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PEER REVIEW OF RELAP5/MOD3 DOCUMENTATION

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Abstract

A peer review was performed on a portion of the documentation of the RELAP5/MOD3 computer code. The review was performed in two phases. The first phase was a review of Volume III, *Developmental Assessment Problems*, and Volume IV, *Models and Correlations*. The reviewers for this phase were Dr. Peter Griffith, Dr. Yassin Hassan, Dr. Gerald S. Lellouche, Dr. Marino di Marzo and Mr. Mark Wendel. The reviewers recommended a number of improvements, including using a frozen version of the code for assessment guided by a validation plan, better discussion of discrepancies between the code and experimental data, and better justification for flow regime maps and extension of models beyond their data base. The second phase was a review of Volume VI, *Quality Assurance of Numerical Techniques in RELAP5/MOD3*. The reviewers for the second phase were Mr. Mark Wendel and Dr. Paul T. Williams. Recommendations included correction of numerous grammatical and typographical errors and better justification for the use of Lax's Equivalence Theorem.

A peer review was performed on a portion of the documentation of the RELAP5/MOD3 computer code[1]. The review was performed in two phases. The first phase was a review of Volume III, *Developmental Assessment Problems*, and Volume IV, *Models and Correlations*. The reviewers for this phase were Dr. Peter Griffith, Dr. Yassin Hassan, Dr. Gerald S. Lellouche, Dr. Marino di Marzo and Mr. Mark Wendel. The second phase was a review of Volume VI, *Quality Assurance of Numerical Techniques in RELAP5/MOD3*. The reviewers for the second phase were Mr. Mark Wendel and Dr. Paul T. Williams. Both phases used the NRC's "Charter for Evaluation of RES Code Documentation" as a guide for the reviews. Some additional review criteria for each phase were added by NRC staff to address concerns specific to these volumes.

The additional criteria added by NRC Staff for the review of Volumes III and IV were those contained in Section 4.4.3 of NUREG-1230, *Compendium of ECCS Research for Realistic LOCA Analysis*[2]. This section describes criteria for documentation in order to support the code scaling, applicability and uncertainty (CSAU) evaluation process. The portions of the NRC's "Charter for Evaluation of RES Code Documentation" which apply to Volumes III and IV are a subset of the criteria given in Section 4.4.3. Therefore, the criteria from NUREG-1230 can be used to provide a concise but comprehensive list of the review criteria for this phase.

The requirements for code assessment reports (i.e., Volume III: *Developmental Assessment Problems*) are set forth in Section 4.4.3.2 of NUREG-1230 which states that it is necessary for the reports:

1. To assess code capability and quantify its accuracy to calculate various parameters of interest such as: cladding temperature, inlet and outlet flows for various components, pressure drops, liquid inventory distribution, temperature distributions, etc.,
2. To determine whether or not the calculated results are due to compensating errors,
3. To assess whether or not the calculated results are self-consistent and present a cohesive set of information that is technically rational and acceptable,
4. To assess whether or not the timing of events calculated by a code are in agreement with experimental data, and
5. To explain any unexpected or at first glance, strange result calculated by the code. This is particularly important when experimental measurements are not available to give credence to calculated results. In such cases, rational technical explanations will go a long way towards generating credibility and confidence in the code.

Futhermore, whenever there is a disagreement between calculated results and experimental data it is necessary:

6. To identify and explain the cause of the discrepancy, that is, to identify and discuss the deficiency in the code (or if necessary, to discuss the inaccuracy of experimental measurements),
7. To address the question of how important the code deficiency is to overall results, that is, to parameters and issues of interest,
8. To explain why this code deficiency may not have an important effect on the particular scenario, or
9. To discuss what changes should be made to code models and correlations in order to obtain better agreement should the discrepancy, that is, the code deficiency, have a significant impact on overall results.

With respect to code input model and sensitivity studies (if performed), it is necessary for code assessment reports:

10. To provide a nodalization diagram along with a discussion of the nodalization rationale,
11. To specify and discuss the boundary and initial conditions as well as the operational conditions for the calculation,
12. To discuss modifications to the input model (nodalization, boundary, initial and/or operational conditions) resulting from sensitivity studies (if conducted),
13. To present and discuss results of sensitivity studies (if performed) on closure relations or other parameters, and
14. To provide guidelines for performing similar analyses.

The requirements for a QA document (i.e., Volume IV: *Models and Correlations*) are set forth in Section 4.4.3.1 which states that the document must:

1. Provide information on:
   - a: Its original source
   - b: Its data base
   - c: Its accuracy
   - d: Its applicability to NPP conditions

2. Provide an assessment of effects, if it is used outside its data base,
3. Describe how it is implemented in the code, that is how it is coded,
4. Describe any modification required to overcome computational difficulties, and
5. Provide an assessment of effects due to implementation (item 3) and/or due to modifications (item 4) on code overall applicability and accuracy.

Each of the five reviewers for Phase 1 prepared an independent report, and these reports were compiled and summarized by W. G. Craddick, D. G. Morris and M. Olszewski of ORNL. A letter report[3] containing the summary plus the full text of each reviewer's report was prepared and provided to the NRC in July, 1992.

While not unanimous in this regard, most of the reviewers felt that Volume III was well written and organized. However, the document has several significant deficiencies when compared to the criteria for acceptance defined in NUREG-1230 for documentation to be used to support the CSAU evaluation process. Modifications in several key areas would be required before the document could meet those criteria. A summary of the reviewer's major recommendations is provided below:

1. All code assessment activities should be performed with a frozen version of the code.
2. A validation plan should be completed. This plan would set forth the logical framework for testing the code. This would lead to a comprehensive set of assessment cases which would demonstrate comprehensive adequacy.
3. Where code results do not match experimental data, more discussion should be offered that details the reasons for the discrepancy. Identified code deficiencies should be evaluated and their impact on the code results assessed.
4. The description of code limitations should be expanded and scaling effects should be addressed.
5. Whenever code features are disabled, the impact on accuracy and code applicability should be discussed.
6. Guidelines for users for performing similar analyses should be included in the report, particularly where difficulties are encountered with code models.

The reviewers' reactions to Volume IV varied from strongly positive (Griffith) to rather negative (Lellouche). The majority felt that the description of what was in the code was fairly clear and understandable, through there is room for improvement. Certainly correction of numerous typographical errors is needed. There were definite differences in the reviewers' reactions to limitations in the description of the applicability and justification of the codes' models and correlations some judging these to be clear deficiencies in the documentation and others more inclined to attribute them to limitations in the code itself or in our knowledge of the physical phenomena. A summary of the reviewers' major recommendations is provided below:

1. Adopt a consistent set of symbols and nomenclature throughout the volume.
2. Provide additional supporting references, justification and explanation for flow regime maps, for applications of correlations and models beyond their original data bases and for modifications made in implementing correlations and models.
3. Provide an explanation for the limits placed on variables and coefficients, particularly in Chapter 4, Section 1.

4. Enhance the readability of Chapters 6 and 7, either by better defining the FORTRAN used or by adopting an alternate presentation strategy.

As was the case for the Phase 1 review, Phase 2 was based on both the NRC's "Charter for Evaluation of RES Code Documentation" plus additional criteria provided by the NRC staff. As before, only a portion of the RES Charter is applicable to Volume VI. Extracting the applicable items produces the following criteria.

1. Is there a description of the capabilities, range of applicability and limitations of the code?
2. Is the numerical solution scheme described? Is time and space averaging described?
3. An executive summary should be supplied which includes objectives, scope, methodology used, conclusions and recommendations.
4. The abstract should contain a brief description of the contents of the document and the sponsoring and performing agencies. Results, conclusions and recommendations should not be included in the abstract.
5. Is the documentation well written, well organized and understandable?
6. Present and discuss results of sensitivity studies on closure relations or other parameters.
7. Address the question of how important the code deficiency is to the overall results, that is, to parameters and issues of interest.

The supplemental criteria provided by the NRC staff address validation of the numerical techniques used in the code and are given below.

1. Volume VI is a self-contained account of the numerical techniques in RELAP5/MOD3.
2. Volume VI establishes the domain of applicability of those numerical techniques by a theoretical nodalization and time step analysis that determines ranges of values of Δx and Δt that lie within the region of stability, convergence, and accuracy for the numerical techniques and correlations used in the code.
3. By combining analytical and computed results, Volume VI meets the regulatory objective to provide RELAP5 documentation sufficiently detailed that the domain of applicability of the numerical techniques and necessary user procedures are both well-defined. That would also provide increased confidence in the ability to distinguish between model deficiencies and deficiencies in numerical techniques.

Wendel reviewed the documentation against the RES Charter criteria and Williams reviewed the documentation against the supplemental criteria. Craddick and Morris compiled and summarized the reviews from Wendel and Williams into a letter report[4] provided to NRC in May, 1993. The major conclusions reached in the review of Volume VI are:

1. Generally speaking, while all criteria are addressed, specific areas require revision and elaboration to meet documentation requirements.
2. Specifically, Chapters 4 and 5 do not meet the requirement of being "sufficiently detailed," and there is insufficient linkage between the theoretical studies presented in Chapter 4 and the computational experiments presented in Chapter 5.

3. Although Volume VI is organized in a logical fashion, significant problems exist with regard to readability due to awkward sentence structure, grammatical and typographical errors, and nomenclature inconsistency.
4. Formalized standards and procedures are rapidly evolving throughout the technical community for software quality assurance. If the term quality assurance is used in this formal sense, Volume VI does not address software quality assurance, despite the appearance of this term in the title of the volume.

Some additional explanation of the second conclusion with respect to the document being insufficiently detailed is warranted. Toward that end, the following four paragraphs are quoted from Williams' review.

Chapter 4 of Volume VI presents a theoretical linear stability analysis for the semi-implicit and nearly-implicit algorithms. The analysis relies upon *Lax's Equivalence Theorem* to provide the fundamental linkage between *well-posedness, consistency, stability,* and *convergence.* This theorem states that given a *properly-posed* linear initial-value problem and corresponding linear finite-difference approximation to it that satisfies the *consistency* condition, *stability* is the necessary and sufficient condition for *convergence.* In other words, in order to prove convergence for a numerical algorithm, it is necessary and sufficient to prove that the parent initial-value problem is well-posed and that the finite difference approximation is consistent and stable. *Well-posedness* requires that solutions to the continuum initial-value problem are unique and continuous functions of the initial data, specifically the initial and boundary conditions. *Consistency* requires that the individual finite-difference approximations converge in some sense to their corresponding continuum partial derivatives in the limit of Δx and $\Delta t \rightarrow 0$. *Stability,* a property solely of the finite-difference approximations used in the algorithm, requires that there should be a bounded limit to the extent to which any component of the initial data can be amplified by the numerical algorithm as it marches through time. *Physical instabilities* are characterized by solutions which have bounded limits, but *numerical instabilities* are unbounded.

Two fundamental issues must be addressed when applying *Lax's Equivalence Theorem* to algorithms for two-phase flow. The first issue is that the Equivalence Theorem has been rigorously proven for *linear* differential and difference operators only. The application of the theorem to nonlinear systems, such as the two-phase conservation law system, represents an extension (albeit commonly made in the computational fluid dynamics literature without justification) beyond its original range of applicability. Such an extension should be justified. This issue is not adequately addressed in Volume VI.

The second issue involves the lack of *well-posedness* of the two-phase conservation law system employed in RELAP5. Quoting from Ransom and Hicks,[5]

> **For some time it has been known that many of the two-phase flow models lead to ill-posed Cauchy problems because they have complex characteristics values. A necessary condition (at least in the linear case) for the Cauchy problem to be well-posed is that it be stable in the sense of von Neumann. For systems of partial differential equations of first order, stability in the sense of von Neumann is essentially equivalent to the condition that the model be hyperbolic (all real characteristics values and complete set of characteristic vectors.)**

This issue is addressed in Chapter 4 but could be expanded with additional background material. The main thrust of Chapter 4 is the theoretical development of conditions for the time-step Δt and nodalization Δx which will ensure that the stated stability condition, Eq. (4.11)$\rightarrow \| U^{n+1} \| \leq \| U^{n} \|$, is met. Since the theoretical treatment, apparently previously unpublished, given in Chapter 4 represents an extension of an analysis reported in the archival literature by Stewart,[6] the detailed comments in Sect. 3.3 of this review suggest a greater rigor and completeness in the presentation of proofs for any new theorems.

Based on the conclusions condensed from Wendel's and Williams' reviews, the set of recommendations summarized below was identified:

1. Include more detailed information in Chapters 4 and 5; specifically, (i) address two theoretic issues when applying Lax's Equivalence Theorem to algorithms for two-phase flow, (ii) provide a linkage between Chapters 4 and 5, and (iii) include geometry, and boundary and initial conditions (or at least a brief summary and appropriate reference) for the computational experiments in Chapter 5.
2. Adopt a consistent nomenclature throughout the volume.
3. Enhance the readability of the volume by correcting numerous grammatical and typographical errors and revising awkward sentence structure.
4. Consideration should be given to retitling the volume or including sections to address the formal requirements of quality assurance.

In conclusion, it is worth noting that the charters for all of these reviews included specific instructions that the review was to be of the documentation only, and not the code itself. This should be kept in mind when considering any of these recommendations. A finding that insufficient justification was presented for any particular model or feature of the code does not necessarily mean that such justification does not exist, but only that we did not find that justification in these volumes.

References

1. K. E. Carlson, et al., "RELAP5/MOD3 Code Manual," Volumes I-IV (DRAFT), NUREG/CR-5535, EGG-2596, Idaho National Engineering Laboratory, June 1990.

2. "Compendium of ECCS Research for Realistic LOCA Analysis," NUREG-1230 R4, Division of System Research, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, December 1988.

3. W. G. Craddick, D. G. Morris, and M. Olszewski, *Peer Review of Documentation for RELAP5/MOD3, Volume III: Development Assessment Problems and Volume IV: Models and Correlations*, ORNL letter report ORNL/NRC/LTR-92/20, July 1992.

4. P. T. Williams, M. W. Wendel, D. G. Morris, and W. G. Craddick, *Peer Review of Documentation for RELAP5/MOD3, Volume VI: Quality Assurance of Numerical Techniques in RELAP5/MOD3,* ORNL letter report ORNL/NRC/LTR-93/10, May 1993.

5. V. H. Ransom and D. L. Hicks, "Hyperbolic Two-Pressure Models for Two-Phase Flow," *Journal of Computational Physics,* Vol. 53, 1984, pp. 124-151.

6. H. B. Stewart, "Stability of Two-Phase Flow Calculation Using Two-Fluid Models," *Journal of Computational Physics*, Vol. 33, 1979, pp. 259-270.

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PEER REVIEW OF RELAP5/MOD3 DOCUMENTATION

SUMMARY PRESENTED BY

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Twenty-First Water Reactor Safety
Information Meeting
Bethesda, Maryland
October 25, 1993

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Review Was Conducted In Two Phases

Phase 1

Reviewed: Volume III, Developmental Assessment Problems
Volume IV, Models and Correlations

Reviewed by: Peter Griffith
Yassin Hassan
Gerald S. Lellouche
Marino di Marzo
Mark W. Wendel

Phase 2

Reviewed: Volume VI, Quality Assurance of Numerical Techniques

Reviewed by: Mark W. Wendel
Paul T. Williams

Both Phases Used Charter For Evaluation Of Res Code Documentation

- Review Completeness and Technical Adequacy of Code Documentation, Not of Code Itself
- Specific Topics for Review:
  - Capabilities and limitations
  - Numerical Solution Methods
  - Models and Correlations
  - User Guidance
  - Quality Assurance

Additional Criteria For Phase 1
Addressed CSAU Needs

- From Section 4.4.3 of NUREG-1230
- For Volume III, Developmental Assessment Problems
  - Quantify Accuracy for Parameters of Interest
  - Identify Compensating Errors
  - Explain Unexpected Results and Discrepancies
  - Assess Implications of Discrepancies
  - Provide Complete Descriptions of Nodalization, Boundary and Initial Conditions etc.
- For Volume IV, Models and Correlations
  - Describe Original Source, Data Base, Accuracy, Applicability
  - Assess Effects of Use Outside Data Base
  - Describe How It's Coded
  - Describe Modifications to Overcome Computational Difficulties and Implications of Those Modifications

Phase 1 Reviewers Sometimes Varied Widely In Their Opinions

Comments on the Same Text:

".....the best written, clearest document of this kind which I've seen and sets a standard for any report of this kind."

".....a hodgepodge of demonstrations but no overview or purpose....writing is often obscure and the grammar is very poor....difficult to follow."

Volume III Clear But Modifications Needed To Support CSAU Process

- Most Reviewers Felt Volume Was Well Written (Readability) and Well Organized
- Modifications Needed to Support CSAU Process:
  - Frozen Version for All Assessment Activities
  - Validation Plan for More Comprehensive Assessment
  - More Discussion of Discrepancies and Their Implications
  - Expanded Description of Code Limitations, Including Scaling Effects
  - Discussion of Implications of Disabling Code Features
  - User Guidelines for Performing Similar Analyses

Overall Reaction To Volume IV Varied Widely

POSITIVE	Griffith	Hassan di Marzo Wendel	Lellouche	NEGATIVE

- Reactions to Deficiencies in Model Justification Differed:
  - Some Judged These to Be Clear Deficiencies in Documentation
  - Some Attributed These to Limitations in Code itself or in the State-of-the-Art of knowledge of the Phenomena, and thus Did Not Consider These as Documentation Deficiencies

Modifications To Volume IV Needed To Meet Both RES Charter And To Support CSAU

- Adopt Consistent Symbols and Nomenclature
- Provide Additional Support and Explanation for :
  - Flow Regime Maps
  - Application of Models Beyond Original Data Base
  - Modifications Made to Models in Implementation
- Explain Limits Placed on Variables and Coefficients
- Enhance Readability Where FORTRAN Source Code is Used
- Correct Numerous Typographical Errors

Additional Criteria For Phase 2 Addressed Validation Of Numerical Techniques

- Self-Contained Description
- Establish Domain of Applicability (Δx and Δt)
- Sufficiently Detailed So Domain of Applicability and User Procedures Are Well Defined

Modifications To Volume VI Needed To Meet RES Charter

- Logically Organized
- All Criteria Addressed
- Significant Problems With Readability:
  - -Awkward Sentence Structure
  - -Grammatical Errors
  - -Inconsistent Nomenclature
  - -Typographical Errors
- Volume Title, "Quality Assurance..." Inconsistent with Formal Use of Term

Modifications To Volume VI Needed To Validate Numerics

- All Criteria Addressed
- Self-Contained
- Better Justify Application of Lax's Equivalence Theorem
    - Justify Extension to Non-Linear Systems
    - Expand Support for Well-Posedness
- Improve Linkage Between Theoretical Studies (Chapter 4) and Computational Experiments (Chapter 5)
- Include Geometry, Boundary Values and Initial Conditions for Computational Experiments