed to the time of interest to the accident analyst. In other cases simple modifications could not be found to fix the underlying code model defect. However, in yet other cases problems were encountered because the underlying physics was not well modelled, e.g. stratified flow in highly sloped pipes. An additional problem noted in the calculations was the occurrence of significant mass error.

The approach of this paper is to describe the kind of problems encountered and some of the ways in which they were overcome. These are classified into six groups based on the problems: non condensables at low pressure, bad time step calculation detection, water packing, physics problems e.g. non-stratified flow in sloping pipes, numerical heat transfer instability and mass error.

2 NONCONDENSABLES AT LOW PRESSURE

2.1 Two Phase Flow Models

Many thermal hydraulics models and codes have a weakness under conditions of low power and pressure and high noncondensable quality. The weakness is that they are designed as a two-phase model, the phases being liquid and gas where the gas is a well mixed mixture of vapour and incondensable gas. Unfortunately, in the conditions mentioned, the partial pressure of the steam in some RELAP5 applications appeared to fall very low, even below the water triple point pressure. There is then no liquid-gas saturation temperature available to drive the codes interfacial mass and energy transfer terms.

In RELAP5/MOD3 and earlier, the water property routines under these conditions give a saturation temperature, 273.16.K. The gas temperature can fall below this resulting in calculation of condensation which further increases the noncondensable quality X_g and reduces the steam partial pressure P_s . Clearly here there is a case for improving the physical modelling. However even if the physical modelling is not improved some amelioration of the problem is possible if it is assumed that in most transients the code will only have cells in these low pressure and high noncondensable quality conditions occasionally. With this assumption it is reasonable to ameliorate the problem by altering the gas state under the low pressure and high noncondensable quality conditions. In principle this will introduce small additional mass and energy errors.

In the case of RELAP5, two major alterations were made which were found to be successful. The first was the gas temperature T_g was restricted to be greater than or equal to the triple point temperature. This prevents the runaway condensation. The second was to merge the gas

conditions with the value corresponding to saturation conditions for the liquid temperature (or system pressure saturation temperature if lower) under conditions of low void α_g and high noncondensable quality X_a . This was not done if the cell was single phase liquid in the previous time step. This alteration was made because code crashes were observed relating to the gas conditions in cells with low void fraction and high noncondensable quality.

The void fraction $\alpha_g^{\#}$ below which the merge is done is given in the following equation:

$$\alpha_g^{\#} = \text{Max} [10^{-4} - 99\alpha_g^n, 10^{-6}] (2X_a^{n+1} - 1)$$

This is less than or equal to zero unless the new time step noncondensable quality X_a^{n+1} is greater than 0.5. Its value can increase by nearly a factor 100 if the old time step void fraction α_g^n approaches zero. The merge fraction ranges from zero to one as the cell new time step void fraction α_g^{n+1} varies from $\alpha_g^{\#}$ to zero. The gas state properties merged with the saturation values at the liquid temperature are the gas specific internal energy U_g and the starting guesses for the gas temperature T_g and the steam partial pressure P_s .

There may also need to be care in the treatment of low quality X_a . It was noted that SCDAP/RELAP5/MOD 2.5 Version 3F had been changed from RELAP5/MOD2 such that noncondensables were ignored for noncondensable qualities X_a less than 10^{-3} (an increase in the limit). This increase was removed to avoid the resulting discontinuity. For noncondensables, individual phase viscosities, thermal conductivities and specific heats have been set to small positive numbers. Some additional state derivatives were also set to their correct values.

It is expected that most codes which model the vapour mass transfer based on the difference of the vapour temperature and the vapour partial pressure saturation temperature (or equivalent enthalpies) will have problems when the partial pressure is below that of the water triple point. The ideal solution would be a new physical model or, if not that, an artificial model to avoid numerical problems.

2.2 Numeric Implementation Problems

At high noncondensable quality, numerical problems can give rise to problems in the calculation of the steam partial pressure. A typical early failure may be a failure in a water property routine for a cell due to a negative steam partial pressure P_s . In these circumstances numerical fixes are required.

In RELAP5/MOD 2.5 the normal code time step rejection and halving fix up did not overcome the problem because the current partial pressure is used as the guess in an iterative equation solution. Since the old time step value of P_s was not stored, the starting guess for the halved step retry was negative. This prevented a solution being obtained. Tests for "bad" values of P_s with a fixup were coded:

```
If (( $X_a^n = 0$ ) || (( $\alpha_g^n > 0$ ) && ( $P_s > P^{n+1}$  ||  $P_s < 10^{-2}(1 - X_a^{n+1})P^{n+1}$ ))) then
```

```
  set  $P_s = (1 - X_a^{n+1})P^{n+1}$ 
```

```
endif
```

The symbol $\|$ denotes a logical "or" and $\&\&$ denotes a logical "and". Superscripts n and $n+1$ denote old and new time step values. X_n is the noncondensable quality, P is the pressure and α_g is the gas void fraction. Basically, this formula resets the partial pressure P , guess if it is greater than the system pressure P or very low or if there was no noncondensable the previous time step.

A problem occasionally seen with the code when the above modifications were included was a sudden large outflow from a cell for no apparent reason. It resulted in a code failure. It was associated with a large increase in noncondensable quality. The sequence of events was that a cell went from single phase liquid to a low void fraction with low noncondensable quality. In the next time step noncondensable gas and steam were transported into the cell and the steam condensed resulting in the calculation of a noncondensable quality of greater than unity. This was cut back to an upper limit of 0.998 and the interfacial mass transfer was changed to account for the estimated gas and saturation temperature changes. This caused the flow problem because the resultant large mass transfer term is used in the relative velocity equation and results in the large jump in mass flow. The adjustment to the mass transfer term was much too large because it ignored the feedback effects that would take place if the gas temperatures were changed. The correction was to remove the adjustment.

While investigating this problem it was noted that the code did not treat the noncondensable quality consistently with the phase specific internal energies for which conservation and non-conservation derived values are sometimes mixed. The code was changed to make the treatment of noncondensable quality consistent.

The generic issues here are:

- The need for careful initialisation of the properties of a phase before any property calculation iteration.
- The need to consider carefully the side effects of altering any property such as the noncondensable quality after the simultaneous solution value has been found because there can be no compensating feedback to adjust the associated properties and transfers. The side effects can show up in unexpected places with delayed effect on the smooth progress of the transient calculation.

3 POOR TIME STEP CALCULATION DETECTION

In thermal hydraulic codes the time step limitation criteria have to be carefully prescribed. In mid-loop applications there may be special criteria which need to be taken into account. In the calculations carried out, an early code failure involved a cell pressure jumping above the critical pressure with conditions such that the code had a state calculation failure. This was found to be a numerical water hammer affect. However it was triggered by a cell further up in a pipe which earlier had a large pressure drop and a void fraction drop greater than 0.8 in a single time step for no apparent physical reason. The cell's other state properties were so odd that the code subsequently ran for 8 infinitesimal time steps before the water hammer failure.

This was an example of the code's failure to detect a "bad" time step calculation. Modifications were made to algorithms which calculate the basic properties for cells, such as pressure and temperature for the case when the semi-implicit integration scheme is invoked.

A time step is now rejected if any of the following additional conditions are satisfied:

- (i) a change in void fraction α_g by more than 0.5.
- (ii) a large estimated increase in liquid superheat, that is if the liquid superheat is greater than 10K and has more than doubled.
- (iii) a large estimated increase in steam subcooling, that is if the steam subcooling is greater than 10K and has more than doubled.
- (iv) any of the state derivatives $\partial\rho_g/\partial P$, $\partial\rho_l/\partial P$ are negative where ρ is a density.
- (v) the state derivative $\partial\rho_g / \partial U_g$ is positive.

There may be analogous criteria for other codes.

The generic point to make is that a code will be more robust if unphysical properties and, for codes which are not fully implicit, changes in properties so large that the first order property extrapolations will break down are detected and rejected immediately. This is particularly important under low pressure conditions with noncondensables because of the nonlinearity of the vapour properties.

4 WATER PACKING

Mid-loop transients often have extensive periods of time where the pressure is not noticeably falling.

In some calculations attempted this allowed problems with the water packing mitigation scheme to become apparent. These showed up as the following sort of sequence. A cell had a pressure rise in a time step sufficiently large to trigger the water packing mitigation scheme. As a result of the mitigation, the final pressure of the cell was a little lower than the pressure in the connected cells. In the next step, this lower pressure caused flow changes so that the cell overflowed and again triggered the water packing mitigation scheme. This persisted for many timesteps. It distorted the flow calculations during this period. In a typical loss of cooling accident the general system pressure is decreasing so that this locking on of the water packing mitigation cannot happen.

One code modification made was to prevent the water packing mitigation being triggered unless the cell pressure increase was greater than 1.5 times the absolute pressure difference along all connected junctions involved in water packing mitigation. This prevented the spurious water packing mitigation lockon.

The water packing mitigation scheme looks for connected cells with a void fraction greater than 0.12. For these it adjusts the velocity calculation in the connecting junction. First it sets

the velocity to be a small outflow (0.01m/s) with consistent material properties. Second, it multiplies the partial derivative of the velocity with respect to the pressure of the water packing cell by 10^6 . This will tend to hold the pressure in the water packing cell constant regardless of changes of pressure in surrounding cells. This was another necessary factor for the occurrence of the water packing mitigation lockon.

A second code modification was made to deal with this situation. This multiplies the partial derivative of the velocity with respect to the pressure of the cell which will receive flow from the water packing cell by 4.10^6 . In this case the water packing mitigation will tend to force the pressure change in the packing cell to be four times the pressure change in the receiving cell. The numerical corrections worked satisfactorily for the calculations attempted but required modification in the light of further experience.

It is not simple to detect water packing events and yet to avoid false detections. The problems of missed or false detection of water packing will be worse at low pressures for any code with such a model. This is because hydraulic pressure pulses are much more significant compared to the system pressure. The problem is exacerbated if the system pressure is steady or rising.

5 FLOW REGIMES: NON-STRATIFIED FLOW IN SLOPING PIPES

The transient analyst noted that one mid-loop shutdown transient was being poorly predicted because stratified flow was not allowed in pipes which had a slope of more than 15° to the horizontal. A code modification had been developed by Dillistone to overcome this problem for RELAP5/MOD2, Sizewell B applications [4]. This was incorporated into a test version of SCDAP/RELAP5 with the other modifications described above. In brief, this model gives a stratified flow regime region to the vertical flow regime map when the following conditions hold:

- (i) the cell is inclined less than 70° to the horizontal;
- (ii) the wall temperature is such that the code would normally use wet wall rather than dry wall correlations for interphase heat and momentum transfer;
- (iii) the liquid velocity is downward;
- (iv) the gas velocity is less than the Taitel-Dukler critical velocity for transition to non-stratified flow.

Model weaknesses will always become apparent as codes are pushed to new uses.

6 NUMERICAL HEAT TRANSFER

The application of codes to mid-loop transients poses additional problems to modelling heat transfer between structure and coolant.

6.1 Explicit Heat Transfer

The analyst found in one application that the code reduced the time step size to a value too small to be practicable and the code eventually failed with an unphysical cell coolant mass.

The obvious problem symptoms were time step size falling below 1 millisecond and eventual code failure with an upper core cell having negative coolant mass. The heat input to the cell was found to be oscillating wildly from positive to negative. The cell gas temperature was also oscillating, 200K peak to peak. The crossflow from an adjacent core section oscillated as well. The relative phases of these oscillations suggested a heat transfer numerics instability involving the heat to coolant and the coolant temperature. The fuel clad surface temperature was nearly constant. The default heat transfer to coolant numerics was explicit and thereby has a time step size limit. An approximation to this limit which ignores connections to other cells is:

$$\Delta t_{\max} = \frac{MC_p}{h_w A_w}$$

where M is the cell coolant mass, C_p is its specific heat, h_w is the wall heat transfer coefficient and A_w is the wall heat transfer area. At the time being considered, the time step size limit given by this formula is about 1 millisecond compared to the Courant time step limit of 16 milliseconds and the average time step size of 1.4 milliseconds. The time step limit was so small because the cell coolant density was small. So the hypothesis adopted was that the explicit heat transfer was being performed at too large a time step and was unstable. This results in large coolant (gas) temperature swings which cause the assumption of linear dependence of gas properties on pressure, specific internal energy and noncondensable pressure to break down causing the excessive relative mass error which reduced the above time step size.

The hypothesis was tested by restarting a particular calculation with a maximum time step size of 1 millisecond and again with a maximum time step size of 0.5 millisecond. The former was still unstable while the latter was stable. The explicit heat transfer time step limit calculated from the stable conditions was 0.8 milliseconds. However a time step size of 0.5 milliseconds was not acceptable for the calculation for practical reasons.

Where a code integrates a term with an explicit scheme, a time step restriction should be included both to prevent oscillation and to warn the user so he/she can demand that the code developers use a more implicit integration if the code is used in circumstances beyond those imagined by the developers such that use of an explicit scheme is no longer suitable.

6.2 Implicit Heat Transfer

The problem can be overcome if the heat lost by the heated structures and the heat gained by the coolant is treated implicitly. This is difficult to achieve rigorously since heat transfer coefficients depend on a wide range of other fluid parameters and are non-linear (e.g. for radiation).

SCDAP/RELAP5/MOD2.5 has an option specifically designed to overcome the numerical heat transfer instability problem i.e. its implicit heat transfer option. The option calculates a

dependence of the heat transfer on the coolant temperature for liquid heat transfer and for gas heat transfer which is used to treat the heat to coolant more implicitly and hence achieve improved stability. There is however no longer exact equality between heat loss by the heated structures and heat gained by the coolant when this option is used. There was some indication that this option was not yet fully implemented but numerical experiments indicated that a "factor of a few" improvement in time step was possible.

The heat transfer for the implicit treatment just mentioned was much smoother than in the original calculation but still had periodic disturbances which prevented a larger average time step size. These were caused because of a discrepancy in the prediction of gas temperature from the linearised state equations compared to the actual state equations as coded. For example, hand calculation using the linearised state subroutines for two consecutive timesteps gave gas temperature changes of 11K and -13K whereas the actual changes in gas temperature were 22K and -18K. These errors are of similar size to the temperature difference between fuel cladding surface and gas coolant.

The reason for the discrepancy is not known. A run was attempted using a water property table in which the pressure and temperature tabular points were four times as dense for the conditions of concern but this apparently had no significant affect. This discrepancy not only affects the stability and time step size for this calculation but possibly also contributes to the generation of mass error.

Unless the heat transfer between fuel clad and coolant is implicit there will be a time step limit which will be very small at conditions of low pressure and high voidage. It may be at least an order of magnitude smaller than the Courant limit under certain conditions occurring in "Loss of RHR" transients. Implicit heat transfer modelling avoids this limitation.

7 MASS ERRORS

Confidence in many of the calculations performed remained limited because the mass error estimated by the code built up to a significant fraction of the system mass. The accident analyst also expressed concern that the nearly implicit heat transfer numerics option might not behave well if used early in the transient.

Below is described the results of an investigation into the problems for a 5 bar case with open steam generator manway (case N5 of [6]). A loss of RHR is assumed to occur while a steam generator manway is open in the primary circuit, and where flow from the manway is initially prevented by the presence of nozzle dams. Calculations were attempted for a case where the nozzle dam in the inlet nozzle fails when the pressure difference across it exceeds 5 bars. These indicated core damage after 4.5 hours. The depressurisation of the primary circuit following dam failure leads to a significant loss of coolant from the vessel, causing a rapid partial core uncover. No mitigative action e.g. alignment of the Refuelling Water Storage Tank (RWST) with the cold legs is considered in this calculation.

Results are sensitive to the modelling by RELAP5 of condensation heat transfer in the presence of incondensables. RELAP5 predictions of the incondensable gas distribution in the primary side of the steam generator tubes, and its effect on local heat transfer coefficients, require validation for the conditions encountered in this transient.

Boiling in the secondary side of the steam generators is a significant heat removal mechanism. The results in this case are affected by assumptions regarding the availability of secondary side relief valves and by the limitations of RELAP5 in representing natural circulation within the secondary sides of the steam generators.

Problems were encountered with excessive running time and mass error. In order to be able to demonstrate that the problems identified were understood, simple code modifications were made to avoid them. These modifications enabled the calculation to proceed to the time of interest to the accident analyst without confidence reducing, large, mass errors.

The obvious problem symptoms were periods of rapidly increasing mass error. This is illustrated in Figure 1. There are three such periods: 0 to 1 hours, 1.5 to 2.5 hours and beyond 4.5 hours into the transient. These are labelled C, B and A respectively. The transient analyst supplied a SCDAP/RELAP5 restart dump file and restart input data for the problem. The mass error periods were considered in the order A, B and then C and investigated using restarts. The time step control part of the Major Edit code output was misleading as to where mass errors were being generated. It is based on cell mass errors as a fraction of cell masses rather than the actual mass errors. In order to locate the cells with a problem, a temporary modification was made to the code so that actual mass error was used to set the counts of when particular cells had the largest mass error. Once a problem cell was identified, the Minor Edit code output was used to show all properties associated with that cell at every actual time step and then appropriate debug prints were inserted into the code.

Each mass error period is considered in the following paragraphs. The entire investigation relates only to the semi-implicit numerics option.

Debug prints showed that in time Period A, Figure 1, the system mass error increase rate output by SCDAP/RELAP5 was inconsistent with and much larger than that obtained by summing the mass error for each cell. This suggested that the problem was in the calculation of the system properties. As a result it was discovered that the hydrogen mass generation, the corresponding water destruction and the input into the circuit of noncondensables from the fuel had been omitted from the system mass calculation. Coding for this was inserted and the excess mass error disappeared. The newer code SCDAP/RELAP5 version 7af was checked and was found not to have the error. The system mass does not affect the calculation (although there may be an occasional time step reduction driven by the system mass error). The conclusion is that this problem is not a real mass error problem and that the code output is misleading. The lesson here is that accounting is important if misleading results are not to be produced.

In time Period B, an offending cell was identified as being in the intact secondary side circuit. It contained no liquid. The mass error was being generated because every time step liquid was calculated to drift into the cell from above and the numerics then threw this liquid away. The liquid is thrown away from a high void cell if one of two conditions are satisfied:

- (i) the void is greater than 0.99999999, or
- (ii) the void is greater than 0.999999 and either the interfacial heat transfer to the gas phase is zero or the gas phase is superheated.

In this case the second condition was satisfied every time step because the interfacial heat transfer to the gas phase is zero when the old liquid fraction is zero. To check this the second condition was removed. Instead a new action was added. 90% of the liquid is thrown away if the void is greater than 0.999999 and the interfacial heat transfer to the gas phase is zero. This will generate mass error for one time step but should not for subsequent steps because some liquid is left. Hopefully enough liquid is removed in the first step to avoid whatever problem the original coding was intended to overcome. It was successful for the transient under investigation here. It removed the excessive mass error increase without cost in running time. The lesson here is that care must be taken in disposing of apparently small amounts of liquid from a highly voided cell.

In time Period C, another problem was found to be associated with a cell or two in the primary circuit containing low void fluid. Every few seconds a negative void was calculated. This was not negative enough to cause time step rejection. The fixup of replacing the negative value by zero is the equivalent of throwing away an amount of liquid proportional to the magnitude of the negative void. The unfortunate aspect of this is that the error is always a loss. Other causes of mass error in the code are likely to give errors of random sign which tend to cancel. There is no cost effective way of changing the code numerics to avoid negative void fractions being calculated. What can be done is to tighten the acceptance tolerance. The magnitude of acceptable negative void fraction was reduced by a factor of 10.

There are several generic points here. The first is that the coding of all system mass and energy totals and discrepancy totals should be carefully checked for errors and omissions (and should be included of course) so that users are not misled about the numerical accuracy. The second point is that the effects of slightly truncating a void or a noncondensable quality after the simultaneous solution value has been found can accumulate to produce noticeable, confidence sapping, errors. The fixup used in the particular case here later threw up the third point to make; that is that a patch for a problem may have a limited range of application in itself (in this case, throwing 90% of the liquid away leaves too much behind under conditions of very high gas temperature). The amount left needs to be no greater than the locally steady state value which decreases as the gas temperature increases. Birchley (private communication) has reported a similar problem where the presence of noncondensable reducing the saturation temperature exacerbated the effect of a high gas temperature to make the flashing of water falling in from above even more violent.

8 TEST CASES

Figures 2-4 show comparative results with and without the modifications described for the mid-loop shutdown transient considered (case N5 of [6]).

A SCDAP/RELAP5 code version was created with all the modifications described above and a long run restarting from time zero was performed to test whether the code would run fast enough. Figure 2 shows a comparison of the mass error before and after the change. Curve 1 is the original, curve 2 the new and curve 3 is a continuation of curve 2 with data taken from the standard output major edits every 500 seconds (the graphics dump was incomplete due to a disk becoming full). The input data for the two cases was identical up to 3.9 hours. At this point the new calculation switched to implicit heat transfer continuing with a 0.1 second maximum time step size. The original calculation switched at 4.6 hours at which time the

maximum time step size was reduced to 0.05 seconds because of concern about mass error. The comparison shows that mass error is much reduced.

Figure 3 compares the cpu times. The workstations used for the two calculations were of almost the same power, a SparcStation 2 and a SparcStation 630MP (with two ROS cpus under Solaris 1 system software). Despite the change described for time Period C which was seen to increase running time in the short term by 15%, there is an improvement overall, especially with using a large maximum time step size after 3.9 hours.

Finally Figure 4 compares clad temperatures at a point part way up the core. The two cases are quite similar with part of the difference being due to the widely spaced plot points on curve 3.

9 CONCLUSIONS

1. It has been found that there are relatively inexpensive code modifications that can be made to codes such as RELAP5 or SCDAP/RELAP5 to make them more robust for conditions of low pressures with noncondensables.
2. The main areas of problems are associated with noncondensables at low pressure, poor time step calculation detection, water packing, inadequate physical modelling e.g. of flow regimes, numerical heat transfer and mass errors. These problems are frequently inter dependent.
3. The work described in this paper is aimed at improving existing models. The corrections start from the assumption of a two-phase flow model in codes of the type of RELAP5. The problem with this approach to date is that corrections can be proposed to patch an existing calculation but the next calculation has a tendency to fail with a new error.
4. Similar problems should be anticipated in other codes and kept in mind when developing new codes. Even a virtually fully implicit code can have similar problems.
5. The authors hope it is not necessary, but feel they should remind code developers to try to avoid discontinuities in correlations, in incorporating models and correlations and, if possible, in the numerics and their solution.

10 ACKNOWLEDGEMENTS

Dr C G Richards was the analyst who provided the mid-loop transient input deck and other information. Dr W M Bryce is responsible for the formulation of the solutions discussed above.

11 REFERENCES

1. Richards, C G and Sweet, D W "SCDAP/RELAP5 Calculations of the Consequences of a Loss of RHR and All Safety Systems During Shutdown: AEA Technology Internal Report", PWR/SUG/P(92)52, RSSD Note 250.
2. Farmer J A "Implementation of SCDAP/RELAP5 Version 3f", AEA Technology Internal Note, RSSD Note 83, Revision 1, July 1991.
3. Lillington J N et al. "SCDAP/RELAP5/MOD2.5 Version 3f, Release 2", PWR/SUG/P(91)17, February 1991, Addendum 1, April 1991, Addendum 2, August. AEA Technology Internal Paper.
4. Bryce W M. "Investigation of Difficulties Encountered in Using SCDAP/RELAP5 Version 3f to Simulate Mid-loop Operation Accident Sequences" PWR/SUG/P(92)55, RSSD Note 255, November 1992. AEA Technology Internal Paper.
5. Richards, C G. "SCDAP/RELAP5 Calculations of the Consequences of a Loss of RHR and All Safety Systems During Shutdown: Final Report" AEA RS 5439, February 1993.
6. Richards, C G. "SCDAP/RELAP5 Investigation of Gravity Drain of the RWST following a Loss of RHR During Mid-Loop Operation: Interim Report", AEA RS 5468, March 1993.
7. Bryce, W M. "Investigation of Numerical Heat Transfer Instability Encountered in Using SCDAP/RELAP5 Version 3f to Simulate Mid-loop Operation Accident Sequences", PWR/SUG/P(93)60, RSSD Note 276, February 1993. AEA Technology Internal Paper.
8. Bryce, W M. "Investigation of Mass Errors encountered in using SCDAP/RELAP5 Version 3f to simulate Mid-loop Operation Accident Sequences", PWR/SUG/P(93)67, RSSD Note 288, March 1993. AEA Technology Internal Paper.

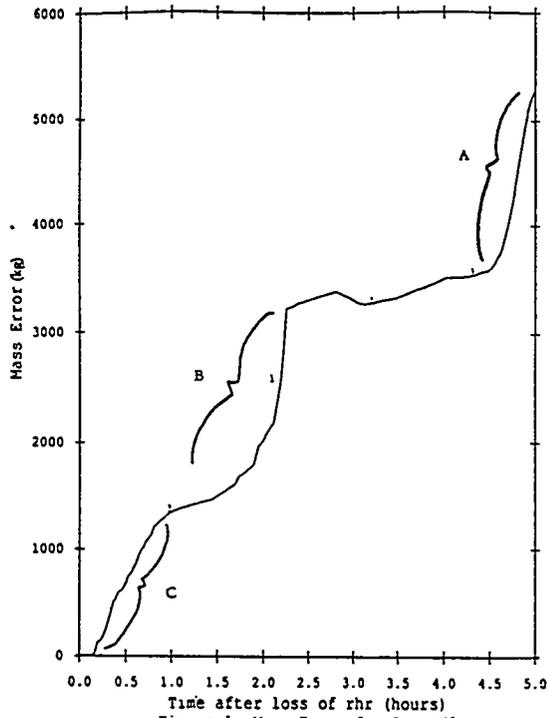


Figure 1 Mass Error for Case N5

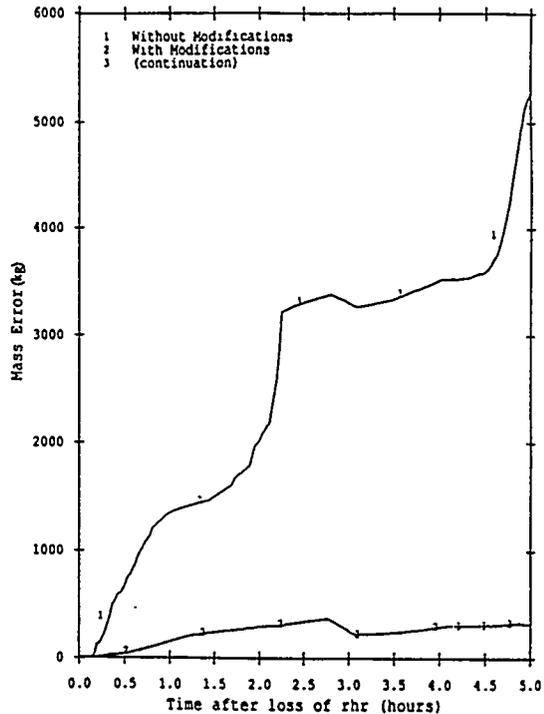


Figure 2 Mass Error Comparison

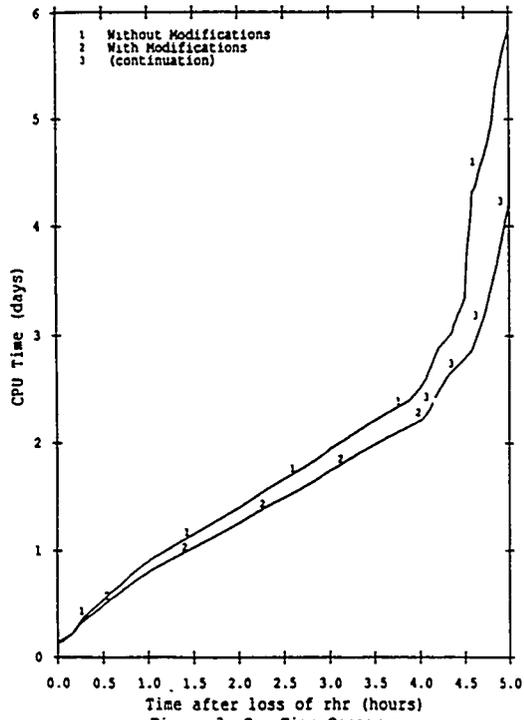


Figure 3 Cpu Time Comparison

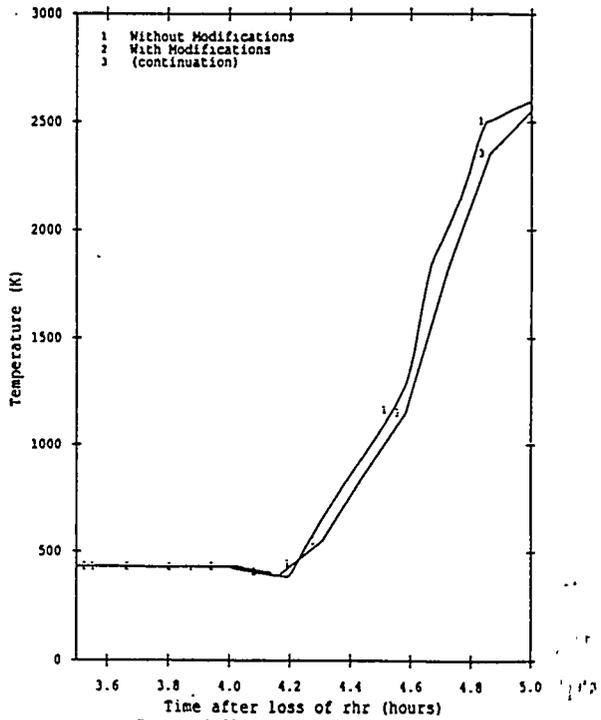


Figure 4 Clad Temperature

Elimination of numerical diffusion in 1 - phase and 2 - phase flows

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Abstract

The new hydraulics solution method PLIM (Piecewise Linear Interpolation Method) is capable to avoid the excessive errors, numerical diffusion and also numerical dispersion. The hydraulics solver CFDPLIM uses PLIM and solves the time-dependent one-dimensional flow equations in network geometry. An example is given for 1-phase flow in the case when thermal-hydraulics and reactor kinetics are strongly coupled. Another example concerns oscillations in 2-phase flow. Both the example computations are not possible with conventional methods.

1. Introduction

An essential problem in computational fluid dynamics is the avoidance of typical numerical errors. These numerical errors cause diffusion and oscillations in the most important parts of the solution. Reliable calculation of any propagated front is very difficult with standard numerical algorithms because numerical diffusion tends to smooth the front. Hence errors in the calculated results for traveling spatial distributions are often of the same magnitude as the spatial variation itself. Although the sufficient accuracy in the case of one transported quantity can be achieved by careful choice of the discretization, the situation is different to several flow channels. Further, in solving the set of the conservation equations needed in the reactor thermal-hydraulics, there are several, varying, unknown velocities which cause several, varying needs and it is impossible to the discretization to satisfy all of them. When several processes, as reactor physics and thermal-hydraulics, are interacted the same discretization may be most convenient in calculation of all of the processes. Therefore, the flow equations of hydraulics should be possible to be solved accurately and as generally as possible in any given reasonable discretization.

The propagation of some disturbances do not obey any velocity appearing in the conservation equations and the characteristic velocities must be employed. E.g. in 1-phase flow, pressure

disturbances proceed in this manner and, in the 2-phase flow, also the velocity of void-fraction disturbances corresponds to the characteristic velocities. Obviously, an algorithm which disregards the characteristic velocities is not applicable to general, accurate calculation of flow phenomena.

A new solution method PLIM^{1,2,3,4} (Piecewise Linear Interpolation Method) has been developed at VTT for the system of time-dependent one-dimensional flow equations. PLIM is capable to avoid numerical diffusion and numerical dispersion in any discretization grid. The work is presently going to attach the latest computer version CFDPLIM⁵ to reactor dynamics code as a part of their hydraulic model.

2. Principles of PLIM

Piecewise Linear Interpolation Method, PLIM^{1,2,3,4} is a shape-preserving characteristics method. Originally PLIM was capable to handle the system of equations as

$$\frac{\partial}{\partial t} U(\mathbf{u}, z, t) + \frac{\partial}{\partial z} F(\mathbf{u}, z, t) + \sum_m [A_m(z, t) \frac{\partial}{\partial t} X_m(\mathbf{u}, z, t) + B_m(z, t) \frac{\partial}{\partial z} Y_m(\mathbf{u}, z, t)] = P_S(z, t)$$

where \mathbf{u} is the unknown vector. It is implicitly assumed that the equations are physical, what means now that the equations form an initial value problem in respect of time.

The particular features of the PLIM algorithm can be described as follows

- PLIM divides the z-t-domain into mesh cells, which are treated in the algorithm separately.
- Within the mesh cell local linear approximations in respect of \mathbf{u} are utilized for the terms of the equations.
- The system of the equations is transformed to the characteristic form.
- The unknown variables $x_i(z, t)$ of the equations of the characteristic form are, firstly, treated independently from each others.
- Their solution is obtained according to the characteristic method where an essential step is to interpolate the value of $x_i(z, t)$ at the incoming boundary of the mesh cell.
- At the interfaces of the mesh cells PLIM forms a piecewise linear approximation using the values of $x_i(z, t)$ at the mesh points and two additional unknown parameters. This allows two types of approximations for the intrinsic behavior: triangles and fronts, shown in Fig. 1.

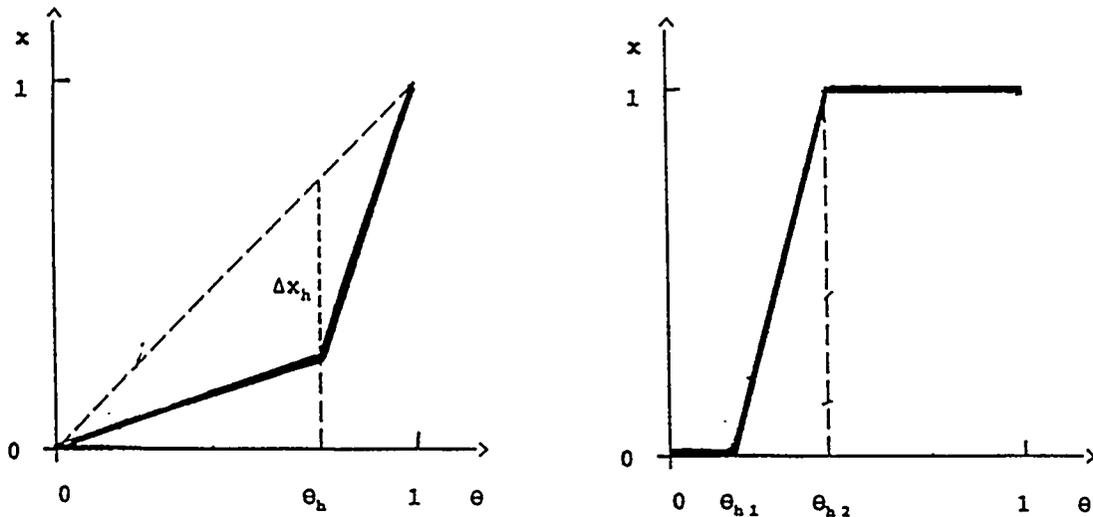


Figure 1. Normalized piecewise linear approximations of PLIM with two unknown parameters

PLIM has useful properties:

- It preserves the shape of the travelling distribution in the sense that when the approximation of the PLIM type travels from one mesh cell to another with a constant velocity it can be reproduced exactly and no additional numerical errors occur as the consequence of the transport^{1,2}.
- Any distribution at the boundary of the mesh cell can be approximated with reasonable accuracy.
- Conservation of x in the mesh cell can be satisfied.
- Overshoots and uncontrolled strong variations can be avoided.
- Also the transport of a front entirely within a mesh cell is described.
- It uses the values of only one mesh interval. Therefore, no extra schemes are needed for the end points or for the discontinuity points of the z -interval. This is a very useful property in the system models, because then the flow networks can be constructed freely but still high accuracy and good applicability to parallel computation can be achieved.
- A good convergence is achieved in solution of any flow conditions of a flow path.
- As a characteristic method, the boundary conditions for a multi-phase flow can be easily defined.

3. The hydraulics solver CFDPLIM

The solver CFDPLIM solves the system of N flow equations in an arbitrary hydraulic network, which is composed freely of nodes and one-dimensional flow paths. Because the numerical diffusion has been eliminated, the effects of diffusion and diffusion-like mixing are not included

at all in the original version. Therefore, the algorithms of CFDPLIM have been developed to take into account general terms of the second order in respect of the spatial coordinate in order to model diffusion-like mixing. The flow path equation is of the form

$$\begin{aligned} & \frac{\partial}{\partial t} U(u, z, t) + \frac{\partial}{\partial z} F(u, z, t) + \\ & \sum_m [A_m(u_G, z, t) \frac{\partial}{\partial t} X_m(u, z, t) + B_m(u_G, z, t) \frac{\partial}{\partial z} Y_m(u, z, t)] + \\ & - \frac{\partial}{\partial z} W_D(u_G, z, t) \lambda(u_G, z, t) \frac{\partial}{\partial z} u = P_s(u, z, t) \end{aligned}$$

where $u_G(z, t)$ is a guess of the unknown vector.

The equation for the nodes with finite volumes have to be defined correspondingly

$$\frac{d}{dt} X_N(u_N, t) + \sum_J F_{NJ}(u_N, t) = P_N(u_N, t)$$

where $u_N(t)$ is the unknown variable vector in the N'th node and F_{NJ} is the flow term from the node N to the flow path J.

The boundary conditions of the flow paths are defined also with functions

$$\begin{aligned} u_J - u_{NJ}(u_J, u_N, t) &= \eta(u_{JG}, t) \lambda(u_{JG}, t) \frac{\partial u_J}{\partial z} \quad \text{or} \\ E(u_J, u_N, t) &= 0 \end{aligned}$$

where one can take into account with u_{NJ} the possibility that quantities leaving the node do not have to receive the same value u_N .

When one considers hydraulic systems, the above partial differential equations are not sufficient as such to describe hydraulics. The description of hydraulic discontinuity behaviors, such as water levels and shock waves, have to be included. The local linearization of the terms, as well as many phenomena, such as carry-over, carry-under and surface evaporation, presuppose that the discontinuity behavior is explicitly modeled

$$F_2(u_2, z_D(t), t) + F_{D2}(u_2, z_D(t), t) - F_1(u_1, z_D(t), t) - F_{D1}(u_1, z_D(t), t) \\ - v_D [U_2(u_2, z_D(t), t) - U_1(u_1, z_D(t), t)] = P_D(u_1, u_2, t)$$

where F_D is the diffusion flow and v_D is the velocity of the discontinuity. When the diffusion-like flow is treated as unknown, the necessary additional relations are taken to be of the form

$$u_2 - u_1 + \eta_2(u_{2G}, t) \lambda(u_{2G}, t) \frac{\partial u_2}{\partial z} + \eta_1(u_{1G}, t) \lambda(u_{1G}, t) \frac{\partial u_1}{\partial z} \\ = P_{uD}(u_{1G}, u_{2G}, t)$$

Appearing and disappearing of discontinuities in any point of the network requires still own description and own particular methods.

The unknown variables are $u(z, t)$, $u_N(t)$, diffusion-like flows and the velocities of the discontinuities v_D .

Besides the normal input, the user has to define the terms of the equations in the own subroutines. The terms are composed of functions of u , z , and t .

The objectives of the development work of CFDPLIM, apart from those satisfied already by the use of PLIM, are the following:

- It solves the unknown quantities when the terms of the equations are correctly defined as functions.
- The geometry of the network is not restricted in any manner. However, the components of the network can be arranged in particular order to produce better convergence.
- The order N of the equations is arbitrary and it can be different in different parts of network. If N is large and all of the variables are not strongly coupled, the system of the equations can be divided into sub-systems.
- Parallel computation can be utilized in evaluation of the function values. Hence rather complicated forms of the terms of the equations may be used.
- As few algorithms as possible are employed in CFDPLIM. Hence diffusion-like terms and discontinuities are assumed to be a part of the normal computation required for the mesh cells. Also this property offers opportunity to apply parallel computation efficiently.

A great advantage of the finite volume method is that the user can build geometry freely and easily from different elementary components. This is consequence from the property that the couplings between these elementary components can be expressed with a simple standardized

way. The mesh intervals and the nodes of CFDPLIM have the same property and, accordingly, CFDPLIM has the same advantage of geometric flexibility. To point out the differences, one can say that within an elementary component the finite difference method uses the spatially averaged terms of the flow equations while PLIM uses the averaged coefficient in the local linear approximations of these terms.

The properties of CFDPLIM are being heavily tested. Some special features of the discontinuity modeling are still under development work.

The extension of PLIM into 3-dimensional flow problems is under development work. Presently, it can be claimed that it is very difficult to create a 3-dimensional algorithm using 3-dimensional piecewise linear approximation functions. However, an obvious opportunity remains, namely to divide the 3-dimensional domain into channels, to integrate equations and to apply the one-dimensional CFDPLIM to them. Then the cross flow terms appear in the source terms of the one-dimensional equations.

4. Example case: Elimination of numerical diffusion in 1-phase flow

In the analyses of RIAs, the thermal hydraulics and reactor kinetics processes in the reactor core are coupled in such a manner that the equations for the processes have to be solved simultaneously by iteration and fully consistent solutions have to be achieved. The iteration is governed simplest when neutronics and thermal hydraulics use the same discretization. Neutronics is very sensitive to any small changes, also to those which happen in numerical errors. Therefore a varying discretization in hydraulics may produce unreliable results.

CFDPLIM has been implemented into the 3-dimensional reactor dynamics code HEXTRAN⁵, which uses originally conventional methods and the new version of the code is here called HEXTRAN-PLIM.

Conventional numerical algorithms have difficulties in simulating the transport of sharp fronts in the coolant channels, e.g. of a local boron dilution front. In the example case of a boron dilution accident simulation, conditions close to natural circulation were assumed. There are many conflicting requirements for the spatial and time discretizations and, as a consequence, the hydraulics calculational grid applied in the calculation in this test case is far from fulfilling the Courant criterion.

The initial reactor power was 1 percent (13.75 MW) of the nominal thermal power and the mass flow through the reactor was initially 742 kg/s, which is approximately 10 percent of the nominal. The volume of the diluted slug was 50 percent of the core coolant volume. The initial and diluted boric acid concentrations were 7.6 and 7.3 g/kg, respectively. The total time of the transient simulation was 20 seconds and at 1.0 seconds the diluted slug entered the reactor core. At 4.5 seconds the boric acid concentration at the inlet of the reactor was increased to its

original value.

The calculated boric acid densities at the inlet node of the reactor core are shown in figure 2a. The results of HEXTRAN show clear signs of numerical diffusion, while the solution obtained with HEXTRAN-PLIM is very accurate. The decrease of the boric acid density seems to be initially steeper in the solution obtained with HEXTRAN because linear approximation between the mesh points is used in plotting.

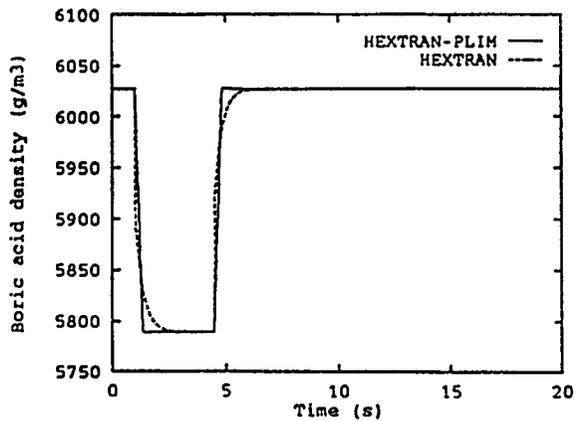


Figure 2a: Boric acid density at the inlet node of the reactor core during a boron dilution.

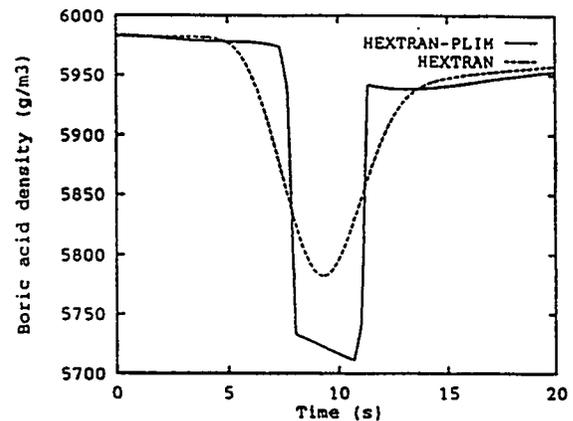


Figure 2b: Boric acid density at the outlet node of the reactor core during a boron dilution

In figure 2b the calculated boric acid densities at the outlet node of the reactor core are shown. Here the HEXTRAN solution is smoothed due to numerical diffusion. The HEXTRAN-PLIM solution is again nearly exact. The boric acid mass is conserved in both solutions. The most serious consequence of the smoothing of the HEXTRAN results is that the reactivity worth of the slug is decreased. Due to the finite volume of the slug, the smoothing of the edges of the slug are combined and the maximum dilution level is not achieved at all in the upper part of the core. As expected the fission power peak produced by HEXTRAN remains clearly smaller than the peak produced by HEXTRAN-PLIM. Also the energy release is essentially smaller.

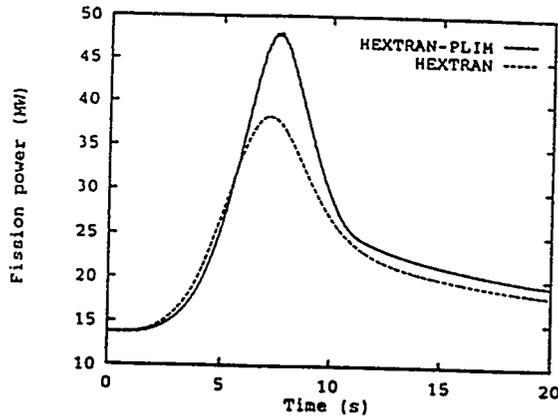


Figure 3: Total fission power during a boron dilution in natural circulation conditions.

In earlier analyses made with HEXTRAN in natural-circulation conditions, this prominent effect on the numerical errors in simulation of finite slugs has been taken into account by using conservative assumptions. The volume of the slug has been enlarged so that the minimum concentration of boric acid has been achieved even in the last nodes at the outlet of the reactor. Using this same conservative assumption here, the power peak was 230 percent greater than the one calculated with HEXTRAN-PLIM. Increasing the volume of the diluted slug with 30 percent was enough to create a power peak in the HEXTRAN calculation as large as in the HEXTRAN-PLIM calculation with the original slug volume. Then the minimum concentration was achieved in the central part of the core but still not in the last nodes at the outlet of the reactor core. Thus the earlier mode of action in the HEXTRAN analyses has guaranteed the conservatism of the results but there has been considerable overconservatism in the analyses.

5. Example case: Application of CFDPLIM to 2-phase flow

CFDPLIM has been used to solve the equations of the SFAV two-fluid approach⁶. The equations for the gas mass, for the liquid mass and for the momentum of SFAV-subflows are of the following forms:

$$M_g = 0$$

$$M_l = 0$$

$$MO_1 + MO_2 = 0$$

$$DMO = \frac{1}{\beta} (MO_1 - v_1 M_1) - \frac{1}{1-\beta} (MO_2 - v_2 M_2) = 0$$

where

$$M_g = \frac{\partial}{\partial t} (A\alpha\rho_g) + \frac{\partial}{\partial z} (A\alpha\rho_g v_g) + S_{gl} - A\alpha S_g$$

$$M_l = \frac{\partial}{\partial t} [A(1-\alpha)\rho_l] + \frac{\partial}{\partial z} [A(1-\alpha)\rho_l v_l] - S_{gl} - A(1-\alpha)S_l$$

$$M_k = \frac{\partial}{\partial t} (A\beta_k\rho_k) + \frac{\partial}{\partial z} [A\beta_k(\rho_k v_k + f_k)] + S_{kk_2} - A\beta_k S_k, \quad k = 1, 2, \quad k_2 = 2, 1$$

$$MO_k = \frac{\partial}{\partial t} [A\beta_k(\rho_k v_k + f_k)] + \frac{\partial}{\partial z} [A\beta_k(\rho_k v_k^2 + 2v_k f_k + g_k)] + F_k \\ + A\beta_k \frac{\partial p}{\partial z} + S_{mkk_2} - A\beta_k S_{mzk}, \quad k = 1, 2, \quad k_2 = 2, 1$$

The velocities of the phases are related with the velocities of the subflows as follows

$$\alpha v_g = \beta\alpha_1 v_1 + (1-\beta)\alpha_2 v_2 - \beta \frac{f_1}{\Delta\rho_{lg}} - (1-\beta) \frac{f_2}{\Delta\rho_{lg}}$$

$$(1-\alpha)v_l = \beta(1-\alpha_1)v_1 + (1-\beta)(1-\alpha_2)v_2 + \beta \frac{f_1}{\Delta\rho_{lg}} + (1-\beta) \frac{f_2}{\Delta\rho_{lg}}$$

In the used SFAV-approach, the f_k and g_k terms have the expressions

$$\begin{aligned}
 f_1 &= - \left[k_{v1r} \beta (1 - \alpha_1) + \frac{\pi}{2} k_{t\rho} k_{tv} \beta (1 - \beta)^3 \Delta \alpha_{12} \right] \Delta \rho_{1g} v_r \\
 f_2 &= - \frac{\pi}{2} k_{t\rho} k_{tv} \beta^3 (1 - \beta) \Delta \rho_{21} v_r \\
 g_1 &= \left[k_{v1r}^2 \beta^2 \frac{1 - \alpha_1}{\alpha_1} ((1 - \alpha_1) \rho_g + \alpha_1 \rho_l) + \frac{16}{3} k_{iv}^2 \beta^2 (1 - \beta)^4 \rho_1 \right] v_r^2 \\
 g_2 &= \frac{1}{3} \left[\eta_{v2} \rho_2 (1 - \beta)^2 + 16 k_{iv}^2 \beta^4 (1 - \beta)^2 \rho_2 \right] v_r^2
 \end{aligned}$$

In a more conventional approach f_k and $g_k = 0$, but then some virtual mass term must be added in order to make the equations well-posed, in other words, to make their characteristic velocities real. Already this non-complete representation is sufficient to show the complexity of the system of the flow equations. The used SFAV-parameters are chosen to produce correctly the sonic velocity, the velocity of void-fraction disturbances, total frictional drag and drift-flux slip in steady state. Particularly, the momentum transfer between the SFAV-fluid was determined to be dissipative.

The application of CFDPLIM to the above system of equations is straight-forward. The terms of the SFAV-equations are equated with those in the CFDPLIM representation, in other words, the functions beneath the derivative signs and the source term function are programmed into the appropriate CFDPLIM subroutines.

The example geometry was a part of a BWR fuel channel between two spacers. No heat transfer was assumed. As the initial conditions, typical BWR conditions were chosen and the boundary conditions were chosen to be possible to realize in experimental work. There are three positive characteristic velocities and one negative. Steam volumetric flux at inlet and pressure at outlet were constant, difference between the SFAV-velocities at inlet was chosen according to drift-flux correlation. Water volumetric flux at inlet was a sine-wave disturbed quantity.

The results calculated with CFDPLIM on the 15 Hz sine-wave disturbance are shown in Figure 4. In the same figure, the results for the corresponding drift-flux equations are also presented. One can see that the front of the void fraction disturbances travels very sharply towards the channel end. Still more remarkable feature at outlet is the increase of the amplitude of void-fraction waves. We have calculated that the change in amplitude at outlet behaves approximately as a function of frequency as (frequency)^{1.5}. The over-all behavior shows to have been calculated with sufficiently dense discretization and we believe that the result is the correct solution to the equations and that the result is not a consequence of the SFAV-approach, although it may be affected with the use of purely convective two-fluid model. However, in the

present paper, we do not try to answer the question: is it correct physically? Also a remarkable thing is that the relaxation time constant of the difference of the SFAV velocities is only 0.02 s, but dynamics of slip becomes observable still in ten times slower variations. Standard numerical methods tend to smooth variations and therefore the present calculation is much easier with them, but they cannot solve the question: which is the correct solution to the used equations?

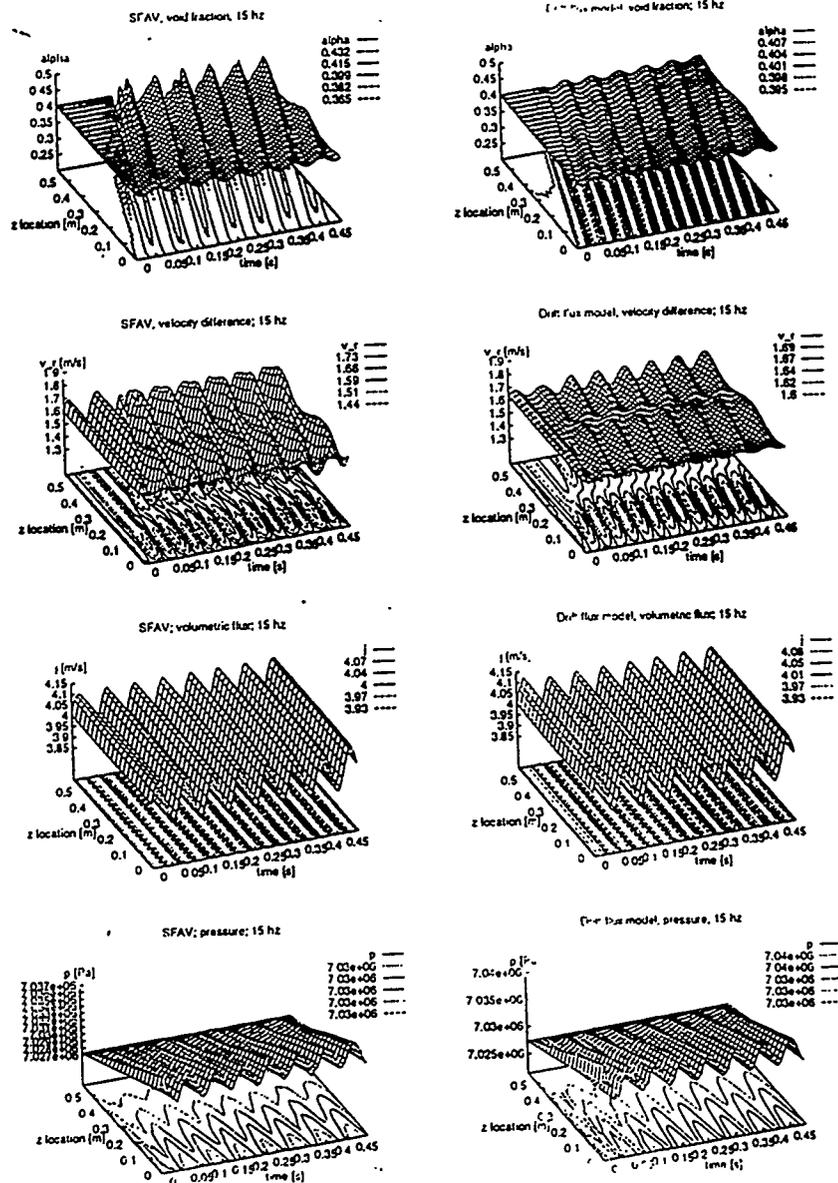


Figure 4: Response of the SFAV-model and the drift-flux model on the 15 Hz sine-wave disturbance in inlet water volumetric flux.

6. Conclusions

When the spatial distribution of a propagating quantity is important, elimination of numerical diffusion is always important. On the other hand, if only the average values in sub-systems are required and they can be achieved without detailed spatial calculation, there is no reason to try to avoid methods amenable to numerical diffusion.

Significance of elimination of numerical diffusion as a natural part of hydraulic computation has to be emphasized when the computation becomes more complex. Then the user of the code may have insufficient experience of calculated phenomena and do not recognize erroneous results. Then also control of computation can become overwhelming. Naturally, there are several phenomena which cannot be computed correctly with deficient methods. As examples of this kind of phenomena, one can mention the temperature and boron concentration fronts in PWR and the momentary accumulation of steam in BWR. The accumulation of steam is originated from sudden power increase or sudden mass flow decrease and its distribution is strongly locally peaked. In addition, it affects the overall dynamic behavior in complicated way when it travels through the steam separation system.

One disadvantage that may result from accurate computation, is the increased difficulty to obtain filtered results and also time of computation may increase unnecessarily.

We have shown that the hydraulic solver CFDPLIM has capability to solve very complex problems without excess numerical diffusion. The use of the solver has been made easy. The user can program the terms of the own flow equations and use CFDPLIM as an advanced solver. Thereafter, the use of the code do not differ from the use of any hydraulic code.

The computation time with CFDPLIM shows increase at least by factor ten in reactor dynamics applications compared with conventional methods, but CFDPLIM solves much more general problems. In addition, the vector and parallel computation will improve the situation.

References

1. Rajamäki, M. & Saarinen, M. PLIM shape-preserving characteristics method for flow equations. International Topical Meeting on Advances in Mathematics, Computations and Reactor Physics. Pittsburgh, PA 28 April - 2 May 1991. La Grange Park: American Nuclear Society, 1991. Pp. 12.1-1 - 12.1-13.
2. Rajamäki, M. & Saarinen, M. Accurate one-dimensional computation of frontal phenomena by PLIM. Journal of Computational Physics, 1994. Vol. 111, no 1, pp. 62 - 73.
3. Rajamäki, M. & Saarinen, M. A numerical study of the withdrawal and return of water following a volcanic eruption at sea. Communications in Numerical Methods in Engineering, 1994. Vol. 10, nro 6, pp. 461 - 468.
4. Saarinen, M. Dynamic model for horizontal two-phase flow predicting low head flooding. Numerical Heat Transfer, Part A, Applications, 1994. Vol. 26, no 4, pp. 471 - 482.
5. Rajamäki, M. & Kyrki-Rajamäki, R. Boron dilution transient calculation with the HEXTRAN code using CFDPLIM. Proceedings of the OECD/NEA/CSNI Specialist Meeting on Boron Dilution Reactivity Transients. State College, PA 18 - 20 October 1995.
6. Narumo, T & Rajamäki, M. Dividing phases in 2-phase flow and modelling of interfacial drag. OECD/NEA/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements
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ADVANCED NUMERICAL METHODS FOR THREE DIMENSIONAL
TWO-PHASE FLOW CALCULATIONS

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ABSTRACT

This paper is devoted to new numerical methods developed for both one and three dimensional two-phase flow calculations. These methods are finite volume numerical methods and are based on the use of Approximate Riemann Solvers concepts to define convective fluxes versus mean cell quantities.

The first part of the paper presents the numerical method for a one dimensional hyperbolic two-fluid model including differential terms as added mass and interface pressure. This numerical solution scheme makes use of the Riemann problem solution to define backward and forward differencing to approximate spatial derivatives. The construction of this approximate Riemann solver uses an extension of Roe's method that has been successfully used to solve gas dynamic equations. As far as the two-fluid model is hyperbolic, this numerical method seems very efficient for the numerical solution of two-phase flow problems. The scheme was applied both to shock tube problems and to standard tests for two-fluid computer codes.

The second part describes the numerical method in the three dimensional case. We discuss also some improvements performed to obtain a fully implicit solution method that provides fast running steady state calculations. Such a scheme is now implemented in a thermal-hydraulic computer code devoted to 3-D steady-state and transient computations. Some results obtained for Pressurised Water Reactors concerning upper plenum calculations and a steady state flow in the core with rod bow effect evaluation are presented.

In practice these new numerical methods have proved to be stable on non staggered grids and capable of generating accurate non oscillating solutions for two-phase flow calculations.

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I. INTRODUCTION

Modeling and numerical simulation of two-phase flow phenomena keep causing complex problems for the development of computer codes dedicated to design or safety studies of nuclear reactors. Generally, engineering two-phase one dimensional or three dimensional calculations require the determination of the velocity, pressure and energy fields for each phase. The usual way to establish physical modeling for two-phase flow, is to start from a single continuous description of each phase such as Navier-Stokes differential equations which represent mass, momentum and energy conservation at a scale larger than some molecular length scales. This initial model is generally well-posed for fluid motion studies and for engineering calculations. Averaging procedures allow calculations of averaged physical variables defined over sufficient control volumes and time steps [1].

This averaging techniques were also applied to derived two-phase flow models but with some difficulties in comparison with single phase flow case. Generally the averaging procedure leads to an ill-posed initial value problem and many differential terms such as added mass or interface pressure terms, are proposed to make the models hyperbolic [2], [3], [4],[5].

An alternative approach in order to obtained satisfactory numerical results is to use numerical methods which have sufficient numerical dissipation to stabilize short wavelengths. These methods, based on staggered grid and donor cell differencing, are used in computer codes like RELAP5 and TRAC. Ransom [6] has shown that this approach leads to convergent results with a practical range of space discretization, meanwhile high frequency oscillations appear with a large number of cells. The non-convergence of the results may be due either to the ill-posed character of the system or to the non-monotone behavior of the numerical scheme.

In this paper we present a new class of numerical schemes for two-phase flow calculations. These numerical schemes are based on a finite volume technique where convective fluxes are deduced an approximate solution of Riemann problem at the interface between two cells. This class of numerical schemes, first developed by Godunov [7] then extended by Roe[8], are now widely used for compressible gas flow calculations, due to their properties of convergence, stability, robustness and monotonicity. For two-phase fluid dynamics, a weak formulation of Roe's approximate Riemann solver has been introduced in [9]. This weak formulation was applied to a homogeneous two-phase flow and to a four equation isentropic two-fluid model [9], [14]. Here, we present this scheme for a one dimensional six equation hyperbolic two-fluid model and we discuss extensions to three dimensional two-phase flow calculations.

II. UPWIND NUMERICAL METHOD FOR 1D TWO-FLUID MODELS

A. Two-Phase Flow model

We consider a one dimensional two-fluid model dealing with a two-component two-phase flow in a straight pipe. The basic system of equations for the two-fluid nonequilibrium model consists in two phasic mass equations, two phasic momentum equations, and two phasic energy equations.

$$\begin{aligned}\frac{\partial}{\partial t} \alpha_l \rho_l + \nabla(\alpha_l \rho_l u_l) &= \Gamma_l \\ \frac{\partial}{\partial t} \alpha_v \rho_v + \nabla(\alpha_v \rho_v u_v) &= \Gamma_v \\ \frac{\partial}{\partial t} \alpha_l \rho_l u_l + \nabla(\alpha_l \rho_l u_l \otimes u_l) + \alpha_l \nabla \cdot p - I + M_{vm} &= F_l \\ \frac{\partial}{\partial t} \alpha_v \rho_v u_v + \nabla(\alpha_v \rho_v u_v \otimes u_v) + \alpha_v \nabla \cdot p + I - M_{vm} &= F_v \\ \frac{\partial}{\partial t} \alpha_l \rho_l E_l + p \frac{\partial}{\partial t} \alpha_l + \nabla(\alpha_l \rho_l u_l H_l) &= Q_l + \Gamma_l h_l^* \\ \frac{\partial}{\partial t} \alpha_v \rho_v E_v + p \frac{\partial}{\partial t} \alpha_v + \nabla(\alpha_v \rho_v u_v H_v) &= Q_v + \Gamma_v h_v^*\end{aligned}$$

In the right hand side of this equation, Γ is the interphase mass exchange, F represents the wall drag and the interphase drag force and Q represents the wall heat flux and the interphase heat exchange. The enthalpies associated with interphase mass transfer Γ in the energy equations are defined in such a way that the interface energy jump conditions are satisfied. For more details on these latter terms, we refer for example to [5], where physical closure laws are given. The system is closed by state functions for the liquid and the vapor phase.

It is well known that the basic two-fluid model is non hyperbolic since the resulting system of equations possesses two complex eigenvalues. In the momentum equations two differential terms have been added:

- The virtual mass force term that describes inertial coupling of the phases in accelerating flows

$$M_{vm} = -\alpha_l \alpha_v c_{vm} \left[\frac{\partial}{\partial t} (u_v - u_l) + u_l \cdot \nabla u_v - u_v \cdot \nabla u_l \right]$$

The inclusion of the virtual mass term change the hyperbolicity of the system. In the case where the relative velocity is much lower than the speed of the sound in two-phase flow, it is demonstrated [14] that the system remains hyperbolic if :

$$c_{vm} \geq (4c(1-c))^{1/2}$$

where : c is the vapor mass concentration

- An interface pressure term given as a spatial gradient of the void fraction. This term must be defined consistently with the physical situation of interest (stratified flows, bubbly flows, ...). Here, we consider the following form for the interface pressure term

$$I = (p - p_i) \nabla \alpha_v$$

with

$$p - p_i = -\alpha_v \rho_v \delta (u_v - u_l)^2$$

where the value of the pressure coefficient δ is defined so as to have a hyperbolic system [15].

Except virtual mass force term and interfacial pressure term which contains partial derivatives, other transfer terms between phases are neglected. The resulting model is a non conservative hyperbolic one.

B. Approximate Riemann Solvers for Compressible Flows

From an original idea proposed by Godunov [6] for gas dynamic calculations, an usual way to define upwind numerical fluxes for inviscid flux is to solve a local one dimensional Riemann problem at cell interfaces. Let the system of conservation laws be expressed as an initial value problem according to the following form :

$$U_t + f(U)_{,x} = 0$$

and

$$U(x,0) \equiv U_i, \text{ for } (x < 0); \quad U(x,0) \equiv U_j, \text{ for } (x > 0)$$

where $f(U)$ is the inviscid flux in the x-direction and U_i, U_j are the vector of extensive flow parameters which are conserved. The system of conservation laws can be exactly solved, over a short time step Δt , because the initial data is piecewise constant and hence defines a sequence of Riemann problems. The exact solution is reached by simply piecing together these Riemann problem solutions, until waves from the neighboring Riemann problems begin to interact. In the 1-D case, the solution is given by :

$$U_i^{t+\Delta t} = \frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^0 U_{i-1,i}^{exact} \left(\frac{x}{t} \right) dx + \frac{1}{\Delta x} \int_0^{+\frac{\Delta x}{2}} U_{i,i+1}^{exact} \left(\frac{x}{t} \right) dx$$

The Godunov scheme can also be written in the following conservative form :

$$U_i^{t+\Delta t} = U_i^t - \frac{\Delta t}{\Delta x} \left[\Phi(U_i^t, U_{i+1}^t) - \Phi(U_{i-1}^t, U_i^t) \right]$$

The numerical flux is then obtained by integrating the conservation law over the domain

$\left[t, t + \Delta t \right] \times \left[-\frac{\Delta x}{2}, \frac{\Delta x}{2} \right]$, this gives :

$$\Phi(U_{i-1}^t, U_i^t) = f(U_i^t) + \frac{1}{\Delta x} \int_{-\frac{\Delta x}{2}}^0 U_{i-1}^{exact} \left(\frac{x}{t} \right) dx + \frac{\Delta x}{2\Delta t} U_{i-1}^t$$

In fact, the Godunov method requires an exact solution of the Riemann problem which is very expensive due to the fact that it is necessary to solve non-linear equations. However the whole structure of the exact Riemann problem is not used because the average over each grid cell. This implies that the exact Riemann problem solution is not worth calculating and that one might obtain good numerical results through an approximate Riemann solution given by cheaper methods.

This is the basic concept of Roe's approximate Riemann solver [7], which is the exact solution of the following local linearization of the conservative system.

$$U_{,t} + [A]_{ij} U_{,x} = 0$$

Where $[A]_{ij}$ is an average Jacobien matrix constructed to satisfy the following properties which traduce respectively the consistency with jump conditions, convective flux definition and positiveness :

$$f(U_i) - f(U_j) = [A]_{ij} (U_i - U_j)$$

$$\Phi(U, U) = f(U)$$

$$[A]_{ij} \text{ has real and distinct eigenvalues}$$

This linear Riemann problem is easy to solve. If λ_p, R_p are respectively the eigenvalues and the right eigenvector, and if we decompose :

$$U_i - U_j = \sum_p a_p R_p$$

then the approximate Riemann solver is given by :

$$U^{approx} \left(\frac{x}{t} \right) = U_i + \sum_p a_p R_p \delta_p$$

$$\text{where : } \delta_p = 1 \text{ if } \lambda_p < \frac{x}{t}; \text{ and } \delta_p = 0 \text{ if } \lambda_p > \frac{x}{t}$$

and, by substitution, one obtains the numerical flux :

$$\Phi(U_i, U_j) = f(U_i) + \sum_p (a_p)^- R_p$$

$$\text{where : } (a_p)^- = \min(a_p, 0), \text{ and } (a_p)^+ = \max(a_p, 0)$$

By using the first property one obtains

$$\begin{aligned} \Phi(U_i, U_j) &= f(U_i) + \sum_p (a_p)^- R_p \\ &= \frac{1}{2} (f(U_i) + f(U_j)) - [A]_{ij} (U_i - U_j) \end{aligned}$$

The matrix $[A]_{ij}$ is defined as : $[A]_{ij} = [R]^{-1} \Lambda [R]$, where the matrices $[R]^{-1}$ and $[R]$ contains respectively the right and left eigenvectors and Λ is a diagonal matrix containing the eigenvalues.

C. Extension to Two-Phase Flows

We still have the problem to determine $[A]_{ij}$ in a reasonable way. Such a matrix is known as a Roe averaged matrix and was first constructed for Euler equations with perfect gas. Several extensions of Roe's linearization to real gases have been proposed [11]. However for our system, the various solutions suggested for real gas extensions will not be generally applicable because of additional difficulties due to the presence of two state equations and nonconservative terms in the momentum equations.

To overcome that difficulty, we will use a weak formulation of the Roe's approximate Riemann solver of a non-linear hyperbolic system in a non conservative form [9]:

$$U_{,t} + A(U)U_{,x} = 0$$

This formulation is based on the definition of non conservative products proposed by Le Floch and Dal Maso [12]. Using this definition, one can define entropy weak solutions for the non-conservative system and get jump relations or generalized Rankine Hugoniot conditions for discontinuous solutions :

$$\int_0^1 [-\sigma I + A(\phi(s, U_L, U_R))] \frac{\partial \phi}{\partial s}(s, U_L, U_R) ds = 0$$

where : $\phi(s, U_L, U_R)$ is a Lipschitz continuous path connecting U_L and U_R in R^m

Our Riemann solver is inspired from the above Rankine-Hugoniot condition. Precisely, we consider approximate solutions of the Riemann problem, which are exact solutions of the following linear problem :

$$U_{,t} + A(U_i, U_j)_\phi U_{,x} = 0$$

where : ϕ is a Lipschitz continuous path connecting U_i and U_j in R^m and $A(U_i, U_j)_\phi$ is an average matrix depending on (U_i, U_j) and on the path $\phi(s, U_i, U_j)$ which satisfy the three following properties:

$$\left\{ \begin{array}{l} \int_0^1 A(\phi(s, U_i, U_j)) \frac{\partial \phi}{\partial s}(s, U_i, U_j) ds = A(U_i, U_j)_\phi (U_i - U_j) \\ A(U, U)_\phi = A(U) \\ A(U_i, U_j)_\phi \text{ has real and distinct eigenvalues} \end{array} \right.$$

One can notice that these conditions imply that a shock wave solution of the linearized system satisfies the Rankine-Hugoniot conditions for the non linear conservative system and it is independent of the path ϕ which is, in this case useful to linearize the jacobien matrix.

To construct such matrix, we follow the method introduced in [9]. The main feature is the choice of a canonical path for a parameter vector w :

$$\phi_0(s, U_i, U_j) = f_0(w_i + s(w_j - w_i))$$

with :

$$f_0(w_i) = U_i; \quad f_0(w_j) = U_j; \quad \text{and } A_0(w) = \frac{\partial f_0}{\partial w}$$

Using this path, we define the Roe's matrix by :

$$A(U_i, U_j)_\phi = C(U_i, U_j)_\phi B(U_i, U_j)_\phi^{-1}$$

with :

$$B(U_i, U_j)_\phi = \int_0^1 A_0(w_i + s(w_i - w_j)) ds$$

$$C(U_i, U_j)_\phi = \int_0^1 A(f_0(w_i + s(w_i - w_j))) A_0(w_i + s(w_i - w_j)) ds$$

D. Application to Two-Fluid Models

To build an approximate Riemann solver for the two-fluid model, we have to find a parameter vector w and to apply the method described above. To derive the parameter w , following Roe [8] we look for a set of new variables w_i such that most of the conservative variables can be written as some quadratic function of the variables w_i . This leads to the parameter vector

$$w = (w_k)_{k=1,6} = \sqrt{\rho} \begin{bmatrix} \sqrt{c_v} \\ \sqrt{c_l} \\ \sqrt{c_v} u_v \\ \sqrt{c_l} u_l \\ \sqrt{c_v} H_v \\ \sqrt{c_l} H_l \end{bmatrix}; \quad \text{and} \quad f_0(w) = \begin{bmatrix} w_1^2 \\ w_2^2 \\ w_1 w_3 \\ w_2 w_4 \\ w_1 w_5 - \alpha_v p \\ w_2 w_6 - \alpha_l p \end{bmatrix}$$

E. Second Order Accurate TVD Scheme

Godunov type numerical schemes are monotone and first order accurate methods. Hence they converge in a nonoscillatory manner to the exact solution. However, they give poor accuracy in smooth regions of the flow. For computations with a coarse meshing, it is necessary to have second order accuracy for the numerical fluxes. The basic idea is to generalize Godunov's method by replacing the piecewise constant representation of the solution by a more accurate piecewise linear representation. From the data (U_i^l, U_j^r) we construct a piecewise linear function $\bar{U}(x)$. Then at the cell interface x_{ij} we have states on the left and right from the two linear approximations in each neighboring cells:

$$U_{ij}^L = U_i^l + \frac{\Delta x}{2} \sigma_i$$

$$U_{ij}^R = U_j^r - \frac{\Delta x}{2} \sigma_j$$

Here σ_i is a vector of slopes on the cell Ω_i which is based on the conservative variables of the neighbors Ω_k . If we make the natural choice

$$\sigma_i = \frac{U_j^r - U_i^l}{\Delta x}$$

for the slopes, the method reduces to the second order Lax-Wendroff method. This is a poor choice of slopes because Lax-Wendroff method produces oscillations near discontinuities. We can rectify this by applying a slope limiter which reduces the value of the slope near discontinuities and extreme points:

$$\sigma_i = \frac{U_j^r - U_i^l}{\Delta x} \phi_i$$

This slope limiter is typically designed to ensure that the method is total variation diminishing (TVD method) [11]. One simple choice of limiter satisfying the TVD property is the so-called minmod limiter. A second order accurate approximation to the flux at the cell interface is then obtained by solving the Riemann problem with left and right states given by the above linear approximations.

F. Numerical Results

Various one dimensional test problems have been computed to validate the approximate Riemann solver previously detailed. In this section we will present to numerical benchmark about a two-phase flow shock tube problem and the water faucet problem.

1. Water faucet problem

This problem proposed by Ramsom [6], consists in a vertical water jet, contained within a cylindrical channel, which is accelerated with the gravity action. At initial time, the pipe is filled with an uniform column of water surrounded by stagnant gas, such that the void fraction is constant and equal to 0,2. The liquid velocity in the column is constant and equal to 10 m/s. Boundary conditions are constant inlet velocities and constant outlet pressure (fig. 1).

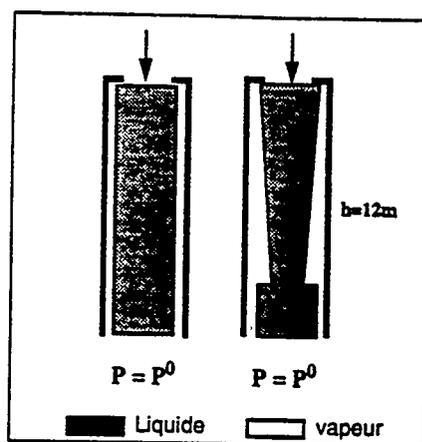


Fig. 1 : Water faucet problem : Schematic description

As illustrated on Figure 1., a void wave develops and is propagated at liquid velocity. Once the void wave exits the pipe, a steady void profile is established. The calculation was carried out with the first order scheme until the steady state is reached, with 96 nodes and a constant CFL number. Several computations with an increasing number of cells have been done to test the convergence and the stability character of the scheme.

2. Edwards pipe Blowdown experiment

This standard test for transient two-phase computer codes concerns the prediction of the blowdown of an initially subcooled liquid from a pipe of 4m length. This test contains features similar to pressurized water reactor loss of coolant accident. The water in the pipe has an initial pressure of 7.0 Mpa. The transient is initiated by opening the right side of the pipe to the pressure environment.

The interfacial heat transfer into phase k is modeled by the relation:

$$Q_k^i = \alpha_v \alpha_l \rho_k \frac{(h_k^{sat} - h_k)}{\tau}$$

where the parameter τ can be considered as a constant rate for the interfacial heat transfer process. The above expression was chosen as a rough approximation.

During the first 10 ms of the transient, a rarefaction wave propagates from the open end into the pipe, leading to a fast depressurization and the onset of flashing of the subcooled liquid. Figure 4. shows a comparison between experimental and predictal values using various rates τ of the interfacial heat transfer process, for the pressure history at the closed end. The results obtained with a simplified model show a reasonable agreement for $\tau = 5 \cdot 10^{-2}$

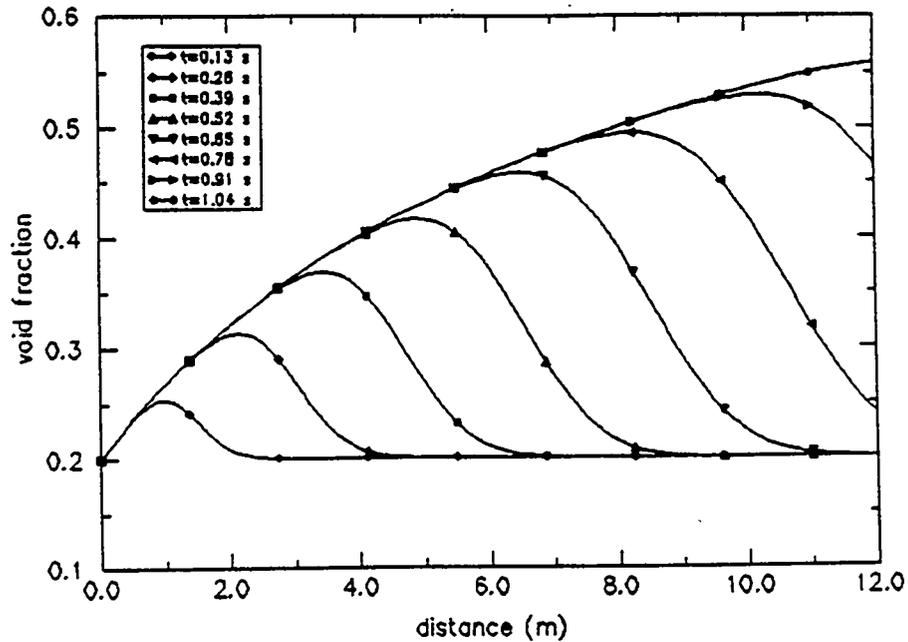


Fig. 2 : Water faucet problem : transient solutions

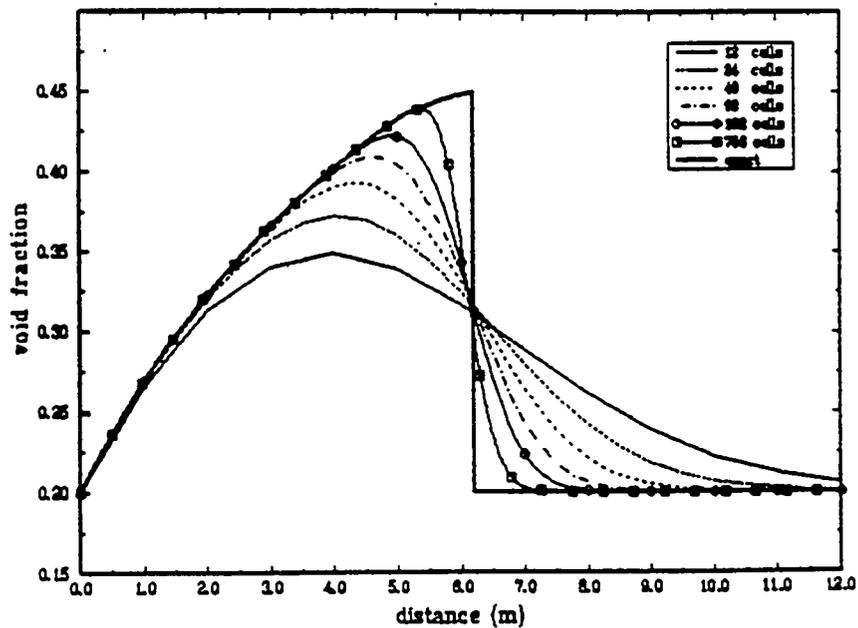


Fig. 3 : Water faucet problem at time $t=0.5s$: spatial convergence

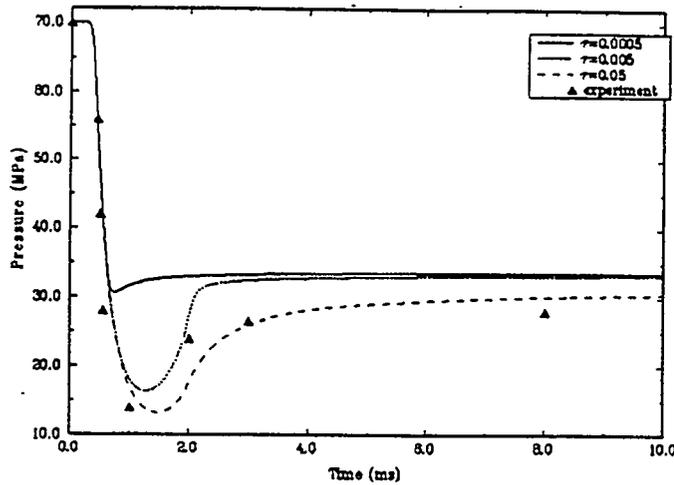


Fig. 4 : Edwards pipe blowdown experiment : closed end pressure versus time.

III. FINITE VOLUME METHOD FOR 3D TWO-PHASE FLOW CALCULATIONS

A. Finite Volume Discretization

We start by considering the system of conservation laws for a set of variables U ,

$$\frac{\partial U}{\partial t} + \nabla \cdot F = S(U)$$

Here $S(U)$ is a source term, and F represents the flux vector associated with the conserved variables and dependent also on the gradient ∇U for viscous fluxes. Finite volume methods are based on the discretization of the integral formulation

$$\frac{\partial}{\partial t} \int_C U d\Omega + \oint_{\partial C} F \cdot n d\Gamma = \int_C S(U) d\Omega$$

for any piecewise smoothly bounded fixed volume C contained in the domain Ω . The finite volume approximation assumes that the conservative variables are constant over each control volume C and the resulting discretization leads to a system of balance equations of the type

$$U_i^t - U_i^{t-1} + \Delta t \sum_j (\Phi_I(U_i^t, U_j^t) + \Phi_V(U_i^t, U_j^t)) = S(U_i^t)$$

where U_i^t denotes the conservative variables for the control volume C_i and $\Phi_I(U_i^t, U_j^t)$, $\Phi_V(U_i^t, U_j^t)$ denote the inviscid and viscous contributions respectively to the flux on the cell C_i in direction of the neighbor cell j .

The evaluation of the viscous contributions requires a knowledge of the first derivatives of intensive variables as velocities, temperature and phase concentration. They are obtained by a centered difference scheme in which the derivatives are represented by piecewise constant functions over computational domain. Full details of the evaluation of dissipative flux terms are given in [10].

The basic point of the numerical method is the use of an approximate Riemann solver for inviscid flux estimation and the implicit integrating step to advance in time.

B. Discretization of Inviscid Fluxes

The inviscid flux in the normal direction to the cell interface ∂C_{ij} is given by

$$\Phi_i(U_i^t, U_j^t) = \iint_{\partial C_{ij}} (F(U) \cdot n) d\sigma$$

Following the one dimensional approach of the above section, this numerical flux is based on the solution of a one dimensional Riemann problem at the cell interface ∂C_{ij} (located at $x = x_{ij}$)

$$U_{,t} + f(U)_{,x} = 0$$

$$U(x,0) \equiv U_i^t, \text{ for } (x < x_{ij}); \quad U(x,0) \equiv U_j^t, \text{ for } (x > x_{ij})$$

In practice, we make a local linearization of this problem and we use Roe's approximate Riemann solver as previously described.

C. Fully Implicit Method for Transient Calculations

Once Roe's matrix $[A]_{ij}$ is constructed, the numerical inviscid flux between control volumes i and j will be given by the following expression :

$$\Phi_i(U_i^t, U_j^t) = \frac{1}{2} (f(U_i^t) + f(U_j^t)) - [A]_{ij}^t (U_i^t - U_j^t) s_{ij}$$

The matrix $[A]_{ij}$ can be split into :

$$[A]_{ij}^t = [A]_{ij}^{t+} + [A]_{ij}^{t-}$$

with :

$$[A]_{ij}^{t+} = [R]_{ij}^{-1} \left(\frac{|\Lambda_{ij}| + \Lambda_{ij}}{2} \right) [R]_{ij} ; \quad \text{and} \quad [A]_{ij}^{t-} = [R]_{ij}^{-1} \left(\frac{|\Lambda_{ij}| - \Lambda_{ij}}{2} \right) [R]_{ij}$$

where : Λ_{ij} is a diagonal matrix containing the eigenvalues of $[A]_{ij}$, and $[R]_{ij}^{-1}, [R]_{ij}$ are matrices which contain the right and left eigenvectors of $[A]_{ij}$. It is noted that $[A]_{ij}^{t+}$ and $[A]_{ij}^{t-}$ have non negative eigenvalues. Then inviscid flux between cells i and j can be expressed according two equivalent ways:

$$\begin{aligned} \Phi_i(U_i^t, U_j^t) &= f(U_i^t) - [A]_{ij}^{t-} (U_i^t - U_j^t) s_{ij} \\ &= f(U_j^t) - [A]_{ij}^{t+} (U_i^t - U_j^t) s_{ij} \end{aligned}$$

Using these two definitions on two opposite surface of the control volume leads to a flux balance equation on the following form :

$$\frac{1}{\Delta t} (U_i^t - U_i^{t-1}) + \left(\sum_l s_{il} C_{il} \right) U_i^t + \sum_l (s_{il} C_{il}^t U_{il}^t) = S(U_i^t)$$

where all involved matrices have non-negative eigenvalues. In order to get U_i^t for all control volumes, we solve this non linear set of equations using a Newton method. In practice, two or three iterations are sufficient for each time step.

D. Implicit Linearized Method for Steady-State Calculations

For steady-state calculations, iterations needed to solve this system of non linear equations at each time step, may not be compensated for the savings gained with the ability to take large time steps. To overcome this obstacle,

the previous equation is linearized by estimating the C matrices at time $t-\Delta t$. Finally, using a delta formulation $\delta U_i = U_i^t - U_i^{t-1}$, one get the following linear system :

$$\left[\frac{1}{\Delta t} + \sum_k s_{ik} C_{ik}^{t-1} - \frac{\partial S}{\partial U} \right] \delta U_i + \sum_k (s_{ik} C_{ik}^{t-1} \delta U_k) = S(U_i^{t-1}) + \sum_k (\Phi_I(U_k^{t-1}) + \Phi_V(U_k^{t-1}))$$

This linearization will destroy the conservative property of the scheme but preserves its unconditional stability. Thus, for transient calculations, a predictor-corrector scheme is used. The first step (predictor) solves the previous linear system. The corrector step uses this estimation to compute fluxes and to solve exactly the balance equations.

For reactor core design or safety calculations, it is necessary to determine with accuracy steady state flow regime which has to be compatible with the transient numerical scheme. A usual way to compute a steady state is to perform transient computations with constant boundary conditions. Generally, this technique leads, after a finite time, to a steady state if the numerical method possesses good conservative properties. To reduce the CPU time cost of this method, a steady-state algorithm was derived [13].

A first remark can be made on the construction of the implicit operator, the right hand-side of the linear system contains a conservative discretization of the steady state equations of the two-phase flow model. It follows that the steady state solution obtained when the time variation of conservative variables leads to zero is:

- consistent with the conservation form
- independent of time step used in the equations
- a spatially first order approximation to the steady state of the partial differential equation system.

Consequently, the second step (conservation step) is not necessary to compute a steady state flow.

A second remark on the implicit scheme comes from an examination of the CPU time distribution between the various phases of the resolution of the predictor step. One can consider three phases :

- the matrix coefficients computations,
- the matrix pre-conditioning,
- the linear system resolution.

If the linear system is solved by using a direct method (LU factorization), the second phase which approximately varies with the square of the number of unknowns is generally the more expensive one. However, the Roe linearization leads to a positive definite matrix for the implicit operator. Since variations of the Roe averaged matrix coefficients between two time steps lead to a second order variation for the solution, it turns out that it is not necessary to update the matrix of the linear system at each time step to achieve a good convergence towards the same steady solution. Consequently, it is possible to significantly reduce CPU time by saving the preconditioned form of the matrix and using it for several time steps.

E. Numerical Results

This numerical method has been implemented in the three dimensional thermal-hydraulic computer code FLICA-4 [9] which is mainly dedicated to core thermal transient analysis. The FLICA-4 computer code is now validated for a great number of steady state and transient calculations in rod bundles and PWR reactor core and assemblies. In this section, we will briefly present results obtained with FLICA-4 for a PWR core with hot fuel rod deformation and a steady state calculations in a PWR upper plenum.

1. Rod bow effect steady state calculation

This calculation was performed in order to estimate the influence of a strong fuel rod deformation on the hot channel coolant flow. The concerned hot channel is delimited by three fuel rods and one guide tube. The deformed fuel rod is assumed to close communications between the hot channel and two adjacent ones between 1.9 m and 2.1 m (fig. 5).

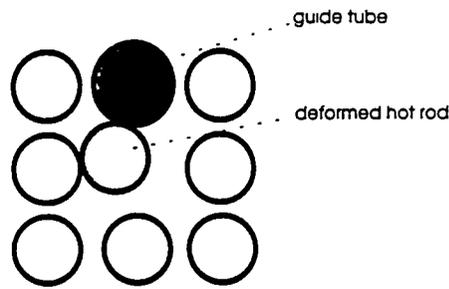


Fig. 5 : Rod position at 2 m level

A two step steady state calculation was performed for this test. The first step was a steady state computation in a quarter reactor core with one radial mesh by assembly and 37 levels. The first step gives transversal boundary conditions for the hot assembly calculation with one radial mesh by channel and 37 axial levels (fig. 6).

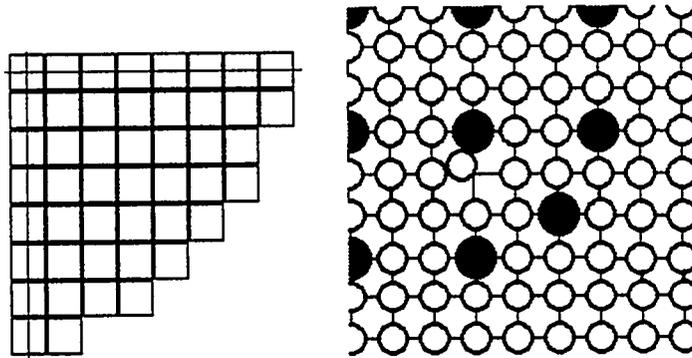


Fig. 6 : Core and hot assembly radial meshing

Figures 7 and 8 give the axial mass flow rate and void fraction distributions in the hottest channels. One can observe an important down flow diminution of the axial mass flow rate in the hot channel due to the cross section diminution this effect leads to coolant vaporization in the hot channel. Mass flow rates in channels becomes equivalent after the hot rod deformation.

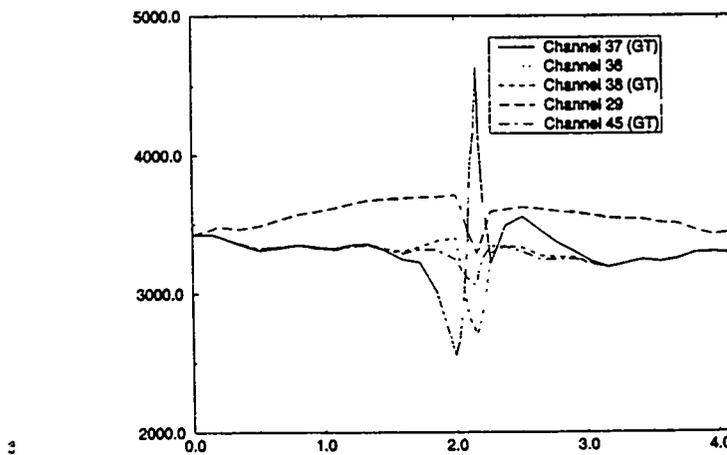


Fig. 7 : Axial mass flow rate in the hottest channels

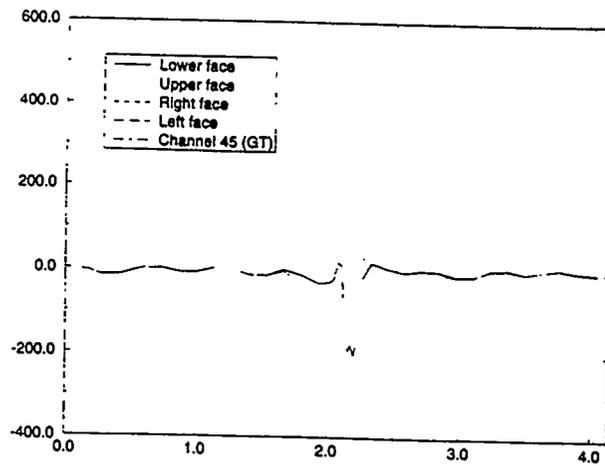


Fig. 8 : transverse mass flow rate in the hottest channels

2. PWR upper plenum calculations

In pressurized water reactors, the knowledge of the fluid flow mixing characteristic in the upper plenum is of main interest. The coolant flow divided in three independent loops enters the vessel by a pipe, flows down to the bottom, then crosses the core before reaching the upper plenum.

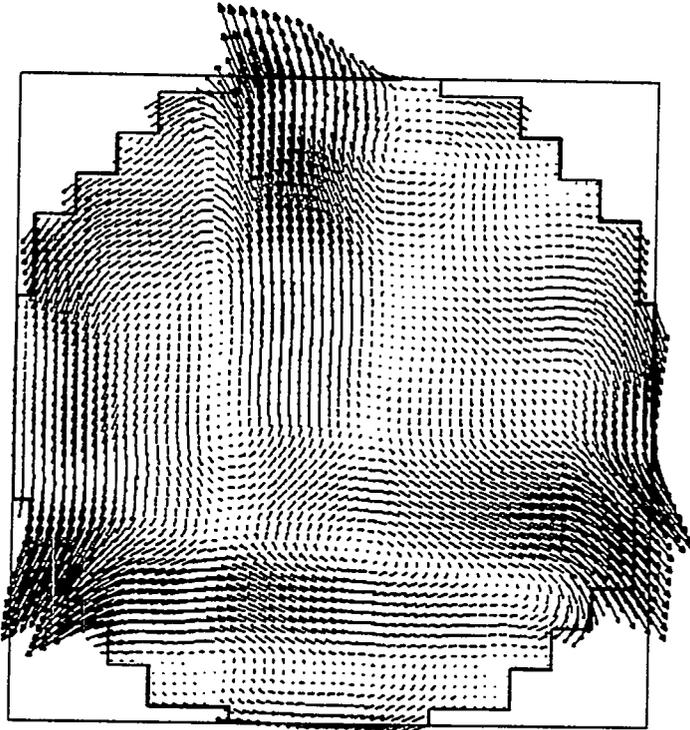


Figure 5: Flow velocity at steady state (cross section)

This computation concerns only the upper plenum. The very complex geometry of the upper plenum with plates and columns supporting the in core instrumentation is homogenized. The boundary conditions are a constant pressure $P = 15.1\text{MPa}$ at the outlet loops and a constant mass flow rate at the outlet of the core. This last boundary condition comes from a steady state calculation in the core. Figure 9 and Figure 10 show the liquid velocity fields at steady state.

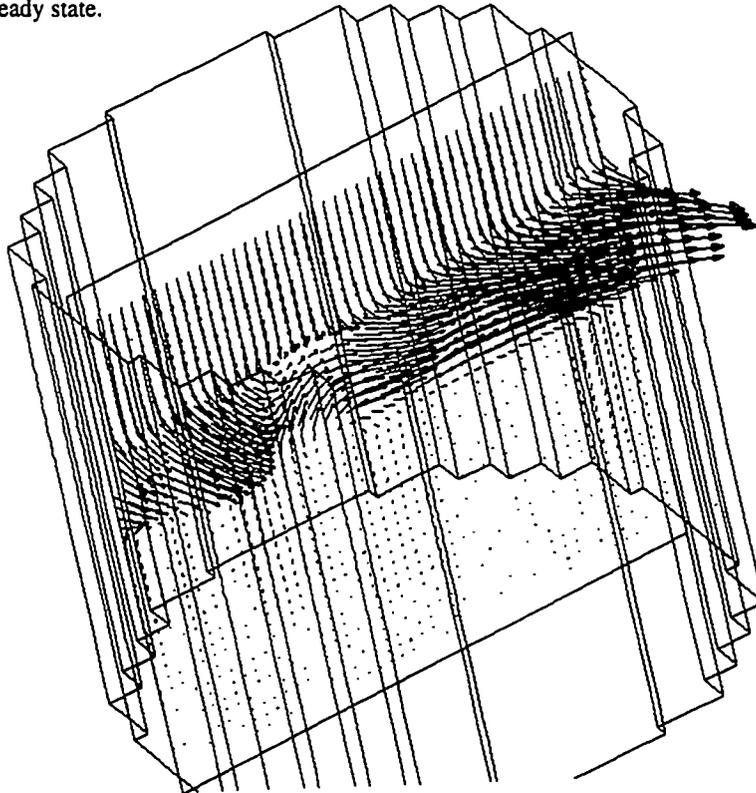


Figure 6: Flow velocity at steady state (axial section)

IV. CONCLUSION

We have presented here an extension of an upwind numerical method to two-phase flow calculations, based on approximate Riemann solvers, which turned out to be very efficient for fluid dynamics. This numerical method seems very promising for the numerical solution of two-phase flows as shown by the numerical results for standard two-phase flow problems.

Compared to standard numerical methods for two-fluid models, this new approach has the following advantages:

- its theoretical basis leads to upwind numerical fluxes, based on the characteristic information, without any heuristic for the upstream or downstream differencing. However, it requires a mathematical analysis for each new system to construct a good approximate Riemann solver.
- the use of staggered grids is not necessary to ensure stability. Consequently, this method can be applied to multidimensional unstructured meshing.
- it has low numerical diffusion and it is designed to calculate strong discontinuities without oscillations.

Improvements of the numerical method are now under development, these studies concern the introduction of this numerical method in the framework of industrial computer codes:

- discretization of nonlinear stiff source terms,
- assessment of this method for unstructured meshes

V. REFERENCES

- [1] M. Ishii
"Thermo-fluid dynamic theory of two-phase flow", Eyrolles 1975
- [2] V.H. Ransom, M.P. Scotfield
"Two-pressure hydrodynamic model for two-phase separated flow", INEL, SRD-50-76 (1976)
- [3] V.H. Ransom, D.L. Hick
"Hyperbolic two-pressure models for two-phase flow", *Journal of Computational Physics*, **53**,1 (1984)
- [4] J.A. Trapp
"The mean flow character of two-phase flow equation", *International Journal of multiphase Flow* **12**,2 (1986)
- [5] J. C. Micaelli
"Document de synthèse CATHARE", CEA internal Report.
- [6] V.H. Ransom, V. Mousseau
"convergence and accuracy of the RELAP5 two-phase flow model", *ANS Topical Meeting on Advances in Mathematics, Computations and Reactor Physics*, Pittsburg Pennsylvania (1991)
- [7] S. K. Godunov, *Math. Sb.* **47**, 217 (1959)
- [8] P.L. Roe
"Approximate Riemann solvers parameter vectors and difference scheme", *Journal of Computational Physics*, **43** 357-372 (1981)
- [9] I. Toumi
"A weak formulation of Roe's Approximate Riemann Solver", *Journal of Computational Physics*, **102**, 360-373 (1992)
- [10] I. Toumi
"Flica-4 - manuel de référence - Methodes numériques", CEA, internal report
- [11] Yee H.C., NASA TM-89464 (1987)
- [12] G. dal Maso, P. Le Floch, F. Murat
"Definition and weak stability of a non conservative product", centre de Mathematiques Appliquées de l'Ecole Polytechnique, internal report
- [13] P. Raymond, I. Toumi
"Numerical Method for three dimensional steady state two-phase flow calculation", NURETH-5 (Salt-Lake City), (1992)
- [14] I. Toumi
"A Linearized Approximate Riemann Solver for a Two-Fluid Model", *Journal of Computational Physics*, **124**, 286-300 (1996)
- [15] I. Toumi
"An Upwind Numerical Method for Two-Fluid Two-Phase Flow Model", *Nuclear Science and Engineering*, (1996)

Recent Advances in Two-Phase Flow Numerics

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ABSTRACT

We review three topics in the broad field of numerical methods that may be of interest to individuals modeling two-phase flow in nuclear power plants. The first topic is iterative solution of linear equations created during the solution of finite volume equations. The second is numerical tracking of macroscopic liquid interfaces. The final area surveyed is the use of higher order spatial difference techniques.

1. INTRODUCTION

Advances in numerical methods for two-phase flow have been slow in coming to the field of Reactor Safety research. The major thermal-hydraulic codes for reactor transient simulation still incorporate old first order (in space and time) finite difference methods [1], but this should not be surprising. Numerical methods are given a strenuous workout by the full range of flow regimes encountered during most reactor transients, and by the particularly challenging flows encountered as ECCS liquid re-enters voided regions. Codes such as RELAP5 [2], TRAC [3,4], CATHARE [5], and RETRAN[6] must be able to complete a transient with little or no user intervention. This has driven a selection of well established, robust numerical methods.

The most significant improvement in these codes in recent years, has ironically been CATHARE's full use of the oldest of the current range of difference techniques, Backward Euler. This has been a necessary step to eliminate both Courant stability limits and various bounded instabilities caused by explicit evaluation of heat transfer and friction coefficients. The obvious price for this stability, a higher cost per time step, is generally more than balanced by larger average time step sizes. However, there is one other cost, developers' time programming and checking the derivatives in the Jacobian, associated with any new model or correlation.

Hand coding of these derivatives cuts the rate at which new models can be tried, and increases problems due to fairly subtle code bugs. The recent maturity of Automatic Differentiation holds significant promise in minimizing these difficulties. Now a developer need only program the basic correlation or other model, and a program such as ADIFOR [7] can be applied to generate the lines

of code for any necessary analytic derivatives. Once a model has been selected for a release version of the systems code, derivatives should be re-coded for optimal speed. However, work is cut from testing of unimplemented models, and validation of the final implemented code.

In recent years more potential improvements have become available as a result of research in other fields. We will survey efforts in three general areas. The first, iterative solution of large sparse linear systems, has direct application to the solution of two-phase flow equations, and recent advances have appeared in CATHARE and RELAP5. The second, interface tracking, has been developed for a number of applications with free surfaces, and has appeared in recent versions of TRAC [8, 9] and RELAP to aid in following liquid surfaces. The third, higher order differencing, has evolved rapidly in single phase shock applications. However, extension of these techniques to conditions and equations typical of reactor safety simulation is just beginning.

2. ITERATIVE SOLUTION OF SPARSE LINEAR SYSTEMS

Reactor thermal-hydraulics codes generate sparse linear systems in two contexts. The first is a nearly block tridiagonal system resulting from the equations in 1-D portions of the system. Direct solution methods have worked well for these systems. However, the details of this approach may need reconsideration, if future codes are to be adapted to massively parallel computers. The second, and more problematic class of sparse matrices are generated by equations modeling two- and three-dimensional regions (usually the reactor vessel). These systems are usually only marginally diagonally dominant, and hence pose a significant challenge to iterative solution methods. Twenty years ago finding a method that dealt with these equations well was extremely difficult. Now the biggest

problem is sorting through a wide selection of methods for the problem to find the most appropriate approach.

About ten years ago enough experience had been gained with matrix preconditioning that variants on the Conjugate Gradient method [10] had come into wide use. Evolution of this methodology has continued with the introduction of several variations on the basic algorithm. The most popular of these is currently Sonneveld's conjugate gradient squared (CGS) algorithm [11]. This class of methods has a rate of convergence that is generally very good, but is not monotonic. Plots of residual versus iteration count can show oscillations. A stabilized CGS method (CGSTAB) [12] has been introduced to mitigate the oscillatory behavior of residuals, but it does not guarantee monotonically decreasing residuals.

Conjugate Gradient methods currently are losing favor to Krylov subspace methods based largely on the GMRES algorithm [13]. As with conjugate gradient, this method is based on the construction of a set of basis vectors, and formally will converge to the exact solution. Rapid convergence in the initial iterations requires preconditioning of the matrix in both approaches. GMRES type algorithms have the advantage that residuals decrease monotonically, and that the algorithms are generally more robust. They have the disadvantage that they must store an additional basis vector for each iteration. The partial solution to this problem has been to restart the solution algorithm after some number of iterations.

Providing a recommendation for a "best" solution algorithm is beyond the scope of this paper. In fact variability of algorithm performance with machine architecture and problem type suggests that

a "best" algorithm exists only in an average sense. Some guidance can be obtained from recent publications. Soria and Ruel [14] provide a summary of the algorithms mentioned above, and comparisons of GMRES and CGS using ILU or diagonal preconditioning to results of Broyden [15], Gauss-Seidel, and Jacobi iterations. The authors clearly illustrate the value of good preconditioning, and conclude that more than one solution procedure should be available in a CFD program. However, they offer no advice on criteria for method selection in such a CFD program.

Chin and Forsyth [16] provide more detailed information for judging relative performance of GMRES and CGSTAB with ILU preconditioning. For their problems, CGSTAB was generally faster than GMRES, but they noted GMRES was not afflicted with the occasional divide by zero observed in the CGSTAB algorithm. They also note (but don't document) the sensitivity of conclusions on relative performance of these methods to the quality of the initial guess for the problem solution.

The interaction between algorithm and machine architecture is always a popular topic. Recent discussions and references can be found in articles by van Gijzen [17] (impact of vectorization on GMRES), Sturler and van der Vorst [18] (GMRES and CG on distributed memory parallel machines), and Xu et al. [19] (GMRES for parallel machines). However, for Reactor Safety codes it is more important to first select a method that performs well without special vector or parallel considerations. This helps to minimize non-uniform behavior across platforms. Special vectorized or parallelized packages should be options that can be activated and checked after initial code validation on a new installation.

We would recommend several key considerations in choosing a linear system solver for reactor thermal-hydraulic codes. The starting point, of course, is a set of problems (probably only segments of transients) that are believed to be representative of the code's work load. Enough solution packages are publicly available that special programming of algorithms should not be attempted for initial tests. LASPack [20] is one resource for testing combinations of preconditioners and solution algorithms. Once a good (based on robustness and speed) iterative solver has been selected, the break-even point (in system size) should be determined between use of the iterative solution and an efficient direct sparse matrix solver. Our experience is that 3-D capabilities are used more in reactor simulations as a simple provision for macroscopic effects of cross-flows, than as a means for detailed analysis of flow patterns. This generally results in 3-D vessel simulations with a relatively small number of computational cells (hundreds not thousands of cells). Both iterative and direct solution packages should be included in the code with an internal check on the geometry of the 3-D mesh to choose between the methods. Given the standard use of coarse "3-D" modeling in these codes, it is likely that the direct solution package will be frequently selected.

3. INTERFACE TRACKING

Discontinuous or abrupt changes in key physical variables are standard features in reactor transient analysis. Key phenomena include flow of ECCS liquid into steam, water levels during steady operation and transients, and propagation of boron and thermal fronts. Boron and thermal fronts are probably more amenable to the use of higher order methods discussed in the next section. However, abrupt transitions from predominantly liquid regions to predominantly vapor regions have caused problems in two-phase flow simulations from the beginning. They have largely driven the continued use of donor-cell differencing to achieve robustness, and have adversely impacted code accuracy.

We will not provide an in-depth discussion of interface tracking, but simply provide a brief list of recent works in the area. Hyman [21] provides an excellent review of some of the pre-1984 work in this area.

The recent work in tracking liquid surfaces in TRAC [8] is based largely on the Volume of Fluid method [22]. The void fractions obtained from the two-fluid model provide the necessary information on the volume of an Eulerian cell occupied by liquid (or bubbly two-phase mixture). In a 1-D simulation, calculation of the surface location is trivial. However, the problem becomes significantly more complex in two and three dimensions. Youngs [23] provides detailed equations for obtaining surfaces on a 3-D Cartesian mesh, and Mashayek and Ashgriz [24] work through a similar problem in Cylindrical coordinates. Welch et al. [25] provide a sub-grid method for locating such interfaces that avoids the complex logic and geometric calculations of the previous two methods. Insufficient information exists for us to choose between the surface equation and sub-grid methods of surface location. However, current research at Penn State on surface tracking is more closely related to the approach of Youngs.

When tracking interfaces in problems with delicate gravitational head balances (advanced passive reactors), more must be done than simply locate an interface and appropriately adjust mass flux terms. Physically based adjustments must be made to momentum equations evaluated at points (or cell faces) adjacent to the interface. The result is a code that runs more accurately and at higher time steps than one without tracking. These adjustments to existing momentum equations are, however, a significant step short of the state of the art in front tracking. Advanced methods create a moving mesh at the interface, and evaluate momentum equations on that interface (including surface

tension terms). An excellent description and review of this methodology can be found in a book by Shyy [26]. Unverdi and Tryggvason [27] provide an interesting application of front tracking to bubble dynamics, including including a calculation of bubble coalescence. Although their level of detail is not appropriate for a reactor systems calculation, it could provide useful information for understanding and extending experimental data, aiding the creation of correlations useful to systems codes.

Lagrangian Hydrodynamics provides another long used method for following interfaces. In multi-phase flow calculations, these tend to appear within mixed Eulerian-Lagrangian schemes. This approach has been applied in OLGA [28,29] to provide improved tracking of liquid slugs within oil and gas pipelines. A similar approach has been applied by Paulsen et al. [30,31] for general reduction of numerical diffusion in a special version of RETRAN-03.

Mixed Euler-Lagrange methods have been used more extensively in multi-phase flow as a method of following dispersed fields (Lagrangian particles) within the flow of a continuous (Eulerian) fluid phase. This approach has been adopted in DISCON [32,33] for modeling basic two-phase phenomena. It is also frequently used when modeling combustion problems and in simulations that model feedback between dispersed particles and turbulence in the continuous fluid. Crowe et al.[34] provide an extensive review of these applications.

An advanced Lagrangian technique, called Smooth Particle Hydrodynamics (SPH) [35], has also been applied to some problems in multi-phase flow [36]. Monaghan [37] and Koshizuka and Oka [38] have demonstrated its capabilities for modeling flows with a free surface. However, the method

is too costly for standard reactor simulations, and utility of the basic method for flows with phase change has not been demonstrated. SPH may be a candidate for enhancing some mixed Euler-Lagrange calculations, and could be useful in calculations to aid in the understanding of basic phenomena.

4. HIGHER ORDER SPATIAL DIFFERENCING

The literature is filled with work on higher order spacial differencing, generally associated with calculations for shock problems. Total Variation Diminishing (TVD) [39,40,41] methods are one popular way to provide a general high order of accuracy while suppressing numerical oscillations near a discontinuity. However, it should be noted that these methods have generally been developed for 1-D test problems, and Goodman and LeVeque [42] proved that linear TVD methods are at best first order accurate in two or three dimensions. Also, Leonard has demonstrated that a different approach, embodied in the QUICKEST difference method and ULTIMATE flux limiter strategy [43] is generally superior to standard TVD schemes (in 1-D)

We noticed problems when adapting Leonard's multi-dimensional work (UTOPIA) [44] to boron transport. As a result we also examined an interesting flux correction technique by Smolarkiewicz [45]. This method starts with an upwind method, then uses additional iterations to improve accuracy, in effect adding terms to the problem's Taylor series expansion. As a check of the methods, we applied a challenging set of problems proposed by Peterson [46]. Figure 1 gives contours for an initial profile on a 2-D Cartesian grid. Concentration is given by the equation:

$$C = 10 * e^{-0.4 (x^2+y^2)}$$

Mesh spacing is equal in the x and y directions. Figure 2 illustrates the displacement of this profile using a standard upwind scheme, and setting the x and y components of velocity equal such that

$$v_x = v_y = .125 \frac{\Delta x}{\Delta t}$$

(material Courant numbers are 1/8 in the x and y directions). Figure 3 illustrates the same propagation using Smolarkiewicz's method. The asymmetry in this case is fundamental to his underlying upwind approach. Figure 4 illustrates the results from Leonard's method. Dispersion of the profile is greater than for Smolarkiewicz, and ringing is evident at lower concentrations. Recent work by Thuburn [47] suggests that the asymmetry (and perhaps ringing) can be minimized for UTOPIA with a revised flux limiter. However, we have not yet implemented this work to test overall behavior, and won't speculate on what to name the next step beyond UTOPIA.

There are few applications of these advanced difference methods to complex problems in two-phase flow. Work is being done in the context of finite element models for geologic reservoirs of oil and gas [48], and the two-phase pipeline code TACITE [49] implements an interesting second order explicit method. TACITE illustrates a standard problem with higher order spatial differencing. These difference methods have been predominantly developed for explicit methods, but authors such as Dai and Woodward [50] have begun looking at more implicit implementations. The higher order explicit methods could be adapted to the semi-implicit schemes found in RELAP5 and RETRAN to improve the resolution of void and thermal profiles. However, analysis by Ohkawa and Tomiyama [51] of a simple model problem suggests that this would cause difficulties when coupled with RELAP's ill-

posed set of field equations. Interestingly, their work suggests that a simultaneous correction to the first-order time differencing could mitigate this problem. We recommend moving to a well-posed equation set before adapting these methods.

6. CONCLUSIONS

We have provided a list of recent work relevant to numerical simulation of two-phase. How does this relate to needs for the development of an advanced systems code? A tool like ADIFOR [7] should be adopted simply on the basis of improved efficiency and reliability. A surface tracking method should be included in any new code, because of known degradation of results when such methods are absent [8, 9].

Any Decision to implement a new equation solution method should begin at a very practical level. All code development efforts should regularly apply some software tool to determine the distribution of computational effort within typical calculations. If an unacceptable percentage of the computer time is spent in the solution of the linearized equations, then a 2-3 staff month effort should be devoted to testing a few current algorithms within the systems code. We expect that the GMRES algorithm [13] will come out at or near the top performance of sampled methods. However, sufficient uncertainty exists that testing on a "typical" problem mix is important.

When the subject turns to selection of improved numerical models for the flow equations our crystal ball becomes very cloudy. Inclusion of special provisions for discontinuities (surfaces) should make robust implementation of higher order methods simpler. We are currently focusing on methods by Leonard [43] and Smolarkiewicz [45]. However, 2 years of research by a several groups is probably necessary to identify a "best" method for this application. Beyond that time period, past experience indicates that another 1-3 years would be required for the method to mature to the highly

robust state required in a production code used to model the full range of conditions experienced in plant transients.

REFERENCES

- [1] Mahaffy, J.H., Numerics of Codes: Stability, Diffusion, Convergence, Nuclear Engineering and Design, Vol. 145 (1993) 131-145.
- [2] C. Allison (Ed.) et al., RELAP5/MOD3 Code manual, US Nuclear Regulatory Commission Report NUREG/CR-5535 (1990).
- [3] N. M. Schnurr et al., TRAC-PF1/MOD2 Theory manual, Los Alamos National Laboratory unpublished Report LA-12031-M, US Nuclear Regulatory Commission Report NUREG/CR-5673 (1992).
- [4] J. A. Borkowski (Ed.) et al., TRAC-BF1: An advanced best-estimate computer program for bwr accident analysis, Idaho National Engineering Laboratory Report EGG-2626, US Nuclear Regulatory Commission Report NUREG/CR-4356 (1992).
- [5] F. Barre, M. Parent, and B. Brun, Advanced Numerical Methods for Thermalhydraulics, CSNI Specialist Meeting on Transient Two-Phase Flow, Aix-en-Provence, France (1992).

- [6] M.P. Paulsen, J.H. McFadden, C.E. Peterson, J.A. McClure, G.C. Gose, and P.J. Jensen, The RETRAN-03 Computer Code, Nucl. Technol., 93 (1991) 105.
- [7] C. Bischof, A. Carle, P. Khademi, and A. Mauer, The ADIFOR system for the automatic differentiation of Fortran 77 Programs, Argonne Preprint ANL-MCS-P481-1194 (<http://www.cs.rice.edu/~adifor>) (1995).
- [8] Aktas, B. and J. H. Mahaffy, "Enhanced Numerical Modeling of Manometer Based Oscillations by Discontinuity Tracking", Eleventh Proceedings of Nuclear Thermal Hydraulics, ANS Winter Meeting, San Francisco (1995) 101-109.
- [9] Aktas, B. and J. H. Mahaffy, "A two-phase level tracking method", Nuclear Engineering and Design 162 (1996) 271-280.
- [10] M.R. Hestenes and E. Stiefel, Methods of conjugate gradients for solving linear system, J. of Research of the National Bureau of Standards, 49 (1952) 409-436.
- [11] P. Sonneveld, CGS, a fast Lanczos-type solver for nonsymmetric systems, SIAM J. Sci. Statist. Comput. 10 (1989) 36-52.
- [12] H.A. van der Vorst and P. Sonneveld, CGSTAB, a more smoothly converging variant of CGS, Technical Report 90-50, Delft Univ. Technology (1990).

- [13] Y. Saad and M.H. Schultz, GMRES: A generalized minimum residual algorithm for solving nonsymmetric linear systems, *SIAM J. Sci. Statist. Comput.* 7 (1986) 856-869.
- [14] A. Soria and F. Ruel, Assessment of some iterative methods for non-symmetric linear systems arising in computational fluid dynamics, *Int. J. for Num. Meth. in Fluids*, 21 (1995) 1171-1200.
- [15] C.G. Broyden, A class of methods for solving nonlinear simultaneous equations, *Math. Comput.* 19 (1965) 577-593.
- [16] P. Chin and P.A. Forsyth, A comparison of GMRES and CGSTAB accelerations for incompressible Navier-Stokes problems, *J. Comput. and App. Math.* 46 (1993) 415-426.
- [17] M.B. van Gijzen, Large scale finite element computations with GMRES-like methods on a CRAY Y-MP, *Applied Numerical Mathematics*, 19 (1995) 51-62.
- [18] E. de Sturler, and H.A. vander Vorst, Reducing the effect of global communication in GMRES(m) and CG on parallel distributed memory computers, *Applied Numerical Mathematics*, 18 (1995) 441-459.
- [19] X. Xu, N. Qin, and B.E. Richards, α -GMRES: a new parallelizable iterative solver for large sparse non-symmetric linear systems arising from CFD, *Int. J. Num. Meth. in Fluids*, 15 (1992) 613-623.

- [20] T. Skalicky, LASPack Reference Manual, Institute for Fluid Mechanics, Dresden University of Technology (<http://www.tu-dresden.de/mwism/skalicky/laspack/laspack.html>) (1995).
- [21] J.M. Hyman, Numerical methods for tracking interfaces, *Physica* 12D (1984) 396-407.
- [22] C.W. Hirt and B.D. Nichols, Volume of Fluid (VOF) method for the dynamics of free boundaries, *J. Comput. Phys.*, 39 (1981) 201-225.
- [23] D. L. Youngs, An interface tracking method for a 3D Eulerian hydrodynamics code, UK Atomic Weapons Research Establishment Report AWRE/44/92/35 (1992).
- [24] F. Mashayek and N. Ashgriz, Advection of axisymmetric interfaces by the volume-of-fluid method, *Int. J. Num. Meth. in Fluids*, 20 (1995) 1337-1361.
- [25] S. Welch, J. Trapp, and G. Mortensen, Interface tracking in two-phase flow simulations using a simple subgrid counting procedure, *Numerical Methods in Multiphase Flows, FED-Vol 185* (1994) 293-297.
- [26] W. Shyy, *Computational Modeling for Fluid Flow and Interfacial Transport*, Elsevier (1994) 372-463.
- [27] S.O. Unverdi and G. Tryggvason, A front-tracking method for viscous, incompressible, multi-fluid flows, *J. Comput. Phys.* 100 (1992) 25-37.

- [28] K. Bendiksen, D. Malnes, T. Straume, and . Hedne, A non-diffusive numerical model for transient simulation of oil-gas transportation systems, European Simulation Multiconference, Nuremburg (1990) 508-515.
- [29] E. Hustvedt, Determination of slug length distributions by use of the OLGA slug tracking model, 6th Int. Conf. on Multi Phase Production, Cannes (1993) 147-163.
- [30] M. P. Paulsen and N. Newman, A RETRAN-03 transport model for time domain analysis of BWR stability events, Proceedings of the ANS-ENS Topical Meeting on Advances in Mathematics, Computations, and Reactor Physics, Pittsburgh, PA (1991).
- [31] M.P. Paulsen, J.G. Shatford, and L.J. Agee, A nondiffusive solution method for RETRAN-03 boiling water reactor stability analysis, Nucl. Reactor Safety, 100 (1992) 162-173.
- [32] J.A. Trapp and G. Mortensen, A discrete particle model for bubble-slug two-phase flows, J. Comput Phys., 107 (1993) 363-377.
- [33] J.A. Trapp, G. Mortensen, and V.H. Ransom, Particle-fluid two phase flow modeling, ANS/ENS Topical Meeting on Advances in Mathematics, Computations and Reactor Physics, Pittsburg (1991).
- [34] C.T. Crowe, T.R. Troutt, and J.N. Chung, Numerical models for two-phase turbulent flows, Ann. Rev. of Fluid Mech., 28 (1996) 11-43.

- [35] L.D. Cloutman, An evaluation of smoothed particle hydrodynamics, *Advances in the Free-Lagrange Method*, Jackson Lake, Springer-Verlag (1990) 229-238.
- [36] J.J. Monaghan and A. Kocharyan, SPH simulation of multi-phase flow, *Computer Phys. Comm.*, 87 (1995) 225-235.
- [37] J.J. Monaghan, Simulating free surface flows with SPH, *J. Comput. Phys.*, 110 (1994) 399-406.
- [38] S. Koshizuka and Y. Oka, Moving-Particle Semi-Implicit Method for Fragmentation of Incompressible Fluid, *Nuc. Sci. and Eng.*, 123 (1996) 421-434.
- [39] B. van Leer, Towards the ultimate conservative differencing scheme, II. monotonicity and conservation combined in a second order scheme, *J. Comput. Phys.*, 14 (1974) 361-370.
- [40] S. Osher and S.R. Chakravarthy, High resolution schemes and the entropy condition, *SIAM J. Numer. Anal.*, 21 (1984) 955-984.
- [41] P.K. Sweby, High resolution schemes using flux limiters for hyperbolic conservation laws, *SIAM J. Numer. Anal.*, 21 (1984) 995-1011.

- [42] J.R. Goodman and R.J. Leveque, Accuracy of stable schemes for 2D scalar conservation laws. Corant Mathematics and Computing Lab., Dept. of Energy Report, DOE/ER/03077-203 (1983).
- [43] B.P. Leonard, The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection, *Comput. Meth. Appl. Mech. Eng.*, 88 (1991) 17-74.
- [44] B.P. Leonard and H. Niknafs, Cost-effective accurate coarse-grid method for highly convective multidimensional unsteady flow, *Proc. of the CFD Symposium on Aeropropulsion*, NASA Lewis Research Center, Cleveland (1990) 227-240.
- [45] P.K. Smolarkiewicz, A fully multidimensional positive definite advection transport algorithm with small implicit diffusion, *J. Comput. Phys.* 54 (1984) 325-362.
- [46] P.F. Peterson, A method for predicting and minimizing numerical diffusion, *Numerical Heat Transfer, Part B*, 21 (1992) 343-366.
- [47] J. Thuburn, Multidimensional flux-limited advection schemes, *J. Comput. Phys.*, 123 (1996) 74-83.
- [48] L.J. Durlofsky, A triangle based mixed finite element-finite volume technique for modeling two phase flow through porous media, *J. Comput. Phys.*, 105 (1993) 252-266.

- [49] C. Pauchon, H. Dhulesia, D. Lopez, and Jean Fabre, TACITE: A comprehensive mechanistic model for two-phase flow, 6th Int. Conf. on Multi Phase Production, Cannes (1993) 29-49.
- [50] W. Dai and P.R. Woodward, Iterative implementation of an implicit-explicit hybrid scheme for hydrodynamics, J. Comput. Phys., 124 (1996) 217-229.
- [51] T. Ohkawa and A. Tomiyama, Applicability of high-order upwind difference methods to two-fluid model: examination based on a linear model equation, Numerical Methods in Multiphase Flows, FED-Vol 185 (1994) 209-215.

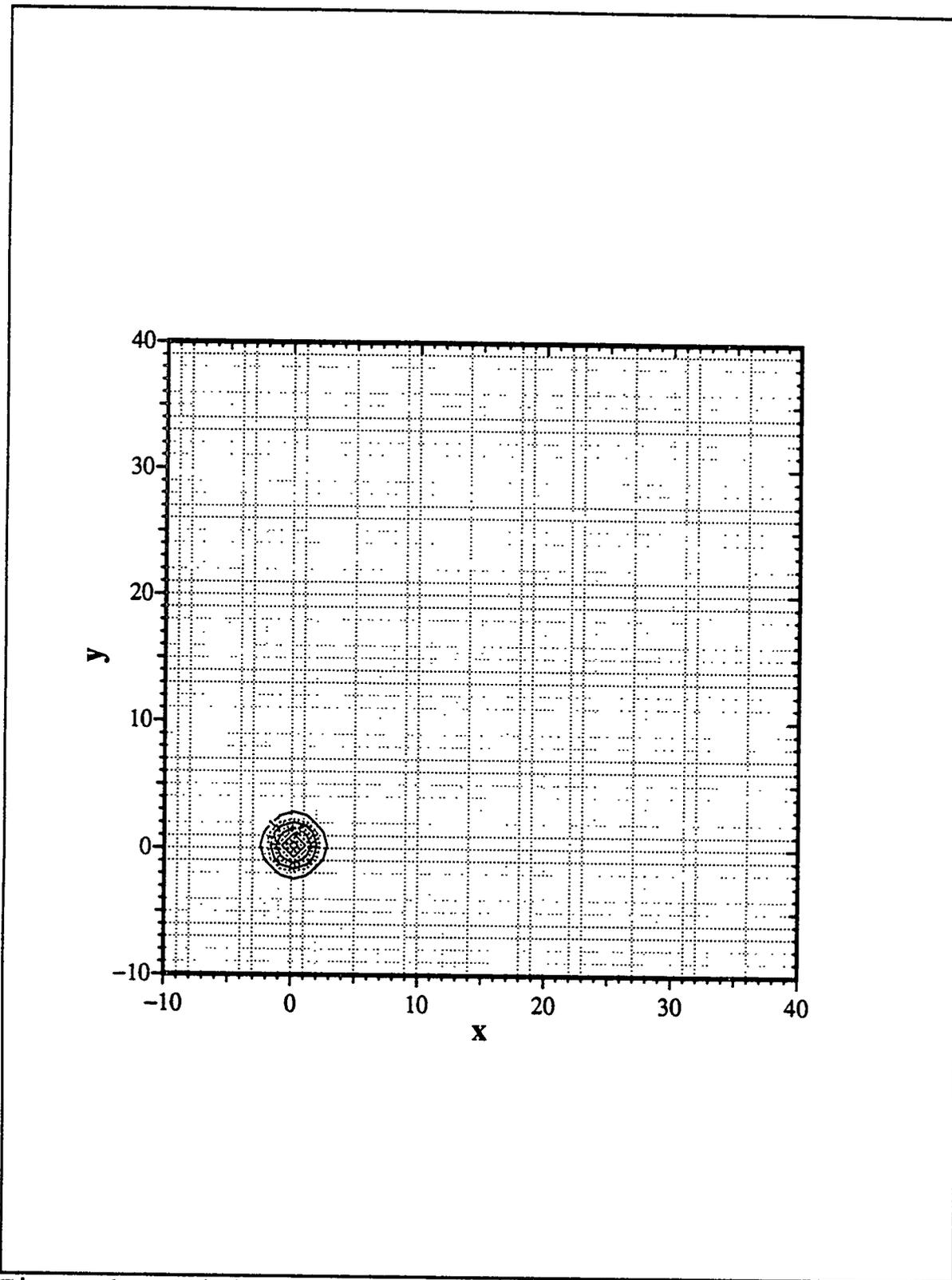
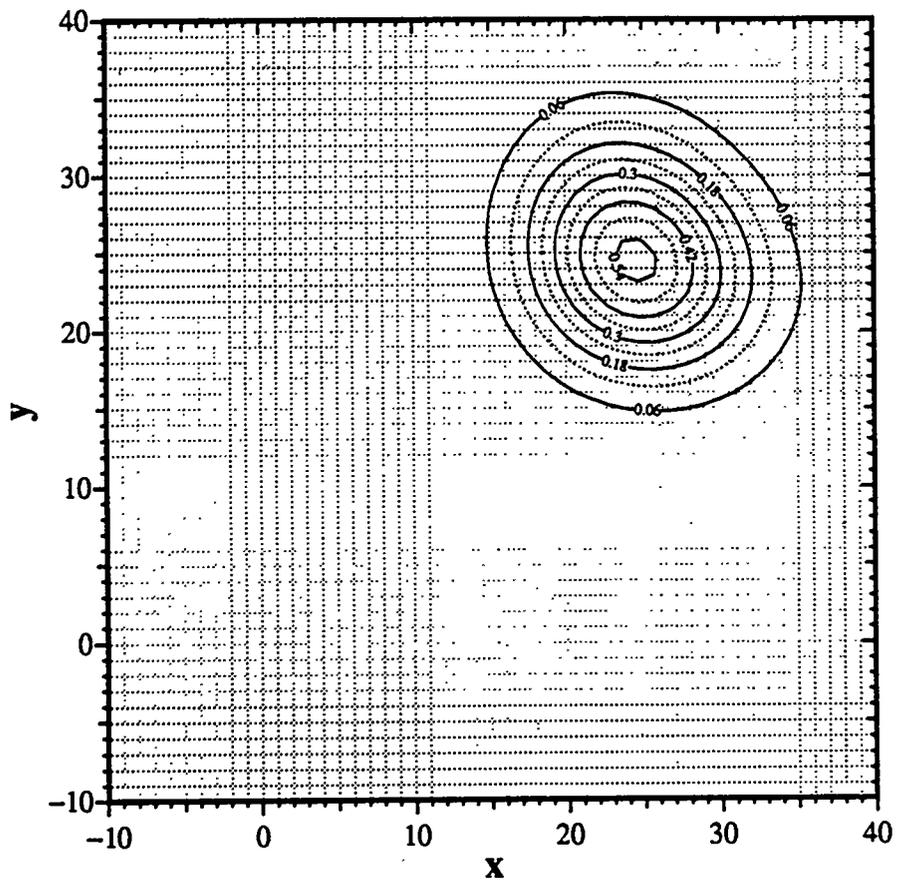


Figure 1. Initial Concentration Profile



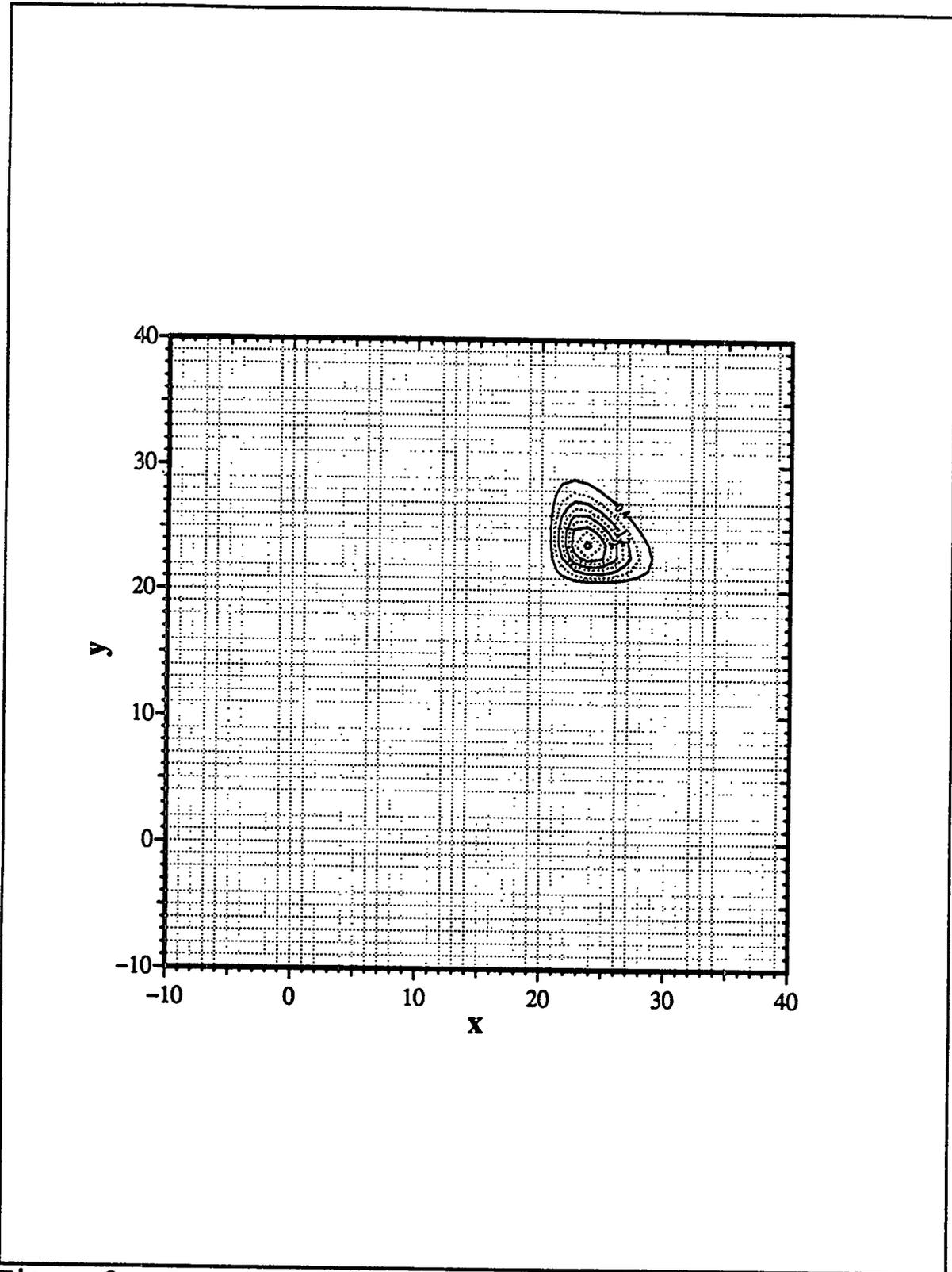


Figure 3. Pure Convection with Smolarkiewicz's Method

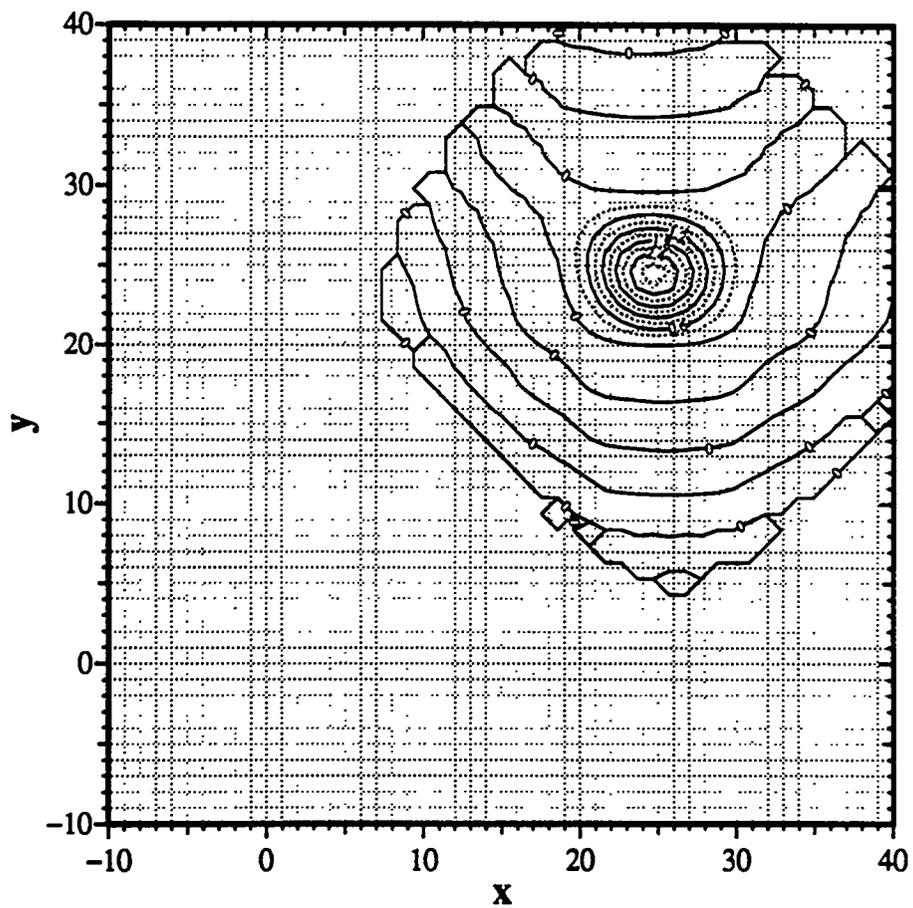


Figure 4. Pure Convection with Leonard's Method.

Figure Captions

Figure 1. Initial Concentration Profile

Figure 2. Pure Convective Transport with Upwind Difference Method

Figure 3. Pure Convection with Smolarkiewicz's Method

Figure 4. Pure Convection with Leonard's Method

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ABSTRACT

This paper presents the current and planned numerical development for improving computing performance in case of Cathare applications needing real time, like simulator applications. Cathare is a thermalhydraulic code developed by CEA (DRN), IPSN , EDF and FRAMATOME for PWR safety analysis. First, the general characteristics of the code are presented, dealing with physical models numerical topics and validation strategy. Then, the current and planned applications of Cathare in the field of simulators are discussed. Some of these applications were made in the past, using a simplified and fast-running version of Cathare (Cathare-Simu); the status of the numerical improvements obtained with Cathare-Simu is presented. The planned developments concern mainly the Simulator Cathare Release (SCAR) project which deals with the use of the most recent

version of Cathare inside simulators. In this frame, the numerical developments are related with the speed up of the calculation process, using parallel processing and improvement of code reliability on a large set of NPP transients.

1 INTRODUCTION

This paper presents the current and planned numerical development for improving computing performance in case of Cathare applications needing real time computing; an example of these applications are simulator applications. Cathare is a thermalhydraulic code developed by CEA (DRN), IPSN, EDF and FRAMATOME for PWR safety analysis.

First, the general characteristics of the code are presented, dealing with physical models numerical topics and validation strategy. The main characteristics of the code will be shortly described. In particular, the fully implicit scheme, used since the beginning of Cathare development, allows potentially large time steps in case of long duration transients.

Then, the current applications of Cathare in the field of simulators are discussed. This need was arising very soon during the Cathare development and some of these applications were made in the past, using a simplified and fast-running version of Cathare (Cathare-Simu); the status of the numerical improvement obtained with Cathare-Simu is presented.

Finally, the planned developments are presented; they concern mainly the Simulator Cathare Release (SCAR) project which deals with the use of the last version of Cathare inside simulators. In this frame, the numerical developments are related with the speed up of the calculation process, using parallel processing and improvement of code reliability on a large set of NPP transients.

2 MAIN CHARACTERISTICS OF THE CATHARE CODE

2.1 Code structure

The code has a *modular structure*. Several modules can be assembled to represent the primary and secondary circuits of any PWR or of any analytical test or system test facility. There are 0-D, 1-D, 2-D, and 3-D modules available. All modules can be connected to walls, or heat exchangers with a 1-D conduction calculation. A 2-D conduction calculation is also available to calculate the quenching of a hot core during a reflooding process. Many submodules are available to calculate the neutronics, the fuel thermomechanics, pump characteristics, accumulators, sources, sinks...

This structure allows to model a large variety of NPP circuits (primary, secondary or auxiliary circuits as RHRS). Using the submodules, it is also possible to connect these main circuits with other NPP systems.

2.2 Physical models

All modules use the *2-Fluid model* to describe steam-water flows and four noncondensable gases may be transported. The thermal and mechanical nonequilibrium are described. All kinds of two-phase flow patterns - bubbly flow, slug flow, churn flow, annular

flow, annular-mist flow, stratified flow - are modeled. Co-current and counter-current flow are modeled with prediction of the counter-current flow limitation (CCFL). Heat transfers with wall structures and with fuel rods are calculated taking into account all heat transfer processes, such as natural and forced convection with liquid, subcooled and saturated nucleate boiling, critical heat flux, film boiling, natural and forced convection with gas, film condensation,...The interfacial heat and mass transfers describe not only the vaporization due to superheated steam and the direct contact condensation due to subcooled liquid, but also the steam condensation or liquid flashing due to metastable subcooled steam or superheated liquid. The effects of noncondensable gases, such as nitrogen, air, hydrogen, are described.

The *range of parameters* is rather large: pressure from 0.1 to 16 MPa, liquid temperature from 20°C to 350°C, gas temperature from 20°C to 1800°C, fluid velocities up to supersonic conditions, duct hydraulic diameters from 0.01 to 0.75 meter.

Mass, momentum, and energy balance equations are written for each phase. Balance equations are also written for the radioactivity and for the mass of each noncondensable gas and of boron.

An important experimental program was carried out as a support for the development and validation of the code.

2.3 Numerics

All Cathare modules, except the 3-D module, use a fully implicit time discretization. This means that the interphase exchange, the pressure propagation and the convection terms are totally implicitly evaluated.

This choice has been done since the beginning of Cathare development in 1979, and has been confirmed before developing the more recent version of Cathare during a market research stage. The purpose is, of course, to achieve the largest time step possible without CFL limit, in particular for long duration transients.

The solution of the non-linear difference equation system is given by a full Newton iterative method.

2.4 Cathare status

The code development distinguishes code Versions and code Revisions. A code Version is an ensemble of modules able to represent reactor components, with a numerical scheme and a solution procedure. A new Version may extend the code capabilities, may add new modules, may change the code architecture or optimize the solution procedure. A Revision is a package of physical closure relationships.

At present, the Version C2 V1.3U contains the revision 5 which is fully assessed. The Version C2 V1.3L contains the revision 5 with some improvements about the Reflood Modeling. The Version C2 V1.4 is delivered only to French users and contains the Revision 5. It has a completely new code architecture, a 3-D module which may be used for the pressure vessel or for the containment. It has also the Discrete Adjoint Sensitivity method, implemented for uncertainty evaluation. The Version V1.4E will be available to other users in autumn 96. The Revision 6 is now defined and will be implemented in the V1.5 Version.

3 CURRENT APPLICATION OF CATHARE TO THE SIMULATORS

3.1 Main purposes

Very early during Cathare development stage, in 1981, the need to implement Cathare models inside training or engineering simulator was arising. The main objective of this work was to benefit of a high level of two phase flow modeling for plant operator or safety staff training.

To achieve this purpose, the requested simulation scope to be covered by Cathare were defined to the primary and the secondary circuits (including main steam lines), with a simulation field including about 40 normal, incidental or accidental transients (up to a 12 inch cold leg break).

After a feasibility study stage, a simplified version of Cathare, named Cathare-Simu, was developed. All these developments were verified against original Cathare calculations for all transients inside the simulation field.

3.2 Cathare-Simu characteristics

The first version of Cathare-Simu, available in 1986, was including :

- a 2-Fluid 6-equation model on *primary side* with some simplifications of the original Cathare correlation set (validated for SBLOCA or transients),
- a 3-equation model on secondary side, also available, at this time in the reference Cathare version,
- the same numerical scheme with fully implicit time discretization as Cathare,
- an improvement of the reliability by an enhancement of physical laws continuity,
- an improvement of the computation speed by an optimization of the data management and an efficient coding on vector processors.

A large amount of work was made to analyze the reasons of convergence failure of Cathare Newton's method during the actual NPP transients and to try to avoid them in using a better formulation of the equation or correlation set. These improvements concern mainly the calculation of the derivatives and the continuity of the transitions between the different correlations.

Cathare-Simu has been implemented since 1991 in the SIPA simulator [6]. It allows operator training or engineering studies with real time interactive simulation for a wide set of transients.

3.3 Recent developments for Cathare-Simu

Cathare-Simu has been recently improved in adding a Drift Flux model to the secondary side 3-equation model and in developing a multi-processor version which allows to decrease the cycle time of the simulator to 100 milli-seconds.

New NPP models based on Cathare-Simu have been defined, validated and used for the new generation of simulators (SIPA or fullscope).

4 PLANNED NUMERICAL DEVELOPMENTS

4.1 Main objectives of the SCAR project

A second stage of Cathare application to simulators is now under way ; it deals with the Simulator CATHARE Release (SCAR) project, whose purpose is to insert standard Cathare models inside engineering or training simulators without any simplification of the original model as it was the case for Cathare-Simu.

This project starts on the basis of the last version of Cathare (V1.4E) and is planned in three main directions:

- 1) implementation of standard Cathare models for several PWR inside SIPA simulator configurations and tests with simulator environment,
- 2) speed up of calculation process, using parallel processing, and improvement of reliability, in particular for low pressure transients,
- 3) development of some additional models needed to achieve an extensive description by Cathare of primary, secondary and auxiliary circuits.

All this work will be validated by a wide set (about 40) of actual NPP transient tests, will be made in close relationship with next CATHARE version (V1.5) development and will benefit consequently of the extensive validation program of CATHARE.

The final objective of the SCAR project is to allow an easy implementation of CATHARE models inside simulators and so, to ensure a maximum level of confidence and flexibility of the simulator software.

Therefore the convergence of safety codes used for safety analysis and for operator or safety staff training will be achieved. The result of the SCAR project will be a unique version of CATHARE inside and outside simulators.

4.2 Improving the elementary calculation time

As it was mentioned in section 2, the solving of one time step of Cathare is done by performing Newton Raphson iterations up to system convergence. This iteration process involves several phases which are systematic at **each iteration** :

(i) for each element constituting the circuit :

- calculation of the water-steam properties and of the physical correlations,
- discretization of the equations and definition of the Jacobian linear system,
- elimination of the internal variables of the element (linear algebra),

(ii) for the circuit as a whole :

- assembling of the « transfer matrix » given by each element,
- solving of the linear system at the element junctions ,

(iii) for each element constituting the circuit :

- calculation of the internal variable increments as a function of the junction increments,
- convergence criteria on the variable increments.

It is obvious that the number of operations and so the CPU time for a Cathare calculation is mainly depending on the iteration number which is, at first approximation, a linear function of the total number of meshes.

The *elementary time* for a Cathare calculation is defined as the CPU time (or elapsed time for a dedicated machine) by iteration and by mesh. This elementary time is approximately independent on the transient, and on the circuit, but depends only on the computer.

The decrease of the elementary time is obviously a good way to achieve real time calculations. This can be obtained by optimization of the most costly routines (for Cathare they are mainly the linear algebra routines) but also by using parallel processing on multi-processor computers.

Due to the modular structure of Cathare it is quite easy to distribute the work to be done for each element (steps (i) and (iii) before) of the circuit between different processors and thus to decrease the elementary time. A preliminary parallel version of Cathare V1.4, using a message passing library (PVM), has shown a speed up of about 4 when using 5 processors, without particular effort to achieve load balancing.

4.3 Improving the code reliability

An other way to reduce the computing time is of course to decrease the number of iteration needed by simulated time step. This can be done in improving the code reliability and avoiding the convergence failures.

This work is planned in the frame of the SCAR project with a particular attention to the physical correlations which will be analyzed in detail in order to achieve their continuity. Only the numerical discontinuities of the physical functions or derivatives will be corrected at this stage ; so, the Cathare validation process will be preserved.

A very large set of transient tests will be analyzed, in particular tests at low pressure with or without noncondensables, to understand and to correct the causes of high number of iterations.

It is obvious that for some transients, a very large amount of calculation time can be saved by this way. This can give locally a very significant speed up of the code (one order of magnitude greater than optimization).

5 CONCLUSIONS

The application of an advanced safety code, as Cathare, to the training or engineering simulators is of prime importance because this allows to associate the high level of thermalhydraulics modeling to the powerful environment and graphical user interface of the simulator.

To ensure a good level of friendliness of the simulator, it is obviously necessary to run the code in real time, and thus to improve its computing performance. This objective has been reached with the Cathare-Simu software which allows today to run real-time Cathare simulations with a cycle time less than 100 milli-seconds.

This work will be extended, in the frame of the SCAR project, to the last version of Cathare and will consist in development of parallel processing and improvement of the code reliability. The preliminary stage to this project which is now under way, has demonstrated the capability of Cathare to benefit in multi-processor computers.

References:

[1] F. BARRE and M. BERNARD "The CATHARE code strategy and assessment" Nuclear Engineering and Design 124(1990) 257-284

[2] J.M. DELHAYE , M. GIOT , M.L. RIETHMULLER "Thermohydraulics of two-phase Systems for Industrial design and Nuclear Engineering" ,McGraw-Hill Book Company, Hemisphere Publishing Corporation

[3] D. BESTION " The physical closure laws in the CATHARE code " , Nuclear Engineering and Design 124(1990) 229-245

[4] M.BERNARD, L.C.BERNARD, J.C.MICAELLI, P.VAN DEN HOVE, " The new modules of Cathare and their specific assessment " , NURETH 4, 1989, Karlsruhe, Germany, SETH/LEML-EM/89-164,

[5] F. BARRE, P.BOUDIER, M.PARENT, V.FIGEROU, M.FLORES, D.KADRI, "New developments in the Cathare 2 code", NURETH 6, 1993, Grenoble, France, STR/LML-EM/94-210

[6] J.COHEN, Ph.CORDEL, F.POIZAT, A.SEKRI, J.M.BERNARD, J.P.KIRCHGESSNER, " SIPA: an advanced project for nuclear accident simulators", CRAY Channels (Spring 1989), 12-15

[7] E.GUINARD, G.HOUDAYER, F.POIZAT, " SIPA-SWORD: a configurable simulator for safety", ENS East-West Topical Meeting, 1992, Prague, Czechoslovakia

**TECHNICAL SESSION 4: PROGRAMMING LANGUAGE AND
A CODE ARCHITECTURE'S AND USER INTERFACES**

Co-Chair: Dr. Vantolla (Finland), Dr. Naitoh (Japan)

**OECD / CSNI WORKSHOP
ON TRANSIENT THERMALHYDRAULIC
AND NEUTRONIC CODES REQUIREMENTS**

Annapolis, Md., USA

5th-8th November 1996

Hosted by

U.S. Nuclear Regulatory Commission

**Current implementation and future plans on new code architecture,
programming language and user interface**

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1. ABSTRACT

Computer technology has improved tremendously during the last years with larger media capacity, memory and more computational power. Visual computing with high-performance graphic interface and desktop computational power have changed the way engineers accomplish everyday tasks, development and safety studies analysis. The emergence of parallel computing will permit simulation over a larger domain. In addition, new development methods, languages and tools appeared the last years.

2. INTRODUCTION

Thermalhydraulic codes, such as CATHARE, have continuously matured during the past 20 years, with new computers technologies and higher demands from the security and regulatory committee, the electricity contractors and the research centres.

Computer technology has improved tremendously during the last years with larger media capacity, memory and more computational power. Visual computing with high-performance graphic interface and desktop computational power have changed the way engineers accomplish everyday tasks, development and safety studies analysis. The emergence of parallel computing will permit simulation over a larger domain. In addition, new development methods, languages and tools appeared the last years.

During the same period, the TMI and Tchernobyl accidents and a better understanding have modified the concern of the development and safety analysis engineers. First safety studies were concerned with dimensional analysis such as a large break LOCA. After the TMI accident, the small break LOCA and Steam Generator Tube Rupture (SGTR) type accidents were intensively studied. Recently engineers have focused their efforts on both severe accidents and residual heat removal from a reactor in shutdown condition. These new accident types have modified the simulated time from several minutes (large break LOCA) up to several days (reactor at shutdown)

Computer technology will continue to change rapidly, especially network and parallel supercomputing. The network is becoming a major component of our computerized world and the supercomputing will permit fine scale multidimensional simulations in large system codes.

Higher demands from the users are expected, and apart from new accident type studies we anticipate several objectives in various domains.

- Adapting the study analysis computer codes to real time computing in order to benefit from the study codes physics in the simulators, but also to lower maintenance and development costs.
- Extending the calculation domain to take into account some critical parts of the plant that may initiate accidents such as Residual Heat Removal System (RHRS) from a reactor in shutdown condition.
- Coupling with other codes to benefit from the finest physics developments in all the fields, such neutronic, mechanic, etc.
- Extending the code capability to study existing VVER, RBMK type reactors but also to design and/or study new generation type reactors such as the EPR (France and Germany joint venture), the American AP600 or the new fusion type reactor (ITER).

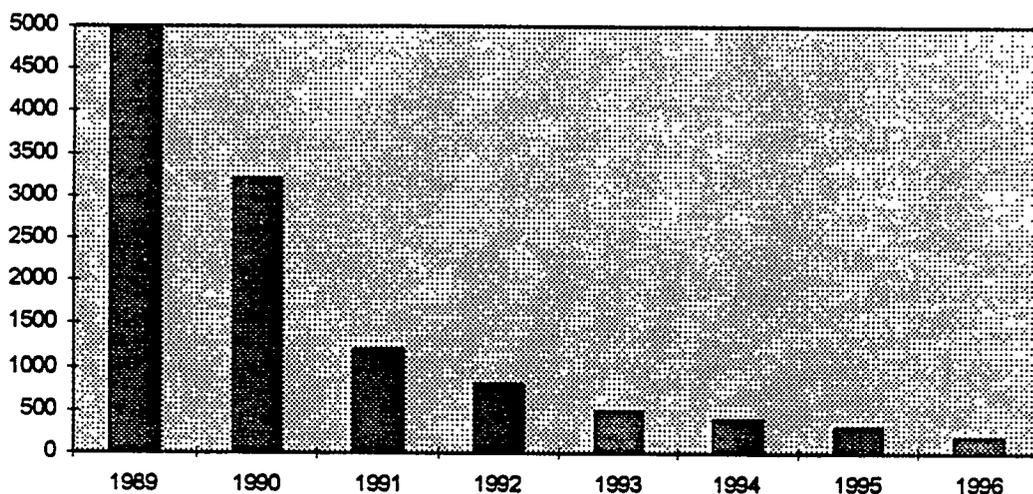
These objectives will require new computational tools, such as parallel computing and algorithm modifications to achieve real time computation over a large calculation domain.

3. AN IMPOSSIBLE CHALLENGE

Defining a new computational tool architecture is not an easy task, neither is the choice of a development method or programming language. The self dynamic and large computing field makes the choices difficult. Computing power doubles every 18 months and this trend is not going to stop before many years [fig. 1]. The architecture of computers is deeply given causes some all 5 years, this evolution is going to accelerate with the emergence of massively parallel machines, heterogeneous clusters, high speed networks, but especially under the effect

of the generalization of object technology. On the other hand the duration of code life is in constant increase. The RELAP, TRAC or CATHARE codes have been used for twenty years or more. The analysis of time constants specific to each area of the computer technology shows, paradoxically, that computer codes are the most stable elements. If they are not regularly updated, they can not exploit efficiently the new computer technologies and become rapidly obsolete. In France the CATHARE code is largely rewritten each 5 years, this effort makes the codes more robust, reliable, flexible, and easy to use.

In this paper attention will be focused on different aspects of the programming technology. First parallelism and coupling will be briefly discussed. In the second part, programming methods will be presented. The last part will be devoted to the user interface.



[fig 1] Evolution of the CPU time needed for a 6 inches break CATHARE calculation (sec/year)

4. PARALLEL PROCESSING

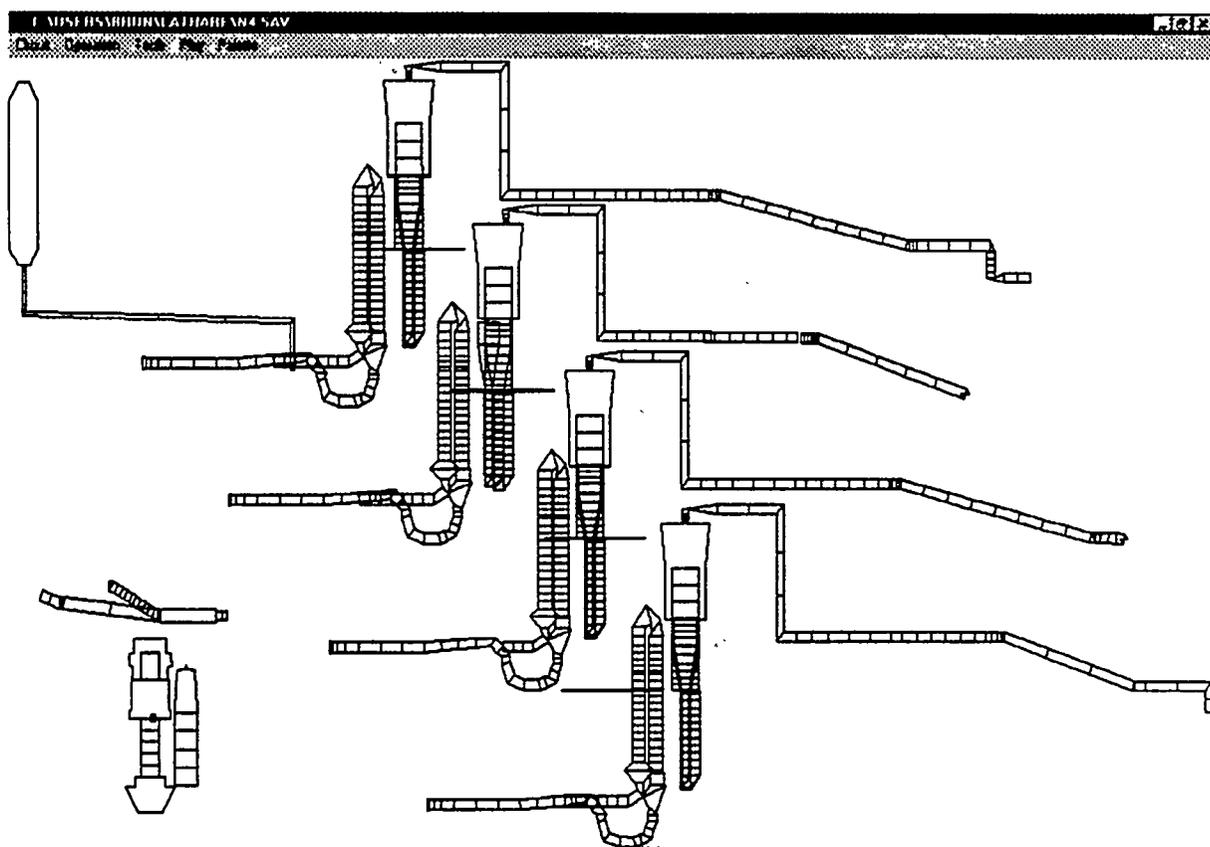
« A saying among some scientific programmers is that they have spent 10 years vectorizing their programs, and that they are not going to spend another 10 years parallelizing them ». Other scientific programmers complain that architecture dependencies and difficult correctness verification, make parallel programming impracticable. These barriers cast doubt on the practicality of parallel programming, despite its potential benefits. New current programming methods were now available to alleviate the frustrations of parallel programming.

There are essentially two programming methods : in one of them, it is the responsibility of the programmer to specify which parts of the program may be executed in parallel. In the second method, this task is left to the compiler.

The main objective, of the first solution, is to hide from the user the exact architecture of the computer on which his program is to be executed. The idea is that knowledge about the computer should be confined to the compiler, the user being responsible only for his algorithm.

It is very tempting to be able to develop a new application sequentially, with the help of a host environments and tools, and then, and only then, to have a compiler construct a guaranteed parallel version.

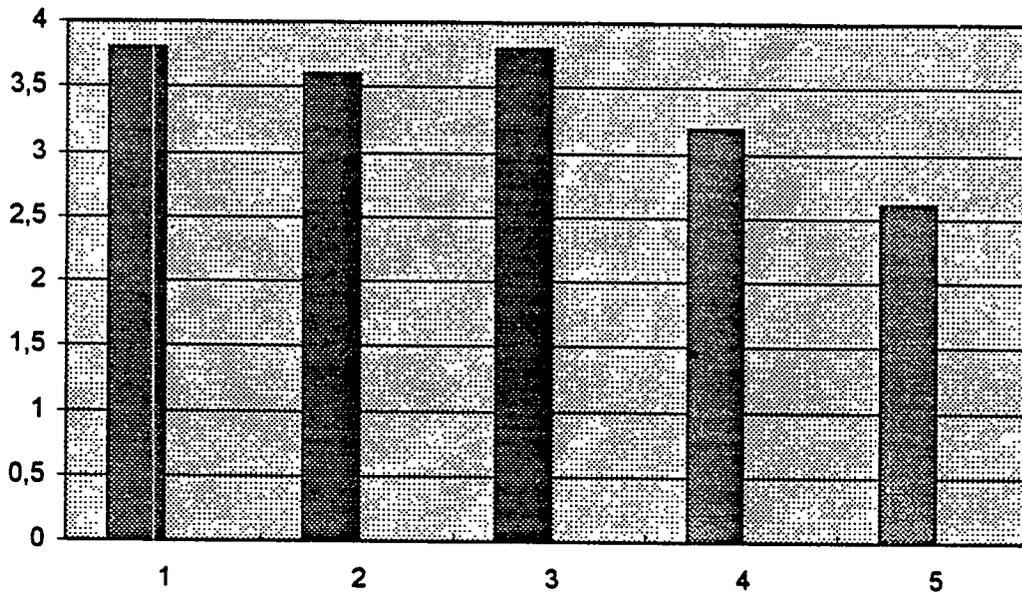
In the second solution, one may use classical sequential languages like Fortran, or C++ in which the sequencing is not specified. This method is used when the needed parallelism cannot be found without help from the programmer, since interactions between different stages of a program are difficult to detect (while the author of the program is aware of them, at least in an intuitive fashion). This solution has led to the development of low level programming languages in which a sequential basis is augmented by parallel constructs. The code can be used on shared (SMP) or distributed memory architectures (MPP) as well as across networks which may be heterogeneous (clustering). Well known examples are PVM or MPI. This solution is used in the very new version of the CATHARE code. The basic paradigm of programming, used in the CATHARE code, is a Data Parallelism approach based on a domain decomposition method. The initial circuit is splitted in P sub-domains, where P is the number of available processors, then each sub-domain is distributed to each processor. The fig. 2 illustrates a typical decomposition, using 5 processors, for a 4 loops calculation. Encouraging efficiency, in term of speed up, is shown fig 3 for different parallel computers.



[fig 2] Example of domain decomposition for a CATHARE calculation. 5 processors are used :
for the vessel

- . for the broken loop (with the pressurizer)
- . for the three intact loops

Due to the modular structure of CATHARE it is quite easy to distribute the work to be done for each element of circuit between different processors and thus decrease the elementary time. A preliminary parallel version of CATHARE V1.4, using a message passing library (PVM), has shown a speed up of about 4 using 5 processors, without particular effort to achieve load balancing . In future versions to ensure that the code is not limited by architectural considerations, we will use the MPI standard to achieve portability to variety of computational platforms.



[fig 3] Speed up of CATHARE calculation. 5 processors are used.

- 1) CONVEX SPP1000
- 2) POWER CHALLENGE SGI R8000-75MHz
- 3) POWER CHALLENGE SGI R10000-200MHz
- 4) DEC ALPHA 300 MHz
- 5) CRAY C98

The two methods are often simultaneously used in computations involving a variety of granularities, ranging from fine-grain parallelism with frequent synchronization between small threads to coarse-grain parallelism with sparse synchronization between large, distributed processes.

5. CODES COUPLING

Numerical codes evolve without ceasing, we have to allow them to communicate between them to avoid a proliferation of tools that are independent and that are in fact only short term solutions.

The more recent CATHARE Users Club meetings (CUC) show clearly that the application field of CATHARE has been considerably enlarged. For several applications, it is necessary to use the code not only in a standalone mode, but also in cooperation with other system codes (i.e. neutronic, fuel, mechanic, SFD, containment, etc.)

This capability of coupling with other codes is particularly improved in the last version of CATHARE. Which allows an easy access to the main data structures. It has been demonstrated that a very small part of CATHARE is modified to achieve the data exchanges with other codes. Most of the applications developed up to now use as coupling package the message passing library (PVM). The major advantage of this tool is to be available on almost all workstations or multiprocessor servers. In the future it is planned to use some normalized and standard tools as CORBA 2 or OLE 2 for coupling purpose.

6. PROGRAMMING METHODS

Software project must be subject to the rigorous design, development, and testing cycle of the engineering disciplines, ignoring this cycle is responsible for most unsuccessful software projects. Software project is studied by dividing tasks into activities associated with the classic life cycle paradigm for software engineering.

6.1.1 Object Oriented application Development

One has assisted, simultaneously to an overproduction of non reusable codes and to a strong increase of development and maintenance costs.

The multiple benefits of the object in term of quality, maintenance, extensibility, reusability, reduction of unfolding costs, etc. are now undisputed. For these reasons object technology makes today passage figure obliged. The question no longer is to know if it is necessary to use the object approach but rather when and how.

The conduct of an object oriented project is more supple than that a traditional project. It will be for example possible to reverberate changes of specifications in belated phases of the development, due to the fact of the modularity of applications and the independence of objects by report to others.

It invites nevertheless to be prudent, projects developed by object technology demand a rigor far more important than with traditional methods, thus to see the object approach as a means to low costs of developments would be a major error.

6.1.2 Methods

In this recent domain difficulties are linked to the great number of available methods (Booch, CR (Class Relation Method), OMT (Object Modeling Technique), Shlaer-Mellor, etc.) and to complex terminologies. The problem of the object technology is due to the fact that it does not

lean on a unique reference model. The convergence of methods is under way, already committed with the OMT and Book methods, the movement will continue under the impetus of the OMG (Object Management Group).

The OMT method, used by more of half of the market, has become, today, a standard. Its convergence with the Block's method is going again to amplify the tendency.

6.1.3 Life cycle

At the present time different approaches are available. Up to now the RAD method is our favorite. The RAD substitutes to the traditional linear sequence of the different phases of the cycle in V a cycle in spiral, each iteration leads to the creation of a prototype submissive to the critic of users, and the process of development unfolds thus by successive refinements. Modularization and parallelisation of tasks become an essential stake.

6.1.4 Programming language

A large number of programming languages are today available, but in scientific area the set of language is limited to Fortran 90 and C++.

Fortran 90 is a true structured language it improves possibility of modular programming of preceding versions, adds the possibility of array manipulation that are well adapted to the parallel and vectorial calculation. It has dynamic management possibilities of memory and benefits from possibilities traditionally reserved to an oriented object language, notably polymorphism and genericity. Fortran 90 support for the FORTRAN 66/77 language specification standards. But Fortran 90 is also a completely new language needing an effort of teaching comparable to the effort needed by C++. Fortran 90, without inheritance capability, is not really an object language.

The C++ revolution has swept oriented object languages academically correct but commercially without success. The richness of C++ is reflected in its suitability to a wide spectrum of applications. These features (especially generic classes and inheritance mechanisms) promote the reuse of code, structure, and verification arguments. This reuse is especially important and useful for new codes development.

For our very new development TRIO_U (3D code for very fine physic) we use an object methodology (OMT) and an object language (C++). The previous version, in FORTRAN 77, was completely rewritten in C++, a posteriori we think that we did not spend more time than in keeping FORTRAN language. Contrarily to false ideas, unfortunately prevalent, C++ is as efficient as Fortran, and its portability has been verified.

An other revolution is under way around JAVA, an oriented object language better than C++ on the theoretical plan.

Whatever the language, the source code must meet open standards for ease of modification and clarity. There should be automatic procedures to verify the adherence of code to the standards. A code style should exist in the documentation for specifying the rules of coding.

6.1.5 Development environment

The development environment enhances productivity by simplifying the tasks software developers do most often : editing, compiling, debugging, and maintaining applications.

The development environment should promote the sharing and reuse of code by all the developers by procedures which make code available to all by coding and documentation standards which enhance the speed with which the knowledge embedded in the code can be understood by others.

The code library must have a well defined and logical structure for both the development and production versions of the code. A document specifying in detail the structure of the library must exist. Each package library should have three identically structured branches of the library signifying three levels of code stability. There should be, a development branch where the day to day development of the code occurs, a public branch, where the code is running, usable and stable for a long period of time, a production branch, where the code is used for production analysis. Rules for migration of code from branch of the library to the next and verification procedures should be specified in the documentation

A source code management system must be provided so that many contributors to the software development can work in a cohesive way without interfering with each other. The code management system should be robust enough so that the library is not damaged in an irreversible way by all the users contributing to the library. All versions should be archived, previous versions must be quickly recoverable. The code management system should be usable locally at the central site and remotely at other developments sites.

Each steps in the code development should have automatic consistency checks to minimize the numbers of errors discovered at execution time.

6.1.6 Quality and metrics

The use of metrics is based on the idea that we cannot manage something that we cannot measure. Software development has long been considered impossible to measure. For a new version of T/H and neutronic code usable for industry and safety studies it is time to take the software process into better control.

Metrics are measurable data points concerning the software process such as :

- The size of the software in terms of lines of code
- The complexity of the software in terms of its control structure
- The portability of the software in terms of its dependence of some hardware,
- The schedule of some activity
- The amount of work needed to achieve some milestone
- The feedback from software testers about the effectiveness of the integration testing environment
- The time needed to assemble a user-specific software

Unfortunately all components of the quality vector are not measurable.

Some technique, as the Goal/Question/Metrics method GQM, has been successfully applied in industrial software development. The method is based on a simple process by which the software and quality engineers and managers first define the goals that the software process and its products must achieve, then refine the goals into a set of questions to be answered, and finally identify the metrics that must be provided to be able to answer the questions. During this process Participation of the software development team members is essential during the process.

Different types of analysis techniques can be used during the prestudy, for example such internationally well known software process assessment techniques as CMM and Spice.

6.1.7 Code documentation

To facilitate use, online documentation will be provided in the form of technical reports, journal articles, and man pages for all algorithms and routines developed as a part of the project. Special attention will be paid to the programming features supporting abstraction and object-oriented programming. The documentation will be available in both form : the printed and the WWW versions. These documents will be simultaneously published.

6.1.8 Portability

Our recommendation is to have a fully portable version, in accordance with current standards in software quality assurance, in order to be sure, that all users use the same version (unique source package) and that all users obtained the same results whatever the computers used.

6.1.9 Data base & code validation

The validation of the code is the most important phase of the development, well led it asserts the confidence of users in results and participates in the use of the code and finally to its distribution. This phase will necessitate the use of very numerous experimental results. The validation will be able to be led efficiently only if these experimental data are easily accessible. The existence of a centralized and unique database, close to the programmers, or reachable by the network, will greatly improve the quality of the work.

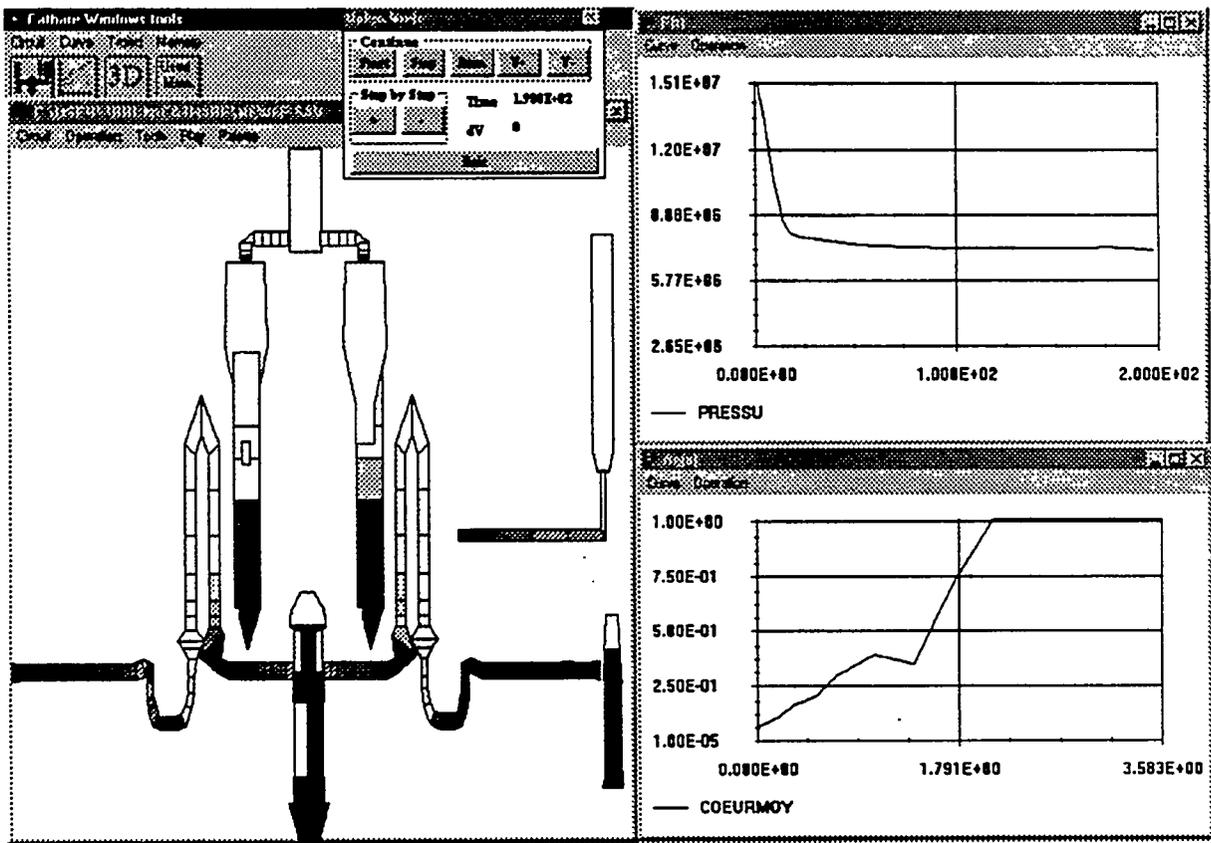
6.1.10 Team location

It has been considered, in France, of prime importance to assemble in a unique team, physical development, numerical development, assessment and maintenance, with a continued existence, allowing a full expertise on the whole problem.

7. USER INTERFACE

7.1.1 Present state

Several tools are currently available with comparable possibilities : multiple windows, schematic circuit representation with sometimes editing and control data possibilities, result animation and curves drawing (A typical view of the current CATHARE GUI is given fig. 4). These tools are not largely distributed, and finally they are little used. It should be very instructive to understand why these tools are not used.



[4] Typical view of the current CATHARE GUI

7.1.2 Future state

Main stages of a calculation are the same whatever is the user :

- preparation of data,
- calculation,
- extraction of results,
- analysis of results,

- writing of reports.

This process is not exclusively sequential and some iterations are necessary to perform a study.

The challenge is to design Graphical User Interfaces that could help the user during all stages of its studies and not only during the phase of result exploitation, as it is often the case today. In particular a GUI must provide complete online documentation to minimize user errors, and produce analysis results quickly. Special effort must be done concerning the user guidelines in order to limit the user effect.

The GUIs must be capable of implementation on a wide range of hardware and operating systems. The respect of standards is, here again, very important if one wants be able to insure the portability of the product. The code must meet critical industry standards, especially those set by X/Open and POSIX. Microsoft Windows workstations must be supported and provide a GUI alternative to X-windows. We want user to be able to select the hardware, operating system, database and user interface that suits him best. So we have to design software to be truly Open.

Future applications will thus demand that interface design goes well beyond graphical representations and interactive dialogues. A new generation GUI will be related to the training of users codes. The objective will be to enhance the communication between code users and developers by providing a user friendly access to all the multimedia documentation which can help the end users to understand the physical basis of the equipment modeling and to better interpret the results and validate the code. This include a data base of theoretical courses, but also videos of specially designed experiments which are aimed at visualizing the basic phenomena, etc.

8. CONCLUSION :

Defining a new computational tool architecture is a very hard challenge, but faced to the needs of nuclear physicists and to the tremendous improvement of the computer technology it's perhaps time to extend the thermalhydraulic code capabilities. Short and medium term objectives are now clearly defined in France around the CATHARE and SCAR projects. These programs would be discussed in other presentations by D. Bestion, F. Barre and B. Faydide. For long term objectives important activities will be devoted to fine scale multidimensional simulations. The emergence of, massively parallel computing, new languages, high speed network, will permit, undoubtedly, to reach this goal. These research activities could be a good field for an international cooperation.

Parallelization and Automatic Data Distribution for Nuclear Reactor Simulations

by Lorie M. Liebrock

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Abstract

Detailed attempts at realistic nuclear reactor simulations currently take many times real time to execute on high performance workstations. Even the fastest sequential machine can not run these simulations fast enough to ensure that the best corrective measure is used during a nuclear accident to prevent a minor malfunction from becoming a major catastrophe. Since sequential computers have nearly reached the speed of light barrier, these simulations will have to be run in parallel to make significant improvements in speed. In physical reactor plants, parallelism abounds. Fluids flow, controls change, and reactions occur in parallel with only adjacent components directly affecting each other. These do not occur in the sequentialized manner, with global instantaneous effects, that is often used in simulators. Development of parallel algorithms that more closely approximate the real-world operation of a reactor may, in addition to speeding up the simulations, actually improve the accuracy and reliability of the predictions generated.

Three types of parallel architecture (shared memory machines, distributed memory multicomputers, and distributed networks) are briefly reviewed as targets for parallelization of nuclear reactor simulation. Various parallelization models (loop-based model, shared memory model, functional model, data parallel model, and a combined functional and data parallel model) are discussed along with their advantages and disadvantages for nuclear reactor simulation. A variety of tools are introduced in Appendices for each of the models. Emphasis is placed on the data parallel model as the primary focus for two-phase flow simulation. Tools to support data parallel programming for multiple component applications and special parallelization considerations are also discussed.

Pilot code development is recommended to explore reactor simulation parallelization using data parallelism, possibly with the addition of some functional parallelism. In particular, the use of High Performance Fortran with an automatic data distribution and transformation system, is recommended.

Introduction

Nuclear reactor simulations are computationally intensive. Simulations of the Westinghouse design for the AP600 have taken as much as 40 times real time. This makes it extremely expensive to run the simulations needed to validate specific design criteria, e.g., the requirement that the reactor can run for three days without human intervention.

Sequential machines near the speed of light barrier. Electrical impulses can not move faster than the speed of light, at about one foot in one nanosecond (10^{-9} seconds). Speed increased in the past through miniaturization, but current supercomputers near the limit of such miniaturization. If electricity can't go faster and the wires can't be shorter, then higher performance must be achieved by running in parallel.

In physical reality, parallelism abounds. Fluids flow, controls change, and reactions occur in parallel with only local interactions. Currently, most reactor simulations run in a sequential manner. Often these simulations exhibit unphysical or physically impossible global instantaneous effects due to the models used to represent the physical reactor. As modelling is revisited with parallelism in mind, advances in understanding in areas such as two-phase flow may improve the correlation between the simulation and the reactor plant operation. Therefore, development of new parallel algorithms provides us with the opportunity to improve not only the speed, but also the accuracy and reliability of the predictions generated.

A number of parallelization efforts have been made over the years for nuclear reactor simulation. Most of the efforts have been focused on shared memory machines using a few (less than ten) processors. These parallelization efforts have, for the most part, approached parallelization from the viewpoint of speeding up existing codes. Attempting to parallelize existing codes is almost always far from the most efficacious approach. As a result, most parallelization of reactor simulations has focused on Fortran loops. A notable exception to this pattern is the large granularity approach used to couple reactor simulators with other models such as NEM 3D (the Nodal Expansion Method algorithm) or Contain (integrated containment analysis). These parallel couplings have typically been made using PVM (a parallel virtual machine library, see Appendix 4 for an introduction). A couple of these parallelization efforts are mentioned here to give further indications of the types of parallelization used and the level of performance that has been reported in the literature.

RELAP5 has a long history of optimizations performed by hand. These include both vectorization and parallelization. As one example, RELAP5 has been parallelized for MIMD (Multiple Instruction Multiple Data) shared memory machines by executing the iterations of individual loops in parallel. Larger grain parallelism was used in the heat structure and hydrodynamic subroutines. A newer equation solver, TRBR, was implemented. Explicit vector and parallel directives were installed. This code, called CERBERUS, achieved speedup of nearly 10 on 16 processors. Even though this appears to be the best speedup published for 16 processors, note this is not a really outstanding speedup result; this is less than 63% efficiency.

TRAC-BF1 has been linked to NEM 3D (the Nodal Expansion Method algorithm) through the use of PVM. This allows TRAC to do the outer hydraulic iterations, while NEM 3D is calculating the current time step 3-dimensional power distribution. {contact knepper@dsknepper.nuce.psu.edu}

At Argonne National Laboratories, preliminary experiments have been performed on parallelization of codes for analysis of thermal-hydraulic and neutronic events in nuclear reactors and nuclear power plants. They developed a hand-parallelized, scaled-down version of a system's analysis code for parallel experimentation. The best speedups they achieved were two on four processors of a Cray Y-MP/464 and three on eight processors of an Alliant FX/80. For details on this work see Tentner, et al.,(1994).

J. Vujic at Berkeley University has been working on a simulator for modelling neutron transport accurately in complex geometries. General Geometry Transport Theory Code in Two Dimensions (GTRAN2) runs on multiple networked workstations through the use of P4 (see Appendix 4). Each workstation gets some of the reactor core assemblies to calculate. Early simulation results are posted on the network {<http://neutrino.nuc.berkeley.edu/neutronics/papers/gtran2.html>}. The experimenters reported "nearly linear speedups were obtained to up to 6 processors." Further experiments showed that "In each case, the modified GTRAN2 program showed close to linear speedup as the number of processors increased from one to four. When more CPUs were added, communications costs began to outweigh the computational improvement."

These results show that parallelization is possible. These results and especially RELAP's long history of repeated optimization indicate that portability is essential. It is wasteful to continually be optimizing these large simulation codes by hand for specific machines. While parallelism holds great potential for these applications, it is time to make development and maintenance costs and portability prime considerations for future developments. Compilers and tools are becoming available that make it possible to write a portable, parallel reactor simulator, which can be optimized taking maximal advantage of both the reactor component connectivity and the code architecture. This paper introduces some of the options available to simulation developers.

Three types of parallel architecture and associated programming models are briefly reviewed as targets for parallelization of nuclear reactor simulation. On most shared memory machines, any variable that must be accessed by more than one processor is equally accessible by all processors. On distributed memory machines, variables are shared only through direct cooperation via communication between processors and there is no extraneous sharing. Networked, heterogeneous systems are similar to the distributed memory machines, but the computers can vary in computational ability as well as memory capacity and the connectivity is often non uniform.

Various parallelization models (loop-based model, shared memory model, functional model, data parallel model, and the combined functional and data parallel model) are discussed along with their advantages and disadvantages for nuclear reactor simulation. The loop-based model considers individual loops for parallelization, with associated overhead for process creation and termination. The shared-memory model declares every variable that must be accessible to more than one process available to all processes. The functional model runs independent functions in parallel. The data parallel model gets its parallelism through parallel computations on large data structures (usually arrays). The combined model uses functional parallelism with each function potentially using data parallelism as well. Each of these models are discussed briefly with emphasis placed on the data parallel model as the primary focus for two-phase flow simulation.

In data parallel computing, the parallel program must, at the very least, specify the parallelism and the mapping of data to processors. The parallelism specification tells what operations may be

done at the same time. The mapping specification tells what processor owns (stores) which data (values of variables). Further, the "owner computes" rule specifies that the processor that owns a piece of data performs all computations that get stored in its memory. Recent work in data parallel languages and compilers has resulted in systems in which other details such as modification of data declarations and loop bounds as well as management of communication are handled automatically for regular applications. In regular applications, fixed offsets are used to access neighbors, e.g., in one dimension the neighbor volumes for volume i in two-phase flow are volume $i-1$ and volume $i+1$. This leaves two essentials for parallel reactor simulator development: 1) parallel model/algorithm development and 2) data to processor mapping. The task of developing new and perhaps revolutionary parallel algorithms is one that must be accomplished by a reactor simulation expert or a team of experts. This is necessary as automatic parallelization technology is not currently capable of either developing new algorithms or recognizing parallelism at a high enough level to be efficient on many processors for complex codes such as reactor simulators. For example, in a reactor simulation, parallel processes should be created once and then communicate (and synchronize if necessary) on each time step; it is not currently possible to recognize this type of parallelism with automatic parallelization systems.

The other task not currently handled by data parallel language compilers is the mapping of the data to the parallel processors. A variety of algorithms, known as data distribution algorithms, have been developed for mapping data to parallel processors. The data distribution problem is to find an assignment of the data (and its associated computations) to the processors that achieves the best load balance (each processor should have the same amount of work), with minimal communication. In the general, heterogeneous setting, the goal becomes to optimize completion time (processors should finish at the same time) including communication time. Many of the available data distribution approaches are not applicable to composite grid problems (problems with multiple components that are computationally linked, e.g., the joined pipes, pumps, vessels, et cetera, in a reactor simulation). Most applicable data distribution algorithms are graph-based. In graph-based algorithms, each piece of data (elements of an array representing the volumes of a component) and all dependencies between data are explicitly represented in the graph. The algorithms attempt to partition the graph into as many sections as there are processors, cutting as few connections (or minimum weight of connections) as possible. The problem with the data distributions resulting from these graph-based algorithms is that they are rarely regular. Regular data distributions, like regular computations, allow fixed patterns of communication between the processors that the data is mapped to. Typically, irregular data distributions and irregular computations involve using index arrays as offsets into other arrays. Codes that use irregular data distributions can not, in general, be optimized at compile time to the same extent that ones with only regular data distributions can. This limitation occurs because the compiler can not determine what the value of an index array will be at run time and therefore can not determine which processor will be storing the data. Communication vectorization is an example of the optimizations that can not be performed at compile time, if there is irregularly distributed data involved in the communication. Therefore, if a problem is essentially regular, regular data distributions should be used to achieve greater efficiency. Although current implementations of reactor simulators are not regular, regular reactor simulators can be developed using modern programming languages. One approach to composite grid data distribution is presented that generates only regular data distributions. A program transformation system is also discussed that could eliminate requiring that the programmer express the data distribution explicitly in the

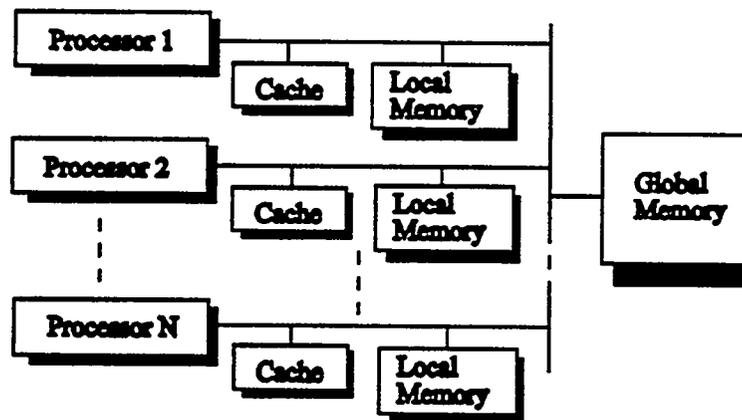
program. For efficient parallelization of reactor simulations, special considerations include: data structure design issues, code architecture issues, and parallel model selection. These will be discussed briefly before recommendations are suggested. The appendices give brief descriptions of a number of tools for parallelization with pointers to further information. In particular, descriptions of parallelization tools mentioned in this paper can be found in the appendices. To simplify reference to tools described in the appendices, an index of tools is included.

Parallel Architectures

Machine architecture has significant impact on the difficulty of parallelization, the performance of the parallel program, and the scalability of the parallelism. Consideration of machine architecture and parallelization models that will support multiple architectures with minimal effort is the starting place for most parallelization efforts.

Shared Memory Machines

Shared memory machines have a global memory that all processors can access over some interconnect mechanism. For example, consider a bus-connected shared memory multiprocessor.



On a machine like the one pictured above, each processor has private access to its own cache and local memory, but all processors have uniform access to the global memory over the bus. Many variations on shared memory machine architecture have been built, but the bus architecture has probably been used most often.

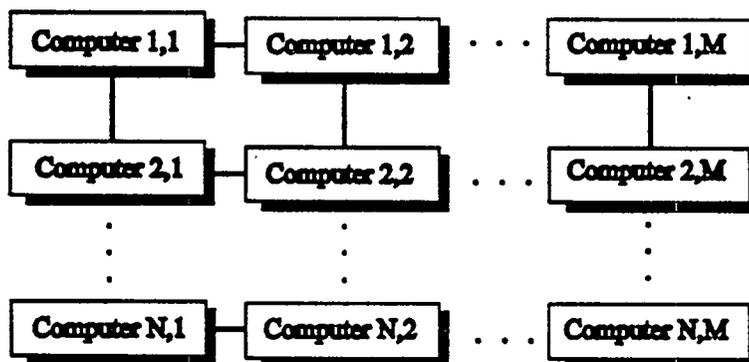
On shared memory machines, each processor has equally fast (or slow) access to the global or shared memory. The shared memory model for parallel computation declares variables that are needed by more than one processor as global shared variables. They are stored in the shared memory and may be accessed by all processors. In many applications, this global sharing is overkill because in physical simulations, there is normally a locality to interactions. For example, a change in one pipe of a nuclear reactor only directly affects neighboring or connected components (usually two components such as a tee and a pump), which in turn later affect their neighbors, and

so on down the line. Therefore, the simulation requires the sharing between neighboring components for this communication; it does not need global sharing. But, in shared memory architectures, if even two processors need access to a value, it is still equally accessible to all. This excessive sharing adds to the computation's cost. For example, although all processors can access the shared variables, their accesses must be synchronized to prevent inadvertent overwriting of values that are still needed and use of out of date values. This coherence support may be provided by the compiler or it may require programmer intervention. On some older machines, shared variables could not be cached unless the programmer controlled the flushing of the cache. On more modern machines, cache algorithms may be sophisticated enough to support caching of global variables and avoid related cache coherence problems. This support costs in terms of cost of machine and speed of execution.

The advantage, or perceived advantage, to the shared memory model is that some programmers consider it to be easier to work with than other models. This is because explicit communication is not required. The disadvantages are numerous. The overhead for sharing is expensive and more general than needed for many applications. The machines and programs written using this model do not scale well. Typically, only up to about eight processors can be used effectively. Further, programs written for the shared memory model do not port easily to distributed memory multicomputers or networks of processors.

Distributed Memory Multicomputers

On distributed memory multicomputers, each machine has its own memory and can access the memory of other processors only with their cooperation. As a simple example consider a 2-dimensional grid of processors.



In the figure above, there are $N \cdot M$ computers with N rows and M columns. Each computer in the grid is equivalent from the viewpoint of computational capability, memory, and cache. The number of neighbors that a computer has is dependent on its position. For any computer, if it has a row number, I , greater than one and column number J , it has a neighbor to the north with identification row $I-1$ and column J . Similar relationships hold for the neighbors in the other three directions. This type of distributed memory multicomputer is particularly appropriate for

simulation of 2-dimensional physical phenomena, because of the match between the topology of the machine and the problem.

Other topologies that have been proposed and/or used for distributed memory multicomputers include 1-dimensional grids, 3-dimensional grids, tori and hypercubes of various dimensionalities.

In distributed memory multicomputers, the ease of programming and the performance of the resulting parallel program will depend on: 1) the match between the topology of the machine and the topology of the problem, 2) the sophistication of the language/compiler/environment, and 3) the various machine parameters, such as the time it takes to communicate a message between neighboring processors.

Originally, the only way to program distributed memory multicomputers was using the vendor-supplied, machine-dependent communication instructions. In the distributed memory model of parallel processing locality, is used extensively as discussed in Heermann and Burkitt(1991). Data are grouped together on a computer to minimize the amount of information sharing between processors, while attempting to assign the same amount of work to each computer. With this paradigm, processes communicate only things that must be communicated and then only with other processors that require the communication. Note, there is *no* extraneous sharing in this model.

New languages and sophisticated compilers are reducing the communication problem to one of mapping the data onto the various computers for execution. This will be discussed further in the section on data parallelism.

The advantages of distributed memory multicomputers include: efficient communication for many physical simulation applications, scalability, portable algorithms (algorithms designed for distributed memory multicomputers can run on shared or distributed memory systems with only syntactic changes). The disadvantage, or perceived disadvantage, is that some programmers consider message passing control to be difficult. This disadvantage is being alleviated by modern data parallel languages, which require data mapping specification instead of complete communication specification.

Distributed Networks

In distributed networks, the connectivity between computers does not fit a fixed pattern. In addition the computers may have greatly varying capabilities, i.e., they may be heterogeneous. The machines on local area networks fit this category. Even small businesses now typically have their own local area network with a few machines. These machines can be used as parallel computer systems with appropriate software support.

Some parallel systems, e.g., PVM, provide support for placing processes on the computers of a distributed network and controlling communication between the various computers. In heterogeneous systems, there still remains the difficulty of writing the program so that the processes all finish at the same time and none of them have to wait long for information from any others. In addition, some of the machines on the network may actually be parallel computers. This will become even more common as multi-CPU workstations become more affordable.

The advantage of using distributed networks is that they are composed of computers that are already paid for and are available for use in solving problems faster. In particular, most organizations have machines that sit idle at night -- these machines may represent a substantial resource that is being wasted. The disadvantages include: communication is more expensive as computers are physically farther apart than in a distributed memory multicomputer, more involved software support or programming is necessary to utilize a distributed network as a parallel computer, and achieving good performance can be more difficult in the presence of heterogeneity.

Options for Parallelization

The type of parallelization used in any effort should match the parallelism available in the algorithm being implemented. To achieve an efficient approach, new algorithm development is often necessary. Parallelism in an algorithm may be expressed in a variety of forms: loop-based parallelism, functional parallelism, data parallelism, or a combination of these.

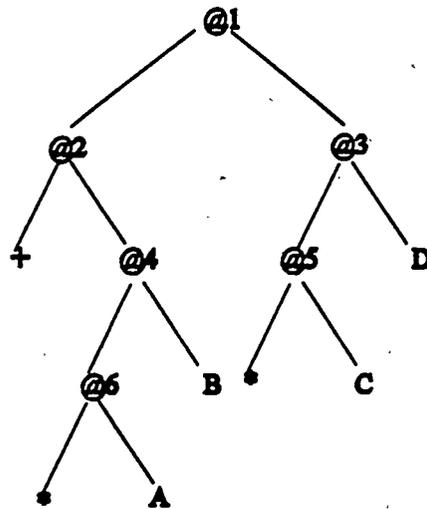
Loop-Based Parallelism

One of the most often used means of parallelization is loop-based parallelism. In loop-based parallelism, each loop nest is independently considered for parallelization. This approach allows extensive work by compilers and/or preprocessors. This was the first area where compilers exhibited some success in automating vectorization and parallelization. Experiments have also exhibited the limitations of this approach. First, most systems could not handle calls to subroutines or functions inside of a parallel loop. Also, when loops are considered separately, parallel processes must be started at the head of the loop and terminated at the end of the loop for each parallel loop or loop nest. This typically involves a substantial overhead for process creation.

Advantages of loop-based parallelism include: 1) it is often the fastest and least costly means of obtaining some performance increase through the exploitation of parallelism; 2) automated tools are available, e.g., KAP. Disadvantages include: 1) the approach targets shared memory machines, 2) usually only a few processors can be effectively used, and 3) the parallelization overhead is high due to the repeated creation and destruction of parallel processes.

Functional Parallelism

A functional program may be represented as a graph, with functional parallel languages executing the program by graph reduction. At a given point, the graph may contain a number of reducible expressions, which could be executed in parallel. Consider the expression graph for the simple expression $(A * B) + (C * D)$:



The expression graph represents the dependencies between sub-graphs (and hence operations). Independent sub-trees represent independent operations, e.g., sub-tree @2 is independent from sub-tree @3.

Initially, @5 and @6 are reducible. The pointer from @3 remains unchanged, but @5 is overwritten with (C*). The pointer from @4 remains unchanged, but @6 is overwritten with (A*). Reductions continue until the entire graph has been evaluated.

This same graph representation can be applied to parallel programs where the subtrees may be independent functions that can be executed in parallel.

Synchronization for functional parallel programs is provided by a shared graph. The parallelism and synchronization is controlled by the dependencies expressed in the graph. Usually, the programmer writes task communication and synchronization mechanisms in terms of explicit communication between the parallel functions, e.g., using MPI or PVM. Some more sophisticated tools have been developed for support of functional parallelism, e.g., HeNCE.

The advantage for functional parallelism is in doing related, but different, tasks in parallel. The disadvantages include: requiring separate functions for different processors, more complicated control (than loop or data parallelism), and difficulty in expression of loop or data parallelism.

Data Parallel Programming

Since automatic parallelization often fails for more complex and sophisticated programs, another approach to parallel programming has been developed, the data-parallel approach. The basis for this approach is that the data are operated on in parallel. In this case, a programmer expresses parallelism in terms of array-assignments and parallel loops(which may contain calls to subroutines or functions).

In the simplest form, using Fortran 90, all computations are expressed in terms of array operations. Given this type of specification for a parallel program, the compiler generates machine dependent code for the target architecture (with shared or distributed memory.).

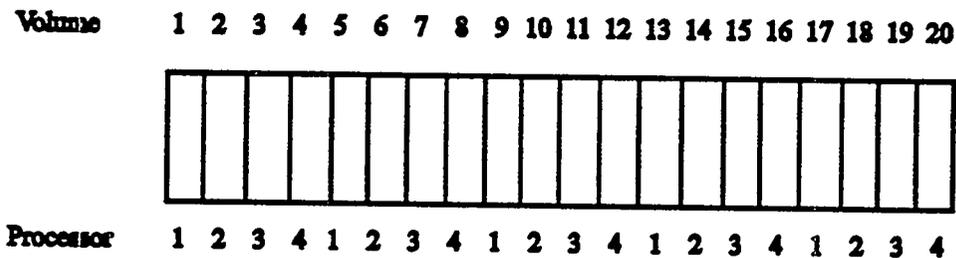
In the data parallel model, operations can be carried out on the entire data structure, usually an array, in parallel. In data parallel programming, DO loops are used sparingly. Where there are no data dependencies, assignment statements may be written in array syntax, which does not imply any element-wise order to the assignments. The compiler is responsible for dividing work among the available processing elements. The compiler is also responsible for fetching off-node data and determining loop index values for the local portion of the array. While this calculation is straightforward (because of the global name space), it is also error prone, when done by humans.

On a distributed memory machine each processor has some local memory on which it can act directly, and the large data arrays must be divided among the many different processors. In the message passing style, this distribution of data across the processors is done explicitly by the programmer, as is the communication of values between processors. However, data parallel languages typically include compiler directives to provide the programmer control over the data layout, but do *not* require the programmer to specify the communication. High Performance Fortran (HPF) is one example of a data parallel language.

Data distribution across processors is critical to the performance of data parallel programs on distributed-memory machines. For example, consider a simple, explicit 1-dimensional conservation of momentum update:

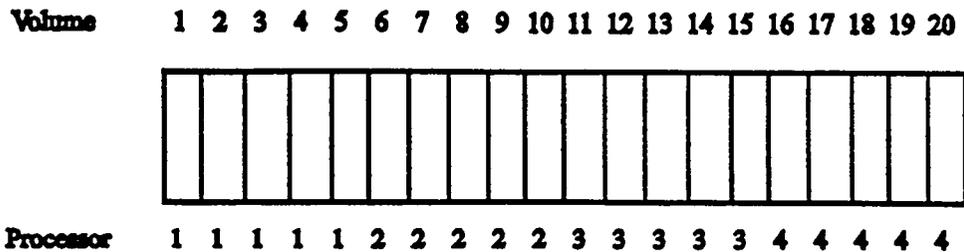
$$SMom(I) = SMom(I) - dt * (Sigma(I) - Sigma(I-1)) / (Mu(I) - Mu(I-1))$$

Consider two data distribution options. If the volumes are evenly distributed over processors in a cyclic fashion, there will be much more communication required than if a block distribution is used. To see this compare the two following figures. In both cases, four processors will be used. A cyclic data distribution results in the volume to processor assignment shown in the next figure.



Cyclic Data Distribution on 4 Processors

A block data distribution results in the volume to processor assignment shown in the next figure.



Block Data Distribution on 4 Processors

Every change in processor number between adjacent volumes implies a communication. Therefore, for only 20 volumes, although the load balance is the same, there is over five times more communication with the cyclic distribution than there is with the block distribution. This simple example illustrates why a good data distribution is so important for performance. The main issue to keep in mind is that the data distribution should maximize the ratio of local computation to communication.

Modern parallel and sequential architectures attain their highest speed when the data accessed exhibits locality of reference, as was just illustrated. The sequential storage order implied by FORTRAN 77 often conflicts with the locality demanded by the architecture. To avoid this, HPF includes features that describe the collocation of data (ALIGN) and the partitioning of data among memory regions or abstract processors (DISTRIBUTE). Compilers may interpret these annotations to improve storage allocation for data, subject to the constraint that semantically every data object has a single value at any point in the program.

The advantages for data parallelism, using a language such as HPF, include: 1) eliminates programming of explicit communication, 2) allows many compile time machine-dependent optimizations, and 3) is portable across a wide variety of architectures. The disadvantages have to do with the data to processor mapping. If irregular data distributions are used, many compile time optimizations can not be performed. Further, in composite grid applications, e.g., reactor simulations where multiple components are present, finding a good data distribution (and expressing it) are non-trivial. Means of overcoming these disadvantages will be discussed next.

Regular Vs Irregular Data Distributions

In regular applications, fixed offsets are used to access neighbor elements or volumes. For example, the following assignment statement is part of a regular application.

$$SMom(I) = SMom(I) - dt * (Sigma(I) - Sigma(I-1)) / (Mu(I) - Mu(I-1))$$

In irregular applications, the location of neighboring elements or volumes is not known at compile time. Often the neighbor index is found via a table lookup as shown in the following assignment statement.

$$SMom(I) = SMom(I) - dt * (Sigma(I) - Sigma(Left(I))) / (Mu(I) - Mu(Left(I)))$$

In the example above, Left(I) is an index array element containing the integer index of the array element that is logically to the left of element I. This use of index arrays can not be analyzed at compile time to allow communication optimizations because the compiler can not tell what the value of Left(I) will be, in general.

Regular data distributions have a fixed, uniform mapping of array elements to processors. Irregular data distributions can have arbitrary numbers of elements mapped to different processors. Further the pattern of mapping is not fixed and uniform, e.g., consider the following table of mappings of blocks to processors.

Block	Elements	Processor
1	20	1
2	5	4
3	50	2
4	24	3
5	31	6
6	15	5

In this small irregular example, the number of elements per block is arbitrary and the processor mapping is also arbitrary. Typically, the number of elements per processor and the mapping to the processors are computed. Therefore, the compiler normally can not analyze them for communication optimization.

When a regular application is parallelized, with a regular data distribution, maximal optimization can be performed. In particular, communications can often be grouped together to reduce the number of communication operations that must be initiated and therefore reduce the overall communication cost.

Composite Grid Considerations

Reactor simulations are partially regular. They are regular inside of each component of the two-phase flow, but irregular in connectivity between components. This implies that communication optimization can be performed for at least some communications, if the data distributions are regular.

None of the current parallelization approaches for these problems, e.g., CHAOS/PARTI as described in Chase, et al., (1992) and Sussman, et al. (1993), save the programmer from having to decipher the component assembly and determine data distributions. Since the description of the grid assembly is normally part of the input, user supplied data distribution would imply user intervention for each new component assembly input. Recently, a number of algorithms have been developed that could be used to automatically determine data distributions for composite grids. These approaches are mostly variations on graph partitioning. A few of the approaches that might, possibly with modifications, be used for mapping reactor simulations onto parallel computers are: simulated annealing, neural networks, genetic algorithms, incremental graph partitioning, recursive single tree bisection, recursive dual tree bisection, greedy algorithms,

minimum bandwidth algorithms, inertia algorithms, and spectral partitioning. These methods are described in Mansour and Fox(1994), Aaafrani and Ito(1993), Ou and Ranka(1994a), Ou and Ranka(1994b), Farhat and Lesoinne(1993), Dagnum(1993), and Pothen, et al.,(1990). Many more references may also be found in these papers.

We see two major problems with the use of these approaches to automatic distribution of data in reactor simulations.

- Graph-based distribution algorithms are inefficient for reactor simulations as each component volume, of which there may be thousands, becomes a vertex in the graph. Even with graph contraction applied, these approaches are still expensive.
- More importantly, these approaches generate irregular distributions. Recall that this implies that the compiler optimizations developed for regular applications can not be used.

Another support development for composite grid applications deserves mention. Researchers at IBM's T.J. Watson Research Center are extending IBM's scientific database package to support composite grid application parallelization. These extensions allow the user to specify array partitioning into sub-blocks and the package then provides automatic distribution of array sub-blocks to processors in a bin packing manner. The user is also required to insert calls to database package routines to manage data exchange [Chesshire and Naik(1993)]. This approach is somewhat similar to that used in CHAOS/PARTI with the exception of the bin packing distribution support. Using a bin packing approach to distribution of sub-blocks at runtime implies that regularity of communication inside of the components is lost and that the compiler can not perform regular optimizations.

None of the data distribution approaches presented to this point generate regular data distributions for nuclear reactor simulations. The next section presents an approach designed specifically for nuclear reactor simulations that generates *only* regular data distributions.

Automatic Data Distribution for Nuclear Reactor Simulations

The automatic distribution approach presented here does not determine distribution on a volume-by-volume basis. The automatic distribution algorithm runtimes are functions of the number and dimensionality of the components and the number of processors. Further this approach preserves regularity and supports maximal optimization at compile time.

This approach is based on the topology of the problem. In this context, topology means the connectivity between the components in a reactor simulation. For simplicity, also note that the sizes and types (PIPE, PUMP, et cetera) of components will be included as part of the topology. A coupling specification tells which volumes in which components are connected together.

For the approach being described, measures of the following are needed in addition to the topology of the reactor:

- the amount of computation per volume in each type of component,
- the amount of communication in each dimension of each type of component, and
- the amount of communication between each coupled pair of volumes in each coupling between component types.

The topology of the reactor is used to determine which volumes in the various components must communicate. The amount of computation for each volume of each component is used in load balancing. The amount of communication in each dimension of each component is used for communication minimization. The amount of communication for each coupling is used to prioritize the order in which coupled components get mapped and to determine the placement of coupled components. In nuclear reactor simulations, these measures may vary by component type, but the nature of the computation carried out for each component of the same type is similar. The computation can also vary by volume according to the material in the cell and the phase of the material.

This approach currently targets a torus-based communications topology. This seems reasonable as many available machines either are tori or can have tori efficiently embedded in the machine topology.

For efficient parallelization of composite grid applications, each component should be distributed according to its dimensionality [Liebrock and Kennedy(1994a)]. Once the number of processors to use on the target machine is fixed, there are only a finite number of possible m -dimensional processor configurations that can be used, where m is between one and the maximum processor dimensionality. This set is limited to only those configurations with at most n dimensions (n is the number of dimensions in the component with the maximum number of dimensions) and is called the *standard processor configurations*. Note that if the target architecture is not configurable, there will be only one standard processor configuration.

All components are classified according to their size relative to the number of processors being used. It makes sense to distribute a component over all processors if such a distribution results in parallel execution that makes efficient use of all processors. Assume for simplicity that the same computation is performed for each volume of every component. Components are *large* if they have enough volumes so that it makes sense to distribute them over all of the processors. Eliminate the large components from further component classification consideration. Components are *small* when they have so few volumes that they have less than the amount of work that should be assigned to one processor. Eliminate the small components and those left are *medium* size components.

Algorithm development began with large component distribution to support applications such as aerodynamics simulations. Next, small components, such as those that represent the many pipes, pumps, et cetera in reactor simulations, were considered. The resulting two algorithms were used for data distribution to obtain the initial results. The initial results lead to development of an algorithm to pack medium size components for distribution.

The large component distribution procedure for selecting a data distribution uses a computational model presented elsewhere [Liebrock and Kennedy(1994c)]. The model provides expected runtimes based on application and machine parameters as well as the selected data distribution.

In large component distribution, all components are distributed over all of the processors in the same dimensionality [Liebrock and Kennedy(1994b)] and the topology is used to reduce communication. Large components are distributed over all of the processors using the following steps. The best mapping and predicted runtime for each large component on each standard processor configuration is found independently, ignoring coupling communication cost. This takes time which is on the order of the number of components times the number of standard processor configurations. The standard processor configuration that produces the minimum total runtime for all large components is found, ignoring coupling communication cost. This takes time which is on the order of the number of standard processor configurations times the number of components. Coupling communication reduction uses the knowledge of topology to reduce communication costs associated with coupling. To do this, the components are aligned with respect to each other in the distribution via transposing, shifting, or folding around the torus. The time for this stage of the algorithm is bounded by the number of distributed dimensions multiplied by $c \log c$, where c is the number of couplings in the system.

After large components are distributed, medium size components are next for consideration. The basic idea is to pack the medium size components into groups, called *bins*, that are large enough to distribute over all of the processors¹. Optimally, the bins should be the same shape as the standard processor configuration selected in large component mapping; when this happens, load balance is improved. The shape is specified in terms of a ratio between dimension sizes. Each bin contains a set of components and all medium components are packed into some bin. Each bin is at least some minimum size -- to ensure that it can be distributed over all of the processors.

To illustrate the idea behind packing, consider the example of packing a load of books and papers into boxes. No books or papers can be bent or folded, but they can be rearranged in any way that packs them together with the least wasted space. Once all of the books and papers are contained in the boxes, you have a packing. The boxes here represent the bins and the books and papers represent the components. To this basic idea, add consideration of box shape and size to arrive at the general problem of packing components into bins for data distribution.

Previously packing was done using a commercial linear optimization package, but that was found to take too long and to produce packings that were not satisfactory in a number of ways. A heuristic algorithm is currently being developed. Preliminary results have yielded packings with predicted performance nearly five times better (for the simulation associated with the medium size components) than the results obtained with the commercial linear optimization package.

After the medium components are packed into bins, the bins are distributed across the full set of processors. By finding a distribution for the bin, a distribution is also specified for each of the medium size components packed in the bin.

¹This is similar to the bin packing problem from Computer Science, except that the components may have different dimensionalities and the bin may have higher dimensionality.

Finally, using load-balance predictions for the large and medium components, the small components can be assigned to processors to improve the overall load-balance. When possible, the small components are assigned to processors with which they need to communicate. When this would make the overall final load-balance worse, they are assigned to the nearest processor that can accommodate the work associated with them.

These algorithms could be used at runtime for dynamic load balancing if computation and communication statistics were collected in the program and the new alignment and distribution specifications were used for data redistribution. This may be useful for applications, such as nuclear reactor simulation, where the amount of computation per cell may change dramatically over time.

This approach to automatic data distribution eliminates the difficulty of determining a data distribution for reactor simulations and other composite grid applications that read the problem topology as part of the input. This form of automatic data distribution has been applied to the input descriptions of a number of reactor designs [Liebrock(1994)], but the results have not been used in a parallel reactor simulation as there is not currently a parallel reactor simulator that can use these distribution specifications. To effectively use these automatically determined data distributions more work is needed. The next section describes an automatic program transformation system that eliminates the need for programming the data distribution specifications in the reactor simulation code.

Automatic Program Transformation

This automatic program transformation approach targets specifically HPF for several reasons including: Fortran is the most widely accepted language for large scale physical simulations, and HPF is capable of supporting runtime input of the topology and distribution specifications. Since the HPF language definition does not require interprocedural analysis, which is needed to perform the transformations that are about to be discussed, the automatic transformation system would add precompiler support for HPF. If interprocedural analysis and this transformation approach is not used, then the programmer must explicitly write code to read and control access to routines for the input distribution specifications as well as handle subroutine clones. The subroutine clones are necessary to support the various data distributions (for different components) that can be active on subroutine entry. With the use of a precompiler, which can be completely machine independent, the user can compile with *any* full HPF compiler.

First a program style is presented for composite grid applications. This style is natural for representing the physical structures in composite grid applications, such as the components in reactor simulations. Programs written using this style enable many compile time optimizations. A program template is also presented. Programs written using this style and template permit automatic program transformation for applications that read the problem topology and automatically generated distribution specifications as part of the input. Finally, the steps needed to support runtime input of data distribution specification are outlined.

Two of the most important language features, for the proposed style, are dynamic memory allocation and user-defined data types. The user-defined data types allow all of the arrays and scalars for a given component to be grouped into one data structure, with the storage for the

arrays allocated at runtime according to the input. Further, an allocatable array of such structures can be used to represent all of the components of a given type. For example, in a reactor simulation code, there could be an allocatable array of structures for all of the pumps, another for all of the pipes, another for all of the vessels, et cetera. This implies that the program would have one allocatable array of structures for each type of component. Alternatively, the user-defined data type may include a type specification and have only one array of structures for each dimensionality. The basic ideas for one model of data structure creation are:

- arrays and scalars for each component type are grouped into a user-defined data structure,
- arrays for each component are dynamically allocated,
- an array of user-defined data structures is created for each type of component, and
- arrays of user-defined data structures are allocated dynamically.

Associated with each type of component there is at least one compute routine that is called with each structure on every time step. In addition, there would be a routine for internal boundary data exchange for each pair of coupled component types. In the case of implicit two-phase flow, the internal boundary data exchange routines also need to compute internal boundary conditions everywhere the system of components crosses a processor boundary.

General good programming practices should be followed: all routines should be written using a structured programming style (e.g., via the use of select case, not computed gotos). Structured programming is recommended as it facilitates compiler analysis and program maintenance.

The program template is outlined next. Note: this organization is *necessary* in HPF to permit the use of input data distribution specifications.

```

MODULE COMPOSITE
C      -- user defined data types go here
C      -- global declarations go here
CONTAINS
SUBROUTINE MAIN
C      -- calls to non-runtime-constant input routines go here
C      -- calls to initialization routines go here
C      -- calls to all computation routines go here
C      -- calls to output routines go here
CONTAINS
C      -- all routines except runtime constant input and storage allocation go here
END SUBROUTINE MAIN
C      -- runtime constant input routines go here
C      -- storage allocation routines go here
END MODULE COMPOSITE

PROGRAM ICRM
USE MODULE COMPOSITE
C      -- calls to runtime constant input routines go here
C      -- calls to allocation routines go here
CALL MAIN()
END PROGRAM ICRM

```

In a nuclear reactor simulator, more than one module would almost surely be used, but this template shows what the nesting must be for the PROCESSORS statements that are inserted by the transformation system to have constant parameters on entry to the module's scope.

Given a program written in this style and an understanding of how the input file relates to the allocation of these structures, the analysis necessary for execution of the automatic distribution algorithm is similar to the interprocedural analysis performed by Rice University's Fortran.D compiler [Hall, et al., (1992)]. Further, this style permits the use of the automatic transformation procedure. An outline of the steps needed for automatic program transformation to support runtime input of data distribution specification is shown below.

- Add distribution specifications to user defined types (UDTs).
- Insert code to read distribution specifications.
- Modify storage allocation to implement data distribution.
- Add a PROCESSORS statement to the main subroutine.
- For each subroutine with distributed data:
 - For each set of distribution types for the various parameters:
 - Clone the subroutine.
 - Replace all UDT parameters with their elements.
 - Add a PROCESSORS statement.
 - Insert distribution specifications for all distributed data.
- For each call to a subroutine with distributed parameters:
 - Replace all UDT parameters in the call with their elements.
 - Add a control structure to select the clone of the callee with the proper distribution specifications.
 - Insert parameters with distribution information.

These steps provide an indication of the complexity of the HPF program that results from the transformation procedure. Of particular importance is that there are potentially many clones of subroutines. Each of the clones can have a long list of parameters and distribution specifications. Therefore, it is vital that the user not have to support the clones directly. Each subroutine has an associated clone for each possible type of data distribution; subroutine clones are a requirement of HPF for efficient compilation to permit optimization without interprocedural analysis. Although not implemented, a more detailed discussion of this transformation procedure, with sample code segments, is presented elsewhere [Liebrock(1994)].

This transformation process, with the automatic data distribution approach described above, overcomes the disadvantages of data parallelism for reactor simulations and other composite grid applications.

Combined Functional and Data Parallelism

For complex problems, possibly one of the most natural approaches may be to use a combination of functional and data parallelism. Functional parallelism has been used previously to link, for example, NEM 3D with TRAC-BF-1. Data parallelism, in various forms, has been used in a numerous reactor simulation parallelization experiments, as were mentioned in the introduction. The combination of these two forms of parallelism provides greater flexibility and opportunity.

In a combined approach, different models would be simulated in parallel, with appropriate communication. Each of these models could potentially express another level of parallelism in the form of data parallelism. This approach should be considered and compared with a strictly data parallel approach to see whether the combined approach is more efficient.

Special Considerations for Parallel Reactor Simulation

Data Structure Design

The design of data structures can have substantial effects. Using data structures that do not correspond with the scientist's vision of the problem can lead to errors and a significant waste of time. Further, the design used for data structures can effect the ability of the compiler to analyze and optimize the program.

For example, in the two-phase flow design, if all of the pressures are represented as offsets in a single array (and similar representation is defined for the other primary variables), then:

1. automatic data distribution is hampered;
2. automatic program transformation is hampered;
3. uniform communication patterns will not be possible in all cases (especially when some components have different dimensionality than others);
4. compilers will not be able to perform communication optimization (and possibly other optimizations as well); and
5. training, maintenance, and new code development are hampered.

In contrast, if the variables associated with each component are grouped in a single user-defined data structure, then:

1. automatic data distribution can use the input problem topology (component sizes and connectivity) to automatically find a good mapping of the components to the parallel machine architecture;
2. automatic program transformation can generate the (regular or uniform) data mapping specifications and control structures to implement the automatically determined data distribution;
3. each component will involve only uniform communication patterns, even though the patterns between different components can vary;

4. compilers will be able to perform communication optimizations such as communication vectorization, provided the data distribution is regular; and
5. the data structures match most scientist's views of the problem more closely, which should make human costs for training, code development, and maintenance significantly lower.

The combination of considerations of scientist and parallelization gives preference to data structures which better reflect the structure of the problem.

Code Architecture

One of the most criticized constructs in Fortran is the GOTO statement. This is a statement that, when overused or wrongly used, can obscure the flow of control in a program. Modern languages include constructs that make the meaning of the program more obvious. Often, overuse of the GOTO can effectively be replaced with CASE statements that have two advantages: 1) the meaning of the program is more easily determined by the next code developer/maintainer, and 2) the program can be more effectively analyzed during compilation thereby allowing better optimization.

Two other constructs, which also have more modern replacements, are the COMMON and EQUIVALENCE statements. The COMMON statement has been used to create global variables. In modern Fortran (Fortran 90 and HPF), the MODULE construct is a more easily analyzed and understood way to express global variables. The EQUIVALENCE statement was used in old versions of Fortran to deal with the lack of dynamically allocatable memory. With dynamic memory allocation in modern Fortran, this need no longer exists and since EQUIVALENCE statements disable many compiler optimizations, they should no longer be used.

Making use of modern programming constructs can improve not only readability, but also allow better compiler optimization. One of the optimizations that can be done automatically with well-structured codes, in most cases, is vectorization. This is an advantage for those parallel machines that have vector processing capability in each processor. It is important to note that vectorization should not be done explicitly because it is often in conflict with efficient parallelization, but it can sometimes provide performance improvement when used as a secondary optimization.

Implicit Two-phase Flow Parallelization

Two approaches for two-phase flow parallelization are: data parallelism and explicit message passing (similar to data parallel, but with explicit programmer control of message handling). Both of these approaches should be tested to compare their efficacy in terms of programmer effort and parallel performance.

Probably the most effective data parallelization strategy for two-phase flow simulation is a data parallel approach with automatic data distribution and program transformation. This allows optimization without explicitly programming the topology of the problem into the simulation. Unfortunately, this data parallel approach will probably require rewriting of solution algorithms, if not development of new algorithms.

In order for the processors to proceed in parallel, a method of decoupling the problem, for a given time step, must be used at each processor boundary. A number of approaches have been developed that should be compared for two-phase flow. For discussions of some of these see Hicks, et al. (1987) and Hicks and Liebrock(1991). These approaches may require extension for multiple component models to address the connectivity between different components.

Interactions between Models: Two-phase Flow, Neutronics, Heat Transfer, et cetera.

Two options should be considered for parallelization that includes the interactions between the various models in a nuclear reactor simulation: strictly data parallelism and data parallelism combined with functional parallelism.

The first option is to attempt to use only data parallelism. Each model would need to be parallelized. Further, the data distribution would need to take the phases of the simulation into account, where a phase refers to the execution of one model. If no single data distribution specification makes this parallelization efficient, then data redistribution would be necessary between phases that can not effectively use the same data distribution. The issue of whether a single data distribution can be used needs further study.

The second option is to use functional parallelism between the various models. Each model would be assigned a set of one or more processors. Inexpensive models could be grouped onto a single processor. For expensive models, data parallelism can be used to run the model on more than one processor. This approach gives great flexibility in the parallelization strategy, but may require more programmer effort than a strictly data parallel approach.

Recommendations and Open Questions

Pilot codes should be used to determine which approach is most efficient in terms of development, runtime, and maintenance. This evaluation must include both human and machine cost considerations.

Pilot code development should include:

- Use of HPF with automatic data distribution and program transformation for data parallel implicit two-phase flow development.
- Use of MPI with explicit communication for implicit two-phase flow development.
- Evaluation of the relative merits of various decoupling options for breaking the implicit two-phase flow equations across parallel processors.
- Evaluation of the relative merits of various strategies for expressing and implementing the parallelism across all models. This should include a purely data parallel approach and a combined functional and data parallel approach.

Appendices

The following appendices present a brief introduction to just a few of the parallelization languages and tools that are available for each parallelization model presented in the main body of the paper. In each case, a reference is provided to assist in finding more information. In most cases, the reference is to a web site for the software or to one with pointers to information on the software.

General web sites to visit for pointers to information on parallel and high performance computing include the following (in no particular order):

<http://www.netlib.org/nhse/>

This site has pointers to a long list of: communication libraries, execution and performance analyzers (including debuggers), parallel input/output systems, parallel programming environments, parallel programming languages and compilers, parallel programming libraries, parallel runtime systems, source code analyzers and restructurers, and miscellaneous parallel processing tools.

<http://www.cs.umn.edu/~hlee/pp.html>

This site includes pointers to parallel processing information such as the top 500 list of the most powerful supercomputer sites, research groups, tools, vendors, and news groups

<http://www-jics.cs.utk.edu/resources.html>

This site has pointers to parallel computing indices, on-line books and courses, general parallel computing information, and some other interesting pages such as a history of parallel computing.

http://www.nersc.gov/doc/Parallel_Processing/Riddle/Parallel-www.html

This site is a "parallel processing information center" and has pointers to: NSF's high performance research highlights; other parallel programming sites; tools; and bibliographies, proceedings, and technical reports.

http://private.yahoo.com/Computers_and_Internet/Supercomputing_and_Parallel_Computing

This search site supports searches specifically aimed at parallel and high performance computing with entries on: commercial software, conferences, institutes, journals, programming, projects, supercomputer manufacturers, systems, user groups, and usenet.

<http://www.lpac.ac.uk/SEL-HPC/>

This site is supported by the London and South-East centre for High Performance Computing. It provides, along with access to high performance computing hardware and software, an article archive including many articles on high performance computing, compiler, and computational mathematics.

<http://www.hensa.ac.uk/parallel>

This site has pointers in the general categories of: internet parallel computing; transputers; Occam; conferences; general help; commercial links; software; contacts and references; theory, research and education. Note this site starts with the line "Over 1,100,000 files served" and it looks like its true.

Appendix 1: Tools for Loop-Based Parallelization

Semi-Automatic Parallelizers

KAP

{<http://www.digital.com/.i/info/DTJF05/DTJF05SC.TXT>}

The KAP (Kuck and Associates Parallelizer) preprocessor is discussed in terms of the Digital Alpha systems. The KAP preprocessor optimizes DEC Fortran and DEC C programs to achieve better performance on Digital Alpha systems. To enhance the performance, engineers selected two challenging aspects of the Alpha architecture as KAP targets: symmetric multiprocessing and cache memory. An additional design goal was to assist the compiler in optimizing source code for the reduced instruction set computer pipeline and multiple functional units.

One key optimization that KAP performs is the parallelization of programs for Alpha shared memory multiprocessors that using DECthreads. The heart of the optimizer is a sophisticated decision process that selects the best loop to parallelize from the many loops in a program. The preprocessor uses data dependence analysis to determine whether a loop is inherently serial or parallel. KAP uses a sequence of modular optimization passes to restructure the program to resolve many of the apparent serializations that are coding artifacts. End users can annotate their DEC Fortran or DEC C programs with directives or pragmas to guide this decision process.

FORGE 90

{http://193.242.86.10/Products/appsdirectory.dir/Applications/Development_Tools/ApplicationNumber5538.html}

FORGE 90's Distributed Memory Parallelizer spreads loops and distributes data arrays for MIMD architectures interactively. The parallelized program is scalable, with calls to APR's (Applied Parallel Research) parallel runtime library, interfacing a number of the popular communication packages such as PVM, MPI, or native message passing systems.

With FORGE's SPMD (Single Program, Multiple Data) parallelization strategy, the same program runs on each processor while selected DO loops are re-written to automatically distribute their iterations across processors.

Appendix 2: Tools for Data Parallel Programming

Languages

ADAPTOR

{<http://www.uni-paderborn.de/pcpc/doc/Adaptor/adaptor.html>}

Adaptor is a tool that transforms data parallel programs written in Fortran with array extensions, parallel loops, and layout directives to parallel programs with explicit message passing.

This tool has been developed at the GMD Laboratory for Parallel Computing where it is used with High Performance Fortran (HPF). GMD is developing efficient and reliable compilation technology to be integrated in currently existing or future HPF compilers.

ADAPTOR automatically generates message-passing statements from data-parallel constructs and distributes the data as specified by the user via directives.

By means of a source-to-source transformation, ADAPTOR translates the data parallel program to an equivalent SPMD program (Single Program Multiple Data) that runs on all available processors. The essential idea of the translation is to distribute the arrays of the source program onto the processors. Thus, parallel loops and array operations are restricted to the local data belonging to a processor (using the owner computes rule). Communication statements for exchanging non local data are inserted automatically. The control flow and statements with scalar code are replicated onto all nodes.

The ADAPTOR system supports the HPF subset and performs optimizations both for handling Fortran 90 array constructs and for improving cache locality, in addition to those for reducing communication costs. ADAPTOR determines communication schedules at run-time.

C / C++ (Syracuse University, npac@npac.syr.edu)

{http://www.npac.syr.edu/NPACoverview/PCRC_Proj.html}

In C or C++, the use of pointers and dynamic memory allocations provide the ability to build more complex and irregularly connected data structures whose size and shape may vary as the computation proceeds. Such dynamic data structures are useful in modeling certain applications such as N-body simulations, adaptive finite element methods, multi-target missile tracking, et cetera. Existing data parallel languages do not provide support for the construction and manipulation of pointer based dynamic data structures on distributed memory multiprocessors.

In a Syracuse University project, language extensions and class libraries are being developed to provide language and runtime support for the dynamic data distribution and load balancing required for these structures in a distributed memory implementation. Task level and data parallel class libraries are being developed for a C++ implementation of an adaptive finite mesh used in a computational fluid dynamics code. Language and runtime support for data parallel pointer-based structures in C and a prototype are also being implemented on the CM5 using the NI interface.

USCD has a C++ library for irregular or dynamically decomposed problems. The library is called LPARX (<http://www-cse.ucsd.edu/groups/hpcl/scg/lparx.html>).

CHAOS/PARTI

{<http://www.cs.umd.edu/projects/hpsl/chaos.html>}

Multiblock CHAOS/PARTI is a runtime support library for distributed memory parallel machines. CHAOS/PARTI provides the support for parallelization of codes in which:

- the data distribution is not known at compile-time,
- the number of processors on which the code is to be executed is not known at compile-time, and/or
- the code involves complex symbolic loop bounds and strides which may make compile-time analysis difficult.

Parallelization of irregular problems using CHAOS/PARTI involves six steps:

Data Partitioning: assignment of array elements to the parallel processors.

Data Remapping: redistribution of array elements to parallel processors.

Loop Iteration Partitioning: allocation of loop iterations to parallel processors.

Loop Iteration Remapping: redistribution of loop iterations to parallel processors.

Inspector: translation of global indices to local indices, identification of non-local references, and generation of communication schedules.

Executor: prefetching of non-local data using schedules from the inspector, and performing the computation.

Charm

{<http://charm.cs.uiuc.edu/descriptions/aboutCharm.html>}

The Charm Parallel Programming System is a machine independent parallel programming system. Charm programs run unchanged on MIMD machines with or without a shared memory. Charm provides high-level mechanisms and strategies to facilitate the task of developing even highly complex parallel applications.

Charm programs are written in C with a few syntactic extensions. It is possible to interface to other languages, e.g., FORTRAN, using the foreign language interface that C provides. Charm++ is the C++-based parallel object oriented language with all features of Charm plus support for multiple inheritance, late bindings, and polymorphism.

A few of the tenets for the design of the system are:

- **Efficient Portability:** Portability is essential for the development of reusable parallel software. The programming model induces better data locality, allowing it to support machine independence without losing efficiency. Charm/Charm++ programs run unchanged on MIMD machines with or without a shared memory.

- **Latency Tolerance:** Latency of communication - the idea that remote data will take longer to access - is a significant issue common across most MIMD platforms. Message-driven execution, supported in CHARM, is a very useful mechanism for tolerating or hiding this latency. In message driven execution, a processor is allocated to a process only when a message for the process is received. This means when a process blocks, waiting for a message, another process may execute on the processor. It also means that a single process may block for any number of distinct messages, and will be awakened when any of these messages arrive. This is an effective way of scheduling a processor in the presence of potentially large latencies.
- **Dynamic Load Balancing:** Dynamic creation of work is necessary in many applications. CHARM supports this by providing static and dynamic load balancing strategies.
- **Reuse and Modularity:** CHARM supports reuse with a well-developed "module" construct and associated mechanisms. These mechanisms allow for compositionality of modules without sacrificing the latency-tolerance.
- **Regular and Irregular Computations:** For regular computations, the system is useful because it provides portability, static load balancing, and latency tolerance via message driven execution. The system is unique for the extensive support it provides for highly irregular computations. This includes management of many medium-grained processes, support for prioritization, dynamic load balancing strategies, handling of dynamic data-structures such as lists and graphs, et cetera.
- **Associated Tools:** **DagTool** allows specification of dependencies between messages and sub-computations within a single process, provides a pictorial view of this dependence graph, and simplifies management of message-driven execution. **Projections** is a performance visualization and feedback tool. Projections has a much more refined understanding of user computation than is possible in traditional tools because it is language-specific. Thus it can provide specific feedback about entities in the user program such as objects and messages. It also incorporates a unique expert performance analysis component which can provide recommendations for improving performance.

Fortran D

{<http://softlib.rice.edu/fortran-tools/fortran-tools.html>}

The Fortran D compiler performs several optimizations like message vectorization, using collective communication, and exploiting pipeline parallelism [Hall, et al., (1992)]. It also performs analysis to eliminate partially redundant communication for irregular computations [Hanxleden, et al., (1992)]. The current version of the Fortran D compiler requires the number of processors to be known at compile time, and supports partitioning of only a single dimension of any array.

Fortran 90D

{<http://softlib.rice.edu/fortran-tools/fortran-tools.html>}

The Fortran 90D compiler exploits parallelism from Fortran 90 constructs in generating a SPMD (single program multiple data) message-passing program. This work has focused on supporting parallel I/O and handling out-of-core programs.

Fortran 90 provides a route forward for modern scientific programming for three reasons:

- **Portability:** The storage size of all variables can be defined in a machine-independent way. Use of COMMON blocks for storage and sequence association of arrays in memory is no longer necessary - this makes programs less risky and more easily parallelized, as well as more portable. Fortran 90 has a growing world-wide user community and compilers are available and supported on most high performance computing platforms.
- **Safer and More Powerful:** The syntax has been rationalized and simplified to incorporate features which are both safer and give the programmer greater expression. Many important features, which are standard in more modern languages such as C, are also included.
- **A Route to High Performance Computing and Parallelism:** This may be achieved by using the HPF extensions to Fortran 90.

Fortran 90 Extensions to Fortran 77

- **Whole Array Notation:** In Fortran 90, the programmer does not need to write code for array indexing or its arithmetic, which removes the necessity of extra levels of DO-loops. Therefore Fortran 90 can allow programs: to be written faster with fewer errors, to express algorithms in less code, to be debugged and maintained more easily.
- **Intrinsic Functions:** Intrinsic functions are provided for many of the common array operations: multiplication, reduction (e.g., ALL), inquiry (e.g., SIZE), construction (e.g., SPREAD), reshape, manipulation (e.g., CSHIFT), and location (e.g., MAXLOC). Ininsics are also provided to inquire and define the precision of variables which improves portability
- **Dynamic Memory Allocation:** Two primitives, ALLOCATE and DEALLOCATE, provide dynamic memory allocation. Fortran programs can then make better use of the machine memory, which can improve readability and compiler optimization.
- **User Defined Types, Derived Types, and Operator Overloading:** Users can build complicated data types that more easily represent what is being modeled. Further, operators can be overloaded to act on these types.
- **MODULES:** These allow users to create program libraries and use them more consistently. MODULEs allow operators to be overloaded in conjunction with user defined types. For example, operations on data could be defined in both polar and Cartesian coordinate systems, and given the same operator names in different MODULEs. The MODULE to use can then be specified in the program, and the relevant operators will automatically be used.

- **Pointers:** These support construction of more complex data types, e.g., linked lists.
- **Modern Control Structures:** A completely new construct, SELECT CASE, has been introduced which allows more concise expression and control over the choices of paths through a program. The DO-loop construct has been extended to be block structured, with CYCLE and EXIT statements for transferring control from the loop.
- **Free Format Source Code Form:** "Pure" Fortran 77 is Fortran 90 compatible, but it is better to convert it to a "mixed" format, acceptable both as free and fixed source form Fortran 90.

In summary, Fortran 90 supports writing code faster, more legibly, and avoiding many bugs. For a new programmers, it is an opportunity to learn a modern language, with most features recommended by computer scientists, and yet to be in line with scientific and industrial engineering communities where Fortran is and is going to remain the predominant language.

HPF (High Performance Fortran)

{<http://www.hensa.ac.uk/parallel/languages/fortran/hpf/index.html>}

The High Performance Fortran Forum (HPFF) is a collection of more than forty organizations including computer vendors, software companies, universities, and national laboratories. Since the first meeting in March of 1992, they have produced several draft versions of the HPF report. The specification of HPF was developed (and continues to develop) as a grass-roots effort by developers and users of Fortran. It is designed to facilitate its potential adoption as a standard sanctioned by ISO and national standards committees.

The HPFF has defined extensions to Fortran 90 to meet the following goals:

- provide a global name space across all processing elements and loosely synchronous parallel computing,
- provide high performance on MIMD (multiple instruction multiple data) and SIMD (single instruction multiple data) computers with distributed memory where the memory read-write time is non-uniform, and
- ensure compatibility across various architectures.

There are four areas where HPF extends Fortran 90. New directives describe data distribution and alignment. New language syntax, chiefly the FORALL statement and the INDEPENDENT directive, extends loop control capabilities. A rich addition of library routines provides information about the processors and adds to the list of intrinsic functions. Finally, language restrictions are included for constructs that make assumptions about the storage and sequence of data.

HPF1 is an extension of Fortran 90 which allows the natural parallelism in many array operations to be parallelized at a high linguistic level. This is provided in three ways:

- **HPF Directives:** Mapping directives support abstract machine description and distribution of arrays onto the abstract machine. The communications for a calculation

may be minimized by proper alignment of the arrays. The INDEPENDENT directive specifies that the iterations of a loop may be executed in any order or in parallel. The directives are machine-independent and help meet the goal of HPF to provide a portable medium for parallel Fortran programs. Another goal of HPF is that sequential F90 programs may be parallelized by the addition of HPF directives: the program should be able to be run either sequentially or in parallel by switching the compiler between ignoring or processing the HPF directives.

- **Additions to Language Syntax:** The main HPF addition is a comprehensive data-parallel array assignment loop statement, FORALL. This extends the whole array notation in F90, and can be used in sequential F90 programs where the compiler supports it. It will also be included in the Fortran 95 standard. Another addition is the PURE attribute which specifies sub-routines as being purely functional, that is without side-effects such as writing to global variables. Purely functional sub-routines may be safely used within pieces of parallelized code because there is no risk of their execution on one processor affecting the results on another processor. There are also a number HPF intrinsic functions which augment the F90 array intrinsic functions for data-parallel operations.
- **Advanced Compiler Technology:** The message passing and synchronization of the program is determined automatically by the compiler, or a pre-processor mapper which produces output for further compilation with a "normal" F90 compiler.

HPF adds directives to Fortran 90 to allow the user to advise the compiler on the allocation of data objects to processor memories. The model is that of a two-level mapping of data objects to memory regions, referred to as "abstract processors". Data objects are first aligned relative to one another and are then distributed onto a rectilinear arrangement of abstract processors.

There is a clear separation between directives that serve as specification statements and directives that serve as executable statements (in the sense of the Fortran standards). Specification statements are carried out on entry to a program unit, as if all at once; only then are executable statements carried out. While it is often convenient to think of specification statements as being handled at compile time, some of them contain specification expressions, which are permitted to depend on run-time quantities such as dummy arguments, and so the values of these expressions may not be available until run time, specifically the very moment that program control enters the scoping unit.

The programmer has many choices in distributing the code's data. The distribution of elements of each dimension in an array must be specified as either cyclic (first element to first processing element, next element to next processing element), block (first n elements to the first processing element), or undistributed (all elements of a dimension on the same processing element). Because assignment statements typically involve more than one array operand, it is necessary to align elements between arrays. Arrays may be aligned one to one, offset, their axes collapsed or replicated with respect to other arrays. The compiler divides the work of an array assignment among the processing elements and fetches any data that resides off the computing processing element. Thus, poor distribution choices can increase communication drastically, but they *do not* change the computation result.

Along with language extensions, HPF requires some restrictions. Many Fortran codes make use of how arrays are laid out in memory. Multidimensional arrays are passed to subroutines and depend on element (i, j) being followed by (i+1, j), and element (N, j) followed by (1, j+1). When data is distributed, these assumptions about the sequence of data storage are no longer valid. Thus, some EQUIVALENCE statements are not allowed, and subroutines must be called with arrays of the same shape (number of dimensions) and size (extent in each dimension) as declared within the subroutine. Failure to observe these restrictions will most likely produce code that is incorrect or halts with an error.

High Performance Fortran has many features to allow the scientist to take maximum advantage of a multiprocessor distributed memory machine, yet still spend most of the effort addressing the science, not the computer.

HPFC

{<http://www.cri.enscm.fr/pips/hpfc.html>}

HPFC is a High Performance Fortran Compiler which is being developed at Centre de Recherche en Informatique in Paris France. This project aims at building a prototype compiler to test new optimization techniques for compiling HPF. It has been supported by PARADIGME. The compiler is implemented on top of PIPS, which provides many program analyses. Realistic codes (hundreds of lines, heavy I/Os, not fully optimizable) are compiled by the prototype and have run on a network of workstations and a Connection Machine. Some experiments were also performed on an Alpha workstation farm.

The compiler generates code for the SPMD (single program multiple data) message passing programming model. It includes many optimizations. HPFC's target programming model is a host-node distributed memory message passing model. The host is in charge I/O and of the process management. The nodes perform the computations. Two programs are generated by the compiler. One for the host, and an SPMD code for the nodes, which is parameterized by the node identification. The generated codes rely on a runtime library. Lower level details for process management and communications are handled by PVM

HPF to MPI

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A translation system is available that works by translating HPF to standard Fortran 90, with calls to an HPF run-time system written in C++; the run-time library is layered on MPI {<http://www.mcs.anl.gov/mmpi-report/mmpi-report.html>}. Besides the standard UNIX utilities, prerequisites for installation are

- a standard Fortran 90 compiler,
- a C++ compiler, and
- an MPI installation.

The combination of these three systems provides a software platform for the HPF installation.

PARADIGM

{<http://roundup.crhc.uiuc.edu/Paradigm/overview.html>}

The PARADIGM compiler is targeted to Fortran 77 programs and provides an option for automatic data partitioning for regular computations. It also supports exploitation of functional parallelism in addition to data-parallelism.

PETSc (Portable, Extensible Tool kit for Scientific Computation)

{<http://www.mcs.anl.gov/petsc/petsc.html>, free; ftp from info.mcs.anl.gov}

Computational science presents a variety of challenges, including the coordination of detailed physical models and various algorithmic approaches. The complexity inherent in these applications may benefit from a framework such as PETSc that provides broad-based infrastructure with provisions for customization and extension. By devoting strict attention to component interoperability, PETSc enables the integration of independently developed application modules, which often employ different coding styles and data structures. In addition, users can replace models as well as combine and nest algorithms.

The PETSc components function similarly to C++ classes in terms of implementation and use. Each component manipulates a particular family of objects, e.g., vectors, through an abstract interface or set of calling sequences and one or more implementations using particular data structures.

Features include:

- Parallel vectors, including code to easily perform scatters, gathers, et cetera.
- Parallel matrices with several different sparse matrix storage formats.
- Easy, efficient parallel matrix assembly routines.
- Sequential sparse matrix direct solvers.
- Scalable parallel preconditioners and Krylov subspace methods, including ICC, ILU, block Jacobi, overlapping Schwarz, CG, GMRES, Bi-CG-stab.
- Scalable parallel nonlinear equation solvers, including line search and trust region Newton-like methods.
- Simple parallel ODE solvers for application of the method of lines to large scale nonlinear (or linear) time-dependent PDEs.
- Distributed arrays.
- Automatic profiling of floating point performance and memory usage.
- Consistent interface for all solvers and data structures.
- Complete documentation including users manual and man pages.
- Intensive error checking.
- Usable from Fortran and C/C++.
- Portable to most UNIX systems.

PIPS (Paralléliseur Interprocédural de Programmes Scientifiques)

{<http://www.cri.ensmp.fr/~pips>}

PIPS is an automatic parallelizer for scientific programs that takes as input Fortran 77 and HPF codes. It emphasizes interprocedural techniques based on linear algebra techniques. PIPS is being developed at Centre de Recherche en Informatique de l'École Nationale Supérieure des Mines de Paris (CRI-ENSMP), Fontainebleau France.

PIPS is a highly modular framework, which can be used to test and implement various compilation schemes, program analyses and transformations, such as automatic vectorization and parallelization (Cray Fortran, CRAFT, CM Fortran, F90 & PVM output), HPF compilation, loop transformations, and partial evaluation.

The compiler is made of independent phases that are called on demand to perform the analyses or transformations required by the user. Consistency and interprocedural issues are dealt with automatically. The phase chaining is driven by an interprocedural make system, **pipsmake**, and internal data structures are automatically stored in a database, **pipsdbm**, which manages persistence through different runs. Persistence is used to avoid the memory bottleneck when large programs are analyzed interprocedurally. It is also used by newcomers to develop new applications without interfering with existing code.

Three interfaces are available: a shell interface (Pips), an X-WindowS interface (wpips) and a hypertextual interface (epips).

SUIF

{<http://suif.stanford.edu/arpa/project2.html>,
http://galileo.eng.wayne.edu/suif_doc/parguide_2.html}

The SUIF (Stanford University Intermediate Format) compiler performs loop transformations for increasing parallelism, and for enhancing uniprocessor performance. The compiler also supports automatic data partitioning. The SUIF compiler system has been released and made freely available.

Some features of the SUIF system include:

- **Interprocedural Analysis for Parallelization:** SUIF research focuses on building a comprehensive suite of analyses for parallelization to measure how effective an aggressive interprocedural system is at locating parallelism across procedure boundaries.
- **Optimizations for Parallel Machines:** Modern scalable multiprocessors can have either a shared address space (e.g., Stanford DASH and KSR-2) or disjoint address spaces (e.g., Intel Paragon, IBM SP-2). Because they all have physically distributed memories, the same compilation techniques can improve performance on both architectures. Investigation is proceeding on three sets of optimization techniques: global parallelism and locality analysis, communication and synchronization analysis, and changing array layouts.
- **Theory of transformations:** A loop transformation algorithm that maximizes parallelism while minimizing communication draws from a large repertoire of

transformations, which include not just unimodular transformations but also loop fission, fusion, reindexing, and statement reordering.

- **Pointer Analysis:** To parallelize C programs, the compiler must have information about the values of pointer variables. Objects reached through pointers may be aliased, and unless the compiler knows otherwise it must assume that all aliases are possible. Using interprocedural pointer analysis, however, aliases that actually occur in the program can be identified, and thus greatly increase the potential for parallelization.
- **SAM:** Run-time and language support are being explored to aid scientific programmers in parallelizing complex programs. SAM is a run-time system that provides a shared name space and automatic caching of shared data in software on distributed-memory multiprocessors and networks of workstations. The Jade language is a parallel programming language (an extension to C) for exploiting coarse-grain concurrency in sequential, imperative programs. Jade is implemented using SAM, and both systems run on the Intel iPSC/860 and Paragon, the Thinking Machines CM-5, the IBM SP1, and on heterogeneous networks of workstations running PVM.

SUPERB

The SUPERB compiler at the University of Vienna represents a second generation compiler using techniques such as message vectorization and overlap regions for shift communication [Zima, et al. (1988)]. The compiler only supports block distribution of array dimensions. It puts special emphasis on performance prediction to guide optimizations and data-partitioning decisions.

Vienna Fortran

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Vienna Fortran is a language extension of Fortran which provides the user with a wide range of facilities for mapping of data structures across processors. Vienna Fortran programs are written using global data references. Thus, the user has the advantages of a global name space with explicit control of data distribution.

Vienna Fortran 90, an advanced data parallel language based on Fortran 90 and Vienna Fortran, enables the user to program distributed memory architectures almost as easily as sequential computers using global addresses only. Vienna Fortran 90 provides a number of new features not found in any other comparable language such as HPF or Fortran D. This includes concepts for distributing user defined data structures, distribution of pointer objects, and a general framework for specifying arbitrary data and work distribution.

Visualization

dtool

{<http://www.npac.syr.edu/copywrite/pcw/node83.html>}

The distribution profiler **dtool** serves to visualize parallel programs that rely on data distribution for their parallelism. The basic idea of this tool is to look at the data distributions that are used with a view to either optimizing their use or looking for places in which redundant transformations are being made. Possible restructuring of the code may eliminate these transformations, thus improving performance. This is particularly useful in conjunction with automatic parallelization tools, which have a tendency to insert redundant communication in an effort to ensure program correctness.

DPV --The Data-Parallel Visualizer

{<http://dis.cs.umass.edu/~wagner/dpv/dpv.html>}

Parallel program visualization and debugging require new techniques for gathering and displaying execution trace and profile data. Interaction with the program during execution is also required to facilitate parallel debugging. The difficulties associated with runtime user/program interaction are non-trivial. This research centers around the data-parallel programming paradigm. The researchers believe that the data-parallel model facilitates much more liberal runtime interaction than typical MIMD-based models, while still providing the performance benefits of asynchronous execution.

A model for data-parallel program visualization and debugging has been developed and a subset of that model has been implemented. Issues being researched include: effective storage and organization of the unordered visualization data, how to visualize multi-dimensional user data, how to view data elements (by physical or virtual processor, or neither), and the granularity required for effective visualization.

Performance Analysis

Pablo

{<http://www.hensa.ac.uk/parallel/performance/tools/pablo/index.html>}

Although correlation of dynamic performance data with the behavior of explicitly parallel message passing programs is possible via the University of Illinois's Pablo performance analysis environment, data-parallel languages such as Rice's Fortran D and High Performance Fortran (HPF) infer parallelism and communication from data distribution directives. In such instances, performance tools cannot meaningfully relate measurements about the key aspects of execution performance to source-level constructs without substantial compiler support.

To provide performance feedback meaningful to a programmer writing in an abstract parallel language such as Fortran D or HPF; performance analysis tools must exploit

information about the translation from the high-level source language to the low-level parallel code. Pablo procedure profiles or communication displays of the compiler-generated code's performance do little to explain how to optimize the original Fortran D code without knowledge of the relation of interprocessor communication to the Fortran D source code.

The current effort is to make it possible for programmers to pose performance questions in terms of the machine-independent programming model used in Fortran D and HPF and use these questions to acquire the performance data needed to produce performance analyses and visualizations that answer these questions in ways that are easily related to the user's program.

Automatic Data Distribution

ddlib

{<http://jane.jpl.nasa.gov/HPCC/ddlib/ddlib.html>}

This library was designed to provide automatic data distribution and redistribution of two dimensional arrays in a MIMD architecture for data parallel applications. The library functions are available for architectures using CrOS, EXPRESS, and NX message passing protocols.

HPF-builder

{<http://www.lifl.fr/west/hpf-builder/>}

The HPF-builder graphical environment goal is to free the HPF programmer of all the syntactic constraints due to the data mapping. All the data distribution and alignment are insured in an interactive and visual way. HPF TEMPLATES and PROCESSORS become the visual support for alignment and distribution on grids of processing elements.

Via an analysis of the source code, HPF-builder extracts the whole set of parallel structures and lets the user map the arrays in a visual way. HPF-builder automatically generates the corresponding HPF directives and inserts them in the Fortran 90 source code. This process results in an HPF code.

From the TEMPLATE distribution on the PROCESSORS, HPF-BUILDER can also visualize the array distribution on the processor grids. According to this visualization, HPF-builder users are able to tune the distribution to improve the balance between the parallelism and the communications.

Appendix 3: Tools for Functional Parallelism

Languages/Compilers

MPI

{<http://www.phy.hr/para/mpi/>}

MPI (Message Passing Interface) was developed as a standard for writing message-passing programs. The MPI Forum goals were to make an interface that was practical, portable, efficient, and flexible. MPI goals include being:

- a widely used standard for writing message-passing programs,
- practical, portable, efficient, and flexible,
- able to "... demonstrate that users need not compromise among efficiency, portability, and functionality." [Gropp, et al., (1994)],
- able to help people writing parallel libraries. MPI targets machines from scalable multiprocessors to networks of heterogeneous workstations.

MPI is a library of functions that support the message passing model. Other MPI features include the following.

- **Collective Communications:** Collective operations such as maximum, minimum, et cetera are supported, with the message-passing library taking advantage of the structure of the machine to optimize performance.
- **Virtual Topologies:** Processes can be conceptualized in terms of application oriented topologies (graphs and grids) to provide a high-level view of process management.
- **Debugging & Profiling:** MPI provides hooks for calls to profilers and debuggers.
- **Library Support:** Use of communicators provides capabilities for making parallel libraries independent of the user code and inter-operable with other libraries.
- **Heterogeneous Network Support:** Data format conversions are done automatically to support parallelization over heterogeneous networks of computers.

Other Tools

HeNCE

{<http://www.hensa.ac.uk/parallel/environments/pvm3/hence/>}

The HeNCE environment provides higher level support for functional programming. In particular it uses a graphical interface to make the construction, debugging, and visualization of functional program more convenient.

The HeNCE environment tool compose supports parallelism specification through graph drawing. Each node in the graph represents a Fortran or C function. Each arc represents data and control flow dependence. Four control construct nodes are available: looping, conditional dependence, fan-out to identical subgraphs, and pipelining. These special control nodes allow dynamic execution of the subroutines based on evaluation of input parameters.

After the dynamic graph is complete, the **configuration** tool allows specification of the machine configuration. This tool supports assignment of tasks to a heterogeneous set of machines.

The **build** tool generates a PVM program to execute the graph, which can run the various routines on the heterogeneous set of machines.

The **execute** tool runs the processes on the machine using the configuration that was determined above.

Finally, the **trace** tool supports visualization of the parallel execution. This provides a dynamic view of the graph as it executes on the heterogeneous machine.

XMPI

{<http://www.osc.edu/Lam/lam/xmpi1.html>}

XMPI is an X/Motif based graphical user interface for running, debugging, and visualizing MPI programs. Extensive MPI information is extracted from a running application on demand, or from a cumulative log of communication. Both sources are tightly integrated with an application overview window and any number of single process focus windows.

After interacting with XMPI to run an MPI application, a honeycomb representation of all processes is displayed in the main window. Icons inside each cell indicate the execution state of the process and alert the user to any unreceived messages. Processes are identified by their rank in MPI_COMM_WORLD. A button click updates the information across the entire application - while the application is running (or perhaps deadlocked or otherwise hung). This simple capability to inspect, at runtime, the synchronization state of processes and messages is a very effective debugging tool. Source code steppers and print statements are often used to get at the same information, but in a more cumbersome manner.

Features include:

- runtime snapshot of MPI process synchronization;
- runtime snapshot of unreceived message synchronization;
- single process focus detailing communicator, tag, message length, and datatype;
- runtime and post-mortem execution tracing, with timeline and cumulative visualizations;
- highly integrated snapshot from communication trace timeline;
- process group and datatype type map displays;
- assembly of MPI applications from local or remote programs; and
- easy startup and takedown of applications.

Appendix 4: Tools for Combined Data and Functional Parallelism

Other Tools

HPF/MPI

(<http://www.mcs.anl.gov/fortran-m/>)

High Performance Fortran (HPF) provides a portable, high-level notation for expressing data-parallel algorithms. An HPF computation has a single-threaded control structure, global name space, and loosely synchronous parallel execution model. Many problems requiring high-performance implementations can be expressed succinctly in HPF.

However, HPF does not adequately address task parallelism or heterogeneous computing. Examples of applications that are not easily expressed using HPF alone include multidisciplinary applications where different modules represent distinct scientific disciplines, programs that interact with user interface devices, applications involving irregularly structured data such as multiblock codes, and image-processing applications in which pipeline structures can be used to increase performance. Such applications must exploit task parallelism for efficient execution on multicomputers or on heterogeneous collections of parallel machines. Yet they may incorporate significant data-parallel substructures.

MPI provides a set of functions, datatypes, and protocols for exchanging data and coordinating the execution of multiple tasks. Previous MPI implementations have supported bindings only for the sequential languages C and Fortran 77. However, there is no reason why MPI functions may not also be used for communication among data-parallel tasks. The HPF binding for MPI makes this possible. It is intended to be used as follows:

- A programmer initiating a computation requests (using some implementation-dependent mechanism) that a certain number of tasks be created; each task executes a specified HPF program on a fixed number of processors.
- Tasks can call MPI functions to exchange data with other tasks, using either point-to-point or collective communication operations. In point-to-point communications, a sender and a receiver cooperate to transfer data from sender to receiver; in collective communications, multiple tasks cooperate—for example, to perform a reduction.

When reading HPF/MPI programs, HPF directives can be ignored, and code understood as if it implements a set of sequential tasks that communicate using MPI functions.

LAM

{<http://www.phy.hr/para/mpi/>}

LAM (Local Area Multicomputer) is an MPI programming environment and development system for heterogeneous computers on a network. With LAM, a dedicated cluster or an existing network computing infrastructure can act as one parallel computer solving one problem.

LAM features a full implementation of MPI. Compliant applications are source code portable between LAM and other MPI implementations. In addition, LAM offers monitoring capabilities to support debugging. Monitoring happens on two levels. LAM has the hooks to allow a snapshot of process and message status to be taken during an application run. The status includes aspects of synchronization plus datatype map / signature, communicator group membership, and message contents. On the second level, the MPI library is instrumented to produce a cumulative record of communication, which can be visualized either at runtime or post-mortem.

Opus

{<http://www.unisys.com/backgrounder/04265804.html>}

Researchers at NASA Langley Research Center have designed language extensions, collectively called Opus, for expressing the outer level functional parallelism exhibited by multidisciplinary codes. The tasking layer can be used to exploit the coarse grained parallelism across disciplines and the interdisciplinary sharing of data. At the same time, parallelism within each discipline can still be expressed via HPF, since the tasking layer is well integrated with HPF. Preliminary work on the programming environment using this tasking layer has begun, along with a runtime system that will support this approach in a heterogeneous environment.

High Performance Fortran is the first step towards a portable programming language for data parallel applications. The extensions and modifications being made at NASA Langley are significant in that they extend this capability to support expression of more complex data parallel applications. These extensions have been presented to the High Performance Fortran Forum which is currently conducting a second round of meetings to generate a set of requirements for future development.

P4 (the source of name is **Portable Programs for Parallel Processors)**

{<http://www.mcs.anl.gov/home/lusk/p4/index.html>}

P4 is a library of macros and subroutines developed at Argonne National Laboratory for programming a variety of parallel machines. The current p4 system includes the following basic computational models: monitors for the shared-memory model, message-passing for the distributed-memory model, and support for combining the two models.

P4 is intended to be portable, simple to install and use, and efficient. It can be used to program networks of workstations, advanced parallel supercomputers like the Intel Touchstone Delta and the Alliant Campus HiPPI-based system, and single shared-memory multiprocessors.

Important features of p4 include:

- support for both message-passing and explicit shared memory operations;
- support for heterogeneous networks;
- World Wide Web version of the manual for on-line help;

- SYSV IPC support for shared-memory multiprocessing on workstations that support multiple processors, and simulating it on uniprocessors;
- instrumentation for automatic logging/tracing;
- automatic or user control of message-passing/buffer-management;
- error/interrupt handling; and
- an optional p4 server for quick startup on remote machines.

A useful companion system is the **upshot** logging and X-based trace examination facility.

PVM

{http://www.epm.ornl.gov/pvm/pvm_home.html,
<http://consult.ncsa.uiuc.edu/docs/consult/Doc/Software/PVM/>}

PVM is a portable message passing system for parallel computing on heterogeneous systems. PVM is in the public domain and is made available by Oak Ridge National Laboratories. It is available from any NCSA system.

The challenges of heterogeneous distributed computing include: architecture, data format, operating system, computational speed, machine load, and network load.

The advantages of heterogeneous distributed computing include:

- Use of existing hardware.
- Use most appropriate hardware.
- Virtual computer can be easily upgraded.
- Program development on familiar platforms.
- Exploitation of the stability of workstations.
- Facilitation of collaborative work.

Some principles underlying PVM:

- User-configured host pool.
- Translucent access to hardware.
- Process-based computation.
- Explicit message-passing model.
- Heterogeneity supported.
- Multiprocessor support.

There are two major components in the system:

- A daemon which runs on every machine in the virtual machine.
- A library of routines (for message passing, spawning and coordinating tasks, modifying the virtual machine, et cetera).

PVM (Parallel Virtual Machine) is a byproduct of an ongoing heterogeneous network computing research project. The general goals of this project are to investigate issues in, and develop solutions for, heterogeneous concurrent computing. PVM is an integrated set of software tools and libraries that emulates a general-purpose, flexible, heterogeneous concurrent computing framework on interconnected computers of varied architecture. The

overall objective of the PVM system is to enable such a collection of computers to be used cooperatively for concurrent or parallel computation.

The PVM computing model is based on the notion that an application consists of several tasks. Each task is responsible for a part of the application's computational workload. Sometimes an application is parallelized along its functions; that is, each task performs a different function, for example, input, problem setup, solution, output, and display. This process is called functional parallelism. A more common method of parallelizing an application is called data parallelism. In this method all the tasks are the same, but each one only involves a small part of the data. This is also referred to as the SPMD (single-program multiple-data) model of computing. PVM supports either or a mixture of these methods. Depending on their functions, tasks may execute in parallel and may need to synchronize or exchange data, although this is not always the case.

The PVM system currently supports C, C++, and Fortran languages. This set of language interfaces have been included based on the observation that the predominant majority of target applications are written in C and Fortran, with an emerging trend in experimenting with object-based languages and methodologies.

The general paradigm for application programming with PVM is as follows. A user writes one or more sequential programs in C, C++, or Fortran 77 that contain embedded calls to the PVM library. Each program corresponds to a task making up the application. These programs are compiled for each architecture in the host pool, and the resulting object files are placed at a location accessible from machines in the host pool. To execute an application, a user typically starts one copy of one task (usually the "master" or "initiating" task) by hand from a machine within the host pool. This process subsequently starts other PVM tasks, eventually resulting in a collection of active tasks that then compute locally and exchange messages with each other to solve the problem.

References

1. C. Chase, K. Crowley, J. Saltz, and A. Reeves(1992), "Compiler and Runtime Support for Irregularly Coupled Regular Meshes", **Journal of the ACM**, July, 1992.
2. G. Chesshire and V.K. Naik(1993), "An Environment for Parallel and Distributed Computation with Application to Overlapping Grids", IBM Research Division, T.J. Watson Research Center, Almaden, **IBM Research Technical Report, RC 18987 (82949)**, June, 1993.
3. L. Dagnum(1993),"Automatic Partitioning of Unstructured Grids into Connected Components", **Supercomputing**, Nov. 1993.
4. C. Farhat and M. Lesoinne(1993), "Mesh Partitioning Algorithms for the Parallel Solution of Partial Differential Equations", **Applied Numerical Mathematics**, V12, N5, May, 1993, pp 443-457.
5. M.W. Hall, S. Hiranandani, K. Kennedy and C. Tseng(1992), "Interprocedural Compilation of Fortran D for MIMD Distributed-Memory Machines", **Supercomputing**, Nov. 1992.
6. W. Gropp, E. Lusk, and A. Skjellum, **USING MPI: Portable Parallel Programming with the Message Passing Interface**, MIT Press, 1994.
7. R. v. Hanxleden, K. Kennedy, C. Koelbel , R. Das and J. Saltz, "Compiler Analysis for Irregular Problems in Fortran D", **Proceedings of the 5th Workshop on Languages and Compilers for Parallel Computing**, Aug. 1992.
8. D.W. Heermann and A.N. Burkitt(1991), **Parallel Algorithms in Computational Science**, Springer-Verlag, 1991.
9. D.L. Hicks, L.M. Liebrock, V.A. Mousseau, and G.A. Mortensen(1987), "Parallelization of Hydrocodes on the Intel Hypercube, Parts 1 and 2", **Idaho National Engineering Laboratories Reports**, EGG-SPAG-7682, 42 pp. and EGG-SPAG-7818, 38 pp.
11. D.L. Hicks and L.M. Liebrock(1991), "Parallel Algorithms for Implicit Material Dynamics Schemes", **Applied Mathematics and Computation**, V46, N3, 1991, pp. 179-209.
12. L.M. Liebrock(1994), "Using Problem Topology in Parallelization", Rice University, **Center for Research in Parallel Computation Technical Report**, TR 94-477S, Sept., 1994.
13. L.M. Liebrock and K. Kennedy(1994a), "Parallelization of Linearized Application in Fortran D", **International Parallel Processing Symposium**, April, 1994a, pp. 51-60.
14. L.M. Liebrock and K. Kennedy(1994b), "Automatic Data Distribution of Large Meshes in Coupled Grid Applications", Rice University, **Center for Research in Parallel Computation Technical Report**, TR 94-395, Apr, 1994b.
15. L.M. Liebrock and K. Kennedy(1994c), "Modeling Parallel Computation", Rice University, **Center for Research in Parallel Computation Technical Report**, TR 94-499, May, 1994c.

16. N. Mansour and G.C. Fox(1994), "Parallel Physical Optimization Algorithms for Allocating Data to Multicomputer Nodes", **The Journal of Supercomputing**, V8, 1994, pp. 53-80
17. C.-W. Ou and S. Ranka(1994a), "Parallel Incremental Graph Partitioning", Northeast Parallel Architecture Center, Syracuse University, **Northeast Parallel Architecture Center Technical Report**, August, 1994.
18. C.-W. Ou and S. Ranka(1994b), "Parallel Remapping Algorithms for Adaptive Problems", Northeast Parallel Architecture Center, Syracuse University, **Northeast Parallel Architecture Center Technical Report**, 1994.
19. A. Sussman, S. Gupta, K. Crowley, and J. Saltz(1993), "A Manual for the Multiblock PARTI Runtime Primitives", Institute for Computer Application in Science and Engineering, **NASA Langley Research Center Technical Report**, Revision 3, 1993.
20. A. Pothen, H.D. Simon and K.-P. Liou(1990), "Partitioning Sparse Matrices with Eigenvectors of Graphs", **Siam Journal on Matrix Anal. Appl.**, V11, N2, July, 1990, pp. 430-452.
21. A.M. Tentner, R.N. Blomquist, T.R. Canfield, P.L. Garner, E.M. Gelbard, K.C. Gross, M. Minkoff, and R.A. Valentin(1994), "Advances in Parallel Computing for Reactor Analysis and Safety", **Communication of the ACM**, V37, N4, 1994, pp. 55-64.
22. A. Zaafrani and M.R. Ito(1993), "Partitioning the Global Space for Distributed Memory Systems", **Supercomputing**, Nov. 1993.
23. H. Zima, H.-J. Bast and M. Gerndt, "SUPERB: A Tool For Semi-automatic MIMD/SIMD Parallelization", **Parallel Computing**, V6, 1988, pp. 1-18.

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TOOKUIL: A Case Study in User Interface Development for Safety Code Application

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Abstract:

Traditionally, there has been a very high learning curve associated with using nuclear power plant (NPP) analysis codes. Even for seasoned plant analysts and engineers, the process of building or modifying an input model for present day NPP analysis codes is tedious, error prone, and time consuming. Current cost constraints and performance demands place an additional burden on today's safety analysis community. Advances in graphical user interface (GUI) technology have been applied to obtain significant productivity and quality assurance improvements for the Transient Reactor Analysis Code (TRAC) input model development. KAPL Inc. has developed an X Windows-based graphical user interface named TOOKUIL which supports the design and analysis process, acting as a preprocessor, runtime editor, help system, and post processor for TRAC. This paper summarizes the objectives of the project, the GUI development process and experiences, and the resulting end product, TOOKUIL.

1.0 Introduction

The majority of present day computational tools used for nuclear power plant systems and safety analysis share some common characteristics. They are fairly general in their applicability and system representation capabilities. They have a great many options which can be invoked (typically on the order of 1000). There are many interdependencies among the options, the various system modeling features, and engineering objectives. These characteristics, while necessary for accurate and effective nuclear power plant (NPP) system modeling, result in a very large number of input parameters and an extremely complex set of rules for generating these input. Traditionally, NPP and safety engineers have had to manually sift through large quantities of data, learn and understand volumes of manuals, and build a high level of expertise in applying manual rules, interfacing with computer operating systems, and processing input and output. The end result is that the cost of modeling and analyzing NPPs is very high. Minimizing the cost (resources) associated with such efforts while maximizing analysis quality is critical to effectively carrying out these tasks.

This paper presents an effort undertaken by KAPL Inc. to improve plant analysts' productivity and model/analysis quality assurance when using the Transient Analysis Code (TRAC, developed

at the Los Alamos National Laboratory) (see References 1 and 2). KAPL Inc. has invested in the development of a graphical user interface (GUI) for TRAC called TOOKUIL because, as numerous studies have shown, GUI technology significantly improves productivity and reduces the number of errors compared to standard text editing. TOOKUIL is a combination of computer programs and methods for enabling the engineer to effectively interact with computer systems. It provides a more intuitive approach to model development and has the ability to incorporate TRAC modeling expertise. Furthermore, TOOKUIL supports the engineer throughout the entire power plant analysis process from input model development to processing and visualizing the output.

The TOOKUIL user interface was developed following a software development life cycle, whereby user needs and requirements are defined; a conceptual design is developed and implemented as a prototype; a final design is coded, tested and released to the user community; and the end product is supported and enhanced as dictated by user needs. The TOOKUIL development process is described in further detail, along with KAPL's experience with graphical user interface development.

2.0 What is a Graphical User Interface

With the advent of window based interfaces, more computer programs are providing graphical user interfaces. A graphical user interface (GUI) uses one or more windows, or panels, to present and collect data. A variety of graphical objects, such as push buttons, scrolled lists, menus, toggle buttons and sliders, may be used to present data. The user interacts with these objects using the mouse and keyboard. The GUI gathers information and passes it on to the underlying program.

A GUI often extends beyond the capabilities of the analysis program to which it is coupled. This extended functionality can include encapsulating expertise for making the system easier to use, adding features to support the whole analysis process, providing an extra layer of quality assurance and quality control, and enhancing data and file management to reduce user burden.

A GUI is not a glorified text editor. Rather, a GUI interprets & analyzes (parses) the input file, has encoded knowledge of the input manual logic and is able to create/interrogate interrelationships among the data as required. It can write various formatted output files for use by the analysis code, data post-processors, visualization tools, etc. Because it has knowledge of the data and logic, expert systems-type functions may also be incorporated to help users with modeling and analysis decisions.

2.1 Ease of Use

The NPP analysis process typically requires the engineer to describe the power plant configuration, geometry, initial conditions, specialized component actions and boundary conditions, and the power plant control system. This information is usually conveyed to the analysis program via a text file containing thousands of lines of input data. Dealing with this large and complex data file presents an array of issues related to data management, intuitiveness, change control, model sharing and the like.

A GUI can be used to organize and present data in a more intuitive manner. For example, an engineer may define a model by drawing a schematic rather than entering blocks of numerical data. This makes it easy to see relationships among model components and the total plant layout. Each component in the schematic can be automatically populated with default data. Model data can be entered through pop-up windows. These pop-ups can be organized to present data in a logical manner. The user interface can dynamically check the data being entered to make sure it is valid and also to determine if there is a relationship between the entered value and other input values. If the entered value causes additional information to be needed, the user can be prompted accordingly.

A GUI can also provide a mechanism for sharing data and supporting top-down design. For example, a component library may be used to supply a standard set of components from which users can build their models. The component library may also include customized components and submodel components. These specialized components can be developed and shared among power plant analysts.

A good GUI provides support for multiple levels of users. Access to functions via menus is useful to the novice user, whereas keyboard shortcuts are convenient for the advanced user. On-line help, tutorials, and guidelines can help users get started or obtain additional guidance during the modeling process.

Another major benefit of a GUI is that it eliminates the need to understand the input file formats and interact with the computer operating system. Once the input has been entered, the required input files for the analysis code as well as geometry information for later post-processing/visualization can be automatically generated. Options for running the analysis program can be included so that the engineer does not need to leave the user interface environment in order to make runs. This can include capabilities for running the program in a batch mode. In this case, the required job control information is automatically generated. The engineer is not burdened with details of creating input files, job control files, and interfacing with the computer on which the analysis is run. The engineer's time is spent doing engineering rather than data processing.

2.2 Support for the Plant/Safety Analysis Process

A well designed GUI creates an environment that supports and seamlessly integrates with the analysis process. This process includes researching and creating models, making numerous sensitivity runs to evaluate changing model conditions, processing and interpreting the output, and documenting the findings. It also includes managing changes to the input model, tracking and managing input and output, and managing links to databases and other components of the analysis process. It may also include linking/integrating the target analysis code with other codes in the overall analysis process.

The task of creating a model may require research into what models have been created in the past and it may also require information from other design and analysis programs. The model building task can be supported by providing access to sources of information such as a database of existing models (e.g., CAD systems) or results from other analysis programs. The user interface can also include a library of standard components, specialized components, submodels and models to use

as building blocks. Artificial intelligence and expert system technology can be utilized to help the engineer build the model more intelligently and to guide the analysis process.

As an engineering tool, a key feature of a safety code GUI is to be able to generate and run parametric cases from a base case model. The base case model may be a plant operating at steady-state. The parametric capability can be used in many different ways. For example, the parametric runs may restart from the steady-state calculation and perform multiple variations of a given transient scenario. Another possibility is that parametric runs use the steady-state restart as a starting point to reach other steady-state operating conditions. The parametric capability may be used to adjust plant operating conditions for a given plant model or may be used to adjust the plant model itself (i.e.- geometry, component characteristics, etc.) for a given operating condition or transient scenario. Consequently, the GUI needs to be flexible enough to adjust multiple input parameters for each parametric case yet remain simple enough for the user to easily understand what parametric studies have been defined and saved. The GUI can directly support the Code Scaling, Applicability and Uncertainty (CSAU) methodology (Reference 5) by automating the calculational matrix for the sensitivity analysis. Such calculational matrices can be made up of hundreds of runs. Each of the runs adjusts input parameters or combinations of parameters over their uncertainty ranges.

The parametric analysis can be further enhanced by integrating optimization software and artificial intelligence technology. This software is particularly useful in the design process where one needs to evaluate the results from a given run, adjust appropriate input parameters and perform further runs so as to arrive at the desired design configuration. It can also be useful in a probabilistic risk assessment role by having the system automatically search for the worst case accident scenario.

A GUI can also improve overall process efficiency by facilitating the coupling of the plant/safety analysis to other analyses. For example, the plant/safety analysis code may be used to drive downstream calculations such as detailed Computational Fluid Dynamics (CFD) calculations or structural analyses. The GUI automates the process of gathering the appropriate output from the plant analysis and coupling it to the downstream analysis. Furthermore, the GUI can be made to automatically initiate the downstream jobs and process their output as well.

Post-processing is another area in which GUIs are useful. The output generated by safety analysis codes is large and not always easy to read. In some cases, the output is in binary format, so that the only way to get at the data is via another program that extracts the data and creates an ASCII file. These output files generally require the engineer to sift through large quantities of numbers and do not give the him/her a clear picture of what is happening in the model. A GUI can solve this problem by reading the output data file and presenting it to the user in an understandable manner such as an x,y plot, contour plot, or a 3-D animation. Access to third party or proprietary visualization and analysis tools can be provided without the user ever leaving the user interface environment. The GUI can be coupled to a statistical software package, as well, for generating performance fits and response surfaces. The user is freed from having to know the numerous file formats used by these visualization tools or how to access these tools. Rather than spending a great deal of time scanning numerical output files, the engineer is able build a deeper understanding of the phenomena and processes occurring in the power plant.

2.3 Quality Control and Quality Assurance

Quality control and quality assurance are important issues when dealing with safety analysis codes. One reason for this is the size and complexity of the input files. A change to a single parameter can change the input requirements for other portions of the model. Checking for data dependencies and making sure a model is correctly and consistently specified is a cumbersome process which can easily be performed by a GUI. As the engineer enters parameter values, a GUI can check the validity of the value and its impact on the model's input requirements. Visual cues, such as prompts or highlights, can be used to indicate changes to the input required. Model inputs often consist of table or array data. Entering this data into a text file is tedious and error prone. A user interface can make this task easier by providing functions to read data from various sources such as files, databases, or other tables. Visualization techniques such as x,y plots or contour plots can be incorporated right into the input pop-up to help the user verify array or table data being input. These features help guarantee correct model input.

Safety analysis codes often contain redundant information. For example, the user may be required to input parameters that could be derived from other input parameters. The user must ensure these parameters are always consistent. A change to one requires a change to the other. Redundant information is often contained in component boundaries. For example, the flow area at the end of one component must match the flow area of the component to which it is connected. A GUI can reduce the amount of redundant data by automatically calculating derived values and updating duplicate values.

Building an input model to an NPP code such as TRAC requires the user to translate a set of plant characteristics into a set of parameters that the safety analysis code understands. This translation process may not be intuitive since there may not be a direct mapping of physical characteristics to model input. The plant analyst may have to set many parameters in order to achieve a single model characteristic. A GUI can help the user by providing a standard set of components with default values from which they can build their model. User defined components having specific characteristics can be added to the standard set. The interface can provide on-line help to guide the user through the model building process. A more sophisticated user interface may incorporate expert system technology so as to allow the engineer to specify higher level or physically based characteristics. The interface then automatically generates the representation required by the NPP code.

Query tools and report generators can be provided so that the user can quickly view the input data. Methods can also be incorporated so that the model is self documenting. In addition to user comments/documentation and the general input variable annotation, facilities can be developed within the GUI that interpret the model input, particularly hardware action scenarios, and print a report describing the sequence of events that are set up in the model. This capability is particularly useful for archival purposes.

3.0 TOOKUIL: A Case Study

TOOKUIL is a graphical user interface developed by KAPL Inc. for the Transient Reactor Analysis Code (TRAC) (see References 3 and 4). This GUI was developed to support the design

and analysis process by providing features for creating TRAC models, running TRAC calculations, managing the resulting output files, and post-processing the output data.

3.1 TOOKUIL Features

The TOOKUIL Main Window is shown in *Figure 1*. It consists of a component library containing the standard TRAC components (e.g., pipe, valve, tee), an "infinite" workspace for drawing a model schematic, and a message window in which warning, error and status messages are printed. At the top of the Main Window is a menu bar that provides functions such as opening and saving models, editing global options, running TRAC, opening on-line documentation and accessing post-processing tools. References (3) and (4) provide detail on the functionality of the Main Window.

Once a model is complete, the engineer can run a TRAC calculation using the model by selecting the Submit option from the Runtime menu (*Figure 2*). The user specifies runtime options such as where to run the TRAC job and where to store the resulting output files. The ability to perform restart calculations is also supported through the submit window. A restart selection pop-up window allows the user to specify which components in the model (if any) are to be resupplied (i.e - redefined) for the transient restart calculation. The components selected to be resupplied are highlighted in the model schematic (Main Window). Before submitting the TRAC job, TOOKUIL checks the model to make sure all required inputs have been specified. Finally, TOOKUIL provides tools for monitoring the progress of jobs that have been submitted.

Once a model is run, the engineer needs to evaluate the results and make decisions based on these results. TOOKUIL provides automated links between the TRAC graphics file and various data visualization and processing tools. The TOOKUIL Output Processor (*Figure 3*) displays a list of the graphics data available from a specific run (the graphics data catalog). The user selects the data to be extracted from the graphics file and specifies how to format this data. The Output Processor extracts this data from the graphics file and reformats it as appropriate. Post-processing and visualization tools (*Figure 4*) are then accessed automatically from within the TOOKUIL Output Processor.

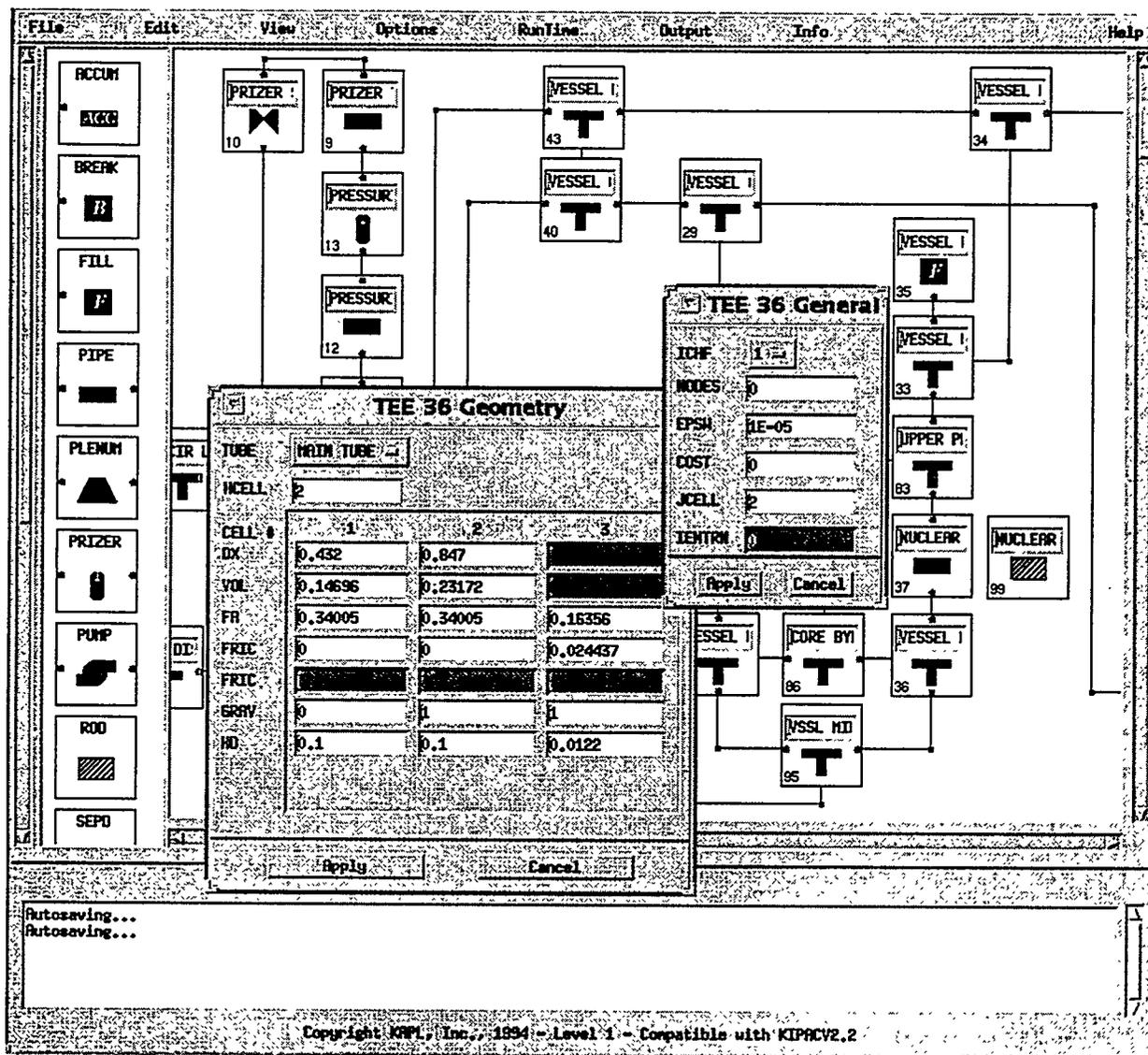


FIGURE 1. TOOKUIL Screen

Submit Info	
Job Control Options	
Machine	C90
Queue	a_default
Time Limit	24
Input Options	
<input type="checkbox"/> Restart	Select Components to Resupply
TRCRST Filename	crst
Output File Options	
Ascii Path	*HOME/loft
TRCOUT Filename	trcout
TRCMMSG Filename	trcmmsg
TRCCBF Filename	trccbf
STDOUT Filename	stdout
DAYFILE Filename	dayfile
INLAB Filename	inlab
Catalog Filename	catalog
Binary Path	*HOME
TRCDMP Filename	trcdmp
TRCGRF Filename	trcgrf
Prefix	User Defined loft.
Suffix	None
XY Plotting Options	
KEX Plot Job File	tecplot.ex
Plot Format	TECPLOT PLOT1/PS PLOT1/Xerox
EJN Plot Dir	*HOME/loft/plots
<input type="button" value="Set Defaults"/> <input type="button" value="Apply"/> <input type="button" value="Cancel"/>	

FIGURE 2. Runtime Editor

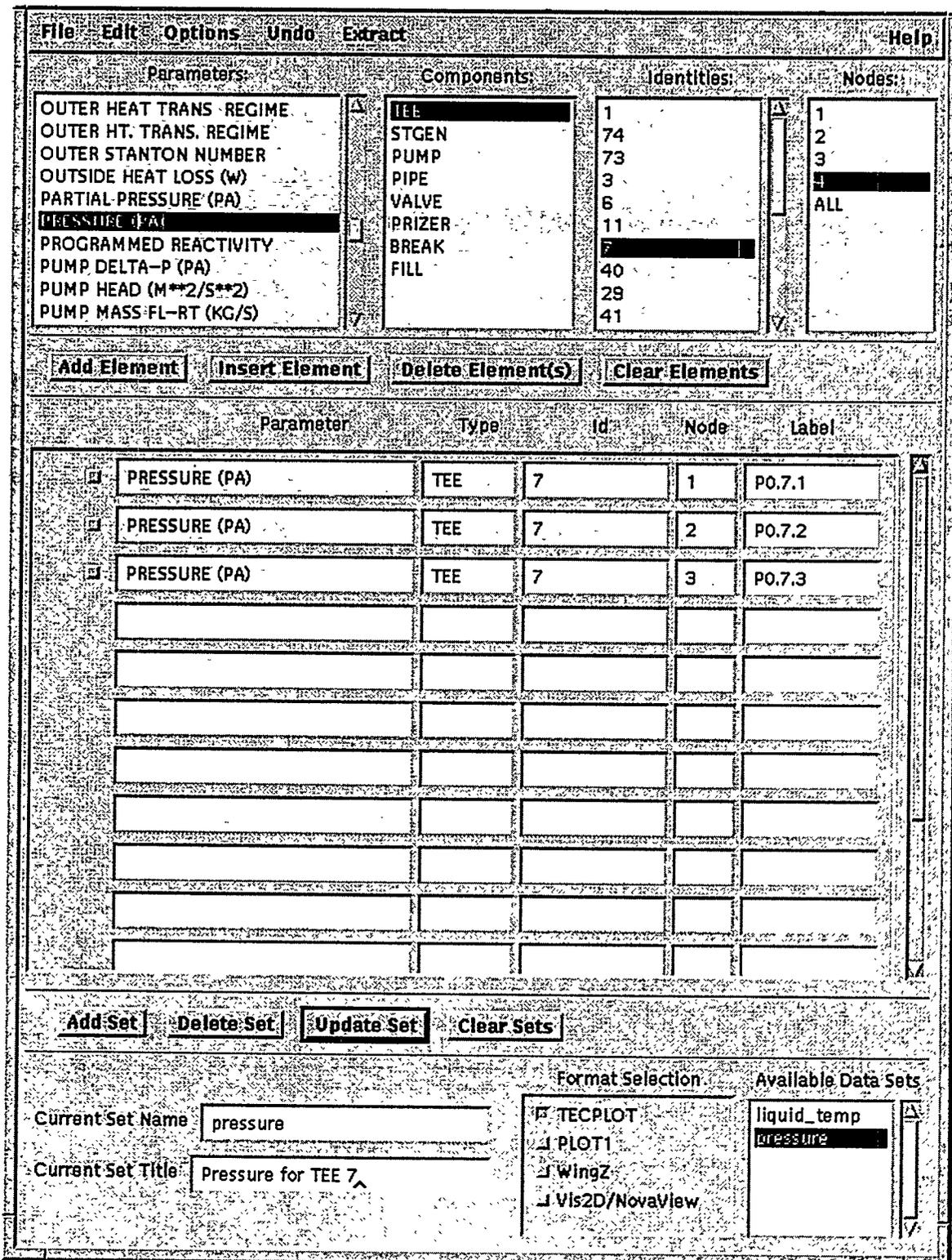


FIGURE 3. TOOKUIL Output Processor

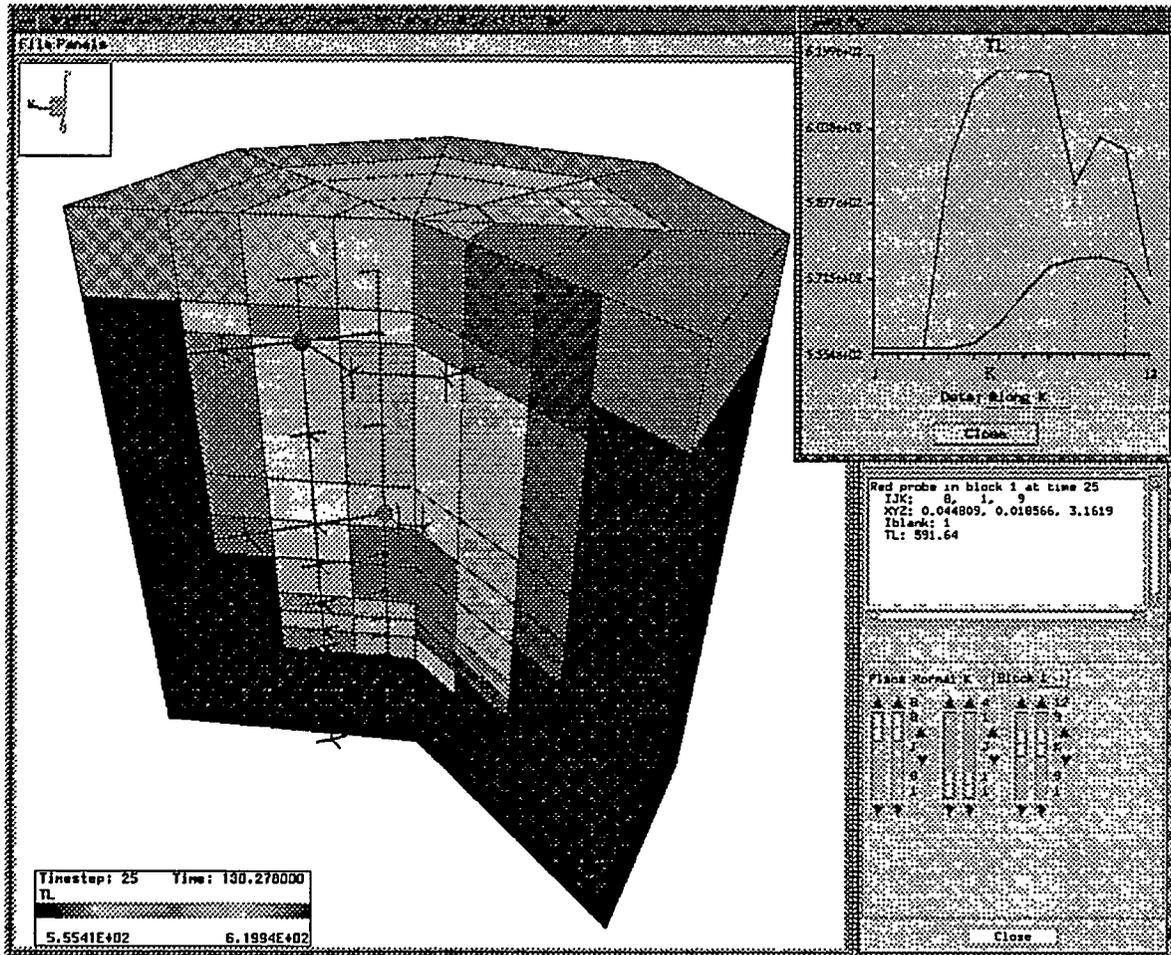


FIGURE 4. 3-D Visualization of TRAC Output Data

3.2 TOOKUIL System Summary

TOOKUIL is a stand-alone program running in a UNIX environment. In its current configuration, there is no direct (i.e. interactive) communication between TOOKUIL and TRAC, which can be run on super-computers or workstations. TOOKUIL generates a TRAC input file and invokes TRAC via a batch queuing system. All job control information is handled by TOOKUIL so that input and output files are transferred and stored correctly.

TOOKUIL, which was implemented in C, uses the X Window System and Motif widgets to perform all graphical user interface capabilities. The GUI requires the X11R5 version of the X Window System. It has been implemented and tested on both Sun and SGI workstations.

3.3 TOOKUIL Data Flow

Figure 5 shows how data flows through the TOOKUIL system. The annotation in the figure shows the order of the data flow. (1) The TRAC model is created via TOOKUIL. This model may be created interactively by reading in an existing TRAC input file or accessing TOOKUIL model

files. (2) When the Submit option has been selected, TOOKUIL generates a TRAC input file and job control file. These files are transferred as appropriate to the computer on which TRAC runs. TRAC will read in the input file, which may be a base model file or a restart file. (3) TRAC produces several ASCII and binary output files. The binary files are generally stored on the machine on which the run was made. The ASCII files are returned to the engineer's workstation area. (4) If the user wishes to use TOOKUIL's Output Processor, an extraction job is run to extract a catalog of graphics information. (5) The catalog extraction program generates an ASCII catalog file that is returned to the user's workstation. This catalog is then loaded into TOOKUIL's output processor. From the output processor window, the engineer can select the data to be extracted and specify the data formats. (6) The output processor runs a second extraction job to extract and format the requested data. (7) The formatted data files are returned to the workstation, where they may be loaded into the appropriate post-processing tools.

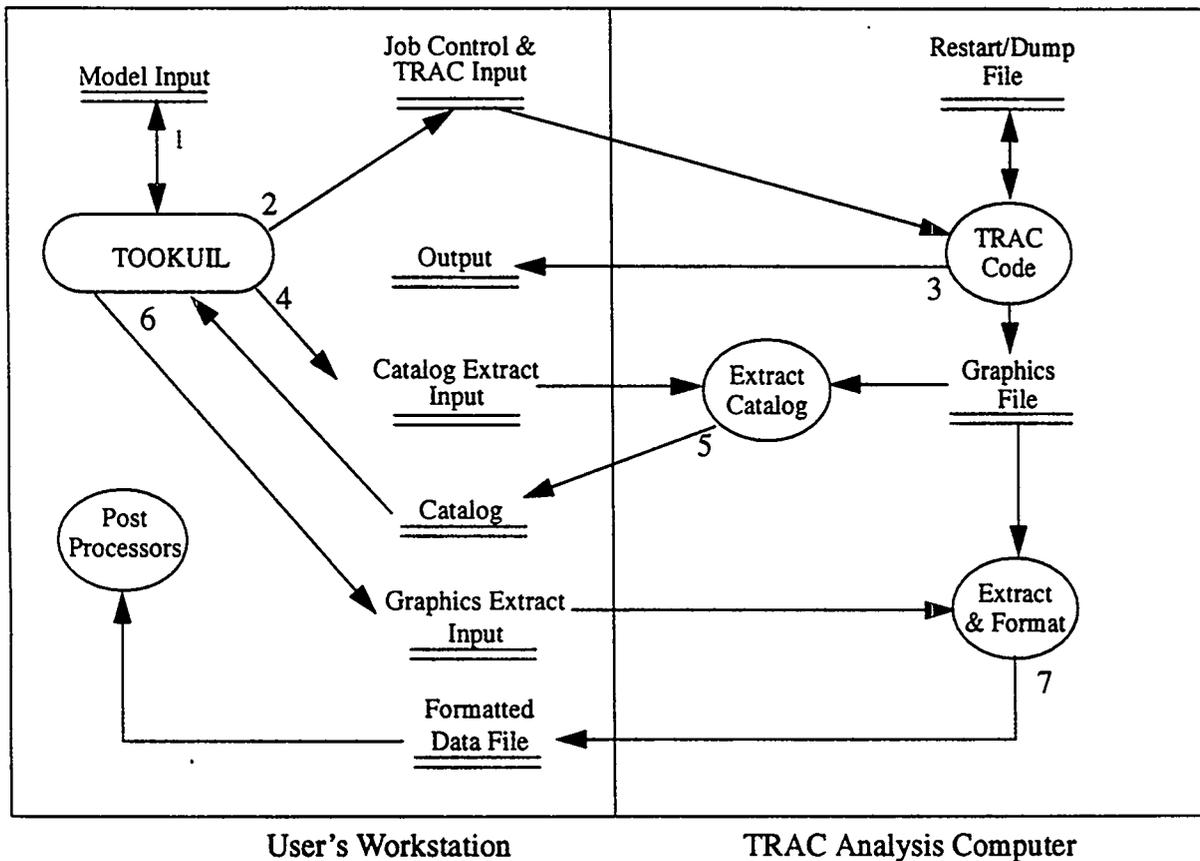


FIGURE 5. TOOKUIL Data Flow

4.0 TOOKUIL Development Process and Lessons Learned

There are many textbooks that define software development methodologies. The standard software development life cycle roughly follows the following steps: (1) user needs and requirements are defined; (2) a conceptual design is developed and implemented as a prototype; (3) a final design is defined and coded; (4) the software is implemented and released to the user community, and (5) the software is continuously supported and enhanced as dictated by user

needs. Throughout the process, the software is tested and user input is sought. In practice, the lines between the steps of the development process are blurred, particularly once the software is initially released. It should be noted that if existing GUI products are available to use as the starting point for further development, the upfront phases of the process may be substantially reduced.

4.1 Defining the Project Team

The first step in any development effort is to pull together the project team. This team will most likely evolve over time. The team should include someone knowledgeable about the safety code and how it is being used within the safety analysis community. The team also needs someone with knowledge about graphical user interface technology. It is useful to have a team member who is familiar with current industry trends and software development tools. Software project management, database, and visualization/post-processing tools skills and knowledge may also be required. In the earliest phases of design, the team is best kept small in order to effectively manage their work. Once the project has been defined, it may be useful to have additional programmers, depending on the size of the project and the schedule.

The TOOKUIL development team consisted of two software engineers familiar with GUI development, a lead engineer responsible for overall project management and an engineer familiar with the details of TRAC use. During the early stages of TOOKUIL development, this team proved to be very effective.

4.2 Process and Requirements Analysis

A big step when designing any software system is to understand the safety analysis process and how the GUI can/should fit into that process. Because many different communities may use the safety analysis code in different ways, the project team must be sure to get input from all of these communities. During this stage, the project team can identify parts of the existing process that may be cumbersome or unnecessary and redefine the process to eliminate these items. The team also needs to determine if the GUI will be specific to a particular safety analysis code or if it will be capable of interfacing with multiple codes.

Another part of requirements analysis is determining hardware and software interface requirements. Some of the questions that need to be addressed include: (1) how is the GUI going to be coupled to the safety analysis code and how will they communicate; (2) are there any other external programs that the GUI must interface with such as a database; (3) from what hardware will the user be accessing the GUI; (4) will the GUI be implemented on a computer network; and (5) what potential hardware platforms may be used in the future and what operating systems and software will this hardware be using? Other issues which need to be addressed at this stage include the organization's policies toward use of third party software and software support, protection of proprietary information, and access to the Internet. All these issues can greatly impact the GUI implementation.

Once the process and requirements are understood, a formal requirements document should be written. This document must be reviewed by the user community to ensure that nothing is missing and that the process and requirements are understood by the project team.

During this stage, the TOOKUIL development team worked with TRAC users at KAPL to understand how TRAC was being used. Some of the requirements that came out of these discussions included the ability to more easily generate a correct TRAC input file, reduce model development time while increasing quality, and provide easy mechanisms to run TRAC, including support for parametric studies. Portability across UNIX workstations was also required. This led to the decision to use X/Motif to develop the GUI rather than a proprietary windowing toolkit. User requirements did not dictate the need for the GUI to interact with the code while it was executing. Thus, TOOKUIL was designed for a batch interface with TRAC. It generates a TRAC input file and provides post-processing for TRAC output. It was also determined that TOOKUIL would initially only provide an interface specific to the TRAC code. The TOOKUIL team generated a comprehensive requirements document that was reviewed by the current user community.

4.3 Conceptual Design

During this stage, the project team must determine how the GUI will meet all the requirements identified in the previous stage. This is the most creative stage of the development process. A small core of developers and users (i.e. users of the safety code) discuss how the GUI might look. There are usually several radically different proposals and "whiteboard" designs. Early decisions such as hardware platform(s), operating system platform(s), etc. are formulated during the conceptual stage. The various approaches are presented to users for feedback. Often, "storyboarding" is used to walk users through each conceptual GUI. These storyboards may be in the form of pictures or prototypes. During this stage, the users and developers can make sure that all the requirements are adequately met.

4.4 Prototype

Once the developers have an idea of how the GUI should look, they may need to do some "proof-of-concept" prototyping. This allows the development team to try out new technology, development tools, and get an idea of what works and what does not. A small subset of the features of the safety code are actually modeled in the prototype and error checking and recovery are not considered (unless that happens to be part of the feature scope). Besides giving developers a test-bed for trying different ways of implementing GUI features, a prototype gives users an early opportunity to test drive the system and provide feedback.

There are several important decisions made during the prototyping stage regarding platform as well. This stage will most likely determine the implementation (programming) language for all further development, the mechanism for interfacing with the GUI platform (i.e. X-Windows library calls, 4GL GUI builder, etc.), and internal data organization, representation, and management. The selection of programming languages and tools should also consider the potential effects of using proprietary software on the longevity of the GUI. The prototype stage will also, formally or informally, introduce the beginnings of the application style.

TOOKUIL started as a prototype. The initial version included just the PIPE, BREAK and FILL components of TRAC. The intent of the prototype was to try out different methods of drawing a schematic using Xlib and Motif. This prototype became the basis for the production version of

TOOKUIL. Because the prototype initially dealt with very simple TRAC components, the development team ran into some obstacles when some of the more complicated components, such as the heat structure, were developed. This required major rework that could have been avoided if the time had been taken to develop a more comprehensive design. In addition, the functions for displaying pop-up tables were developed specifically for inputting geometry data. It was difficult to use these functions for creating more general purpose tables. As a result, TOOKUIL contains many different routines for creating tables. In hindsight, it would have been helpful to identify the generic objects needed for the GUI. This experience made it apparent that a fair amount of design work needs to be done in the prototype stage. A prototype should not necessarily include the easiest elements to implement, but rather those elements that may be the trickiest. Error handling must be included during this stage because it is very difficult to back fit it into the code.

4.5 Initial Development

The prototype is usually used for demonstrative sessions with users and management. After prototyping, initial or "Phase-I" implementation begins. The term "Initial" is used here because it is usually not realistic to produce a working GUI that meets the entire set of requirements in the early releases. The initial implementation expands the prototype in scope to include enough features to run the safety analysis code. During this stage, added error checking makes the GUI more robust. As with the prototype, user feedback is very valuable at this stage and is one of the principle reasons for this development stage. The user feedback obtained during this stage may actually change the requirements or at the very least, the method of implementation for some of the requirements.

Undoubtedly the most difficult step in the initial development stage is deciding which of the features identified in the requirements analysis stage to leave out of the GUI. The importance of different features can vary dramatically depending on the user and how they are using the analysis code. For example, some users may have very complex models and require extensive model building capabilities. Other users may need to make hundreds of runs so runtime features, such as support for parametric studies and data management, take a higher priority. Another set of users may need output processing support for report generation.

The TOOKUIL initial development effort has incorporated most of the features necessary to create a model, run TRAC and perform 2-D and 3-D visualization and spreadsheet related post-processing. Features include reading an existing TRAC input file and converting it to TOOKUIL model files, building a schematic of the model, automating TRAC input manual logic in the data entry panels, TRAC input file generation, and TRAC job submittal and data access tools for use in post-processing. Data entry panels were developed for the most commonly used components. Components such as the TURBINE and VESSEL, as well as TRAC control procedures, were implemented as text editors in which the user was required to enter the component data by following the TRAC input manual specifications. Other features that were also put off for future development included several schematic editing features such as zooming and group editing, more sophisticated model checking and model management, schematic-based control procedure definition, and support for parametric runs.

TOOKUIL development during this stage progressed more slowly than the prototype development. There is much more to a GUI than appears on the screen. Most computer-aided GUI

development tools can improve the developer's productivity when designing the layout of a GUI. However, the development team must still contend with designing efficient data structures; memory management logic; input file parsing and generation logic; cut, copy, paste, drag-drop, and undo logic; file management (i.e. autosave, creation of backup files, etc.); and the like. All of this development must be done and maintained regardless of the complexity of the GUI's interface with the user. Thus, there was a relatively large initial development cost to arrive at TOOKUIL's current level of capability. Future enhancements, however, do not need to incur such a heavy cost, as they can build significantly off of the existing infrastructure.

Prior to the initial release, TOOKUIL was tested out by the development team. This testing focused on two major categories. First and foremost, the TRAC features that were implemented in TOOKUIL were tested to show that they were indeed operational. The members of the development team that were experienced TRAC users were crucial for this testing. The second type of testing performed by the development team focused on trying to find incomplete logic (i.e. trying to break the system). This involved performing operations in various sequences, pressing various key sequences, etc. Many bugs were found and eliminated through this testing. At this point, TOOKUIL was released to a subset of users. These power plant analysts were used to identify bugs which could only be found through real production use. This stage is extremely valuable and close user-developer interactions are key to its success.

Once the first version of TOOKUIL was released, several things became apparent. First and foremost, the GUI had a significant positive impact on bringing new users up to speed on the code. TRAC is a very complex code and the manuals are daunting. TOOKUIL encapsulates the manual logic/requirements within it and helps guide new users in model creation and data post-processing. However, the initial release of TOOKUIL met with a significant level of resistance from engineers who were experienced with using TRAC. These users were/are very proficient at editing the input deck by hand (with a text editor), interfacing with the various computer operating systems, and utilizing the available post-processing tools. Initially, the GUI actually slowed down these experienced users. Furthermore, these users also utilize the safety code in an advanced (efficient) manner that was not supported by initial releases of the GUI. The experienced users desired features such as model management, parametric analyses and expert systems type capabilities, many of which are being worked on now. Most of the users issues associated with the initial release of TOOKUIL have been resolved. Advanced development work is proceeding in parallel with production use of the GUI.

Finally, a ripple effect of the release of the GUI was that new development essentially stopped for a period of time following the first release of TOOKUIL. During this period, a great deal of time was spent fixing bugs and helping users learn the new system. Team members spent a lot of one-on-one time with users as well as giving group demonstrations. A walk-through tutorial in the TOOKUIL User's Manual would have been helpful for users who were basically familiar with the TRAC code and creating TRACIN files.

4.6 Advanced Development

Initial development work is focused on getting a robust, capable working system into production. Once the GUI has been in production for a period of time, the developers get a sense for what the next step should be. The next set of features to be implemented can be identified and an

implementation plan developed for the next set of releases of the GUI. During the more advanced stages of development, more consideration can be given to issues such as process integration, integration with other codes, model data management, version control (of both the safety code as well as the GUI), model sharing, etc.

These considerations are very broad in scope and difficult to design in adequately during early development stages. However, once this advanced point in the development cycle is reached, substantial system changes are more difficult, costly, and functionality may need to be downgraded through compromise. During advanced development phases, user needs are reassessed, development priorities are solidified, and functional capabilities updated to incorporate key computer system and safety code upgrades that have occurred. This work often must take precedence over larger usability related development tasks. As usage grows, the development plans must begin to consider legacy data where they had not previously. Coupling the GUI to the design process or implementing a data management scheme may require changes to the storage of both the data for the safety code as well as the enhancing data the GUI captures and maintains. It must be decided whether the GUI will be backward compatible with these older formats or whether a conversion utility should be developed. Incorporating advanced functionality becomes increasingly complex.

TOOKUIL is currently in an advanced development stage of its life cycle. Most of the basic model building capabilities exist, along with support for running TRAC and performing data post-processing functions. TOOKUIL fully parses the input deck and all user manual logic has been encoded. This positions the GUI to implement expert system type functions to act as an Engineering Assistant. TOOKUIL has the potential to act in an interactive manner with the code as dictated by user requirements. TOOKUIL has access to substantial 2-D and 3-D post-processing capabilities and tighter integration between the model generator and these visualization tools is possible. The data structures in TOOKUIL are designed for implementation on top of a database (library) of component/model information which will facilitate additional user capabilities and increased configuration control of modeling information. A model validation database was implemented which uses a commercial database system (Oracle) and TOOKUIL's knowledge of the data in the verification model database to dynamically assess a user's model against the base code validation matrix. Model diagnostic information is also available to help users assess the complexity of their model against others of a similar type. TOOKUIL's schematic drawing capability also lends itself for use as an interactive control procedure generator to automate use of the TRAC signal variable and control block input.

During the advanced development phase, there is increased pressure on the development team due to support/maintenance related needs. In order to keep both production code support and development moving forward concurrently, it is crucial to ensure that the development team is staffed properly and has the necessary mix of skills (e.g. GUI programming, safety code use and model building, data management, process integration and mapping, and software development for maintainability).

4.7 Software Validation

Verification and testing of an interactive GUI such as TOOKUIL is a challenging task. The process is dependent upon the type of capability to be tested. There are two primary categories of

capabilities which require different types of testing. The first is a change to TOOKUIL to support enhancements to the underlying code, TRAC. The second is a change to elements of the GUI which are independent of TRAC. In both cases, modifications are tested individually and in conjunction with other modifications and the base code.

Modifications to TOOKUIL to support new features in TRAC require several common types of changes and as such, several common testing procedures. Typically, new TRAC modifications require a new input. The internal data structure in TOOKUIL needs to be modified to include a place to hold the value of this input. The routines that parse and build the input deck (TRACIN) must be modified to understand this value and write it out properly. These changes are usually made before any GUI elements of TOOKUIL are changed. This allows for easier testing since this portion can be coded, compiled and tested completely without significant GUI changes. Once the new input is able to be read in from the input deck, stored internally, and rewritten to the input deck, the changes to the GUI can begin to allow the user the ability to view / update the value of this input. Once completed, this new GUI input field capability can be verified visually and through inspection of the resultant input deck.

There are numerous routines in TOOKUIL that define the characteristic nature of the system and are not related to TRAC input model options. For example, the routines that generate a pop-up dialog for querying geometric inputs from the user or routines for cutting and pasting components are TOOKUIL features that have no bearing on the nature of the communication with TRAC. Changes of this nature to portions of the system that are used in only one location of the GUI are relatively simple to test. For example, when rearranging the layout of a pop-up dialog window, testing the changes can be done by displaying the window. If however, a generic routine was developed to automatically layout a pop-up dialog window, a change to this would require more testing. Cut and Paste logic is an area that is generic to all components but requires extensive testing. This logic must account not only for the differences between the component types, but must also account for the states of the components. For example, if the user attempts to "Cut" out a component and a pop-up window associated with this component is currently open, the cut logic must be able to detect the presence of this window and know how to eliminate it.

The overall validation process involves several steps. The first level of testing is referred to as unit testing. Unit testing is how the individual programmers test specific code modifications. Typically a release of TOOKUIL involves the integration of several modifications, potentially from multiple developers. Prior to a release of the system, the developers use the system with all of the changes integrated and retest specific updates as well as many of the (base) general system functions. This is usually referred to as an integrated system test. The purpose for this is to ensure that the modifications from the multiple enhancements do not conflict with each other or improperly impact other GUI functions. After an integrated system test, the system can be given to users for testing. TOOKUIL development has typically made the new version of the system available for a limited number of users initially for a Beta testing period. Following successful completion of user testing, the system is then released for production use.

5.0 Summary

It is generally recognized that a well organized and functionally comprehensive graphical user interface can significantly improve the productivity and quality assurance of data entry and processing tasks. This observation provides the rationale for the development of an integrated graphical user interface for nuclear power plant and safety analyses codes such as TRAC. An overview of the requirements and potential benefits of a TRAC GUI have been discussed in this paper. A graphical user interface developed by KAPL, TOOKUIL, has been described and the development process reviewed in terms of TOOKUIL's requirements, architecture, key features, and implementation. TOOKUIL provides an integrated environment for engineers to build a TRAC input model, interface with computers in a client/server environment, and process and visualize analytic results. Stages of the development process include team formation, process/requirements analysis, conceptual design, prototyping, initial development, and advanced development. Key components in a successful GUI development effort include development of a detailed and comprehensive design which accurately addresses both short-term and long-term requirements, constant user review and feedback during all stages of the process, and proper project staffing, including both number and skill mix.

REFERENCES

- [1] N.M. Schnurr, et al., "TRAC-PF1/MOD2 Code Manual User's Guide," Los Alamos National Laboratory, Los Alamos, New Mexico (1992).
- [2] J.C. Lin, V Martinez, J.W. Spore, "TRAC-PF1/Mod2 Developmental Assessment Manual," Los Alamos National Laboratory, Los Alamos, New Mexico (1993).
- [3] A.E. Kelly, "Development of an Interactive Model Generator for the TRAC Plant Safety Analysis Code," Transactions of the American Nuclear Society, 71, 554-558 (1994).
- [4] A.E.Kelly, C.K. Harkins, R.J. Smith, "Development of a Graphical User Interface for the TRAC Plant/Safety Analysis Code," Proceedings of the 7th International Meeting on Nuclear Reactor Thermal-Hydraulics NURETH-7, NUREG/CP-0142, Vol. 3, 2003-2010 (1995).
- [5] B.E. Boyack, et al., "Quantifying Reactor Safety Margins: Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large-Break, Loss-Of-Coolant Accident," Idaho National Engineering Laboratory, Idaho Falls, Idaho, NUREG/CR-5249 (Dec 89).

REQUIREMENTS FOR A MULTIFUNCTIONAL CODE ARCHITECTURE

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Abstract

The present paper studies a set of requirements for a multifunctional simulation software architecture in the light of experiences gained in developing and using the APROS simulation environment.

Introduction

The huge steps taken in the development of computer hardware and software during the last ten years are changing the status of the traditional nuclear safety analysis software. The affordable computing power on the safety analysts table by far exceeds the possibilities offered to him/her ten years ago. At the same time the features of everyday office software tend to set standards to the way the input data and calculational results are managed.

The current needs for a nuclear safety analysis code are not any more limited to correctly predicting the plant primary circuit behaviour in certain anticipated operating conditions. A large number of possible severe plant transients start from minor malfunctions in automation or electrical power supply systems. These systems affect the plant behaviour significantly through the secondary systems often left outside the scope of the typical safety analysis.

Additional features would include a possibility to use the same software as a tool for plant design and personnel training. Design data including actually used decision criteria might also be part of the information collected during the plant model life cycle and used in planning plant modifications and in training plant personnel.

Therefore a multifunctional simulation environment would be of advantage in the toolbox of a nuclear safety analyst. The term multifunctional is here understood as wide range simulation software useful in most phases plant lifetime and having capabilities of simulating the full plant behaviour in all operational and accident conditions.

Many of the features listed as requirements have been tried in the APROS simulation environment, some are included in the code development plan.

Requirements for modern safety analysis code

The main subjects to be considered in defining the requirements for a modern safety analysis code architecture are:

General

- wide range multifunctional code
- all models based on first principles
- a choice of different physical models for comparison
- extensive validation through real applications (wide range)
- models for auxiliary systems, automation and electrical systems

User interface

- graphical user interface for model building and modification
- tools for high level component definition
- versatile output systems including database visualisation
- extensive on-line documentation of the software and the model

Architecture

- open layered architecture
- database structure
- fast calculation
- model initialisation
- interconnectivity
- advanced applications

Programming languages and standards

- Fortran-90 or HPF, C, C++
- UNIX, Windows NT
- Windows, X-Windows

Wide range multifunctional code

One of the visions emphasised throughout the APROS development process is the ability to use and extend the same model specification for a plant, from the pre-design phase through the lifetime of the plant. Having access to a model, that from the beginning can be made with simple component specifications and later on be upgraded in more detail, makes this possible. The model can also help to transfer design knowledge to the users of the plant. Accordingly, it is important that the modelling environment provides for computerised collection of source data, where and how all the parameters given to the model have been found, and by whom. Here is an excellent opportunity also to ask for the design criteria for the different components, to have them

forwarded to the users. Later on when changes and updates to the plant design have to be made, much less re-engineering work is needed. Also all changes to the design can be tested in advance on the simulator, before application to the real plant.

Physical models

The physical models in a modern multifunctional analysis tool must be uniform in the sense they can be interconnected to each other using a certain set of simple rules. Wide application range is important as well. It is difficult to obtain meaningful results, if the analysis task must be explicitly cut into sections of time, in which separate codes or models have to be used. The actual models have to sustain their known fidelity over the whole range of a transient. Another feature is the robustness of the solution algorithm, especially during abrupt changes of the actual model structure e.g. when a new component is added to simulation or a large leakage is introduced.

The basic entities should be as few as possible, the nodes and branches of a conventional flow network can actually describe flow of any material, if the parameter and correlation system can be adjusted accordingly. Thus the basic network model is applicable in flue gas network as well as in a primary circuit.

Thermal hydraulic models applicable in a pipe network are in general one-dimensional. Three dimensional calculation capability is necessary in certain parts of the nuclear power plant primary circuit (downcomer, lower plenum). The actual models should range from homogeneous to five and six equation models, depending on the needs (speed, accuracy, etc.) of current analysis task. For single phase flows a simplified homogeneous model can be used.

Reactor models with two (three) energy groups should range from 1-D (as fast as point model, when set against the calculation time required by the rest of the model) to full 3-D models, all with user selectable amount of flow channels, including a set of hot channels to be calculated on-line or afterwards with all necessary adjustment parameters. The reactivity level and axial power distribution should be tuneable as well as the feedback effects, which should have additional conservativity factors to be used according to safety analysis needs.

A modern analysis tool must have proper facility to describe all the present day automation systems including digital and model based systems. A possibility to actually use the manufacturer specific components or software would be an advantage.

The electrical system to solve the electrical power parameters in the plant network is often useful considering the amount of transients actually initiated by a fault in the network. The voltage in the nodes and the current, the active and the reactive power in the branches should be calculated as well as the frequency in the separate parts of the network.

Validation of the code is essential. The standard model of validation is still valid: physical model verification, comparison with separate effects tests, studies of a full plant behaviour.

A multifunctional code brings along a much larger set of validation cases, if its wide application area as a design tool can be exploited properly.

User interfaces

The usefulness of a multifunctional code depends much on the quality of the available user interfaces. The requirements are very stringent: the user interface should be informative, self-explanatory, easy-to-use and at the same time support the needs of standard procedures in building the models and using them. The building of the model is the most error prone phase of the use of the analysis tool or simulator. The software should be capable of telling the user about configuration errors he/she has made or is about to make. Also questionable modelling should cause some kind of a warning.

After completing a model for a component or a subprocess the user should be able to easily test its operation in steady state and with a desired form of excitation. Thus a reasonable set of excitation tools should be readily available. The software should be able to store the tuned state of the component as a set initial values for later use. This is also a point where the model documentation should be updated with written information on the component, its intended usage and possible guidelines followed in building the component.

In the course of building the model the user interface should support different visualisation modes, which could be used to show and highlight certain model parameters used around the model in order to help the user to detect possible inconsistencies in the model. During the simulation the interesting parameters should be available in the same manner.

Especially in nuclear safety related work one aspect of the analysis is 'playing around' with the simulator and using it as tool for creating and testing new ways of thinking. This kind of use requires an interface, which really integrates the simulator with the user.

Open layered code architecture

The modern simulation environment should have a multilayer architecture. The code consists of a kernel part in the centre, which includes the database, solvers, basic physical models, communications and the server part of the user interface. This layer is closed to the users of the software. The main reason is the validation problem, if changes are allowed in the code. The next layer is the configuration layer, where the higher level process components are defined for each application. This layer can be changed by qualified users and compensates for the closed kernel. The outer level is the application model layer.

The openness requirement includes the possibility for users to gain added value by developing their own component libraries with the tools available. Also, it should be possible to re-use previously developed external programs by connecting them to the simulation environment with a flexible communication interface.

In order to increase the computational speed the user should be able to configure the system to run on several workstations or parallel processors simultaneously. By means of the layered software structure employed, it is easy to transport the models developed between different computers having different operating systems or even different bit or byte patterns used to reflect the values of data.

Database

The database system is evidently the basis of all the functionality of the simulation software. It must be capable of taking care of interconnections between models, cutting models apart, copying and renaming them and at the same time storing not only process related data but also the relevant data for the graphical user interface. These data must be stored in the same database as the model data in order to provide strict correspondence between the actual process model and the picture, which in turn is used as part of the model documentation.

The possibility to exploit the database to define which models are actually included in the simulation also facilitates the alternate use of fast simpler models and slow accurate models in the same simulation system.

In addition to the standard features the database language should include extensions, which enable a qualified user to define higher level parametrizable process components. These objects are capable to create calculational level structures according to a set of instructions stored along with the component type definition. The structure may include any number (defined by a parameter value in the process component parameter list) of low level components including automation and electrical system components. The process component parameter list shown to a casual user can depend on the first choices made, e.g. the level of the thermal-hydraulic flow model and the set of substances being considered. The instructions should also define the calculations needed to transfer high level input data to the calculational level and vice versa.

The database should have facilities for referencing component/model/plant/project related data, which describes sources of input data, design and modelling criteria and also sources of validation data, validation results and the statement of validity range of the model.

The database should also have system to define a set of access rights for the project personnel indicating the components and subsystems, which are open for modifications by a certain person. This feature facilitates continuous development of a model during the plant life cycle.

Advanced applications

The multifunctional simulation software system can find many advanced applications along with the development of affordable computing power. A training simulator is already possible on the most powerful workstations. The really challenging applications include a tracking or a prediction

simulator. The former is used to estimate the state of the plant even through accident sequences and to provide up to date initial conditions to a prediction simulator used to study possible choices in operational procedures.

Simulation system requirements set by new computer architectures

A full scope plant analyser model with one dimensional reactor and turbine plant models included runs presently on a desktop workstation computer faster than real-time with a reasonable time step. The same plant model provided with a detailed fully three dimensional reactor representation may reach real time. To run the code at speeds needed in tracking or prediction simulators one must resort to extensive use of parallel processing. The problem is that a general code made for sequential computing cannot usually benefit much from traditional, medium grain vectored or parallel processing. The algorithms used have to be adapted for parallel processing and the code reprogrammed, which is a major effort. Also distributing the overall model on several computers for coarse grain parallelism requires advanced computerised tools for efficiency and database consistency.

An interesting feature is that code optimised for parallel and vector processing also runs more efficiently on a single processor due to the fact that all high-end workstation processors have some amount of parallel execution units on chip. Optimising the code already at the compiler level structures also the low level metalanguage so that the optimising code generator can produce more efficient code. This effect will be more evident in future as the single processor architecture develops with inherent fine grain parallelism. Future Very Long Instruction Word processors provides already for massively parallel operation.

Programming languages and standard tools

The question of relevant programming languages and standard tools has prevailed in discussions for more than 20 years. It seems that Fortran is difficult to overcome is tasks requiring maximum performance in pure calculation. The C and C++ languages have traditionally provided much more flexibility for more system-oriented tasks, communication and databases. The differences are however vanishing along with the Fortran-90 standard. In order to reach a reasonable decision one has to consider two facts: On the one hand the old program material available to the nuclear community is by far Fortran-based, on the other hand the young generation programmers know much better the usage of C or C++ than Fortran. In any case, both the languages will coexist and communicate with each other in the foreseeable future.

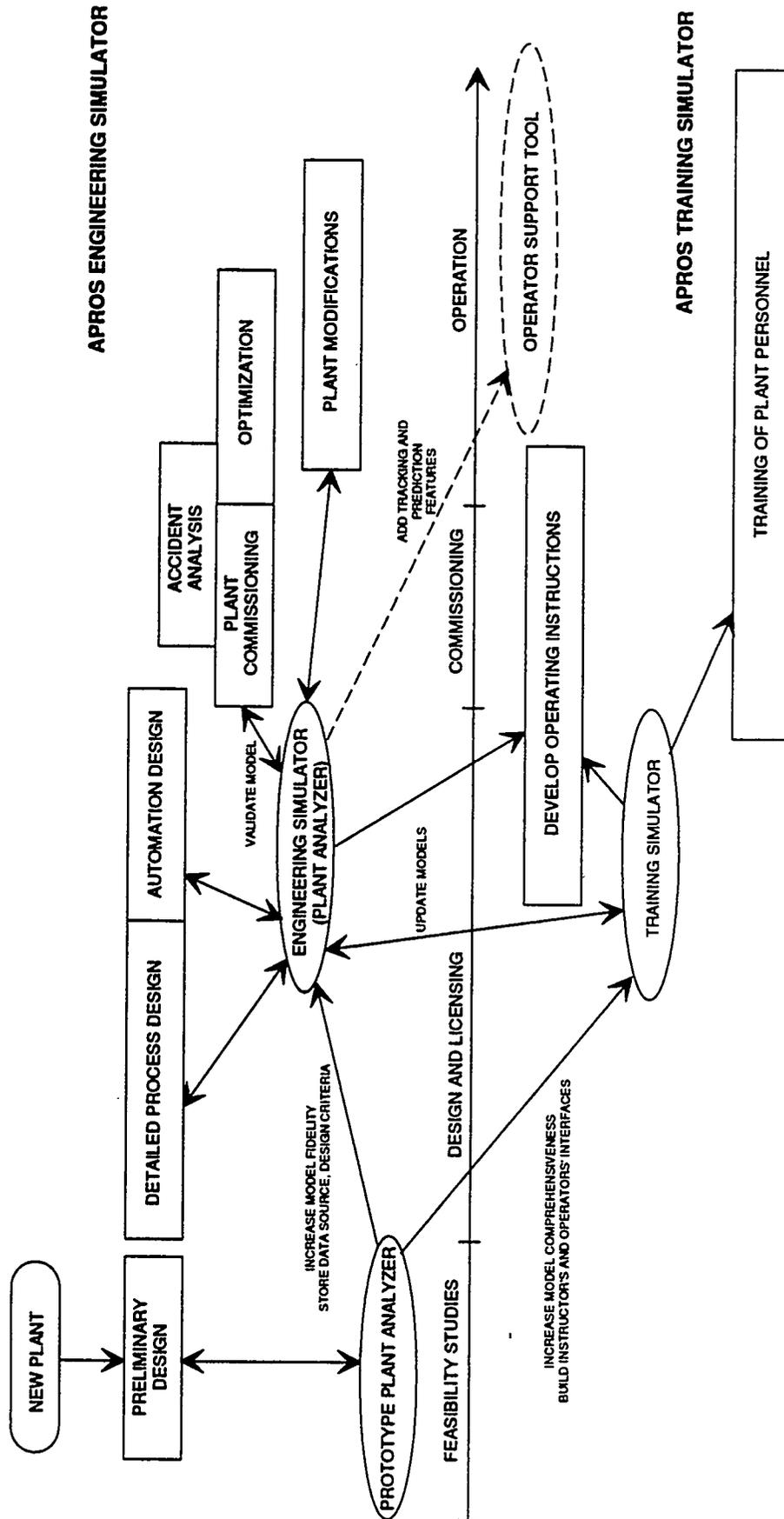
The standard tools, computer operating systems and graphical display software will develop at an unknown but fast pace. To cope with the changes it is essential to develop the basic kernel and the application dependent part of the code in strictly modular way, taking care of well defined interfaces between the modules.

References

- [1] Juslin, Kaj. Experience on Using an Object Oriented Language for Specification of mechanistic Models of Industrial Processes. UKSS'93, Conference of the UK Simulation Society. Chiswick, Cumbria, UK, September 13-15,1993. Edinburgh: United Kingdom Simulation Society, 1993.5p.
- [2] Porkholm, Kari; Hänninen, Markku, Shutov, Viktor; Ovtcharova, Ivanka. APROS-based Kola Nuclear Power Plant Analyser, SCS Simulation Multiconference, April 11-13, 1994, Hyatt Regency Aventine, La Jolla, San Diego CA, 6 p.
- [3] Juslin, Kaj. An Advanced Testbench for MMI Experiments, Goals and Technical Aspects. Enlarged Halden Programme Group Meeting, Bolkesjö, Norway, October 30 - November 3, 1994. Halden: OECD Halden Reactor Project, 1994. 6 p.

Figure: The range of current applications of the APROS simulation environment

A/PROS MULTIFUNCTIONAL SIMULATOR



DEVELOPMENT OF THE SIMULATION SYSTEM "IMPACT" FOR ANALYSIS OF NUCLEAR POWER PLANT SEVERE ACCIDENTS

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ABSTRACT

The Nuclear Power Engineering Corporation (NUPEC) has initiated a long-term program to develop the simulation system "IMPACT" for analysis of hypothetical severe accidents in nuclear power plants. IMPACT employs advanced methods of physical modeling and numerical computation, and can simulate a wide spectrum of scenarios ranging from normal operation to hypothetical, beyond-design-basis-accident events. Designed as a large-scale system of interconnected, hierarchical modules, IMPACT's distinguishing features include mechanistic models based on first principles and high speed simulation on parallel processing computers. The present plan is a ten-year program starting from 1993, consisting of the initial one-year of preparatory work followed by three technical phases: Phase-1 for development of a prototype system; Phase-2 for completion of the simulation system, incorporating new achievements from basic studies; and Phase-3 for refinement through extensive verification and validation against test results and available real plant data.

1. INTRODUCTION

Computer codes to analyze phenomena appearing in nuclear power plants have been developed and used for design and safety evaluation. Many of the traditional codes, especially codes for safety evaluations, employ empirical equations, empirical constants, and tuning parameters based on experiments.

For safety evaluation, the range of conditions which must be considered now extends beyond the traditional scope of design basis accident conditions to include hypothesized accident conditions. In addition to fluid flow and heat transfer events occurring under design basis accident conditions, phenomena to be evaluated include fuel melt and relocation, behavior of radioactive fission products, response to loads on the reactor pressure vessel and the containment vessel, numerous other events, and associated coupling effects.

To ensure the safe operation of a nuclear power plant even under hypothetical severe accident conditions, understanding of the phenomena involved and tools to calculate such

events must exist. The safety of nuclear power plants under such hypothetical severe accident conditions has been confirmed using traditional codes. However, such codes give more severe results for hypothetical severe accident conditions and can not give quantitative safety margin of the plant system, because they employ simplified models from restriction of traditional computer performance such as memory capacity and computing speed, and conservative assumptions for phenomena which comprehension is insufficient due to lack of experimental data.

Considering above situation, the Nuclear Power Engineering Corporation (NUPEC) has initiated a ten-year program from 1993 to develop a simulation system named IMPACT, an acronym for "Integrated Modular Plant Analysis and Computing Technology", with financial sponsorship from the Japanese government's Ministry of International Trade and Industry (MITI) [1, 2]. IMPACT is designed as a large scale system of interconnected hierarchical modules covering a wide spectrum of scenarios ranging from normal operation to hypothetical, beyond-design-basis-accident events with a final target to verify

quantitative safety margin of light water nuclear power plants.

- (6) Fast running analysis modules for parametric survey and detailed analysis modules with high-accuracy for verification of safety margin.

2. OVER ALL DESIGN

2.1. Unique Features

The basic policy was first established to develop the IMPACT software system for analysis of quantitative safety margin under a wide spectrum of scenarios ranging from normal operation to hypothetical, beyond-design-basis-accident events. The key features are as follows.

- (1) Minimization of use of empirical correlations and constants,
- (2) Maximization of use of mechanistic models and theoretical-base equations,
- (3) Utilization of a parallel processing computer, (currently use of IBM Power SP-2 with 72 processors),
- (4) User assistance from input generation to comprehension and retention of results,
- (5) Modular structure for easy development and maintenance, and

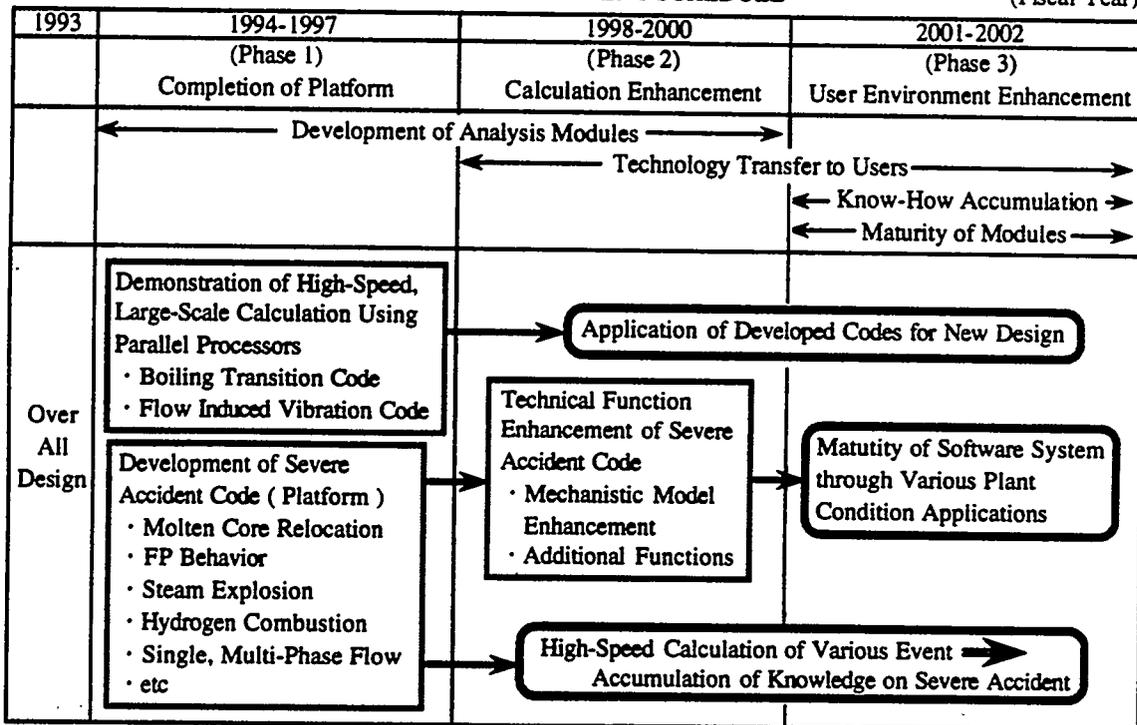
2.2. Development Plan

IMPACT was formulated into a ten-year program. To justify continuation of the long term project, it is important to provide check points for verification of the results obtained. For this purpose, the program is divided into an initial one-year planning phase followed by three technical development phases, as shown in Table 1.

Phase-1 is a period of technology acquisition for parallel computing software and understanding detailed phenomena to plan for incorporation of mechanistic modeling. It will be demonstrated at the end of Phase-1 that high-speed and large-scale calculations with existing mechanistic models can be realized using the parallel processing computer. For this purpose, the Boiling Transition Code and the Flow induced Vibration Code are now under development within the IMPACT program. Since many of the mechanistic models for these phenomena exist,

Table 1. DEVELOPMENT SCHEDULE

(Fiscal Year)



efforts can be put into effective parallel processing. As for the Severe Accident Code, a prototype version will be completed during Phase-1. The prototype version will consist of fast-running analysis modules with models which are mainly experimentally based.

Phase-2 is a period of software enhancement. Models in the prototype version for severe accident analysis will be replaced with mechanistic models to enable safety margin calculation. The Boiling Transition Code and the Flow-induced Vibration Code will be completed within Phase-1, and these codes will be

transferred to users for application.

Phase-3 is a period of user environment enhancement. The Severe Accident Code will be put to practical use. The software will be brought to maturity through various applications.

3. SEVERE ACCIDENT CODE STRUCTURE

The groups of modules shown in Fig. 1 will make up the IMPACT Severe Accident Code system. Three of the main module systems are described as follows.

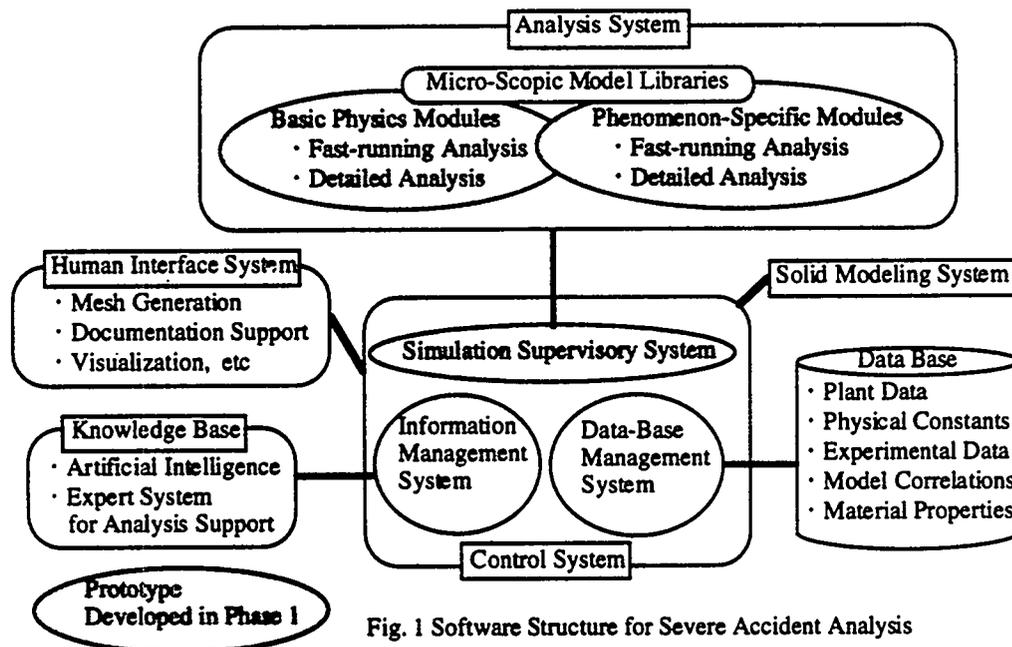


Fig. 1 Software Structure for Severe Accident Analysis

3.1. Control System

The IMPACT Severe Accident Code structure will differ from traditional codes in that the various functions will be performed by independent groups of modules, or "systems". These systems will be managed by independent control systems which also consist of several modules each. The Control System will also be able to retrieve and distribute information necessary for simulation in full scope. It will obtain information from the input data, data bases, and knowledge bases including simulation conditions, accident scenarios, and various criteria such as conditions for initiating safety devices.

Based on these data, the system will call analysis modules and input/output modules, etc. Scenarios and various criteria will be recorded without being programmed into the code and will be able to be changed freely. Such control and management will be possible even when the various modules are executed in parallel. Consequently, the control system manages multiple modules while appearing to the users to be a single code.

The major portion of the Control System, the Simulation Supervisory System will manage the Analysis System. It will call and terminate analysis and input/output modules as appropriate, with

respect to time in the event and to physical location, as shown in Fig. 2.

The system will enable modules to run in parallel or time-sequentially. With these capabilities, the Simulation Supervisory System will make possible integration of multiple modules for unified, efficient calculations. The Simulation Supervisory System will also have knowledge of event scenarios, simulation conditions, and various criteria and call analysis modules and output modules as they are required. In order to realize these functions, the Simulation Supervisory System will make consistency of time steps among various modules and have a function for parallelization control, that is dynamic allocation of processor elements to optimize simulation elapsed time, as shown in Fig. 3.

3.2. Human Interface System

The Human Interface System supports the Analysis System and the Control System. It will assist with automatic mesh generation and include

expert systems which can integrate data from several information management systems and from previous numerical simulations. As examples, boundary and initial condition data may be derived from results of previous simulations and material properties may be obtained from information banks, all of which have been stored in the Data Base. To support the Control System, the Human Interface System will assist in creating scenarios by scheduling operating directives, malfunctions, and other events. Operator actions will be input.

3.3. Analysis System

The Analysis System will be a highly flexible system, capable of simulating any plant component or system at any time during an event. This flexible structure will also readily accommodate changes in the calculational degree of detail, function and range of scale.

The modules have been divided into two broad groups, namely, "basic physics modules"

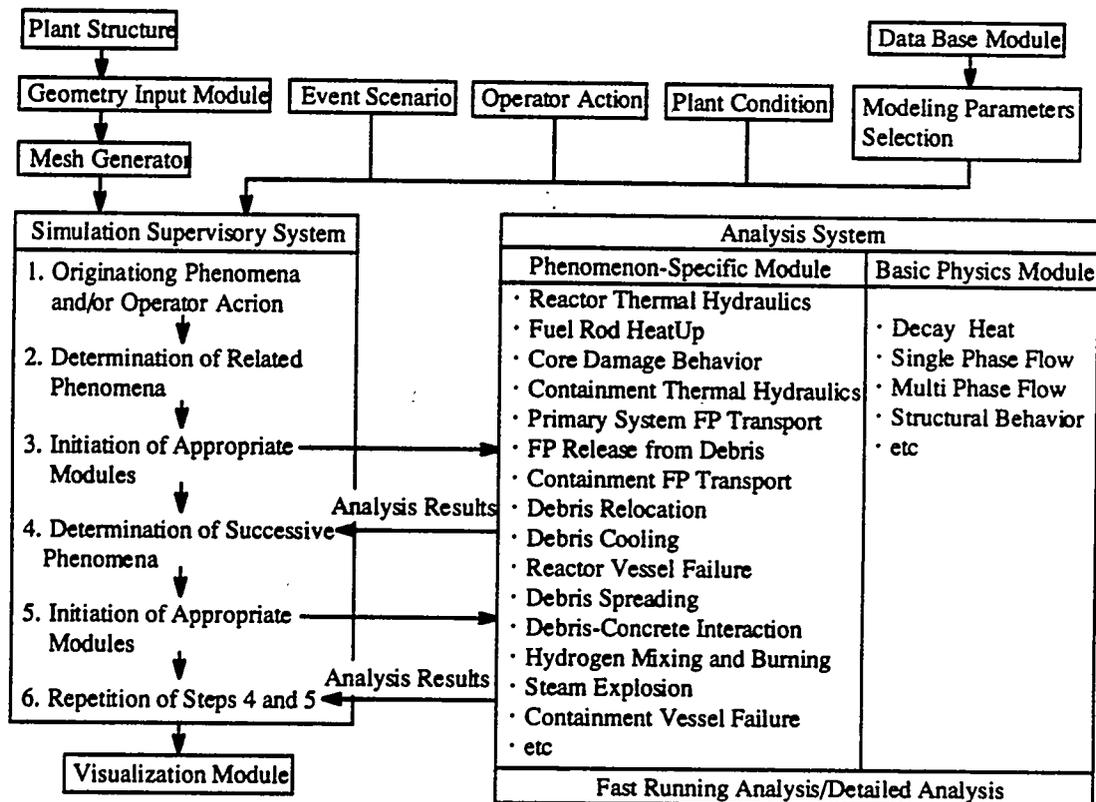


Fig. 2 Function of Simulation Supervisory System

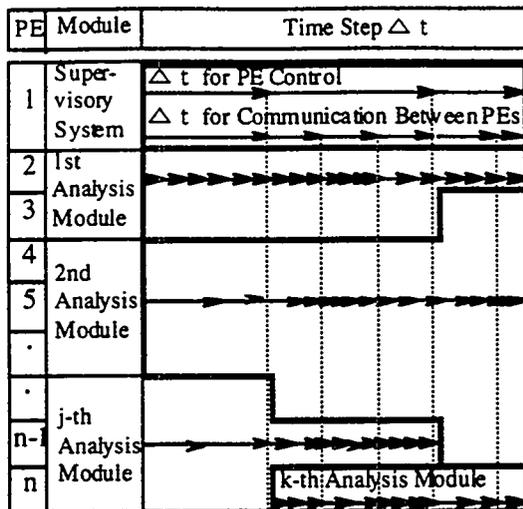


Fig. 3 Time Step Control and Dynamic Allocation of Processor Elements

and "phenomenon-specific modules". The former modules will analyze basic physics phenomena, such as three-dimensional single- and multi-phase flow, which will appear not only in a specific plant component and specific event but also in various components, accident scenarios, and events. The latter modules will treat phenomena specific to accident scenarios such as debris relocation, fission products release, steam explosion, hydrogen burning, etc. These modules are described in Fig. 2.

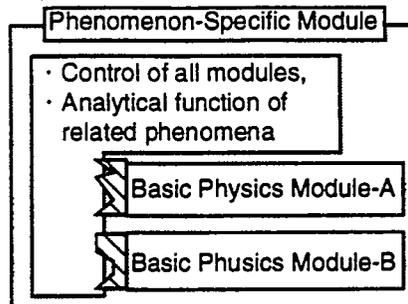
The basic physics modules are currently not used as independent modules, but are incorporated into related phenomenon-specific modules as their sub-modules, as shown in Fig. 4A. Pending an increase of the number of processor elements, they will be, in future, independently installed on processor elements as independent modules and data will be transferred by communication between the processor elements, as shown in Fig. 4B.

To reconcile the calculation speed and the degree of detail in the model, "detailed analysis modules" and "fast-running analysis modules" in both module groups will be developed.

3.3.1. Fast-running Analysis Modules

The fast-running analysis modules will be completed within Phase-1 period. The models for the fast-running modules will be mainly

A. Incorporated into a phenomenon-specific module as sub-modules, resulting in a independent phenomenon-specific module



B. Data Transfer by communication between independent modules

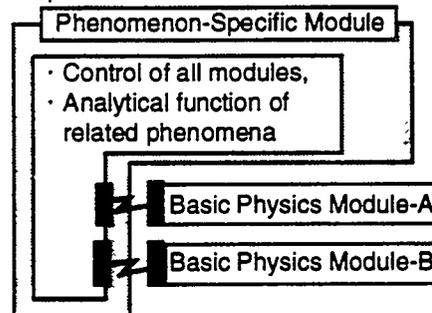


Fig. 4 Incorporation of Basic Physics and Phenomenon-Specific Modules

experimentally based, because the mechanistic models, in general, will require a lot of CPU time and further research work will be required for the development of some mechanistic models. Using these fast-running modules, extensive parametric surveys will be performed for various event sequences to accumulate knowledge on severe accident scenarios.

3.3.2. Detailed Analysis Modules

The Detailed Analysis Modules will be completed within Phase-2. The experimentally based models in the fast-running modules will be replaced by the mechanistic models. For phenomena which are not yet fully understood, structural and physics models will be selected so as to rely as little as possible on experimental data.

Increase in analysis reliability is being attempted for better quantification of safety margin and for optimization of accident management procedures.

3.3.3. Microscopic-Model Library

Microscopic-level simulations such as molecular dynamics and cellular automaton are in the research phase. Since their application to the large system of nuclear power plants and reliable physical interpretation of their calculation results will require further several years, the microscopic models are currently not introduced to the IMPACT software. In future, they will be used as standard for verification of empirical models. For example, applicability of empirical models over the confirmed range by experiments will be verified by the microscopic-level simulations.

4. CURRENT STATUS AND RESULTS

In April, 1994, the IMPACT program entered into the initial four-year technical development phase. The NUPEC has initiated the technical development and contracting work out to IMPACT team members. Software is being developed on an IBM POWER SP-2 parallel computing system having 72 processor elements with total performance of 18.7 GFLOPS, which was installed in October, 1995.

4.1. Basic Physics Modules

Current emphasis is put on development of three dimensional single-phase and two-phase flow analysis modules as the basic physics modules. These are being incorporated into the Boiling Transition and Flow Induced Vibration Codes as their sub-modules. These flow analysis modules are based on the existing code for single processor, vector computers, named " α -FLOW".

Parallelization was completed for the incompressible single phase flow module, which is contained in α -FLOW code series [3], for analysis in cartesian and cylindrical coordinates. In parallelization, a domain decomposition method was used. Emphasis was put on the parallel solution of the discrete Poisson equations, because it consumes most of the execution time. The parallel Block ordering was used as a preconditioner in the Simplified Marker and Cell (SMAC) scheme. The speed up ratio by parallel

calculation was evaluated by the model problem of the standard three-dimensional square lid driven cavity flow. Calculation speed of at least 30 times by parallel processing was currently attained in case of large number of meshes, as shown in Fig. 5. In Fig. 5, the speed up ratio was based on the speed when one processor element was used, and it was assumed to be "n" when the minimum number of processor elements used was "n" in case of large number of meshes which requires more than one processor element.

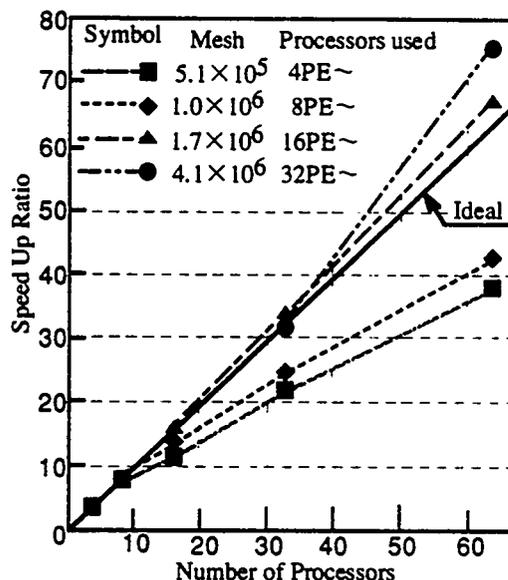


Fig. 5 Speed Up by Parallelization of Three Dimensional Incompressible Single-Phase Flow Analysis Module

4.2. Phenomenon-Specific Modules

The fast running analysis modules are now in the stage of detailed design. They will be combined to a single prototype code, namely the prototype or the platform of the Severe Accident Analysis Code, which can analyze overall behavior of nuclear power plants under severe accident conditions by once-through manner.

As one of detailed analysis modules, steam explosion analysis module has precedently been developed. The two-phase flow analysis module, as one of the basic physics module, was expanded to four-phase flow; water, steam, particle molten debris, and continuous phase of molten debris.

The phenomena of steam explosion can be divided into four stages; Pre-mixing, Triggering, Propagation, and Expansion [4]. The Pre-mixing sub-module with a particle breakup model and a jet breakup model [5] was completed. Comparison of calculation result with the MIXA test result [6, 7] is shown in Fig. 6. In the MIXA test analysis, the particle breakup model was used and the test data of the steam generation rate of about 0.2 m³/s at time 0, which is written in the reference [6], was given as an initial condition for the calculation. All of other sub-modules will be completed and unified within Phase-1 period.

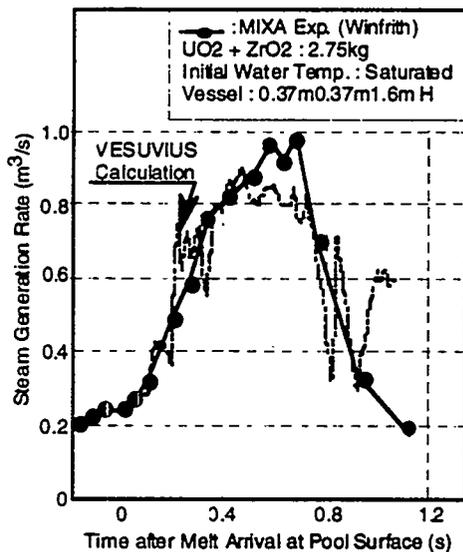


Fig. 6 Verification of Steam Explosion Module, VESUVIUS

4.3. Simulation Supervisory System

The system is under detailed design. The following questions are specifically addressed.

- Necessary input data and data format for complete simulation,
- Required input data for each module,
- Out put data to be visualized, and
- Form for visualization.

The system to support input generation, mesh division, and selection of initial conditions are also under detailed design.

4.4. Boiling Transition Code and Others

The Boiling Transition Analysis Code has also a module structure, as shown in Fig. 7. All of

analysis modules have mechanistic models. The detailed design was completed and coding has been initiated. Some of mechanistic models were verified with basic experiments. The basic physics modules for analysis of single- and two-phase flow are incorporated into the Code as the sub-modules, as shown in Fig. 4A. The code will be completed within the fiscal year of 1997.

The situation of the flow Induced Vibration Code is almost the same as of the Boiling Transition Code. The Code developed within Phase-1 period is to analyze coupling phenomena of structures and single-phase flow.

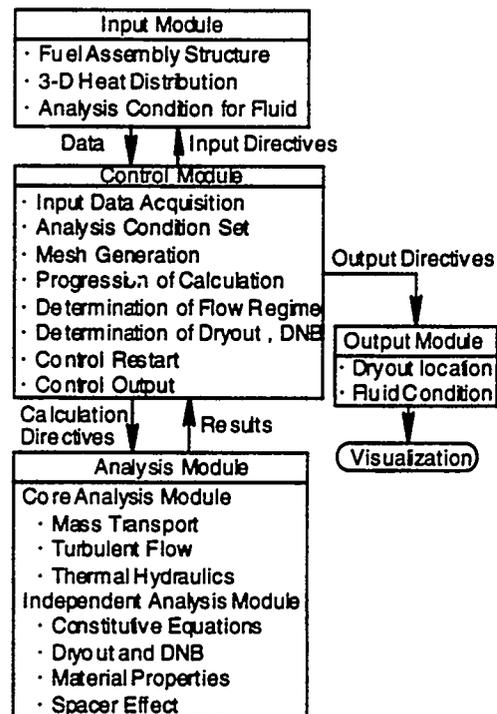


Fig. 7 Boiling Transition Code Structure

5. CONCLUSIONS

Three years of the IMPACT project have been completed with financial sponsorship from the Japanese government's Ministry of International Trade and Industry (MITI).

The final result of the IMPACT program will be an integration of software modules for nuclear power plant simulation, capable of analyzing conditions ranging from normal operation to

hypothesized accidents. Multiple modules will be executed simultaneously while appearing to the user to be a single code.

Three major sections of the software have been described herein. In the initial four-year technical development phase, work has begun on these sections of the software, namely, the Control System, the Human Interface System, and the Analysis System.

Current results on single-phase flow and steam explosion analyses showed effectiveness, or fast calculation for large system with mechanistic models, of parallel processing.

Vessel Steam Explosion", Proc. of Int'l. Conf. on Nuclear Engineering - ICONE-4, Vol. 1, Part A, New Orleans, LA, March 10-14, 1996, pp. 333-341.

REFERENCES

- (1) Vierow, K. et al., "The IMPACT Supersimulator - Conceptual Design", Proc. of The Second Workshop on Super Simulators for Nuclear Power Plants, Nuclear Power Engineering Corporation, Tokyo, JAPAN, December 1994.
- (2) Vierow, K. et al., "The IMPACT Super Simulator-Basic Framework", '95 Simulation Multi Conference, Phoenix, AZ, April 9-13, 1995
- (3) Akiyama, M. et al. "Development of Advanced Fluid-Dynamics Analysis Code: α -FLOW", 1990, Proc. of Int'l Conf. on Supercomputing in Nuclear Applications.
- (4) Corradini, M. L., Kim, B. J., Oh, M. D., "Vapor Explosions in Light Water Reactors: A Review of Theory and Modeling", Progress in Nuclear Energy, Vol. 22, 1988, pp. 11-17.
- (5) Ginsberg, T., "Liquid Jet Breakup Characterization with Application to Melt-Water Mixing", Proc. of Int'l. ANS/ENS Top. Mtg. on Thermal Reactor Safety, San Diego, CA, 1986, pp. II.4.1-18.
- (6) Denham, M. K., A. P. Tyler, D. F. Fletcher, "Experiments on the Mixing of Molten Uranium Dioxide with Water and Initial Comparisons with CHYMES Code Calculations", Proc. of the 5th Int'l. Top. Mtg. on Teactor Thermal Hydraulics - NURETH-5, Vol. VI, Salt Lake City, UT, Sept. 21-24, 1992, pp. 1667-1675.
- (7) Vierow, K., Naitoh, M., Nagano, K., Araki, K., "Development of the VESUVIUS Model and Analysis of the Premixing Phase of an Ex-

BREAK-OUT SESSIONS

Thermal Hydraulic Codes for LWR Safety Analysis - Present Status and Future Perspective -

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Abstract

The aim of the present paper is to give a review on the current status and future perspective of present best-estimate Thermal Hydraulic codes. Reference is made to internationally well-established codes which have reached a certain state of maturity. The first part of the paper deals with the common basic code features with respect to the physical modelling and the numerical methods used to describe complex two-phase flow and heat transfer processes. The general predictive capabilities are summarized identifying some remaining code deficiencies and their underlying limitations. The second part discusses various areas including physical modelling, numerical techniques and informatic structure where the codes could be substantially improved.

1. Introduction

The Workshop on "Transient Thermal-Hydraulic and Neutronic Codes Requirements" is not the first time to discuss this matter in some detail. During the last decade there have been many debates with regard to the future of nuclear thermal-hydraulics and in particular to the status and further development of thermal-hydraulic and neutronics codes. This includes for example the "CSNI Specialist Meeting on Transient Two-phase Flow" at Aix en Provence in 1992 which was specifically dedicated to this subject. The same matter has also been discussed (often controversially) at most of the NURETH meetings or other reactor safety related conferences, however, the conclusions drawn have been often rather vague.

The present paper on the "status and future perspective of thermal-hydraulic codes" represents the opinion of the author. It is based on long-term involvement in the development, verification and application of various codes including RELAP4, RELAP5, ATHLET and CATHARE. The aim is not to judge any of these codes rather than trying to summarize their principal prediction capabilities and limitations and to explore possible future developments in this area.

There is certainly no other field of engineering which depends so strongly on "numerical process simulation" as nuclear technology. This is mainly due to two major reasons (1) the impracticality of executing full-scale safety related experiments and (2) the absence of simplified scaling laws for the governing processes which would allow a direct transfer of results from small scale test facilities to the full size plant. The only way to close the gap between the mostly small scale separate effects or integral test facilities and the full size plant is via the use of system codes which are capable of describing the governing processes and which have been sufficiently verified against experimental data from differently scaled test facilities. It is evident that each model or code represents an approximation of the real system or plant. The final use of these codes will therefore largely depend on the progress in quantifying the uncertainty associated with the prediction of the plant behaviour which will not be addressed in this paper.

2. Current status of TH-codes

Although starting from rather different approaches, there has been a remarkable convergence over the last few years and at present the basic modelling strategies and numerical techniques used are rather similar in most TH-codes. It is therefore not surprising that all the codes produce similar results and (consequently) suffer from the same deficiencies and limitations. For this reason, the following section will not distinguish between the different codes but rather concentrate on the common code features and the underlying modelling and numerical strategies.

2.1 Review of basic modelling in present TH-codes

By far the most challenging part in the codes represents the modelling of transient two-phase flow and related heat transfer processes. A lot of work was therefore dedicated specifically in the late sixties and in the seventies to study complex two-phase flow phenomena like non-homogeneous flow conditions, thermal non-equilibrium processes, critical flow, boiling/condensation heat transfer including critical heat flux and rewetting processes. Most of the results obtained form the basis of our present best-estimate computer codes for the description of the LWR system behaviour. The following review therefore concentrates on the basic approach for the description of transient two-phase flow conditions as is commonly used in most of the second generation of TH-codes.

Governing equations of transient two-phase flow

In the past there have been many debates about the advantages and disadvantages of the drift flux models and the two-fluid approach to represent transient two-phase flow. However, most of the present best-estimate codes are based on the two-fluid model using separate balance equations for mass, momentum and energy for the two phases. This approach allows to model the time evolution of local (generally unequal) phase velocities on the basis of the physical processes (interfacial friction). The drift flux model instead prejudices the resulting "slip velocities" using highly empirical drift flux correlations which are valid only in case of steady state and fully developed flow conditions which,

strictly speaking, never exist in reactor transient situation. However, this does not mean that codes based on the two-fluid model give a priori better results.

The basic conservation equations of the two-fluid model as given by equations (1) to (3) are derived by a spatial and time averaging procedure where most information of the local flow processes (especially at the interface or near the wall) are lost and higher frequency time fluctuations have been completely filtered out [1,2,3,4]. The transport processes at the interface including heat transfer, evaporation/condensation or interfacial friction are modelled by corresponding source terms on the right-hand side of the separate balance equations. At best, the two-fluid model can provide information only on the average flow behaviour, assuming that sufficiently accurate correlations are used to describe the heat, mass, and momentum transfer processes at the interface and at the wall.

mass:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla \cdot (\alpha_i \rho_i \bar{v}_i) = \sigma_i^M \quad (1)$$

with $\sum_{i=g,l} \sigma_i^M = 0$

momentum:

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_i \rho_i \bar{v}_i) + \nabla \cdot (\alpha_i \rho_i \bar{v}_i \bar{v}_i) + \nabla(\alpha_i p) - \nabla \cdot (\alpha_i \bar{\mathbf{T}}) \\ = \bar{F}_i^{\text{int}} + \sigma_i^M \bar{v}_i^{\text{ex}} + \alpha_i \rho_i \bar{f}_i^{\text{ex}} \end{aligned} \quad (2)$$

with $\sum_{i=g,l} \bar{F}_i^{\text{int}} = 0$

energy:

$$\begin{aligned} \frac{\partial}{\partial t} \left[\alpha_i \rho_i \left(u_i + \frac{1}{2} \bar{v}_i^2 \right) \right] + \nabla \cdot \left[\alpha_i \rho_i \bar{v}_i \left(h_i + \frac{1}{2} \bar{v}_i^2 \right) \right] + (p) \frac{\partial \alpha_i}{\partial t} - \nabla \cdot (\alpha_i \bar{\mathbf{T}}_i \cdot \bar{v}_i) \\ = \sigma_i^Q + \sigma_i^M \left(h_i + \frac{1}{2} v_i^2 \right) + \bar{F}_i^{\text{int}} \cdot \bar{v}_i^{\text{int}} + \alpha_i \rho_i \bar{f}_i^{\text{ex}} \cdot \bar{v}_i + Q_i^{\text{ex}} \end{aligned} \quad (3)$$

with $\sum_{i=g,l} \sigma_i^Q = 0$

In many flow conditions the two-fluid model just represents a rough approximation of the real flow situation. This might be already the case for rather well structured flow regimes like bubbly flow with a continuous distribution of bubble sizes. It is obvious that lumping together all the bubbles into one pseudo fluid cannot describe the size-dependent behaviour of individual bubbles (or classes of bubbles) and the associated dispersion of the gas phase. Similar consideration might be valid for dispersed droplet or mist flow. The situation becomes even more critical in case of less structured or more complex flow

regimes like annular mist and inverted annular flow. It is also clear that this inherent limitation of the two-fluid approach cannot be compensated by "improved" interfacial transport models.

The interfacial transport processes for mass, momentum and energy are generally described by algebraic, flow regime dependent expressions. The resulting system of equations is (in most cases) characterized by complex conjugate eigenvalues even in the case when all viscosity or diffusion terms are dropped. This indicates that the model represents an ill-posed initial/boundary value problem which has been extensively (and controversially) discussed in the past with respect to the prediction accuracy and numerical stability [5]. However, experience in applying these models has shown that in most applications stable solutions can be obtained since the present numerical techniques used in all the codes provide a sufficiently large damping mechanism but at the expense of large artificial diffusion or viscosity effects. In some cases, additional time and space derivative terms have been included in the two separated momentum equations to account for additional (non-viscous) forces resulting from virtual or added mass effects which makes the two-fluid model hyperbolic. However, the effect of these terms has always been rendered negligible due to the overwhelming damping and artificial diffusion effects of the numerical method used.

Closure laws for interfacial transport processes

The general balance equations for the separated phases have to be completed by additional closure relations describing the transport processes for mass, momentum and energy at the contact area (interface) between the phases. For the corresponding source terms for mass, momentum (interfacial friction) and energy (heat transfer) at the interface, σ^{int} , simplified mechanistic models are widely used which often have the form

$$\sigma^{\text{int}} = C'' f(\alpha) \Delta X \quad (4)$$

where ΔX represents the "driving force" for the transport process, e.g. temperature or velocity difference between the phases, or the difference between an actual state parameter and a corresponding equilibrium value. The void fraction dependent function $f(\alpha)$ describes indirectly the available contact area between the phases. The highly empirical transport coefficient C'' is generally used to match experimental data or to provide "reasonable" values for the predicted deviations from the mechanical or thermal non-equilibrium state.

In principle different correlations of the form (4) have been derived for various well-structured flow regimes like bubble flow, droplet flow, annular flow or stratified flow. Flow regime boundaries are characterized by threshold values for specific flow parameters (often just void fraction and mass flow density) within simplified "flow regime maps". As an example, the flow regime map for vertical flow conditions is shown in Fig. 1. as is generally applied in the RELAP5/MOD2 [6] and (slightly modified) in RELAP5/MOD3 for pre-CHF conditions [7]. Similar (even more simplified) flow maps

are used in various TRAC code versions [8]. Criteria for the flow regime boundaries are either completely empirical or are derived from Kelvin-Helmholtz or Rayleigh-Taylor instability limits. More complex or less well-structured flow regimes and flow regime transitions are dealt with by purely mathematical interpolation procedures using linear or higher order interpolation functions.

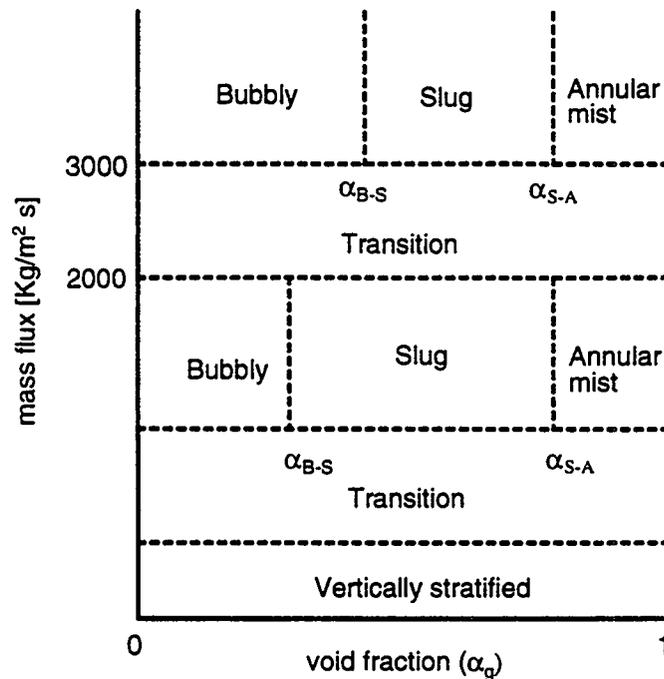


Fig. 1: RELAP5 flow regime map for vertical flow conditions

As outlined above, the modelling of the interfacial laws represents the weakest point in the two-fluid approach to describe transient two-phase flow and no large progress has been made in this area over the last ten years. The major problem comes from the fact that, up to now, there is no way to directly measure the interfacial transport processes. Therefore, the verification of the model can only be made in an indirect way using basic or separate effect experiments performed in (mostly) small scale facilities.

Wall friction and heat transfer

Further constitutive relations are needed to describe the interaction of the fluid with the solid structures in the primary and secondary system including wall friction and wall heat transfer. Compared with the interfacial processes, the situation is somewhat simpler due to the fact that the fluid-wall contact area is a well known parameter and that the corresponding physical phenomena like pressure drop and wall heat fluxes can be rather accurately deduced from pressure or wall temperature measurement. In all the codes (almost exclusively) empirical correlations are used for frictional pressure drops in pipes and for heat transfer coefficients or heat fluxes including all important boiling regimes like sub-

cooled/nucleate boiling, transition boiling, film boiling and critical heat flux. The correlations used are based on a large data base which to a certain extent cover also relevant reactor geometries like fuel rod assemblies, influence of rod spacers or SG tube geometries. The overall uncertainty for two-phase boiling heat transfer has often been estimated to be in the order of $\pm 30\%$ which is attributable to various contributions:

- ◇ heat transfer conditions can depend on often unknown wall surface conditions like wall roughness or oxidation layers
- ◇ all correlations are derived for steady state and fully-developed flow conditions which are not always applicable, e.g. in fast transients or under conditions where heat transfer regimes change over extremely small spatial distances (local dryout phenomena, quenching or reflood processes)

Another source of uncertainty originates from the fact that the evaluation of the measured data require additional modelling assumptions. The specific models try to correlate measured frictional pressure drops or heat fluxes with local (bulk) flow parameters (like void fraction, vapour quality, phasic velocities or temperatures) which are not *a priori* known. Additional models are therefore needed to calculate these parameters from known inlet conditions. In many cases, rather simplified assumptions have been used (e.g. homogeneous and thermal equilibrium flow conditions) which are no longer consistent with present best-estimate thermal hydraulic codes which require a partitioning of the overall wall friction and heat fluxes with respect to the individual phases. A re-evaluation of the measurements might be advisable in order to reduce the uncertainty band for the correlations if the original data base is still available.

Numerical methods

All of the presently well-established codes are using finite difference, first-order numerical methods based on staggered grid and donor cell techniques. Although this method is known to introduce a substantial amount of numerical (artificial) diffusion or viscosity, it is preferred due to the inherent numerical stability. This is of specific importance since most codes are using two-fluid models having complex characteristics which suffer from small wave length (high frequency) instabilities. Therefore, often additional damping has been introduced (e.g. by the way in which the momentum flux terms are formulated in RELAP5) which may further contribute to the numerical diffusion or viscosity in the predictions.

Apart from the staggered grid and donor cell approach numerical methods largely differ in the degree of implicitness for the time integration. The NRC sponsored codes RELAP5 and TRAC are using an extension of the Implicit Continuous Eulerian ICE method originally developed for the solution of single phase gas dynamic problems [9] and later extended also for transient two-phase flow conditions [10]. The ICE technique is expected to provide stable results for time step sizes below the material Courant limit, however applying the method for two-phase flow predictions often shows a rather high level of numerically induced (unphysical) oscillations. A further problem of the ICE technique is that it does not a priori guarantee the conservation of mass and energy. In RELAP5 [6], the appearing mass error is used as a parameter for the time step control. In

the TRAC code [8] a "two-step" method is applied where an ICE type approach is used only as an intermediate step, followed by a "stabilizer step" to provide conservation of mass and energy for the two separated phases.

Of large importance in the numerical approach is the way the interfacial transport processes are dealt with which might be characterized by rather small time constants. In RELAP5 and TRAC the related source terms are treated only in a partially implicit manner (e.g. using new time values for phasic velocities or temperature) which might result in numerical instabilities. For this reason additional damping procedures like an "under-relaxation" are often applied (as in the RELAP5) where the related source terms are averaged between the old and the new time values.

The above mentioned problems with respect to time step limitations and/or numerical stability can be largely avoided if fully implicit time integration techniques are used as in CATHARE [11] and ATHLET [12]. However, the principal advantage of fully implicit methods might be compromised by the large numerical effort needed for the matrix inversion in particular for large (3-dimensional) systems. For this purpose a partially implicit "two-step" numerical method is presently applied also in the CATHARE code for the 3-dimensional reactor pressure vessel module.

Nodalization schemes and spatial resolution

Only few attempts have been made to systematically investigate the effects of the nodalization or the convergence of the predicted results in case of a continuous increase of the number of computational cells or control volumes. Such studies have always been hampered by several reasons including economic constraints and stability problems in particular in case of small cell sizes. Another problem is related to the fact that many highly empirical models and correlations have been adapted to a specific range of control volume size and, consequently, the use of very small control volumes will not always produce better results than a coarse nodalization. For this reason, rather coarse nodalization diagrams are usually applied where even complex reactor systems are represented by a relatively small number of nodes, often in the range of 200 to 300. From this it is clear that important local phenomena can not always be described.

Multi-dimensional effects

Three-dimensional flow processes are generally expected in large test facilities or full-size plants in particular with respect to large break LOCA, where they can strongly influence the overall system behaviour, for example the delay in the delivery of ECC water into the core (ECC bypass problem). However, a more detailed analysis of data from integral scaled facilities indicates that multi-dimensional effects are present also (and often governing) in many other accident scenarios even in small scale facilities. This is in particular the case in the upper head and upper plenum region of the pressure vessel with the multiple connections of hot and cold leg pipes, within the upper downcomer regions of the pressure vessel, the lower plenum as well as in the inlet/outlet plena and steam dome of the steam generators.

There are at present two different ways to deal with these multi-dimensional effects:

- ◇ strictly one-dimensional codes like RELAP5 or ATHLET try to handle this situation by multiple junction connections to a (one-dimensional) computational cell or by using a parallel channel representation with cross junction connections). The results obtained are very sensitive to the chosen nodalization details, and other input parameters like flow resistance and form loss coefficients. Since no general guidelines exist, a large freedom is left to the code user to make best use of the various possibilities for his specific problem.
- ◇ explicit 3-dimensional modules exist as an option in the codes TRAC and CATHARE for the reactor pressure vessel. They represent a straightforward extension of the one-dimensional modules for cylindrical coordinates. Due to the heavy computational effort needed, the 3-dimensional modules are used only for fast (short) transients like large break LOCA. In most applications, extremely coarse nodalization schemes are applied and consequently the advantage of a 3-dimensional modelling of the flow processes might be largely lost. As for all attempts to simulate 3-dimensional two-phase flow processes, the modules suffer from the large numerical (artificial) diffusion/viscosity effects and the lack of appropriate bulk (physical) diffusion and turbulence models. To a certain extent both shortcomings might compensate each other in a non-physical manner.

2.2 Present practice of code assessment and verification

Our present knowledge on the capabilities and limitations of present TH-codes is based on the huge amount of work that has been executed in many countries on the assessment and verification of internationally well-recognized codes or code families like RELAP5, TRAC, CATHARE or ATHLET. This includes developmental assessment programmes performed by the code development institute and their associated partners, international code assessment programmes like ICAP and CAMP, carried out for codes like RELAP5 and TRAC, and the large number of code applications for reactor licensing or audit calculations and the extensive use of the codes in the framework of experimental programmes like SEMISCALE, LOFT, LOBI, ROSAIII/IV or BETHSY. An additional source of information represents the large number of International Standard Problems exercises (ISPs) organized by the CSNI over a period of more than twenty years. However, despite this large effort, the present picture with respect to the codes' status is still not very clear and far from a consensus among experts in this field. There might be different reasons for this situation including:

- ◇ most of the assessment studies are based on experiments performed in scaled integral test facilities. The comparison of measured and predicted parameters for these tests often provides a good overall picture of the code performance, however, the large number of coupling phenomena and the often coarse resolution of the measurement information largely prevent a more detailed analysis of the reasons for existing discrepancies between the experiment and the prediction.

- ◇ the strong influence the user still has (also for present “best estimate” codes) on the quality of the predicted results. These “user effects” have been identified in nearly all ISP exercises when a group of participants using the same code or code version produced significantly different results [13].
- ◇ the often practiced “code tuning” strategy used to produce “good results” with respect to experimental data by trial and error choices of code input data, initial and boundary conditions, specific nodalization diagrams, or even worse, by ad-hoc changes to code models or correlations. This is often misleading since it gives the impression that an existing problem can be fixed just by a small “code improvement”.

Nevertheless, in the following section it is intended to give a broad overview on the prediction capabilities of present TH-codes and to identify the reasons for still existing deficiencies and limitations.

2.3 Prediction capabilities, existing limitations and underlying modelling deficiencies

The major outcome of the large number of assessment studies can be summarized as follows

- ◇ despite the in some parts rather poor or ad-hoc physical models and the limitations in the numerical methods used, all the well-established codes like RELAP5, TRAC CATHARE or ATHLET have demonstrated their principal capability to qualitatively describe most of the governing phenomena and the general system behaviour for a large variety of accident scenarios including Loss of Coolant Accidents, Steam Generator U-tube Ruptures and Special Transients such as Loss of Power or Loss of Heat Sink. This generally indicated that these codes have reach a rather high degree of maturity.
- ◇ the quality of the predictions is strongly user dependent which results not only from the care taken to correctly describe initial and boundary conditions but also from the chosen nodalization details. Often the code user has to introduce ad-hoc decisions in order to compensate for a lack of (or not fully applicable) modelling in the codes.
- ◇ in the framework of present modelling concepts, as summarized in section 2.1, the potential with respect to a further improvement of the predictive capability seems to be largely exhausted. This is specifically indicated by those codes which have reached their major state of development already some years ago (like RELAP5 and TRAC). Further “code improvement” programmes as were conducted for example in the ICAP or CAMP programmes have only marginally changed their prediction capability and new releases were not always better than previous ones.

Although the overall system behaviour is generally well described, deficiencies still exist in the prediction of safety relevant local processes which is often related to limitations in the modelling of the constitutive relations in the two-fluid model like interfacial friction or the non-equilibrium evaporation or condensation processes. However, as will be explained later this is only one part of the problem. The interfacial transport processes are largely governed by the contact area (interface) between the phases which is only indi-

rectly modelled. In all codes attempts are made to correlate this interface with void fraction and some other local parameters like mass fluxes, which at best give only a static or instantaneous description of the process and, therefore, cannot model the time evolution of the processes. This is the case in particular for the modelling of flow regime transitions and the time needed for predicting the corresponding spatial re-distribution of the phases.

All the codes show great difficulties to represent flow conditions with large spatial gradients either in axial or radial directions. Examples include the occurrence and tracking of mixture levels in various components of the primary and secondary systems in case of slow transients like small break LOCA, the steep pressure gradients associated with the occurrence of critical flow conditions in large and small break LOCA, or the conditions related to a partially uncovered core where local flow and related heat transfer conditions can drastically change within extremely small spatial distances (e.g. in case of quench front propagation).

A realistic description of steep parameter gradients or quasi-discontinuities would require a rather fine local discretization (possibly down to a centimeter or even less) in the vicinity of a (generally) moving front or discontinuity, which with present codes is not feasible due to the heavy computational effort or stability limits of the numerical method applied. However, even if such a detailed nodalization could be realized, the result might be largely compromised due to the numerical diffusion effects of present numerical methods.

As was shown by many assessment studies, the deficiencies as described above might become even more dominating factor for low system pressures. This is caused by the fact that with decreasing pressure the difference between the state properties of the phases, and such the inhomogeneity of the two-phase mixture, increases. This results in a further decoupling of the phases and consequently thermal and mechanical non-equilibrium effects like phase separation become more important. In addition, flow regime transitions at the low pressure region might be accompanied with an extreme change of evaporation/condensation rate or interfacial friction over some orders of magnitude which becomes difficult to handle by the numerical schemes used in the codes. For this reason predictions at near atmospheric pressure values are often characterized by strong unphysical oscillations or numerical instabilities.

3. Potential areas for code improvement or development

There are three major driving forces which might demand future improvements of existing TH-codes or even for a new attempt in the development of best-estimate thermal-hydraulic codes:

- ◇ the continuous extension of accident scenarios for which the code was not originally developed, like very slow (nearly steady) transients, long term heat removal conditions, coupling of primary system and containment, transients resulting from accident management procedures or application to non-standard plant designs. This often goes far beyond what the codes have been developed for.

- ◇ the increasing interest in new advanced reactors which will largely rely on passive safety features and processes characterized low driving forces and low system pressure values. Many of the related phenomena have a distinct three-dimensional nature and are beyond the predictive capability of physical models and numerical techniques in present codes.
- ◇ the fast development of computer hardware and the tremendous growth in computing capabilities over the last few years which would principally allow a much higher spatial and time resolution in the prediction of complex thermal-hydraulic phenomena compared with present practices.

In the following a number of new approaches for physical modelling, numerical strategies and code structure enhancements are briefly reviewed which have at least the potential for a substantial improvement of the prediction capability of TH-codes.

3.1 Physical models

Fully hyperbolic system of governing equations for transient two-phase flow

As has been stated before, the use of a fully hyperbolic system of partial differential equations will not provide *a priori* improved results, however, it will be essential for a class of advanced numerical methods providing low numerical diffusion or viscosity. There have been various attempts to extend the system of governing equations for the two-fluid model into a hyperbolic set of partial differential equations. This is generally done by including additional terms in the two separated momentum equations like interfacial pressure (difference) terms as is done in case of CATHARE [11] or by specific formulations of the added or virtual mass effects [14]. In most cases the existence of only real eigenvalues could be verified only by numerical evaluations, and algebraic solutions for the characteristic velocities could be derived only for specific flow assumptions as for example for constant phasic densities. It is also often overlooked that the presence of exclusively real eigenvalues is a necessary but not sufficient condition for a hyperbolic system of equations. Of equal importance is the existence of an independent set of eigenvectors. The perhaps only existing two-fluid model covering the whole range of void fraction for which a rigorous characteristic analysis has been performed is that of H. Städtke et al [15] resulting in an algebraic formulation of the eigenvalues and the corresponding set of eigenvectors. This allows the coefficient matrix representing the set of governing equations to be decomposed with respect to individual characteristic velocities in a purely algebraic way which is of large advantage for a class of advanced numerical techniques described below.

Multi-field representation of specific flow regimes

As has been outlined in section 2.1 the two-fluid model approach which represents the basis for most TH-codes might reach its limits of validation when dealing with increased inhomogeneity of the two-phase mixture. Occasionally it has been proposed to extend the two-fluid model by a further subdivision the individual phases into clearly identifiable parts which could then be described by separate balance equations. This would imply for example for the prediction of dispersed particles (bubbles or droplets) flow regimes a

need to distinguish between specific classes of particle sizes. Another application might be related to the one-dimensional description of heterogeneous two-phase flow regimes in pipes like annular-mist, slug or inverted annular flow regimes. In all these cases the liquid or vapour fraction concentrated near the wall (liquid or vapour film) behaves rather differently than the dispersed fraction (droplet or bubble) in the core of the pipe. Separate balance equations for the wall film fraction and the dispersed fraction could principally describe important deposition or entrainment processes assuming that corresponding source terms can be adequately modelled. A further benefit of such a multi-field approach is that it would allow a more physically based description of flow regime transitions.

Explicit modelling of interfacial area transport processes

The idea to explicitly model the transport of the interfacial area concentration in two-phase flow systems is not new, however it was never brought to a stage where it could be applied in engineering calculations. The only attempt to implement such a model into a transient two-phase flow code was the Advanced Fluid Dynamics Model (AFDM) developed by a group of international scientists at the Los Alamos National Laboratory [16] which, however, was not advanced to a state where it could be applied for reactor safety relevant applications.

The interfacial transport model consists of a balance equation for interfacial area concentration a^{int}

$$\frac{\partial}{\partial t}(a^{int}) + \nabla \cdot (a^{int} \bar{v}^{int}) = \sigma^A \quad (5)$$

which can be derived either in a very general form by an averaging of the spatial gradient (divergence) of a phasic distribution function [17] or, for specific cases of dispersed particles (bubbles, droplets) from the transport of the particle density distribution function [18].

As is true for all time and space averaged approaches, the crucial point is always the formulation of the corresponding source or sink terms σ^A including processes like nucleation, particle (bubble/droplet) break-up or coalescence and flow regime transitions which is discussed in some detail by Kocamustafaogullari and Ishii in [18]. The authors give a rather optimistic view on the potential of interfacial transport modelling, however, some work is still needed in particular in dealing with flow regime transitions and less well structured flow regimes like annular mist, inverse annular or churn-turbulent flow conditions.

Bulk viscosity and/or turbulent diffusion models for multi-dimensional two-phase flow processes

Although most two-phase flow processes are known to be of a highly stochastic nature, all present TH-codes do not include any direct modelling of turbulent diffusion or viscosity processes. Turbulent effects are only indirectly accounted for, e.g. in form of wall friction and/or interfacial friction correlations, which seems to be fully adequate as long

as highly diffusive numerical methods are applied. However, with the introduction of advanced numerical techniques with low artificial viscosity, a strong need will emerge for the modelling of physical diffusion and turbulent effects for multi-dimensional two-phase flows. Since a direct simulation of turbulence, or a filtered statistical approach like large eddy simulation are (and most certainly will remain so for the near future) prohibitively expensive, any modelling of turbulence effects in two-phase flow systems will be related to more engineering approaches based on simplified eddy viscosity concepts or more sophisticated k- ϵ models. Sufficient knowledge exists today which allows to derive such simplified turbulence models for relatively well structured two-phase flow regimes like dispersed bubbly and dispersed droplet or mist flow. However, further research is certainly required to extend these models to more complex two-phase flow conditions.

3.2 Numerical methods

Low numerical diffusion methods based on Flux Vector Splitting or Approximate Riemann Solvers

Any further improvement in the prediction capability for multi-dimensional two-phase flow will largely depend on the success in the development of numerical techniques providing low numerical diffusion or viscosity. These kinds of techniques, also known as essentially non-oscillatory high resolution methods, have been developed within the last decade for single phase flow and have become a standard for many gas dynamics calculations. They include for example the Split Coefficient Matrix method, the Flux Vector Splitting technique or the method based on the Approximate Solution of a corresponding Riemann Problem.

Common to all these methods is the concept of "upwinding" which combines the preservation of wave propagation processes along characteristic directions with the conservation property for mass, momentum and energy, for the solution of the advection problem. The less challenging diffusion processes are then handled with a standard central differencing scheme or a related finite volume equivalence. Furthermore, what makes these methods attractive is the fact that they are principally based on a "true" finite volume concept which allows a rather straightforward application also for unstructured grids. These methods can also be relatively easily extended to higher order accuracy in space following the concept of Monotonic Upwind Scheme for Conservation Laws (MUSCL) of Van Leer [19]. The methods have been successfully used to provide a high resolution of flow discontinuities like shock or detonation waves without the need of additional explicit shock capturing algorithms.

Application of the methods described above for two-phase flow processes has been largely hampered by the requirement for hyperbolicity of the governing system of equations which is not *a priori* the case for the two-fluid model. However, within the last few years, new hyperbolic two-fluid models have been developed which principally allow to extend these techniques also to transient two-phase flow conditions [20]. A numerical example is shown in Fig. 2 for the Oscillating U-tube manometer problem as proposed by Ransom [21] where the amount of damping gives a measure of the numerical viscosity effect in the calculation. The comparison with a standard method (in this case

RELAP5/MOD3 is used as an example) clearly indicates the superiority of the Flux Vector Splitting technique.

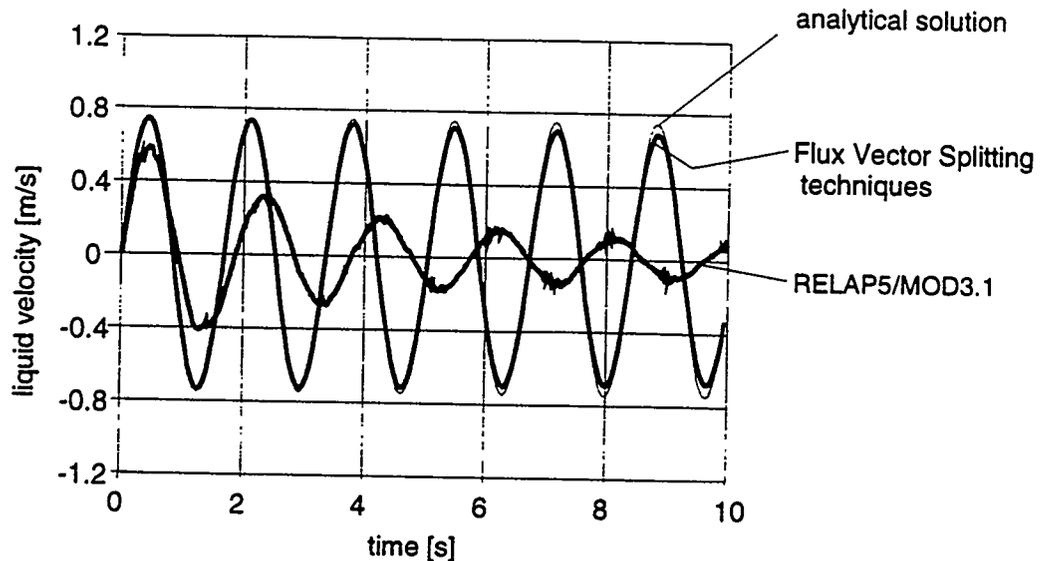


Fig. 2 Liquid velocity at bottom leg of U-tube manometer

Automatic grid (nodalization) adaptation techniques

As outlined in section 2.3 extremely small cell sizes might become necessary to accurately describe the occurrence and tracking of flow discontinuities such as mixture levels or quench fronts. With respect to reflood processes the use of moving meshes for the two-dimensional calculation of heat conduction in fuel rods might be helpful, however, the same resolution would be required also on the fluid side in order to provide the necessary local heat transfer conditions at the rod surface. Even in case that the numerical method applied could handle such small grid sizes, their practical use is in most cases not feasible due to economic constraints.

A possible solution to this problem is the implementation of automatic grid adaptation schemes as were developed and successfully applied for gas dynamic calculations in order to better follow the propagation of shock or detonation waves [22]. The method includes three basic steps: (1) the identification of the region in the flow domain where additional grid points should be introduced based on information of local gradients of pre-selected flow parameters, (2) the introduction of new grid points and (3) the corresponding interpolation procedures providing conservation of mass, momentum and energy. The whole process can be made completely reversible which means that, after a front has passed, the original grid will be regenerated. The implementation of these methods is largely supported by numerical techniques based on "true" finite volume schemes and the use of unstructured grids.

Applications of automatic grid adaptation methods have shown that the additional numerical overhead can be made rather small compared with the overall gain due to a dras-

tic reduction of the number of grid points needed to achieve a given spatial resolution of the prediction. Apart from the increased economic performance, such automatic grid adaptation systems might also drastically reduce the "code user effect" since the final nodalization used in the code will be based on the actual physical needs rather than on the imagination of the code user.

3.3 Code structure

In most of the existing TH-codes the physical modelling and the numerical solution of the system of partial differential equations are largely interwoven which often results in a less transparent code structure. This makes it often rather difficult if not impossible to implement improved physical models or new features into the code. For any new developments, strong emphasis should therefore be given to maintaining a high degree of modularity in the code structure which would also require clearly defined interfaces between the description of the basic set of governing equations, the various physical models and the numerical solution strategy. Such a code structure would then facilitate possible future extensions of the modelling approach like an increase of the number of field equations for the description of more complex two-phase flow regimes, the use of additional balance equations for the transport of interfacial area concentration, the inclusion of turbulence models, as well as the modification or even complete replacement of the numerical solution scheme.

A highly modular approach would also permit a different degree of modelling sophistication for various sub-domains of the overall system. This could imply for example the use of a more complex multi-field approach only in some restricted parts or components while the remaining system is described by more simplified models based on a reduced number of balance equations. However, such a strategy will require a robust numerical method which can be sufficiently generalized to handle advection-diffusion problems with an arbitrary number of conservation equations.

4. Conclusions and recommendations

Present best-estimate TH-codes have reached a high degree of maturity as indicated in the principal capability to describe qualitatively and in many cases also quantitatively a wide spectrum of accident scenarios in Light Water Reactors. To a large extent these codes synthesize the experience and the know-how gained over a period of more than thirty years from extensive reactor safety research programmes as were carried out in many industrialized countries.

There still remain, however, shortcomings in the codes which are often related to limitations of the basic modelling approach or the numerical methods applied and as such cannot always be solved by minor changes to the code. These more basic deficiencies are in many cases partially compensated by simplified highly empirical "engineering" solutions which are usually tuned to the experimental data from separate effects and integral test programmes. These (sometimes ad-hoc) engineering models largely contribute to the uncertainty of the prediction if the code is applied outside the validity of the experimental

data base from which these models have been derived. Therefore, specific care has to be taken if the codes are used to extrapolate results obtained for small scale facilities to full size plants.

There is some evidence to suggest that most codes have reached a level of "saturation". This is indicated by the observation that "code improvements" have only marginally changed the quality of the prediction as long as the underlying basic physical modelling concept and numerical method applied are maintained. On the other hand, more fundamental changes to the modelling like the use of multi-field equations, interfacial area transport models, or the use of new low diffusive numerical methods can hardly be realized in the framework of the present code structure.

The future perspective of TH-codes will largely depend on the time frame considered. Although the present TH-codes no longer represent the "state-of-the-art" in many aspects, they will certainly continue (at least in a short term view) to play an important role for the safety assessment of LWRs with standard or evolutionary design. Major efforts in the near term might concentrate on making them easier to use and on quantifying uncertainties associated with the predictions.

The longer term perspective of these codes is certainly connected to the future of nuclear energy in general. New fields of applications and new innovative reactor designs might demand a new attempt for the development of thermal-hydraulics codes for two reasons:

- ◇ new reactor concepts are expected to largely rely on passive safety features which are often characterized by low head driven flow processes like natural circulation or convection processes with distinct 3-dimensional nature. This goes beyond the prediction capability of present TH-codes.
- ◇ extensive experimental programmes as were performed in the past for the present standard PWR and BWR might be prohibitively expensive. New reactor designs will therefore require a more generic approach for the numerical simulation of basic reactor features in order to reduce the necessary experimental back-up to a minimum.

As suggested in the present paper, there are many promising new approaches with respect to the physical modelling, numerical method and informatics which could justify a new attempt for the development of a "third generation" of TH-codes. On a long term view, such a project might be the only way to maintain the (still) existing large competences in reactor thermal hydraulics and in related fields like transient two-phase flow and boiling heat transfer or neutron kinetics. However, the final decision on this subject will certainly be driven by the future needs in this field coming from nuclear industry or safety authorities.

Nomenclature

Variables

a^{int}	interfacial area concentration
C^{tr}	coefficient for transport processes at interface
f_i^{ext}	specific external forces for phase i
\bar{F}_i^{int}	interfacial force for phase i
h_i	enthalpy of phase i
p	pressure
Q_i^{ext}	external heat source for phase i
$\bar{\mathbf{T}}_i$	viscous stress tensor
u_i	internal energy of phase i
t	time
\bar{v}_i^{ex}	exchange velocity for phase transition
\bar{v}_i^{int}	velocity vector of interface
\bar{v}_i	velocity vector of phase i
α_i	volumetric concentration of phase i
ρ_i	density
ΔX	driving force for interfac. transp. processes
σ_i^M	source term for mass of phase i
σ_i^Q	source term for heat of phase i
σ_i^A	source term for interfacial area concentration

Subscripts

g	gas
i	liquid or gas
l	liquid

References

- [1] M. Ishii, *Thermodynamics of Two-Phase Flow*, Eyrolles, Paris, 1975
- [2] J. Bouré, *On a Unified Presentation of the Non-Equilibrium Two-Phase Flow Models*, Proceedings of a ASME Symposium, New York, 1975
- [3] J.M. Delhayé, J.L. Achard, *On the Averaging Operators Introduced in Two-Phase Flow Modelling*, Proceedings of a CSNI Specialist Meeting in Transient Two-Phase Flow, Toronto, 1976
- [4] D.A. Drew, R.T. Lahey, *Application of General Constitutive Principles to the derivation of Multidimensional Two Phase Flow Equations*, Int. J. Multiphase Flow 5, 243-264, 1979
- [5] D. Gidaspo (chairman), *Modelling of Two-Phase Flow*, Round Table Discussion RT-1-2, proceedings of the Fifth International Heat Transfer Conference, Tokyo, Japan, September 3-7, 1974, also in Heat Transfer, 3 (1974)
- [6] V. Ransom, *RELAP5/MOD2 Code Manual*, Idaho Engineering Laboratory, NUREG/CR-4312, EGG-23986, 1985
- [7] RELAP5 Development Team, *RELAP5/MOD3 Code Manual, Models and Correlations*, NUREG/CR-5535, Vol. 4, 1995
- [8] J.A. Borowski, N.L. Wade, *TRAC-BF1/MOD1: An Advanced Best-Estimate Computer Program for BWR Accident Analysis, Model Description*, NUREG/CR-4356, EGG-2626, Vol.1, 1992
- [9] F. H. Harlow, A.A. Amsden, *A Numerical Fluid Dynamics Calculation Method for all Speeds*, Journal of Computational Physics, 8, (1971), 197-213
- [10] F. H. Harlow, A.A. Amsden, *Numerical Calculation of Multiphase Flow*, Journal of Computational Physics, 17, (1975), 19-52
- [11] J.C. Micaelli, D. Bestion, et al., *The new Improved Thermal-Hydraulic Code CATHARE for Safety Reactor Studies*, Conference on Thermal Reactor Safety, Avignon, 1988
- [12] M. Burwell, G. Lerchel, G. Miro, V. Teschendorff, K. Wolfert, *The Thermal-Hydraulic Code ATHLET for Analysis of PWR and BWR Systems*, Proc. 4th Intern. Topical Meeting on Nuclear Reactor Thermal-Hydraulics, NURETH-4, Karlsruhe, Vol.2, pp. 1093-1102, 1988
- [13] S.N. Aksan, F. D'Auria, H. Städtke, *User Effects on the Thermal-Hydraulic Transient Code Calculations*, Nuclear Engineering and Design 145, 1993, 159-174
- [14] D.A. Drew, R.T. Lahey, *Application of General Constitutive Principles to the Derivation of Multidimensional Two Phase Flow Equations*, Int. J. Multiphase Flow Vol. 5, p. 243-264, 1979

- [15] H. Städtke, R. Holtbecker, *Hyperbolic Model for Inhomogeneous Two-Phase Flow*, Intern. Conference on Multiphase Flows, '91 TSUKUBA, Univ. of Tsukuba, Japan, September 24-27, 1991
- [16] D. Wilhelm, *AADM: An Advanced Fluid-Dynamics Model, Vol. II: Topologies, Flow Regimes and Interfacial Areas*, Los Alamos National Laboratory, LA-1692-MS, Vol. II, September 1990
- [17] W.G. Gray, P.C. Lee, *On the Theorems for Volume Averaging of Multi-Phase Systems*, Int. J. Multiphase Flow, Vol. 3, p. 333-340, 1977
- [18] G. Kocamustafaogullari, M. Ishii, *Foundation of the Interfacial Area Transport Equation and its Closure*, Int. J. Heat Mass Transfer, Vol. 38, No. 3, p 481-493, 1995
- [19] B. Van Leer, *Towards the Ultimate Conservative Difference Scheme, a Second-Order Sequel to Godunow's Method*, J. Computational Physics, Vol. 32, pp. 101-136, 1979
- [20] H. Städtke, G. Franchello, B. Worth, *Numerical Simulation of Multi-Dimensional Two-Phase Flow based on Flux Vector Splitting*, 7th Intern. Meeting on Nuclear Thermal Hydraulics, Saratoga Springs, NY, USA, September 10-15, 1995
- [21] B. Spalding et al, *Problem Specifications and Collated Solutions of the Two-phase Numerical Benchmark Exercise 1987-87*, Proceedings of DOE,/EPRI Workshop on Two-Phase Flow Fundamentals, Rensselaer Polytechnic Institute, Troy, NY, USA, March 16-20, 1987
- [22] T.J. Barth, *On Unstructured Grids and Solver, Lecture Series on Computational Fluid Dynamics*, von Karman Institute, Brussels, March 3-9, 1990

Views on the Future of Thermal Hydraulic Modeling

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I. Introduction

It is essential for the U.S. NRC to sustain the highest level of the thermal-hydraulics and reactor safety research expertise and continuously improve our accident analysis capability. Such expertise should span over four different areas which are strongly related to each other. These are:

- 1) Reactor Safety Code Development
- 2) Two-phase Flow Modeling
- 3) Instrumentation and Fundamental Experimental Research
- 4) Separate Effect and Integral Test

The NRC is already considering a new effort in the area of advanced thermal-hydraulics effort. Its success largely depends on the availability of a significantly improved two-phase flow formulation and constitutive relations supported by detailed experimental data. Therefore, it is recommended that the NRC starts significant research efforts in the areas of two-phase flow modeling, instrumentation, basic and separate effect experiments which should be pursued systematically and with clearly defined objectives. It is desirable that some international program is developed in this area. This paper is concentrated on these items in the thermal-hydraulic area which eventually determine the quality of future accident analysis codes.

II. Significance of the Problem

The simultaneous flow of two-phase occurs in most of the important accident conditions in LWR's. If we recall that the singular characteristic of two-phase flow is the presence of one or several interfaces between the phases, it can be noticed that many of the two-phase systems have a common structure, or a common topology of the interface. Furthermore, whereas single-phase flows can be classified according to the geometry of the flow in laminar, transitional and turbulent flow, the flow of two-phases can be classified according to the geometry of the interface into three main classes; namely, separated flows, transitional or mixed flows and dispersed flows.

The major characteristic of the gas-liquid two-phase flow is the existence of the deformable interface and significant evolutions of interfacial structures along the flow. The coalescence and disintegration of fluid particles, entrainment or deposition of droplets from a continuous liquid film, and instability of an interface are common problems. The change in the interfacial structures, which depends on the flow field, is the major difficulty in modeling two-phase flow.

The design of nuclear reactor systems and the ability to predict their safety and performance depends on the availability of experimental data and of conceptual models which can be used to describe a physical process with a required degree of accuracy. From a scientific, as well as from a practical point of view, it is essential that the various characteristics and properties of such conceptual models and processes should be formulated clearly, on a rational basis, and supported by experimental data. For this purpose, specially designed instrumentations and experiments are required which must be conducted in conjunction with and in support of analytical investigations.

The conceptual models which describe the steady state and dynamic characteristics of structured multi-phase media should be formulated in terms of the appropriate field equations and closure relations. However, the derivation of such equations for the flow of structured media is considerably more complicated than for single-phase flow. In multi-phase or multi-component flows, the presence of interfaces introduces great difficulties in the mathematical and physical formulations of the problem. From the point of view of physics, the difficulties which are encountered in deriving the field and closure equations appropriate to multi-phase flow systems stem from the presence of the deformable interface and the fact that both the steady and dynamic characteristics of multi-phase flows depend upon the structure of the flow.

The weakest link in the two-phase flow formulation is the constitutive equations for the interfacial interaction terms. The difficulties arise due to the complicated motion and geometry of interfaces in a general two-phase flow. Furthermore, these constitutive equations should be expressed by the macroscopic variables based on proper averaging.

The interfacial transfer terms are strongly related to the interfacial area concentration and to the local transfer mechanisms such as the degree of turbulence near interfaces. Basically, the interfacial transport of mass, momentum and energy is proportional to the interfacial area concentration, a_i , and to a driving force. This parameter, a_i , having the dimension of the reciprocal of length, represents the available interface area per unit volume and characterizes the geometrical effects on the interfacial transport processes. The driving forces for the interfacial transport depend on the local turbulence, transport properties, driving potentials and some length scale at the interfaces. This length scale may be related to a transient time such as the particle residence time or to the interfacial area concentration and void fraction.

One of the major difficulties in developing a reliable one or quasi-one dimensional two-fluid formulation is modeling of the constitutive relations for the interfacial transfer of momentum and energy which does not have a counterpart in a single phase flow analysis. For three-dimensional two-fluid model, the mechanistic modeling of the constitutive relations for the interfacial transfer and turbulent transfer in two-phase flow requires detailed local measurements of the interfacial area, interfacial velocity, phase velocities and turbulence which were not available until quite recently. In the last five years, tremendous advances in the local instrumentation technology for two-phase flow have been accomplished. These developments came by due to the advances in electronics, local multi-sensor techniques, and optical methods. Now the local interfacial area concentration, void fraction, interface velocity, Sauter mean diameter, phase velocities and turbulence in two-phase flow can be measured. These parameters give great insight

into the interfacial transfer and turbulent transfer mechanisms. Many of the three-dimensional transfer phenomena can be measured and quantified such that modeling of the constitutive relations for the interfacial and turbulent transfers becomes realistic.

From the standpoint of analysis, there exists a need for improved methods of accounting for the structure and local phenomena in two-phase systems. From the standpoint of experimentation, there exists a need for new and improved measurements for local phenomena to support constitutive equation development. The two must proceed in concert if we are to be successful in producing new computational methods that are based upon first principles.

The new approach for modeling of the interfacial structure that replaces the conventional flow regime maps and criteria should be one of the focal points of the research. The introduction of the interfacial area transport equation or multi-field approach is now possible. The modeling of the interfacial structure is directly related to the foundation of the new two-fluid model.

III. Recommendation for Two-phase Flow Modeling

1) Interfacial Area Modeling

For predicting the thermal-hydraulic behaviors of two-phase flow, the interfacial structure is one of the most important factors. This is because all the transfers of mass, momentum and energy between phases occur at the interface. Both the available interfacial area and the transfer mechanisms strongly depend on the structure of interface. Traditionally, the effects of the interfacial structure have been analyzed using the two-phase flow regimes and regime transition criteria. However, this traditional approach has a number of shortcomings. First, the flow regime transition criteria are algebraic relations which do not fully reflect the true dynamic nature of changes in the interfacial structure. Hence the effects of the entrance or boundary cannot be taken into account correctly, nor the gradual transition between regimes. Secondly, the method based on the flow regime transition criteria is a two-step method which requires the regime dependent closure relations for the interfacial area effects. Normally, the effects of these are imbedded in the correlations implicitly, therefore, the compound errors from this approach can be significant.

In view of this, it is recommended here to develop an interfacial area transport equation for the first-order characterization of interfacial structures. The basic ideas are presented below. The transition from bubbly flow to slug flow occurs mainly due to agglomeration and coalescences of smaller bubbles into cap bubbles. Once a cap bubble is formed, further coalescences follow in the wake region of a cap bubble. These observations indicate that for a good mechanistic modeling, it is necessary to study bubble coalescence and break-up criteria. The latter will give information on the maximum bubble size and bubble size distribution. These are important in the formation of a link between the flow-pattern transition and the characteristics of the interfacial structure, such as interfacial area concentration and void fraction distributions.

In the recommended research, bubble coalescence and break-up processes are considered explicitly to develop a more mechanistic model. For this purpose, the use of the interfacial area transport equation for two-phase flow appears to be most suitable. The concept of the interfacial area transport equation was suggested by Ishii in 1975 and subsequently applied for annular mist flow by Kataoka and Ishii to predict the entrainment and deposition processes. The mechanism of the transition from bubbly to slug flow can be considered as the elimination of the dispersed phase by the coalescence mechanism, whereas in the annular to annular-mist flow transition the dispersed phase is created by the droplet entrainment process. Therefore, the processes are almost in the complete opposite direction. Hence it can be concluded that once the rate processes of the coalescence and bubble break-up are modeled, the gradual transition from the bubbly to slug flow can be predicted through the interfacial area transport equation. In the three-dimensional formulation it is given by

$$\frac{\partial a_i}{\partial t} + \nabla \cdot a_i \vec{v}_i = \phi_{dis} - \phi_{co} + \phi_{ph}$$

where a_i is the interfacial area concentration, and \vec{v}_i is the mean interface velocity. The right hand side represents the source and sink due to the bubble break-up, coalescence and phase change or compressibility.

The fluid particle disintegration occurs mainly due to the turbulent fluctuation and interfacial stability, hence it should depend on the continuous phase Reynolds number, Re_c , fluid particle size, r_d , and relative velocity, v_r .

$$\phi_{dis} = \phi_{dis}(Re_c, r_d, v_r)$$

The coalescence process mainly depends on the random collisions and the systematic wake entrainment. The collision frequency is a strong function of the void fraction and the turbulent fluctuations, whereas the wake flow depends on the particle Reynolds number, Re_d . The coalescence probability after a collision depends on the particle size and fluctuation velocity components. Thus,

$$\phi_{co} = \phi_{co}(\alpha_d, r_d, Re_c, Re_d)$$

The phase change effect depends on the nucleation, temperature difference and the flow field. For a simplified one-dimensional model, the interfacial transport equation becomes

$$\frac{\partial \langle a_i \rangle}{\partial t} + \nabla \cdot \langle a_i \rangle \langle v_i \rangle = \langle \phi_{dis} \rangle - \langle \phi_{co} \rangle + \langle \phi_{ph} \rangle + \langle \phi_w \rangle$$

where $\langle \phi_w \rangle$ represents the source due to wall nucleation. These constitutive relations

ϕ_{dis} , ϕ_{co} and ϕ_{ph} or their one-dimensional forms should be modeled using basic experimental data and mechanistic models.

2) Pilot Code Development using Interfacial Area Transport Equation

The effect of the interfacial area transport equation on the overall two-fluid model formulation and numerical solution method should be studied through a simple one-dimensional pilot code. This will give us the insight to the dynamic effects of the transport equation, stability of the differential equation system, accuracy of the constitutive relations and efficiency of the numerical method.

3) Two-phase Flow Turbulence Modeling

For a three-dimensional two-phase flow formulation, the constitutive relation for the two-phase Reynolds stress becomes necessary. As in the case of single phase flow, the Reynolds stress determines the transverse momentum transfer and velocity profile in the fluid. The simplest form of the constitutive relation is a two-phase mixing length model. A higher order turbulence model such as the $k - \epsilon$ model is also possible. In the state-of-the-art of the two-phase flow modeling, there are no well established or reliable turbulence models. Thus, as a long term goal, some effort in this direction should be made for a three-dimensional model. The two-phase turbulence may be divided into two main categories: the flow shear-induced turbulence (macroscopic) and the interface-induced turbulence (microscopic). Turbulence is a non-linear phenomenon; however, as a first step, a linear combination of these two turbulence effects can be considered and modeled separately.

4) Two-phase Flow Instability at Low Pressure

At low pressure, two-phase flow systems tend to be quite unstable due to several mechanisms. In particular, a natural circulation two-phase flow at a low pressure is highly unstable due to manometric, density wave, chugging and flashing-induced instabilities. This is because the flow and void generation are closely coupled in a natural circulation system. Furthermore, due to the large density ratio between liquid and vapor, small fluctuations in heat transfer result in significant void fluctuations. However, two-phase natural circulation is a key in most of the advanced LWR designs which use the automatic depressurization systems and depend on the gravity induced flow. Most of the existing studies have been performed for a forced flow system at relatively high pressure, hence it is necessary to carry out some basic research to understand these instabilities.

5) Constitutive Relation Development

The constitutive relations and correlations are used in the two-fluid model to close the two sets of conservation equations of mass, momentum and energy. In particular, the interfacial transfer terms couple the mass, momentum and energy of phases. There are several areas where improved constitutive relations can make a large difference in the accuracy and reliability of code predictions based on the two-fluid model formulation. These are listed below.

a) Interfacial Heat Transfer at Low Pressure

The current algebraic heat transfer model for the interfacial energy transfer is too sensitive to the instantaneous changes in the system pressure through the use of the saturation temperature of the interface, particularly at low pressure. This leads to considerably fluctuating energy transfer between the liquid and vapor and oscillatory void fraction predictions. The actual physical process involves the transient thermal boundary layer development which should exhibit some effects of time delay. Either a time lag model which leads to a difference differential equation or an exponential relaxation model may be used to fix this problem.

b) Interfacial Momentum Transfer

The constitutive relations for the interfacial drag and shear for certain regimes require further study. These are i) inverted flow regimes in the post dryout region, ii) annular flow at high pressure with the effect of entrainment and deposition, and iii) developing flow where void distribution changes rapidly and the drag force, lift force and turbulent diffusion force interact with each other.

c) Thermal Non-equilibrium Model

Significant thermal non-equilibrium occurs during flashing, direct contact condensation and post CHF heat transfer. Among these, flashing and direct contact condensation are particularly important for advanced LWR and severe accidents. A mechanistic model of the flashing based on the nucleation site density is in the early stage of the development; however, it has a good potential to eliminate the large uncertainty of the existing empirical correlation or the shortcomings of the thermal equilibrium model.

The condensation of large volume of steam with non-condensable gases by injected subcooled water is an important problem, yet there are no reliable models or data to analyze it with confidence. Similarly, the condensation of steam with non-condensable gases in a heat exchanger or in a pool of subcooled water is not understood well and has a scaling problem.

IV. Recommendation for Instrumentation and Fundamental Experimental Research

1) Instrumentation Development

An advance instrumentation development for two-phase flow systems is a necessary component of the thermal-hydraulic research. These instrumentations are the basic tools for the fundamental experimental research focused on the important phenomena in two-phase flow. Recommended instrumentation development programs are listed below.

- Multi-sensor conductivity probes for the measurement of local interfacial area, void fraction, particle size and interfacial velocity, particularly for a boiling system

- Turbulence measurement in two-phase flow
- Measurement of entrainment rate, deposition rate and droplet size at high velocity two-phase flow at relatively high pressure
- Measurement of mass flux and vapor quality
- Accurate measurement of break flow
- Flow visualization and characterization of interfacial geometry
- Measurement of liquid flow rate using modified magnetic flow meter or other methods
- Global void sensors based on impedance measurement with dynamic information such as the histogram, cross correlation, etc.
- Incorporation of artificial intelligence, fuzzy logic and neural network methods in processing the data.

2) Fundamental Experiments

Using the state-of-the-art instrumentations, fundamental experiments focused on the outstanding important problems and phenomena can be studied and a data base for a model development effort can be established. Some of the recommended experiments are listed below.

- Interfacial area measurements focused on developing a data base for the coalescence sink term and disintegration source term in the area transport equation. This should be performed for both the vertical and horizontal flow at several hydraulic diameters
- Single phase and two-phase natural circulation, dynamics and instability experiments
- Flashing phenomena in stagnated fluid or in a natural circulation system
- Annular flow experiment focused on the entrainment rate, deposition rate, droplet size, film thickness and interfacial shear
- Two-phase flow turbulent experiments focused on bubbly and churn-turbulent flow using the hot film measurement and interfacial area measurement.

V. Recommendation for Separate Effect Test Using Integral Test Facilities

Some of the integral test facilities can be used to perform useful separate effect tests which are valuable bases for the verification of the thermal-hydraulic models and constitutive relations in safety analysis code. In order to be specific, this is discussed in terms of the one facility.

The PUMA facility at Purdue was originally designed for the confirmatory integral test for the GE SBWR design. However, this facility has a large number of instrumentations including local void measurements and flow visualization capability. Furthermore, each of the components exhibit some fundamental characteristics of various two-phase

flow systems. In view of these, it is quite possible to run the PUMA facility for various separate effect tests to obtain some fundamental data focused on particular phenomena.

The recommended separate effect tests which can be performed without any major geometrical modifications are given below.

(1) RPV and ADS

- Single Phase Natural Circulation Benchmark Test

It is focused on the natural circulation rate, two- and three-dimensional energy distribution and flow instability.

- Two-phase Quasi-steady Natural Circulation Test

It is focused on the void distribution, relative velocity, two-phase level, natural circulation rate, void generation by flashing and various flow instabilities.

- Rapid Depressurization and Flashing Test

It is focused on the flashing phenomena and void generation, void distribution, relative velocity, transient behaviors of void fraction, flow, temperature and two-phase level, and flow instabilities.

- Critical Flow at Low Pressure Test

It is focused on the break flow and its measurement for both the large breaks (MSL, DPV and SRV breaks) and small breaks.

- Downcomer Mixing Experiment

It is focused on the cold water injection into RPV through GDCS, IC or FWL nozzles, mixing of the subcooled water with saturated water and two-phase mixture, void collapse, condensation, re-establishment of natural circulation and transition between single phase and two-phase flow.

- Boiler-Condenser Mode Operation Test

Using the RPV and ICS, the steady boiler-condenser mode of core cooling is studied. By some modifications, reflux condenser mode operation is also possible.

(2) Condenser System Test (Quasi-Steady Mode)

- It is focused on the ICS with and without non-condensable gases. The RPV, ICS and SP are used in this test. The single unit and parallel unit operations are studied. The effect of the non-condensable gas (air or helium) in the RPV and the function of the purging system are evaluated.

- PCCS Performance Test with/without Non-Condensables

The RPV, DW, PCCS and SP are used in this experiment. The focus is the PCCS performance with the non-condensable gas (air or helium) and the purging mechanism. A single unit and parallel unit operations and interaction between units are studied.

(3) **Suppression Pool Dynamics Test**

This experiment has several focuses such as the direct contact condensation of steam injected through SRV lines, the horizontal vent condensation, thermal stratification of the pool, effect of non-condensable gas and single phase flow mixing in the pool.

(4) **Drywell Phenomena**

The major focus is the steam mixing with the non-condensable gas in DW. The inertia regime, transition regime and plume regime are studied separately. Other focus is the effect of the vacuum breaker operation on the non-condensable gas distribution.

VI. Recommendation for Other Separate Effect Tests

1. **Large Volume Vapor Condensation with Water**

The direct contact condensation of large volume of vapor such as in the containment by the injection of subcooled water is the focus of this separate effect test. The phenomenon is a major importance for the severe accident phenomena and containment cooling in the advanced LWR. This phenomena is studied with and without the existence of the non-condensable gas. The rapid depressurization and large pressure wave generation are the potential problems.

2. **Counter-Current Horizontal Flow with Phase Changes**

The current code is not very good to analyze the counter-current flow with significant interfacial condensation. Such a flow can be potentially unstable and even may lead to a water hammer problem. This phenomenon is studied with and without the non-condensable gas. Based on the experimental observations, a proper model to handle this flow will be developed.

VII. Summary and Conclusions

For a successful research, both proper focus and good strategy are necessary. For improving our predictive capability for various transients and accidents in LWRs, the most critical element is the improvement of the thermal-hydraulic models, in particular two-phase flow models and constitutive relations. The model improvements and advancement in predictive capability should have four key elements; namely, instrumentation and fundamental experimental research, separate effect and integral tests, two-phase flow model development and reactor safety code development. The present paper is focused on the first three aspects which are the foundation of a reliable safety code. Specific recommendations on modeling, instrumentation developments, basic experiments and separate effect tests are made.

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10. SUPPLEMENTARY NOTES

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11. ABSTRACT *(200 words or less)*

This is a report on the CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements held at Annapolis, Maryland, USA, November 5-8, 1996. This experts' meeting consisted of 140 participants from 21 countries; 65 invited papers were presented. The meeting was divided into five areas: (1) current and prospective plans of thermal-hydraulic codes development; (2) current and anticipated uses of thermal-hydraulic codes; (3) advances in modeling of thermal-hydraulic phenomena and associated additional experimental needs; (4) numerical methods in multi-phase flows; and (5) programming language, code architectures and user interfaces. The workshop consensus identified the following important action items to be addressed by the international community in order to maintain and improve the calculational capability: - preserve current code expertise and institutional memory; - preserve the ability to use the existing investment in plant transient analysis codes; - maintain essential experimental capabilities; - develop advanced measurement capabilities to support future code validation work; - integrate existing analytical capabilities so as to improve performance and reduce operating costs; - exploit the proven advances in code architecture, numerics, graphical user interfaces, and modularization in order to improve code performance and scrutibility, and - more effectively utilize user experience in modifying and improving the codes.

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