Recent efforts in MELCOR development to incorporate CORCON-Mod3 models for core-concrete interactions, new models for advanced reactors, and improvements to several other existing models have resulted in release of MELCOR 1.8.3. In addition, continuing efforts to expand the code assessment database have filled in many of the gaps in phenomenological coverage. Efforts are now under way to develop models for chemical interactions of fission products with structural surfaces and for reactions of iodine in the presence of water, and work is also in progress to improve models for the scrubbing of fission products by water pools, the chemical reactions of boron carbide with steam, and the coupling of flow blockages with the hydrodynamics. Several code assessment analyses are in progress, and more are planned.

1. INTRODUCTION

Recent activities in the MELCOR development project have led to the release of MELCOR 1.8.3,1 a much-improved version of the code. Several important modeling improvements and other new features have been incorporated into the code and are described in Section 2. Concurrent with code development efforts, continuing assessment of the code has resulted in a significantly expanded database of calculations and sensitivity studies. These efforts have demonstrated the ability of the code to successfully calculate a variety of phenomena important to severe accident analyses, and they have also identified many problems with the code and phenomenological models that have subsequently been corrected. These analyses and modeling improvements have resulted in substantially increased credibility of the code. Three assessment studies23,4 completed in the last year are described in Section 3.

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Work was completed shortly after the MELCOR 1.8.3 release on two additional models related to reactor vessel failure. Work is now in progress in a number of additional areas related to fission product transport and chemistry, and efforts are continuing to couple the effects of flow blockages during late-phase melt progression to the hydrodynamic models. Furthermore, new models are being developed at Oak Ridge National Laboratory (ORNL) for phenomena important in boiling water reactors (BWRs) during early core heatup and degradation. These efforts are all described in Section 4.

2. MELCOR 1.8.3 IMPROVEMENTS

MELCOR 1.8.3 was released to the international reactor safety community in August 1994 following substantial testing on a suite of plant calculations to demonstrate its robustness and reliability for many different accident scenarios on a variety of computer systems. This version of the code incorporates a number of new features, corrections, and other changes that have been made since the release of MELCOR 1.8.2.

Perhaps the most significant modification has been the incorporation of CORCON-Mod3 into MELCOR. This implementation was part of a joint effort to simultaneously implement CORCON-Mod3 into CONTAIN and it included significant restructuring of CORCON to minimize future duplication of effort. No changes were made to the basic phenomenological models, but now the central phenomenological routines are identical in the stand-alone, MELCOR, and CONTAIN versions, and additional modeling improvements to CORCON can now be made in all versions with a minimum amount of effort. During the course of implementation, previous modifications made to MELCOR and CONTAIN to address difficulties with CORCON in a systems code environment were retrofitted to the new version. Several other numerical deficiencies with CORCON-Mod3 have also been addressed, including instabilities in the interlayer mixing model and a general lack of robustness. The numerical implementation of the interlayer mixing model was completely redone, and the oscillations that have been observed in calculations that utilized this model have been eliminated.

A few CORCON modeling issues that have previously been identified are still unresolved. Releases of fission products calculated by the VANESA model as a metal phase vanishes are still incorrect, but a possible modification to the model developed by the Nuclear Safety Institute (NSI) in Russia may be incorporated that will remedy this problem. The adjustment made to the oxygen potential in VANESA to account for unequal metal and oxide temperatures is inadequate; a patch has been made to prevent code aborts, but a more permanent modeling fix is still needed. Finally, the nonideal oxide chemistry model is not functional in CORCON-Mod3, but investigations by others (e.g., NSI) have questioned the need for and practicality of this model.

Another major improvement to MELCOR has been the upgrade of the hydrodynamics solution algorithm to include the mass and energy transfer terms associated with bubble separation from a two-phase pool in the implicit numerical solution scheme. This was needed to stabilize computed void fractions and pool surface elevations, which had exhibited severe oscillations in many calculations that had a strong negative impact on the functioning of several other models. As a part of this effort, many of the low-level hydrodynamic modeling algorithms were
completely recoded to enhance their future maintainability. Other hydrodynamic improvements include adding the capability for the user to define momentum flux terms for a two-dimensional network of control volumes for use in fine-scale natural circulation calculations in the core region. A new input format for mass and energy sources has been added to allow direct reference to external data files and to allow scaling. Also, the option to write various flow variables to external data files has been added.

A number of improved modeling capabilities and new input options have been added to the heat structure models. The model for film condensation and evaporation on heat structure surfaces has been substantially enhanced by modeling the water film surface as an additional temperature node and explicitly accounting for the thermal resistance across the film. The mass transfer expressions were generalized to remove inappropriate limitations so that they would be applicable to both pure steam and noncondensible gas mixture environments. A new film tracking model was also added to allow condensate to drain from one structure to another, thus allowing modeling of passive containment cooling systems proposed for certain advanced light water reactors (ALWRs). New optional input to allow scaling of heat and mass transfer coefficients for specified surfaces has been added, and an option to allow the use of the maximum heat transfer coefficient given by the correlations for forced and natural convection and for laminar and turbulent flows has been added as an alternative to the existing interpolation scheme for transitions between those flow regimes. (Late in MELCOR 1.8.3 testing, we discovered situations where the default scheme can significantly underpredict the true heat transfer coefficient.)

Several new modeling features have been added to other packages as well. The capability to initialize the core in a degraded state with debris materials and oxidized cladding and canister materials has been added to the Core package, and the high-pressure melt ejection model in the Fuel Dispersal Interactions (FDI) package has been extended to treat oxidation and heat transfer for debris that is deposited on heat structures. Automatic mass conservation accounting for fission products has been implemented in the RadioNuclide (RN) package. New input has been added to the Containment Sprays (SPR) package to allow spray sources to be associated with control volume pools, thus permitting a recirculation mode of operation.

Many additional changes have been made to correct errors of varying degrees of severity. These include fixes to errors that caused the code to abort in one or more calculations, such as floating point numbers divided by zero or array subscripts out of range. They also include logic errors that led to code shutdown, poor execution performance, numerical sensitivity, or incorrect phenomenological behavior. Additional improvements to the user interface and code input/output capabilities have been made. User input has been provided for additional control and flexibility in some models, and input checking in a number of areas has been strengthened to ensure consistency and prevent later problems from arising due to bad input. Several control function arguments and plot variables have been added, and output for some packages has been improved. Several more enhancements to warning and error message processing have been made.

New modeling capabilities specific to BWRs have been added as well to the BWR Lower Plenum Debris Bed (BH) package by ORNL MELCOR development staff. Treatment of radiation heat
transfer among the lower plenum debris, the core plate, the core shroud, and the vessel wall has been added, and a model to simulate the melting of heat structures used to treat the core shroud has been added (but is currently only available in conjunction with the BH package models. A model to calculate the effects of water interacting with the debris bed has been added, and fission product release from the debris using either the CORSOR or CORSOR-M models has been added. Mass and energy conservation accounting is now calculated within the BH package, though it has not yet been fully integrated with the global MELCOR accounting scheme. New models have been added to the BH package to simulate operation of the PCCS and ICS in ALWRs.

In preparation for distribution to external MELCOR users, MELCOR was subjected to a number of tests as required by our Software Quality Assurance Plan (SQAP). This testing was done primarily to ensure robustness of the code; however, calculations were also quickly reviewed for physical reasonableness and plausibility. The following full-plant calculations were selected for this testing:

1. Grand Gulf large break loss-of-coolant accident (LOCA) during shutdown (POS 5) with 40-day decay heat levels.
2. Grand Gulf low pressure boiloff during shutdown (POS 5) with open containment, closed upper head vent, 2 safety relief valves open, and 24-hr decay heat levels.
3. Surry S2D sequence (hot leg small break LOCA).
4. Surry AG sequence (hot leg large break LOCA).
5. LaSalle high-pressure short-term station blackout with failed emergency core cooling and automatic depressurization systems.
6. Advanced boiling water reactor (ABWR) loss of all core cooling with failure to depressurize.
7. DEMO calculation distributed with the software (simplified coarse nodalization for idealized plant).

MELCOR 1.8.3 was required to run each of these calculations to completion without aborting, terminating prematurely (necessitating restart with a different time step), or using an excessive amount of computational time because of numerical difficulties. These calculations collectively were run on various machines (IBM, HP, and SUN workstations, and IBM PC), although any individual calculation was run on only one or two machines.

3. MELCOR ASSESSMENT

Significant progress continues to be made in MELCOR assessment, and most phenomenological areas within the code have been or are being assessed against at least one experiment. Recently completed assessments include the MP-1 and MP-2 late-phase melt progression experiments
conducted at the Annular Core Research Reactor at Sandia, the General Electric large vessel level swell tests, which measured void fraction distributions and bubble rise velocities, and the containment spray experiments conducted in Pacific Northwest Laboratory’s Containment Systems Experiment vessel. The SURC-2 core-concrete interactions test conducted at Sandia was used to verify the correct implementation of CORCON-Mod3 in MELCOR, a more complete assessment against this test was conducted for stand-alone CORCON-Mod3. All assessments conducted at Sandia include a systematic search for and identification of numeric effects from time step and machine dependencies, in addition to the identification of other code problems and limitations requiring developer attention. Extensive sensitivity studies also provide the basis for development of user guidelines.

The GE large vessel blowdown and level swell experiments are a set of primary system thermal/hydraulic separate effects tests studying the level swell phenomenon for BWR transients and LOCAs. This experiment series includes both top blowdown tests with vapor blowdown, characteristic of accidents such as steam line breaks, and bottom blowdown tests with liquid and two-phase blowdown, more characteristic of recirculation line breaks. The test facility includes a 4.5-m³ steel-shell vessel containing saturated steam/water at 7 MPa and a 10-inch diameter blowdown line with a dip tube extension. Assessment against this data allowed an evaluation of the ability of MELCOR to predict the inventory loss, and hence time to core uncoverage and heatup, in the early stages of transients and accidents in BWRs. Also, an implicit bubble separation algorithm has been implemented recently in the MELCOR hydrodynamics models, and analysis of the GE tests was intended to validate this algorithm for general use.

MELCOR was able to calculate reasonable agreement with the depressurization and break flow data for all tests. Although the code predictions for the liquid level showed good agreement with experimental data for the bottom blowdown tests, MELCOR underpredicted the level swell for the top blowdown tests with the base case nodalization and model parameters, generally reaching a maximum value that is significantly below the maximum two-phase levels in the test data and then beginning to decline earlier in the calculations than in the tests. Sensitivity studies showed that the break flow and depressurization rate were sensitive to the time step during the two-phase portion of the calculated blowdown and that the calculated level swell is very sensitive to nodalization and bubble rise model parameters.

Eight experiments have been performed in the CSE containment vessel to evaluate the performance of aqueous sprays as a means of decontaminating containment atmospheres. The 595-m³ steel-shell vessel is subdivided into a dome, lower drywell, middle and lower rooms, and wetwell. Uranium aerosols were generated to represent core materials that have very low vapor pressures and low solubilities in water, and cesium aerosols were generated to represent volatile solids highly soluble in water. Iodine was injected as both elemental iodine and methyl iodide. Six intermittent, multiple spray experiments conducted after the aerosols and iodine had been injected involved either STP air or steam/air at 3 atm and 400 K, different spray rates and timing, both fresh and recirculating sprays, different spray solutions, and different nozzle types and distributions. Two continuous spray tests were conducted with concurrent aerosol/vapor injection.

Results of MELCOR assessment analyses demonstrated that MELCOR correctly reproduces the qualitative thermal/hydraulic, aerosol washout, and vapor decontamination response to
containment spray injection. In particular, MELCOR reproduced the relative responses observed when the spray flow rate and droplet size distribution were varied. Also, the accuracy and reasonableness of the predicted results generally improved as more MAEROS components and sections were used to model the aerosol size distributions. Quantitatively, MELCOR predicts more efficient steam condensation and equilibration of drops with the atmosphere than shown by experimental data. Removal of aerosols and vapors by sprays is generally underpredicted by the code, which also shows the same proportional effects for each spray period, while the data shows the first spray period being much more effective in removing contaminants than later spray periods. Major sensitivities include the fraction of the spray assumed to interact with the atmosphere, the spray droplet size and distribution, and the fog water droplet evaporation and condensation.

The major purpose of our calculational efforts for SURC-2 were to verify the correct implementation of CORCON-Mod3 in MELCOR by comparing MELCOR results for the same analysis with those of stand-alone CORCON-Mod3. This verification effort showed no significant differences; most results showed no distinguishable differences at all in the plots, and the few minor observable differences were readily traced to unavoidable coding differences associated with the interface to MELCOR. One sensitivity study was performed to examine the effects of the input options for multiple debris layers vs. a single homogeneous layer (now the default in MELCOR). Results with multiple layers and using the interlayer mixing model were different only at very early times when the debris was stratified. Results with the old CORCON-Mod2 layer configuration agreed with those using the interlayer mixing model.

Work is currently in progress to assess code thermal/hydraulic behavior for Surry plant calculations with pressurizer surge line failure. Assessment calculations of aerosol scrubbing by water pools are to be conducted for two sets of Electric Power Research Institute experiments, one set involving superheated steam and the other involving noncondensible gases.

4. POST-1.8.3 MODEL DEVELOPMENT ACTIVITIES

Work was completed shortly after MELCOR 1.8.3 release on two additional models related to reactor vessel failure. The capability to treat heat transfer from the exterior surface of the lower head to a liquid pool surrounding the lower vessel has been added, using boiling heat transfer correlations specifically applicable to downward-facing surfaces. This model is needed for simulation of flooded reactor cavities for accident scenarios involving advanced reactor designs. Experimental correlations relating the critical heat flux and the film boiling heat flux to the surface orientation are used to determine the heat transfer coefficient from the external surface of the vessel, and several user control options were added to provide additional flexibility, as this is an ongoing area of research still with large uncertainties.

Also, models for creep rupture failure of the lower head were implemented in the code after 1.8.3 release. These models are based on Larson-Miller time-to-rupture correlations and application of a life fraction rule to calculate the cumulative damage fraction for transient conditions. Options in the model include the ability to treat the lower head stress as a zero-dimensional membrane stress or to calculate the one-dimensional stress distribution through the thickness of the head.
Fission product chemistry models are being developed to treat the chemical deposition of cesium and tellurium compounds on structural surfaces. Preliminary design of the model calls for the modeling of chemisorption as an addition to the current mass transfer processes. Experimentally based mass transfer coefficients for CsOH and Csl chemisorption on stainless steel and Inconel surfaces would be factored into the TRAP–MELT equations used in MELCOR for normal condensation and evaporation. The chemisorbed mass would not be considered for release from the structure unless very high temperatures were reached, in which case a general refractory vapor pressure curve could be utilized to return vapor to the atmosphere. We do not propose applying the model for tellurium, hydrogen iodide, or iodine by default, as the mass transfer coefficient values are not based upon sufficient data, but we plan to incorporate the capability to perform these calculations at the user's option.

Models are also being developed to capture the important chemical reactions of iodine in the presence of water. Preliminary design of the model includes submodels to calculate release of I₂ from a water pool to the atmosphere in the presence of steam condensation or evaporation, which will either inhibit or enhance iodine diffusion through the boundary layer, and to calculate the pH of the water pool based on the concentrations of boric acid and alkali metal hydroxides. Radiolysis and pyrolysis processes may also be considered in the pH model, and the formation, release, and destruction of methyl iodide will be modeled.

Fission product vapor scrubbing is being implemented by incorporating updated models from SPARC–90. The enhanced modeling capabilities will be demonstrated through testing, which will verify that the new models are giving reasonable results. Implementation of these models should also lay to rest questions about the decontamination factors predicted by the aerosol scrubbing models.

Coupling of flow blockages to the hydrodynamic models by automatically reducing flow areas and increasing loss coefficients is being developed to enhance natural circulation capabilities during late-phase melt progression. We have proposed a limited model for the increased flow resistance associated with formation of core debris ("core blockage") based on correlations developed for flow in porous media. Consistency of representation between core models and hydrodynamic models will require that much of the geometry now defined by flow path input will have to be derived internally from core input.

Finally, new equilibrium chemistry models for the reactions of boron carbide with steam and the partitioning of those reactions with competing eutectic reactions of the boron carbide with steel are being implemented. The advanced chemistry models are based on minimization of the Gibbs free energy and have been taken from models developed by Oak Ridge National Laboratory. The methane produced by these models will be provided to the fission product iodine chemistry models for determining the formation of methyl iodide in water suppression pools and its release to the containment atmosphere.

Oak Ridge National Laboratory is also working on models for the allocation of steam among core components during oxidation and for gamma heating of other core components, particularly those in the interstitial region in boiling water reactors. These model upgrades should give a more accurate simulation of the internal heating rates and oxidation of BWR canister walls and control blades.
Longer term development plans include the examination of models developed by the Nuclear Safety Institute under a cooperative agreement with the Russian Research Center for in-vessel fuel-coolant interactions, ex-vessel debris coolability, melt spreading, and reflood hydrodynamics, followed by the development of simplified models for implementation in MELCOR. Additional improvements in a few areas are also needed to address some residual concerns identified during the MELCOR peer review.

5. REFERENCES


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