

Progress on the MELCOR Code

Kenneth Bergeron, Randall Cole Jr., Arnold Elsbernd,
Salvador Rodriguez, Russell Smith, and Mark Leonard*

Modeling and Analysis Department

Sandia National Laboratories

Albuquerque, NM 87185-0739

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Abstract

Sandia has made considerable progress in the past year on the MELCOR code for integrated severe nuclear reactor accident analysis:

Boron-Carbide Steam Reactions. We completed an upgrade of our treatment of chemical/physical interactions among water, B_4C , and stainless steel. These processes are important for tracking iodine inventories in BWRs.

Fission Product Vapor Scrubbing by Water Pools. We have upgraded the treatment of fission product scrubbing by replacing the earlier SPARC models with the more recent SPARC-90 models.

Core Flow Blockage and Generalized Axial Gradient Model. Perhaps the most fundamental improvement to MELCOR is our modified treatment of the effect on coolant flow of blockages due to core melt movement. A closely related model improvement was to extend MELCOR's sub-grid axial thermal gradient feature to conditions of arbitrary flow direction (e.g., reversed axial flow or radial flow).

VANAM (ISP-37). We have completed the calculations for the International Standard Problem, and have submitted them to the coordinator at Battelle Frankfurt.

Westinghouse Large-Scale Tests. We have assessed MELCOR's models for containment thermalhydraulics that are relevant for the passive containment cooling concept.

Accident Sequence Analyses. In view of the current interest in steam generator tube rupture (SGTR), we have conducted a series of studies of SGTR-induced accidents in the Surry plant. We have also completed an extensive series of accident sequence calculations for the Westinghouse AP600 reactor in support of the current ALWR certification process.

Current Work in Progress. We are currently in the process of implementing several new or improved models for MELCOR. These include models of fission product chemical reactions with surfaces, aqueous fission product chemistry, and an improved treatment of core structure support failure. We have two ongoing efforts to validate MELCOR against experimental data: an analysis of the Phebus FPT-0 experiment, and an evaluation of the new pool scrubbing model against EPRI experiments.

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*Innovative Technology Solutions, Inc.

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Introduction

The MELCOR code is a computational system for simulating the progression of events and phenomena in a nuclear power plant undergoing a hypothetical reactor accident. It was developed at Sandia National Laboratories (with important contributions from Oak Ridge National Laboratory and others) for the U.S. Nuclear Regulatory Commission. MELCOR is being developed with strict attention to configuration management, with numerous distinct versions released over the years. The most recent major release was version 1.8.3, which was released (with entirely new documentation) in September 1994.¹ To date, the code has been distributed to forty-eight organizations in twenty-two countries (see Table 1). Sandia personnel provide limited levels of assistance to these users. In addition, Los Alamos National Laboratory manages the MELCOR Code Assessment Program (MCAP) for the USNRC. Recent activities of MCAP are discussed in the paper by Boyack et al. in these proceedings.

Table 1. Countries (other than U.S.) to which MELCOR 1.8.3 has been distributed

Austria	Belgium	Croatia
Czech Republic	Finland	France
Germany	Hungary	Italy
Japan	Korea	The Netherlands
Republic of China	Russia	Slovak Republic
Slovenia	Spain	Sweden
Switzerland	Ukraine	United Kingdom

Considerable progress has been made at Sandia in the past year on MELCOR. In this paper, we will briefly describe the progress. The remainder of the paper is organized into five sections: *Recent Improvements to MELCOR*, *Code Development in Progress*, *Validation of MELCOR*, *Validation Work in Progress*, and *Accident Analyses*.

Recent Improvements to MELCOR

The MELCOR project at Sandia (and corresponding work at Oak Ridge) follows a strictly controlled software development procedure, that incorporates a design phase, an external peer review phase, and an implementation phase that includes a limited degree of developmental testing. Releases of new versions of MELCOR also require, in addition, an extensive formal testing program. In this section, we will describe all the major code modifications that have been fully implemented since the release of MELCOR 1.8.3.

Boron Carbide Steam/Reactions. In MELCOR 1.8.3 there is a simple model for oxidation that has been found to be adequate for many situations, but which gives unsatisfactory results for reducing environments — it tends to seriously underpredict the methane generation rate, leading possibly to underestimation of the risk from the release of volatile methyl iodide. For this reason, we have developed an optional advanced boron

carbide reaction model, based on work done at Oak Ridge for the BWRSAR code and SCDAP/RELAP5.

This model uses a free energy minimization calculation that is constrained by limitations on the available masses of boron carbide and of steam. The boron carbide available is limited by a variety of processes, depending on the configuration of the core at the time of the calculation. For example, in the early stages of melt progression, no reactions will occur until a specified fraction of the stainless steel clad has been removed. Also, boron carbide that dissolves into the eutectic phase is not available for reaction. Steam available for reaction is limited by diffusion through oxidized layers for the geometry appropriate to the state of the core at the time of the calculation.

Fission Product Vapor Scrubbing by Water Pools. Numerous analyses and experiments involving the performance of pressure suppression pools have shown that removal of fission products from the primary system discharge is a very important mitigating process. An extensive experimental database exists upon which to base theoretical models. The modeling approach in MELCOR 1.8.3 is based on modifications of the SPARC code developed at Pacific Northwest Laboratories. Since their incorporation into MELCOR, improvements in the SPARC code have been made, culminating in the SPARC-90 code.² These improvements have now been incorporated, with as little modification as possible, into MELCOR.

Models for several aspects of fission product removal in SPARC-90 represent a significant upgrade to modeling capability and fidelity to measured data from that provided by the earlier release implemented in MELCOR. Among the more significant enhancements to modeling capability are the treatment of removal of iodine species that would be transported as vapors under typical reactor accident conditions (e.g., I_2 and organic iodides) and an explicit recognition of the dependence of bubble hydrodynamics and aerosol particle deposition efficiency on pool entrance geometry.

The capture of volatile iodine species in water pools is now represented in two regions of a water pool: local deposition upon entering the pool, resulting from thermodynamic equilibration with conditions in the neighborhood of the vent exit; and deposition at bubble/pool interfaces as the bubble swarm rises to the pool surface. Deposition in both regions of the pool is assumed to be limited by iodine species solubility at the interface. Changes in pool pH due to high radiation fields [which lowers the $H(I_2)$ partition coefficient] is not accounted for in the SPARC-90 models.

Numerous enhancements to the treatment of bubble hydrodynamics and aerosol particle deposition have been made in SPARC-90, most of which are based on observations and measurements from experiments performed by Battelle under the auspices of the Electric Power Research Institute (EPRI).^{3,4} SPARC-90 (and MELCOR) currently offer the user a choice of three distinct pool entrance geometries, from which unique correlations for bubble breakup are applied, i.e., multi-hole vent such as the BWR T-quencher, horizontal vent, or vertical downcomer. Improved models are also implemented to describe the

hydrodynamics of, and particle deposition in, bubble swarms. Among the more important of these improvements is the recognition of the work of expansion generated by bubbles in the rising swarm. This term in the treatment of bubble thermodynamics produces conditions that favor enhanced particle condensation growth under certain thermodynamic conditions, thereby greatly increasing the potential for deposition.

Core Flow Blockage and Generalized dT/dz Model MELCOR's strongly modular architecture treats core behavior and fluid flow separately, even allowing different nodalizations of the core region within the two modeling areas. This has several advantages for the code user, including modeling flexibility and the opportunity to trade off detail against calculational expense. It also simplifies maintenance for the code developer. There are some drawbacks: the flexibility of input imposes greater demands on the analyst, and separate modeling with the resulting numerically explicit interfaces imposes timestep limits for stability of the solution. Code improvements since release of MELCOR 1.8.3 have involved two areas affected by this structure: (1) the calculation of heat transfer between core structures and fluids and (2) representation of the effects of degraded core structures and/or relocated core materials on the resistance to fluid flow.

The first of these involves a model that has come to be called the " dT/dz " model. This model solves, within the core package, a numerically implicit representation of fluid flow and heat transfer using the core nodalization and boundary conditions from the hydrodynamics package. The resulting net heat transfer is passed as a numerically explicit source to the subsequent flow calculation. Although previous discussions of the model have tended to emphasize its function in allowing the core package to infer a more detailed temperature profile within a single hydrodynamic control volume, the implicit numerical method also stabilizes the calculation, permitting longer timesteps. The entire approach fails, however, if the flow patterns calculated by the hydrodynamic calculation are significantly inconsistent with those assumed by the heat transfer calculation.

In previous versions of MELCOR, the model was based on the assumption of upward axial flow. If the assumption was violated, calculated temperature profiles often appeared nonphysical and code performance suffered, sometimes to the point of a code abort. In addition, user input was required to define the source of upward flow, which proved a common source of errors. Improvements to the model have eliminated the need for user input and also removed the restriction on flow directions, allowing consistent treatment of flow patterns involving upward, downward, and radial flows. The improved model produces far more realistic results and, by reducing discrepancies between core and hydrodynamic temperatures, eliminates the cause of many previous numerical instabilities.

The second area of new modeling involves the hydrodynamic effects of relocation of materials in the core. This can substantially change flow geometry and alter the resistance to flow of coolant and/or coolant vapors through the core region, thus affecting the ability of the coolant to remove heat and also the ability of steam to reach and oxidize hot metal surfaces.

Previous versions of MELCOR have the capability to represent the increased flow resistance resulting from blockage of flow paths by core debris. However, this capability relies on a knowledgeable user defining effective valves based on appropriate control functions, and was rarely employed. For a flow path involving potential flow blockage by core materials, the new model calculates an additional friction term based on a correlation for flow in porous media in addition to adjusting the flow area; the only input required is a specification of which core cell or cells are associated with the flow path.

One anticipated effect of the new blockage model is that, by reducing the flow through highly blocked regions of the core that contain little fluid, it will relax the timestep limitation imposed by the material Courant condition in these regions. This may make it possible to run calculations with relatively detailed hydrodynamic nodalizations in the core region without the extreme performance penalties that have been observed with earlier versions of the code.

The new models allow greater fidelity in representing the behavior of a reactor system during a severe accident, while reducing the burden on the user to provide appropriate, often obscure, input. In addition, they have resulted in a much more robust code.

Code Development in Progress

Besides the completed code development work described above, we have a number of code improvements in progress.

Fission Product Reactions with Surfaces. Fission product releases from the primary system depend not only on generation and deposition mechanisms, but also on re-vaporization of volatile fission products from surfaces after deposition has occurred. Chemisorption at these surfaces can significantly inhibit re-vaporization. New models for chemisorption have been designed for MELCOR and, in addition, some improvements in the equations of state of fission products have been made to give more realistic re-vaporization behavior. The design report for this improvement has been externally reviewed and work on implementation has begun.

Fission Product Aqueous Chemistry. Accurate tracking of iodine inventories in the atmosphere and water pool requires improved modeling of aqueous chemical processes. Work has been initiated on a new model that treats diffusion through the pool surface boundary layer, radiolytic chemical reactions, and selected equilibrium chemistry. A key feature is tracking the pool pH, which is known to be a strong determinant of iodine chemistry equilibrium.

Core Support Structure Failure Model. MELCOR 1.8.3 has a model for failure of the core support plate that tends to affect accident progression results when the user changes timestep size, machine platform, or other variations to the code runs that should not impact the results. A thorough analysis of the reasons for these problems has been conducted, and a design for an improved model has been developed and documented. The improvements involve more careful treatments of axial and radial heat conduction, integral

incorporation of a creep-rupture failure model, and a user-controlled treatment of crust formation of the debris supported by the core support plate. Implementation of this model will take place following completion of the external peer review of the design document.

Validation of MELCOR

A major finding of the MELCOR Peer Review Committee⁵ was that, given the importance of the code to safety and regulatory issues, there was inadequate documentation of systematic validation of the predictions of the code against experimental results (or against other codes that themselves were well-validated). In the past several years, Sandia and numerous other organizations have greatly expanded the base of validation results to address this deficiency. Below, we discuss two important new contributions.

International Standard Problem 37—the VANAM Experiments. VANAM M3 was a multi-compartment aerosol depletion test with hygroscopic aerosol material that was performed in the Battelle Model Containment (BMC) in Germany by Battelle Frankfurt in April 1992.⁶ The experiment was intended to investigate thermal-hydraulic conditions and aerosol behavior in containment following a core meltdown accident with depressurization by pressurizer relief valve discharge (ND* scenario of German Risk Study B). The experiment was conducted in five phases that lasted a total of 29 hrs. Each phase was characterized by different combinations of air, saturated or superheated steam, insoluble aerosol, and soluble aerosol (NaOH). A key purpose of the experiments was to investigate the importance of hygroscopic aerosol behavior — i.e., the tendency of soluble aerosols to take up water even when the relative humidity is less than one.

MELCOR 1.8.3 does not have a model for hygroscopic water uptake by aerosols. For the purpose of this study, we developed a simple model and implemented it in a special version of the code. Our intention was not to establish a complete and robust implementation, but rather to create a minimal operational capability within the integrated MELCOR framework so that we could evaluate the importance of the effect and also the expected difficulty of a full implementation.

This interim model is based on the Mason equation, which gives the time rate of change of the particle radius as a function of aerosol composition and atmosphere conditions. The Kelvin effect, which modifies the equilibria to take account of the curvature of the particle surface, was also treated. The numerical implementation required coupling between the results of the water uptake process and the atmospheric conditions (which are calculated in a different module of MELCOR). Rather than attempting a careful implicit treatment, we used a "quasi-implicit" method, that during the aerosol calculation estimates thermal-hydraulic conditions at the end of the time step. This method was expected to generate some degree of numerical instability, and the results shown in Figure 1 are evidence of this. Fortunately, however, the oscillations in the results were bounded, and we successfully achieved numerical convergence throughout the calculation. Given the

oscillations, the accuracy of the solution is uncertain, but in general, this is an encouraging result with respect to the feasibility of implementing a model more rigorously.

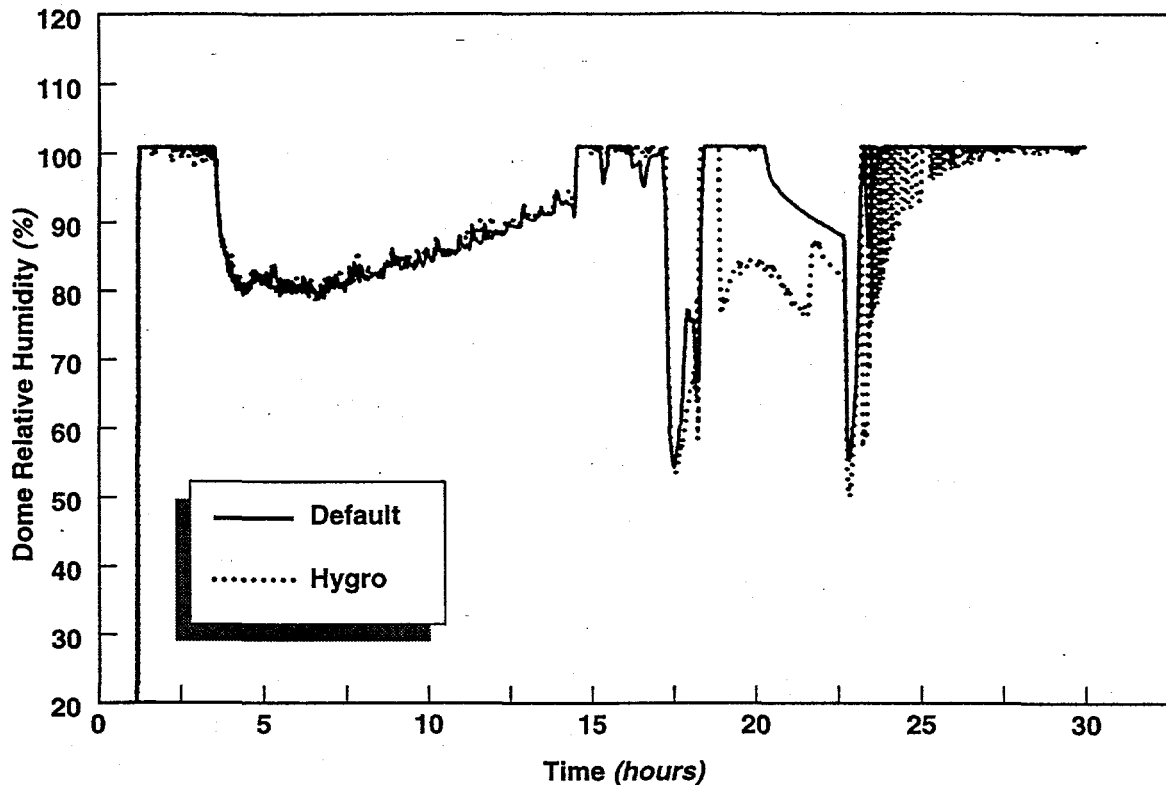


Figure 1. Relative humidity in the dome as predicted by MELCOR.

Figure 2 illustrates the calculated results of including the hygroscopic effect. As seen, the new (Hygro) model is closer to the experimental results for suspended soluble aerosol than is the default model. The new model successfully captures the trend seen in the experiments for accelerated water uptake to increase the rate of gravitational settling. No particular attempt was made to improve agreement for these calculations, because the severe numerical chatter seen in Figure 1 could be responsible for much of the deviation seen in Figure 2. Whether a proper numerical implementation of a hygroscopic model would give better agreement than shown here remains to be seen.

Westinghouse Large-Scale Tests. In order to provide confirmation of the Passive Containment Cooling System concept utilized in the AP600 advanced reactor design, Westinghouse has carried out a large number of tests at a scaled experimental facility. These experiments are known generically as Large-Scale Tests (LST), and provide an opportunity to validate a variety of MELCOR models, including recently developed capabilities for tracking water films on structure surfaces.

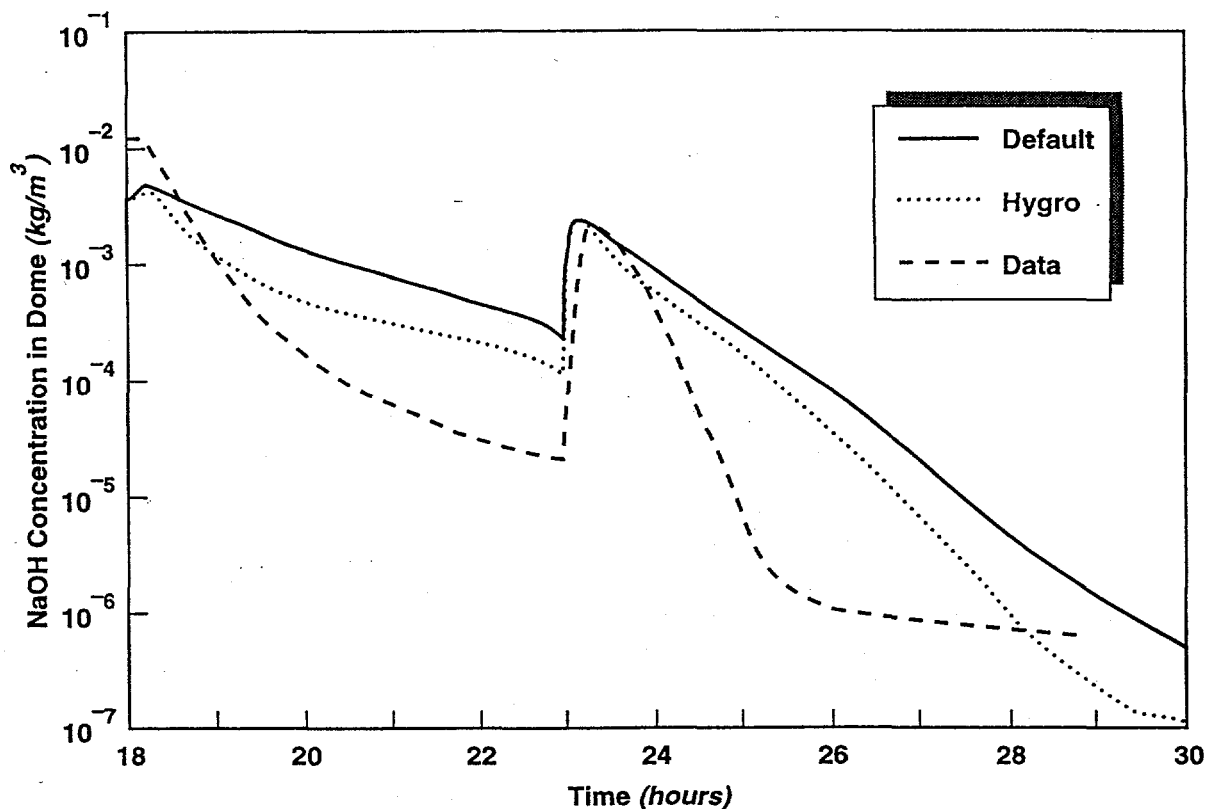


Figure 2. Soluble aerosol mass in atmosphere of the dome region of the VANAM experiment.

Post-test calculations were completed for Tests 202.3, 212.1, and 220.1 using MELCOR 1.8.3. The primary emphasis of the simulations is to demonstrate the adequacy of MELCOR to simulate containment phenomena and, secondly, to provide quantitative evaluation of the new film-tracking model in MELCOR. The film-tracking model is used to simulate the water flooding as it flows down from the top of the outer shell of the dome wall, carrying away sensible heat, and computes the amount of evaporation occurring in the liquid film. In addition, the model tracks the liquid film that develops as condensation occurs inside the dome wall.

During Test 212.1, steam was injected into the LST vessel until a quasi steady-state was reached. The process was repeated three times, with progressively higher steam-injection rates. Figure 3 shows the normalized measured and calculated pressure history (because of the proprietary nature of the data, pressures and time are shown only in arbitrary units). The figure shows that the calculated pressure remained mostly within 5% or less of the measured value. The dome vapor-temperature was typically calculated within 2 K or less of data. The measured temperature drops across the dome shell were calculated within 0.3 K of data and the calculated condensation rate was within 1.5% of data. The calculated inner- and outer-vessel heat transfer coefficients followed the data trend (i.e.

hand-calculated heat transfer coefficients based on measured data), were mostly inside the data band, and for the values outside the band, the coefficients were within the typical experimental error of $\pm 25\%$ found in the literature.

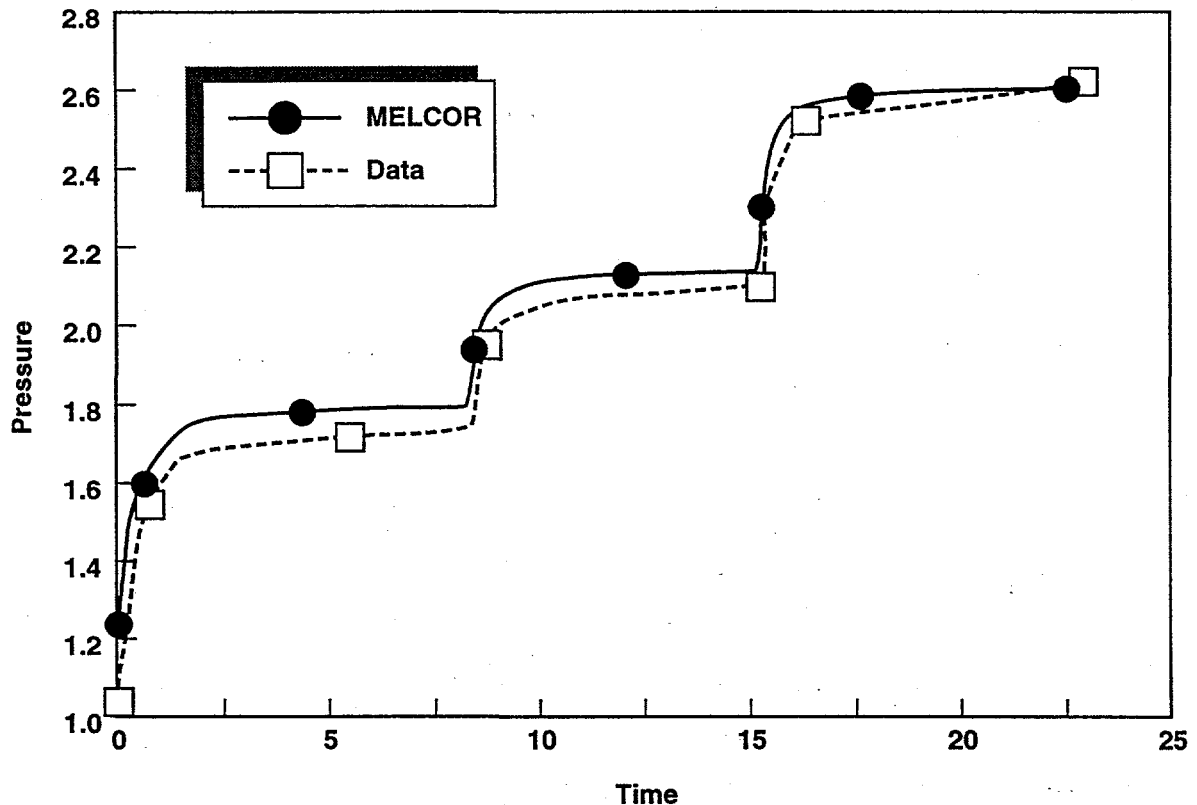


Figure 3. Normalized calculated and measured pressure for large-scale tests.

The adequacy of the film-tracking model was assessed by performing a code-to-code comparison (MELCOR-to-CONTAIN). The comparison was made because (1) no experimental data for the thickness was available and (2) the CONTAIN film models have been assessed previously and found to be in good agreement with data. The comparison showed that the MELCOR and CONTAIN film thickness were within 0.75 mm. Finally, as the MELCOR condensation film flowed downward, the film thickness increased at a consistent rate, as expected, and the evaporation film thickness decreased at a consistent rate as the film flowed downward, as expected.

Validation Work in Progress

Two MELCOR validation studies are currently underway at SNL. First, we are using EPRI data on fission product scrubbing in pools to assess the improved models (discussed above) from SPARC-90. Second, we are performing a series of calculations of the Phebus

FPT-0 integral severe accident experiment. For the latter, we have benefitted from the cooperation of several organizations that have previously performed MELCOR/Phebus studies. In particular, we have been provided with the MELCOR decks that were constructed by personnel at NUPEC in Japan; the Polytechnic University of Madrid, Spain; and KEMA in the Netherlands. We intend to pursue a series of calculations that will complement, rather than duplicate, the work already done by these institutions, and we are grateful for their cooperation.

Accident Analyses

Steam Generator Tube Rupture Sequence at the Surry Plant. Calculations have been performed with MELCOR to examine several aspects of severe accident progression during a postulated Steam Generator Tube Rupture (SGTR) accident sequence in a typical Westinghouse 3-loop PWR system. A key objective of these calculations was to provide thermal-hydraulic boundary conditions for a detailed assessment of fission product transport and deposition with the VICTORIA computer code⁷ discussed in a paper by Bixler *et al.* in these proceedings. A second objective was to assess the potential for counter-current, vapor phase natural circulation flow patterns within hot leg piping during a single-tube SGTR. If natural circulation flow patterns could develop, the extent to which they influence fission product deposition was of interest. MELCOR calculations addressing natural circulation behavior are in progress, and are not discussed in the current paper. The discussion below is limited to results of preliminary (uni-directional flow) MELCOR calculations.

The calculations performed for the current study were restricted to an SGTR accident sequence in which only one tube is assumed to rupture as the accident initiating event. It is assumed that operator actions to depressurize the primary coolant system in response to detection of a ruptured U-tube (as directed by emergency operating procedures) are not successful. Under these conditions, the primary coolant system pressure remains elevated (~300 psia) during the period of core degradation and initial fission product release. A release path for fission products directly to the environment (i.e., bypassing the containment pressure boundary) occurs prior to the onset of core damage as a consequence of a presumed failure (in the open position) of a single relief valve on the faulted steam generator. Automatic actuation of the high-pressure emergency coolant injection system is assumed to occur when demanded to make up primary coolant mass lost through the ruptured tube, until the Refueling Water Storage Tank (RWST) inventory is depleted.

The preliminary MELCOR model used to simulate this accident sequence is based on the Surry plant configuration because a functioning MELCOR input deck was readily available from prior analyses performed by Sandia.⁸ Modest modifications to this model were necessary to represent the SGTR accident sequence producing the hydrodynamic nodalization scheme shown in Figure 4. The faulted steam generator was arbitrarily selected to be "loop C" which contains the pressurizer. The combined volume and

behavior of the other two "intact" coolant loops are represented by a single, but separate, coolant flow circuit.

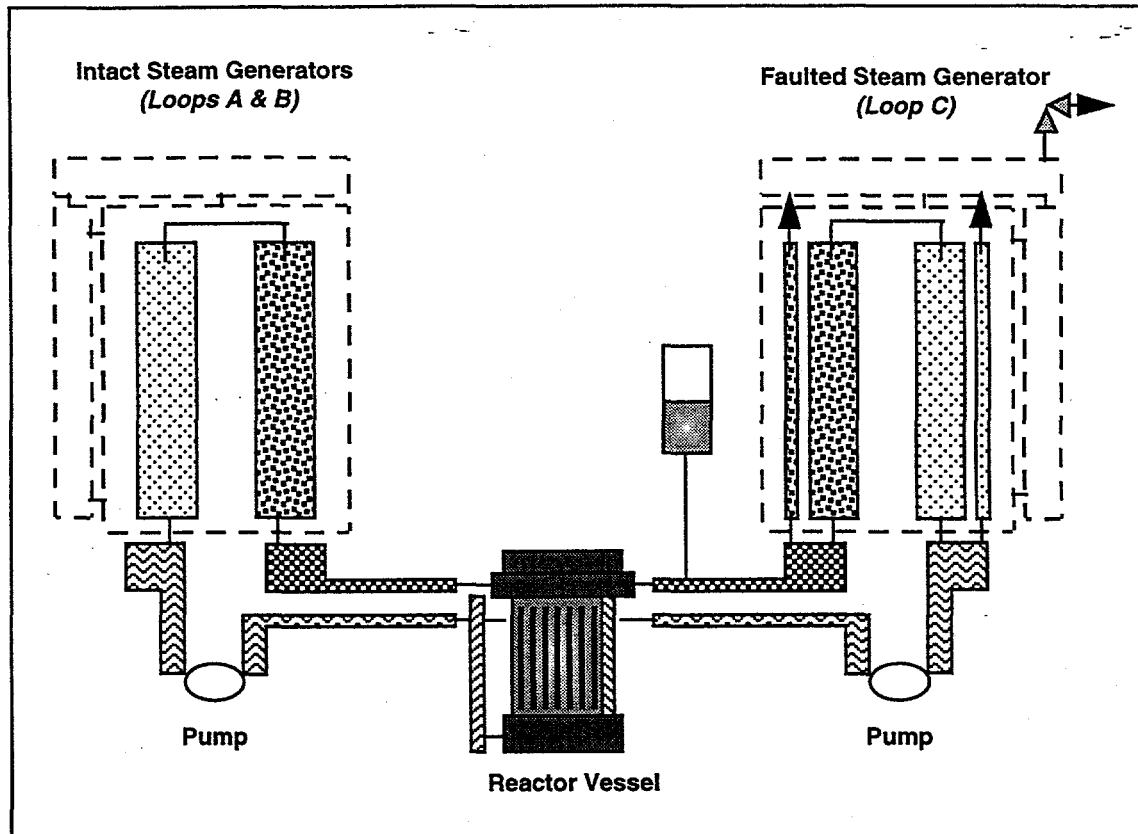


Figure 4. Nodalization for Surry SGTR sequence with "one way" hot leg.

The times at which key events in the SGTR accident sequence are calculated to occur are listed in Table 2. Due to the relatively small size of the break in the primary system, and the large volume of water in the RWST, the accident is very slow in evolving. For example, it takes approximately 16.2 hrs for the RWST inventory to be depleted, and the reactor vessel water level decreases below the top of active fuel at approximately 19 hrs after the initiating event.

Table 2. Timing of Key Events: MELCOR SGTR Simulation

Accident Event	Time After Initiating Event (s /hrs)
Guillotine rupture of one tube in the Loop C steam generator	0.0 / 0.0
Reactor scram on low pressurizer pressure	353.6 / 0.10
Main feedwater terminates/reactor coolant pumps trip and auxiliary feedwater initiates	358.7 / 0.10
High Pressure Injection (HPI) starts on low pressurizer pressure	376.0 / 0.10
Auxiliary feedwater terminates in Loop C due to high water level	1919.6 / 0.53
First cycle of the Loop C steam generator secondary coolant relief valve (RV)	3770.0 / 1.0
Secondary RV sticks open in the Loop C steam generator on the 55th cycle	7619.0 / 2.1
RWST depleted—HPI flow terminates	58,408.1 / 6.2
Reactor water level below top of active fuel	~68,000 / ~18.9
Gap release in Rings 1 & 2	105,671 / 29.4
Core Support Plate Failed	113,755 / 31.6
Lower head penetration failed -- debris ejected to cavity	113,804 / 31.6

The calculated pressure response of the primary coolant system, as well as the intact and faulted steam generator secondary coolant systems, are shown in Figure 5. Following an initial depressurization in response to the break, the primary coolant system stabilizes at a pressure of approximately 95 bar (1375 psia). When the RWST is depleted at approximately 58,000 s, the pressurizer water level drops below that allowed for pressurizer heater operation and primary coolant system pressure decreases sharply. The subsequent thermodynamic state of the primary coolant system becomes closely coupled to the response of the steam generator secondary systems after this point in time.

Accident Analyses for the Westinghouse AP600

In support of NRC's effort to review the AP600 design certification analysis, Sandia performed independent MELCOR analyses of accident progression and associated containment performance for a wide range of postulated severe accidents. Where meaningful, comparisons were made between results of the MELCOR calculations and corresponding MAAP4 calculations performed by Westinghouse in support of the AP600 Standard Safety Analysis Report (SSAR). Although the objective of the MELCOR calculations was to provide a general technical basis for NRC to evaluate the analyses presented in the SSAR, specific MELCOR calculations were also performed to examine

unique aspects of the AP600 design that are designed to mitigate severe accidents. For example, calculations were performed:

- To characterize the importance of hydrogen igniter system, Passive Residual Heat Removal (PRHR) system and Passive Containment Cooling System (PCS) operation to severe accident progression and containment loads;

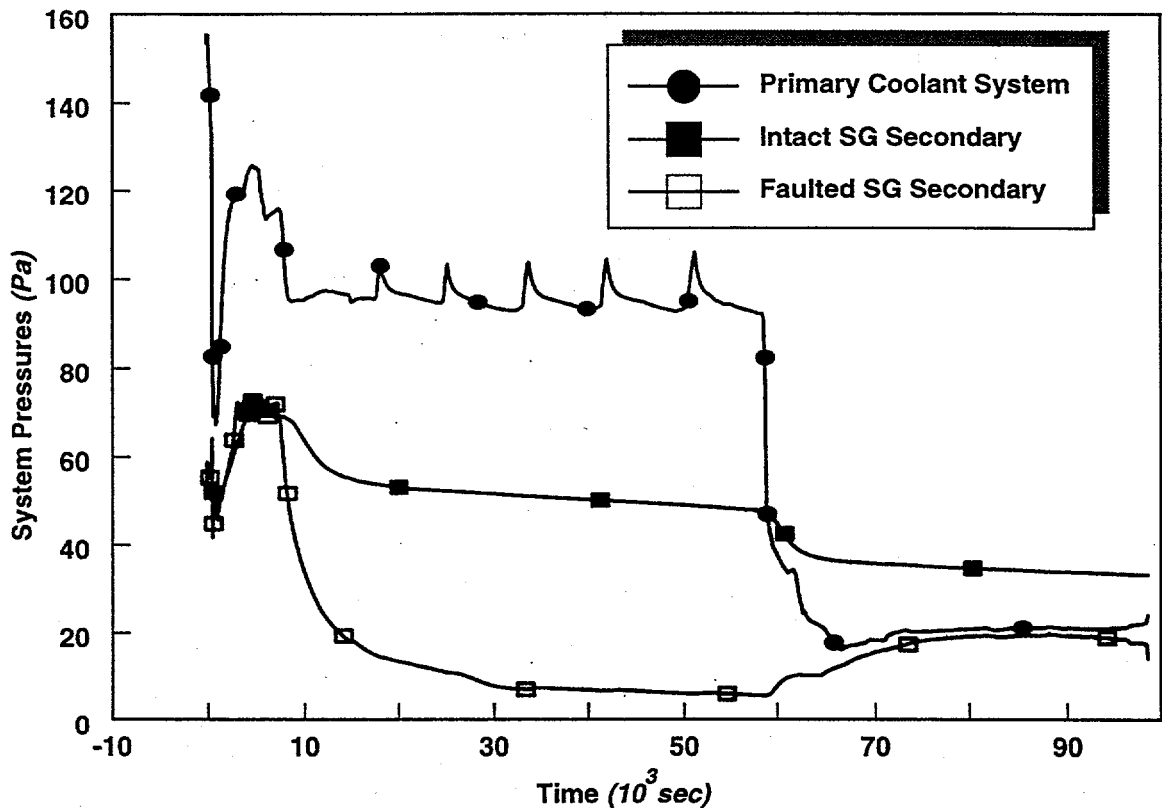


Figure 5. MELCOR calculations for Surry SGTR sequence with "one way" hot leg.

- To examine the conditions under which sufficient water would be available for maintaining external cooling of core debris via heat transfer to a flooded cavity (thereby preventing vessel breach); and
- To examine the impact of alternative modeling assumptions regarding corium-concrete interactions on long-term containment loads under conditions in which vessel breach would occur.

Results of these calculations are documented in a proprietary report.⁹

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