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# Quicklook Overview of Model Changes in MELCOR 2.2: Rev 9496 to Rev 11932

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# ABSTRACT

This document summarily provides brief descriptions of the MELCOR code enhancement made between code revision number 9496 and 11932. Revision 9496 represents the last official code release; therefore, the modeling features described within this document are provided to assist users that update to the newest official MELCOR code release, 11932. Along with the newly updated MELCOR Users' Guide and Reference Manual, users will be aware and able to assess the new capabilities for their modeling and analysis applications.

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# ACRONYMS AND DEFINITIONS

| Acronym | Definition |
|---|---|
| BWR | Boiling Water Reactor |
| COR | Core (Package) |
| CV | Control Volume |
| CVH | Control Volume Hydrodynamic (Package) |
| EOS | Equations of State |
| FLiBe | Lithium Fluoride Beryllium Fluoride, Molten Salt EOS (Filename: tpffi) |
| He | Helium, EOS (Filename: tpfhe) |
| HS | Heat Structure (Package) |
| N2 | Nitrogen, EOS (Filename: tpfn2) |
| Na | Sodium, EOS (Filename: tpfna) |
| NRC | U.S. Nuclear Regulatory Commission |
| Pb-Li | Lead Lithium, EOS (Filename: tpflipb) |
| PWR | Pressurized Water Reactor |
| RN | RadioNuclide (Package) |
| SNL | Sandia National Laboratories |
| TMI | Three Mile Island |

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# 1. INTRODUCTION

MELCOR is a fully integrated, engineering-level computer code designed to analyze severe accidents in nuclear power plants and nuclear fuel cycle facilities. Created at Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (NRC), MELCOR's primary purpose is to model the progression of accidents in light water reactor nuclear power plants. Development of MELCOR was motivated by WASH-1400[1], a reactor safety study produced for the NRC, and the Three Mile Island (TMI) nuclear power plant accident. Since the project began in 1982, MELCOR has undergone continuous development to address emerging issues, process new experimental information, and create a repository of knowledge on severe accident phenomena.

MELCOR 2.2 is a significant official release of the MELCOR code with many new models and model improvements. This report provides the code user with a quick review and characterization of new models added, changes to existing models, the effect of code changes during this code development cycle (rev 9496 to rev 11932), and a preview of validation results with this code version. The user is referred to the MELCOR User Guide[2] and Reference Manual[3] to provide clarification of existing code parameters or models.

# 2. MELCOR CODE IMPROVEMENTS

## 2.1. New Defaults

### 2.1.1. Gravitational Settling on Horizontal Cylinders

Deposition in a horizontal cylindrical pipe is calculated as the deposition velocity multiplied by the total surface area. This velocity is the terminal velocity which is independent of the surface area. In this way, deposition is calculated over the entire cylindrical surface and not just the upward facing portion (floor). By default, the surface area is multiplied by $1/\pi$ for horizontal cylinders to correct for this effect. A user can arbitrary change this correction factor on the HS_LBS (and HS_RBS) records as a new field (4th word).

### 2.1.2. Sensitivity coefficients

The default value for SC1502(3) adjusted TRACE_HCR (C1502(3)) from 1.e-6 to 1.e-5.

## 2.2. Significant code corrections since revision 9496

Many code corrections have been made since the last official code release. Some of the more important changes are outlined here. However, many other corrections have been made and are documented on both the Bugzilla site as well as the changelist that is provided with the code release.

### 2.2.1. Corrections for Flow Blockage

A Control Volume Hydrodynamic package (CVH) robustness issue was traced to problems with control volumes (CVs) that become isolated when all flow paths in/out are blocked due to material relocation. Isolated CVs are now identified (including up to two contiguous CV's) and changed to equilibrium thermodynamics as long as the conditions persist. In addition, if unphysical pressures are detected, over-pressurization is mitigated by auto adjusting friction factors. Default values for PORMIN and POR_THRESH were also adjusted as part of this correction.

### 2.2.2. Corrections for Disappearing Films

A typically rare but potentially fatal code failure mechanism was identified when "film" disappears from a Heat Structure (HS) surface. Under specific conditions this could cause convergence failure of the temperature iteration. The simple correction assures that when no film exists on a HS, that the previously saved values of the outer node temperatures are equal to the newly calculated outer node temperatures.

### 2.2.3. Corrections to the Stefan Model

Misbehavior of the Stefan model in certain calculations led to a careful review of the model and a subsequent set of small corrections. These included (1) the removal of a "heat_to_melt_point" term from the qnet calculation; (2) the removal of a small erroneous term in the "B" coefficient in CORCRS; (3) the restoration of a "lost" division by delx in Q12long term in CORCLP; (4) an improved method for checking convergence check in CORTZR; and (5) an adjustment for how the "trace-amount" case is handled to avoid unwarranted failures.

## 2.3. New or Extended Modeling

Several models have been added to the code or extended to satisfy user needs. The user is referred to the changelog provided with each code release for information about other code changes.

### 2.3.1. COR Eutectics Model [r9849-r11043]

Though the MELCOR eutectics model was implemented prior to MELCOR 1.8.5, it has not functioned in the code since it was first implemented. Changes made for versions 1.8.6 and 2.0 made correcting those problems even more difficult. This model now runs properly and has been tested for both pressurized and boiling water reactors (PWRs) and (BWRs) without any significant mass or energy errors. The current update to the assessment report will evaluate this model against appropriate test cases. Early evaluation with the TMI accident and the MELCOR/MAAP cross-walk were encouraging. It is intended that this new model will become the default treatment in MELCOR, eliminating the need for users to specify an effective eutectic melt temperature for UO2-INT and ZRO2-INT with a reasonable eutectic melt temperature based on experiments. However, for this release, the eutectics model will be optionally specified on the new COR_EUT input record.

### 2.3.2. Sodium Fire Models [r10430, 10455, 10457]

Two sodium fire models have been implemented into MELCOR, a spray fire model (NACOM) and a pool fire model (SOFIRE II). These models were based on models found in the CONTAIN/LMR code. Several improvements/adaptations to these models have been added for allowing radiation from a pool surface to heat structures, allowing for an upward sodium spray, and adding control function options to control pool diameters as well as various reaction parameters. Two equations of state options for sodium were added to the code based on implementation of properties from the Simmer code as well as an option for reading EOS libraries from the Fusion Safety Database.

### 2.3.3. Improved CORSOR-Booth Model [r11164, 11325, 11334]

Previous versions of the CORSOR-BOOTH model implemented in MELCOR scaled the release of all RadioNuclide (RN) classes to the release calculated for cesium. However, as cesium is depleted from a component (loses numerical precision) then cesium release stops as well as release from all RN classes, even less volatile classes. This places a maximum on release for all classes that is determined by the scaling factor. The new model scales the diffusion coefficient for each RN class rather than the calculated release fraction. In this way, the diffusion release from each class is independent.

### 2.3.4. Helical coil heat transfer coefficient [r10080]

Helical steam generator heat transfer correlations (inside tubes) were added to the code, with user input option to select from correlations for subcooled water flow, two-phase flow, or superheated steam flow.

### 2.3.5. Dimensionless Numbers [r10182, 10208, 10214]

Dimensionless number across the CVH, HS, and COR package have been added to provide easy validation for users.

### 2.3.6. RN Condensation Algorithm

A new algorithm for remapping particle sizes after condensation (or evaporation) was introduced to improve resolution of the aerosol mass within a section (particle size bin). This new algorithm is deactivated by default until fully validated. Either "NEW" or "OLD" algorithms can be selected using the commandline argument, MAEROSNumerics.

### 2.3.7. Support for new EOS files

The ability to read EOS files from the Fusion Safety Database was added in revision 10276. The following libraries are now readable with the current version of MELCOR: Na (tpfna), FLiBe (tpffi), Pb-Li (tpflipb), He (tpfhe), N2(tpfn2), though testing has only been performed for Na and FLiBe.

## 2.4. Minor Code Improvements

### 2.4.1. Activity Model (BONUS) [11269]

The activity model (BONUS) was updated to allow comment lines in the isotope library files. A plot variable was added to plot the activities for each isotope summed over all locations (all CV volumes, COR components, deposition surfaces, etc.) for model evaluation. Plot variables were also added to provide simple estimates of doses from a surface or from a volume.

### 2.4.2. Turbulent Deposition Model [11164]

The turbulent deposition model was expanded to include pipe transitions such as contractions and venturis.

### 2.4.3. Radiation Enclosure Model [11164]

In the original implementation of the radiation enclosure model, view factors were input as constant real values. This has been extended to allow the user to specify control functions for view factors by specifying either a control function name or number in place of the constant value. In addition, if a pool forms on a floor heat structure, radiation to/from the submerged heat structure is replaced by radiation to/from a pool surface using the same view factor that was specified for the heat structures. Finally, for large networks, it may be necessary to extend a view factor input record (from a heat structure to all other heat structures in the network) onto additional records. The ampersand '&' is used as a continuation symbol to indicate a record that continues onto the subsequent record.

# 3. VALIDATION CASES

The MELCOR validation report[4] has not been updated at this time but will be at a later date. Even so, preliminary results are provided here to help the code user understand any impact on important validation cases. Many code corrections have been made that affect specific models such as the hygroscopic and reflood quench models. Consequently, changes in validation tests that assess these models are of interest. In addition, other code changes can affect core degradation or heat transfer and hence, oxidation and generation of hydrogen. Plots from several validation tests are provided to demonstrate that the code continues to predict reasonable agreement.

## 3.1. Hygroscopic Model

Several changes have been made to the hygroscopic model have been made. Revisions 9445 and 9446 changed the precision of a variable used for testing convergence to double precision to correct a runtime convergence error. Revision 8611 corrected a mass conservation error that occurred when both the hygroscopic and flow path flashing model were enabled simultaneously. The AHMED tests show no significant change with these changes. The LACE LA-4 experiments included both hygroscopic (CsOH) and non-hygroscopic (MnO) aerosols, which are shown in Figure 3-2 and Figure 3-3, respectively. The new comparisons are shown with and without the new MAEROS numerics model and with 20 and 30 sections. The new coding overestimates the hygroscopic aerosol removal but has an improved prediction of the non-hygroscopic aerosol removal rate.

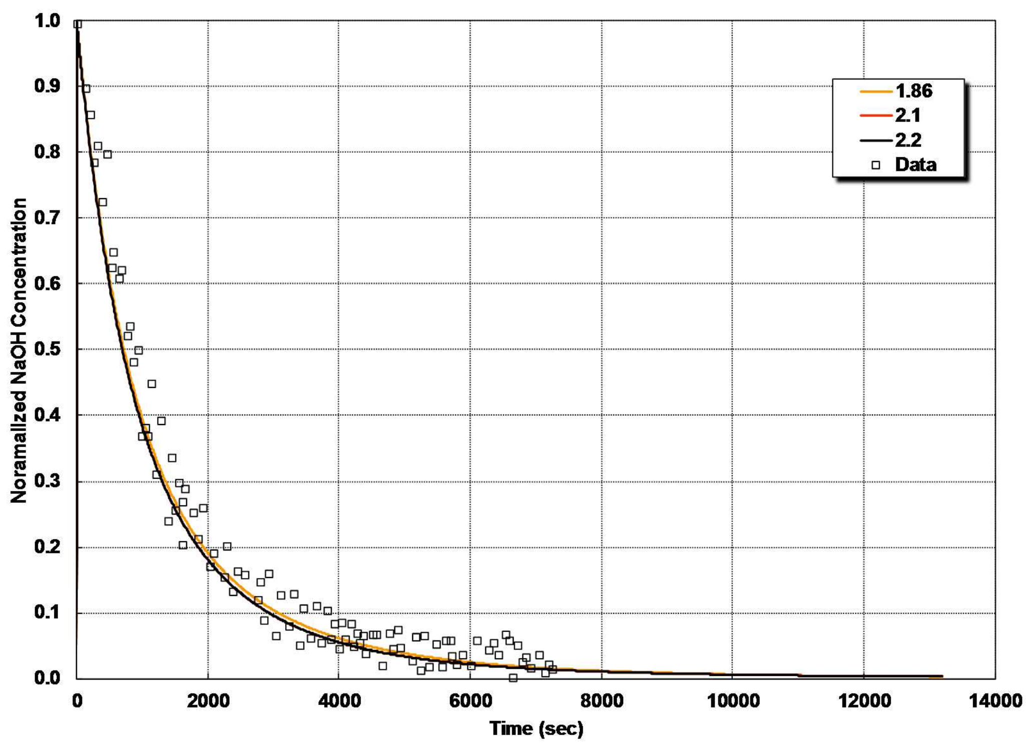


**Figure 3-1 AHMED Experiments (82% RH)**

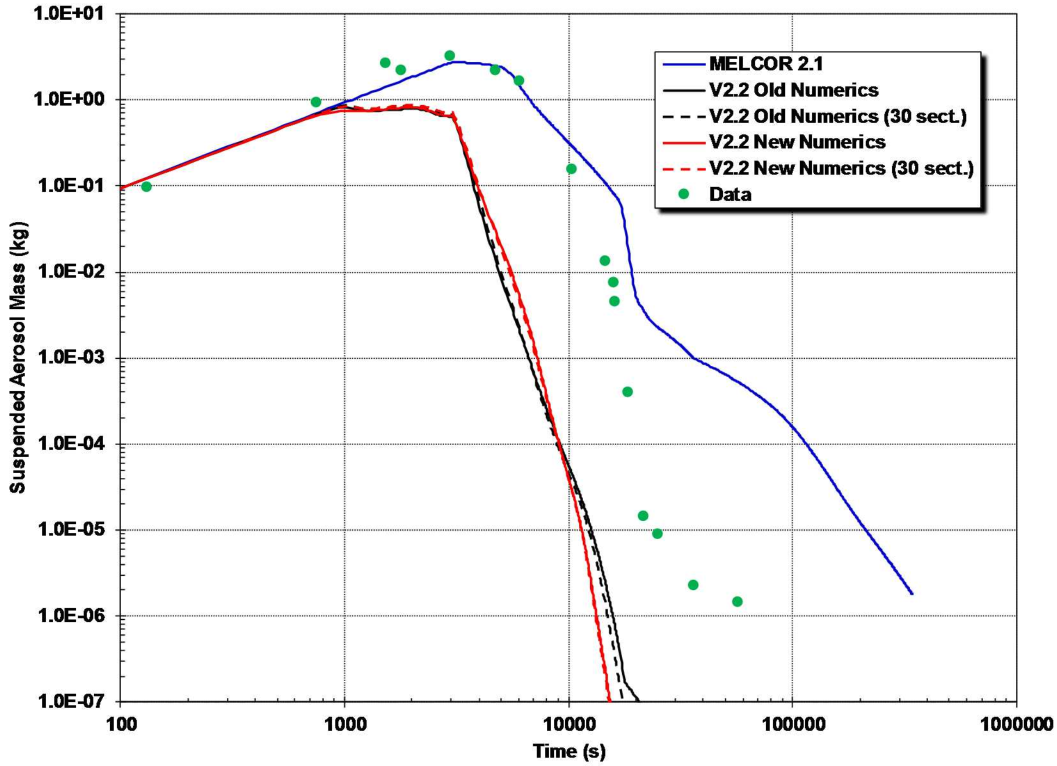


**Figure 3-2 LACE LA-4 Experiment (CsOH)**

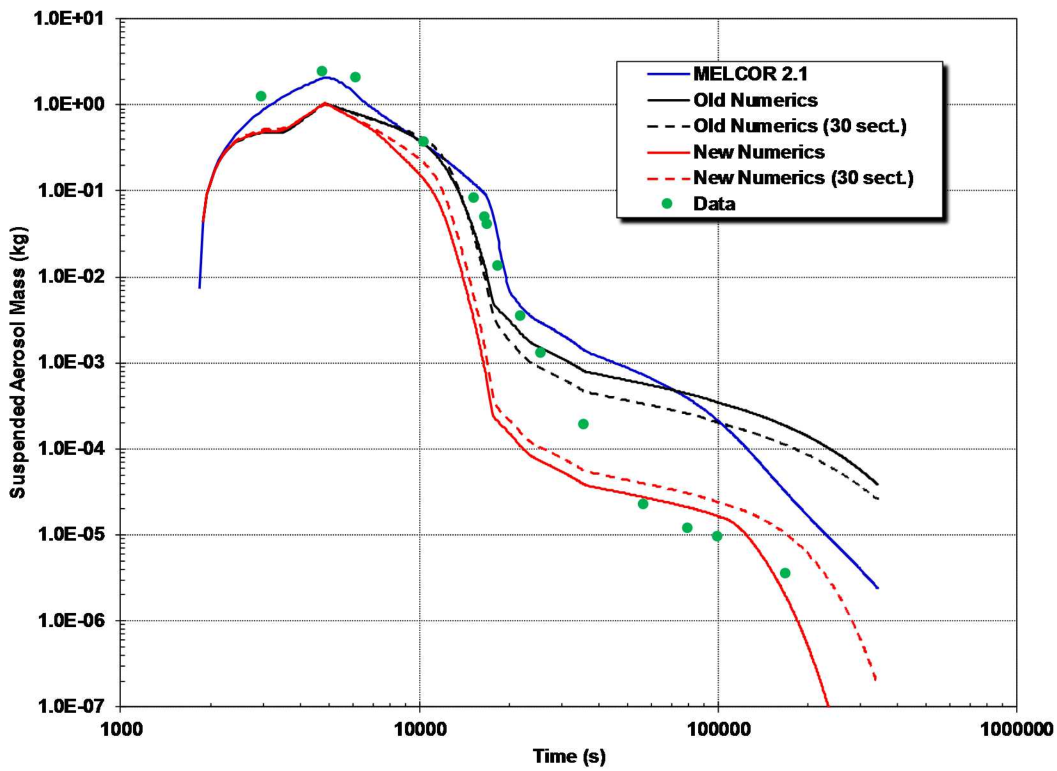


**Figure 3-3 LACE LA-4 Experiment (MnO)**

## 3.2. Oxidation Models

Many code corrections addressed the reflood quench model which effects component surface temperatures and hence oxidation rates. In addition, many changes can have an impact on core degradation, which can also affect surface areas available for oxidation. No changes were made directly to the oxidation models. The plots below demonstrate that oxidation is still well-predicted for the FPT-1, CORA-13, and Quench-6 tests.

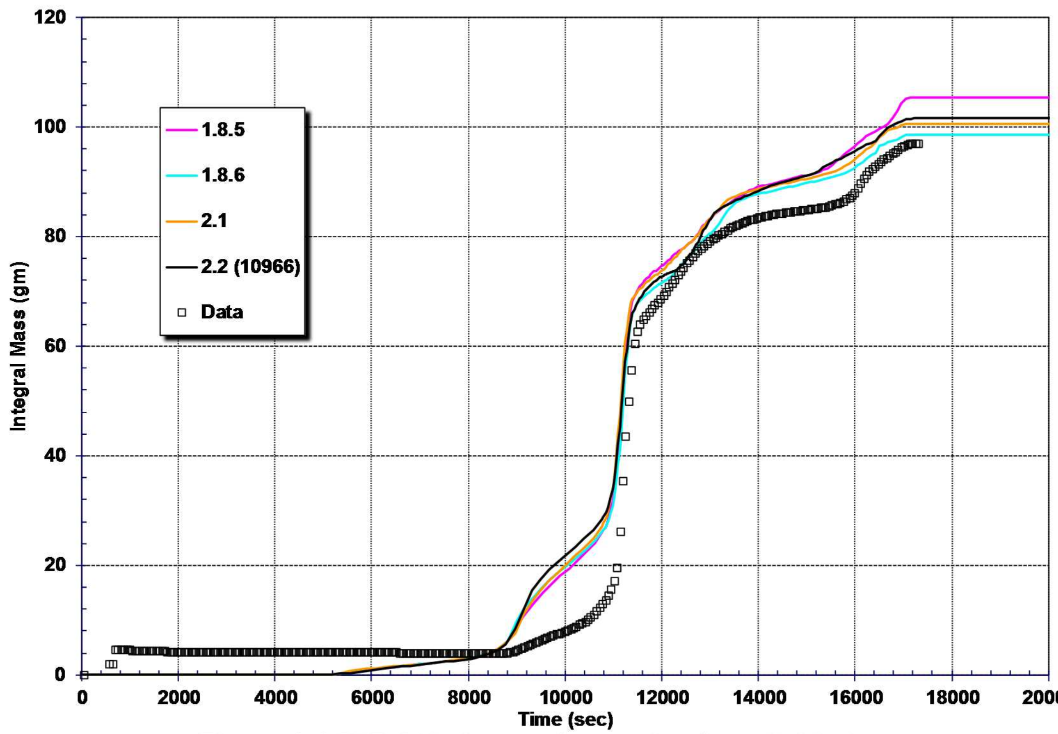


**Figure 3-4 FPT-1 Hydrogen Generation from Oxidation**

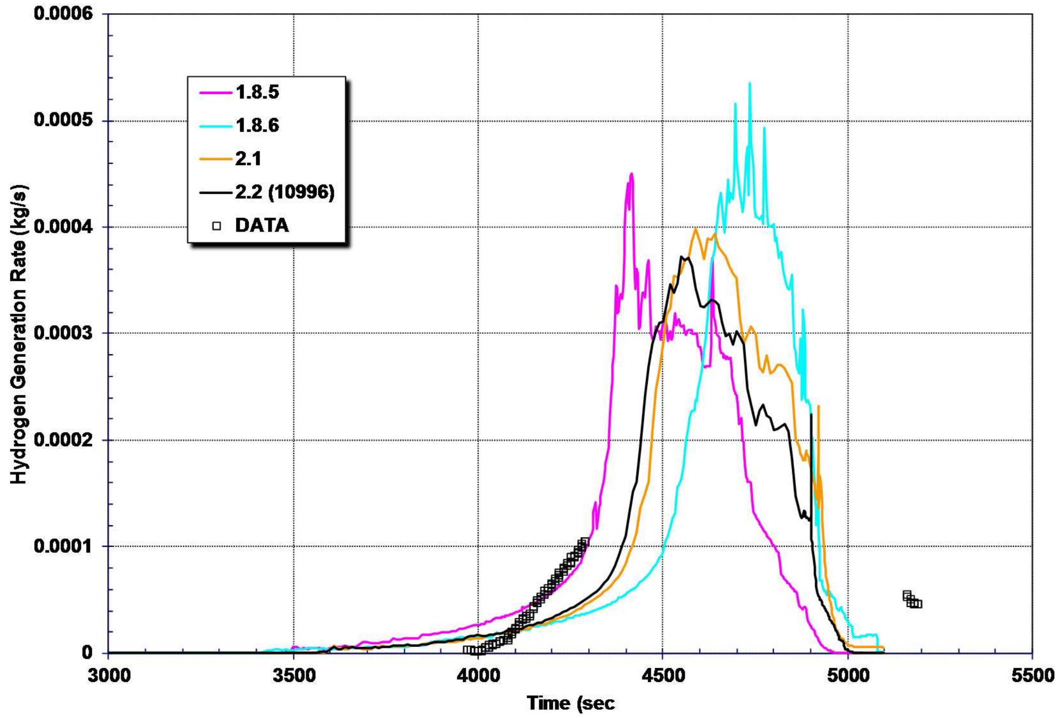


**Figure 3-5 CORA-13 Hydrogen Generation from Oxidation**

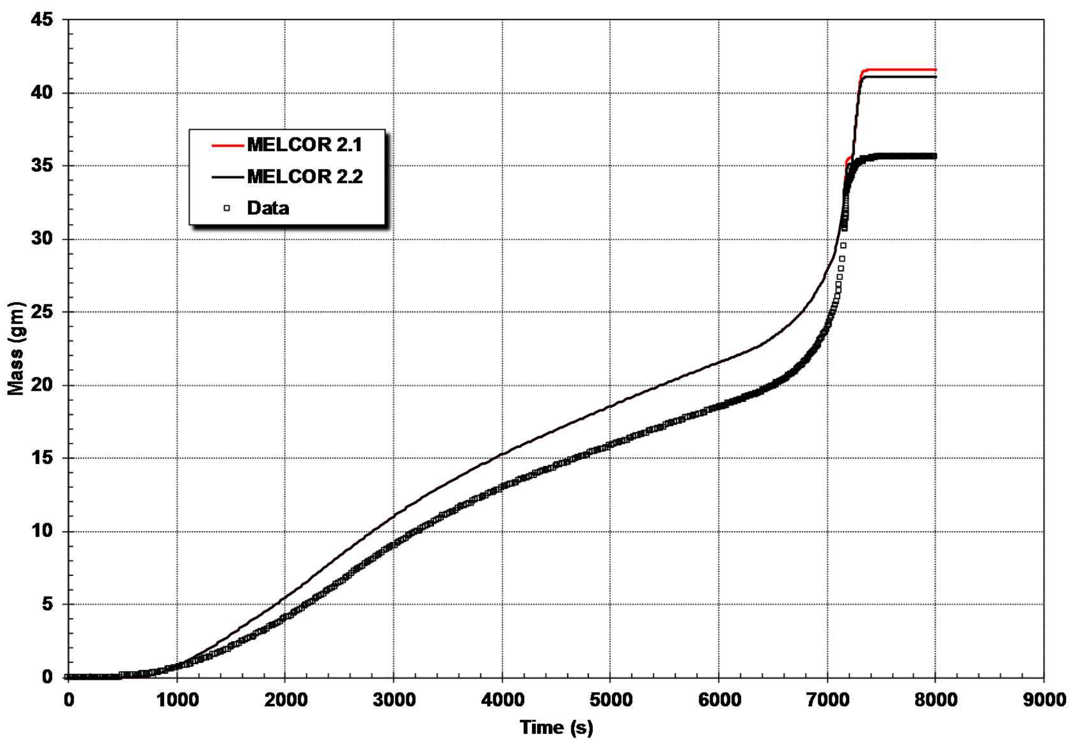


**Figure 3-6 Quench-6 Hydrogen Generation from Oxidation**

## 3.3. Condensation Improvements

Previously, the DEMONA test results showed a strong sensitivity to the application of the hygroscopic model to the airborne aerosol concentration. DEMONA test B3 was a non-hygroscopic aerosol test. Consequently, the results were not expected to be sensitive to inclusion of the hygroscopic model. Figure 3-7 shows the new model gives the same result whether the hygroscopic model is active or not.

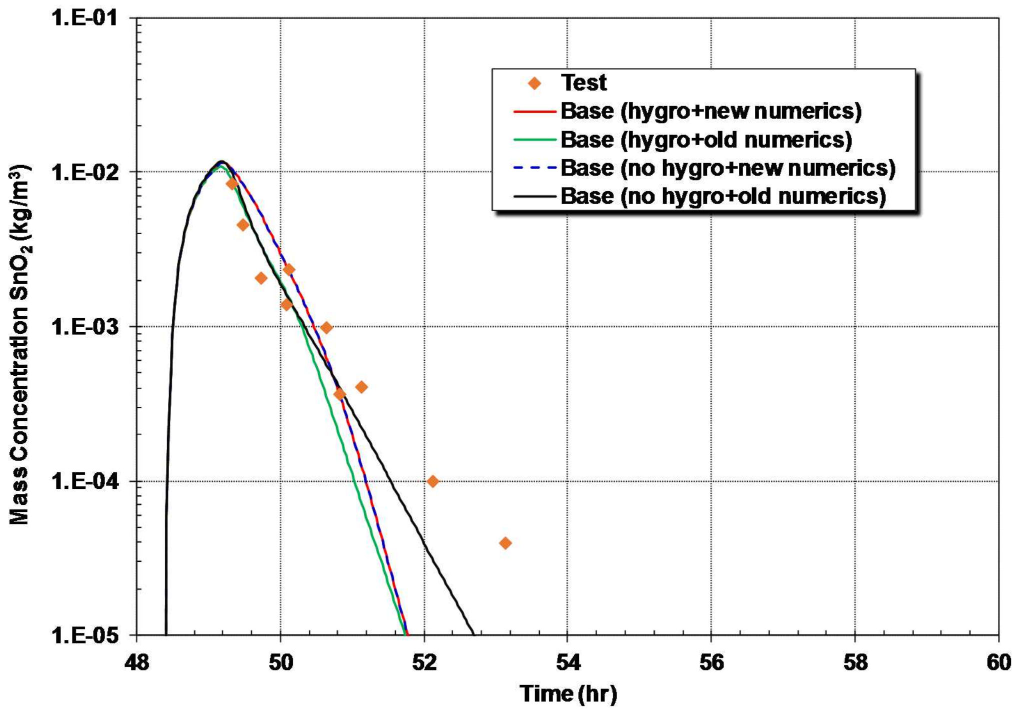


**Figure 3-7 DEMONA B3 Experiment (non-hygroscopic aerosol)**

## 3.4. New CORSOR-Booth Release Model

A new CORSOR-BOOTH model was implemented that did not rely on release fractions calculated for cesium. The new model scales the diffusion coefficient for each RN class rather than the calculated release fraction. In this way, the diffusion release from each class is independent. Figure 3-8 through Figure 3-11 from the Phebus FPT1 experiment shows the volatile releases are still xenon, cesium, iodine, and tellurium are still well calculated. The Barium release is different with the new model and is in line with the reported response with the CORSOR-Barium model documented in Reference [5]. The total Ruthenium response in Figure 3-13 is consistent between the models but the release rate is better calculated by the older CORSOR-Booth model. The new CORSOR-Booth formulation is expected to be particularly important in low decay heat accidents (e.g., spent fuel pools) where the cesium could be completely exhausted and therefore all releases stop.

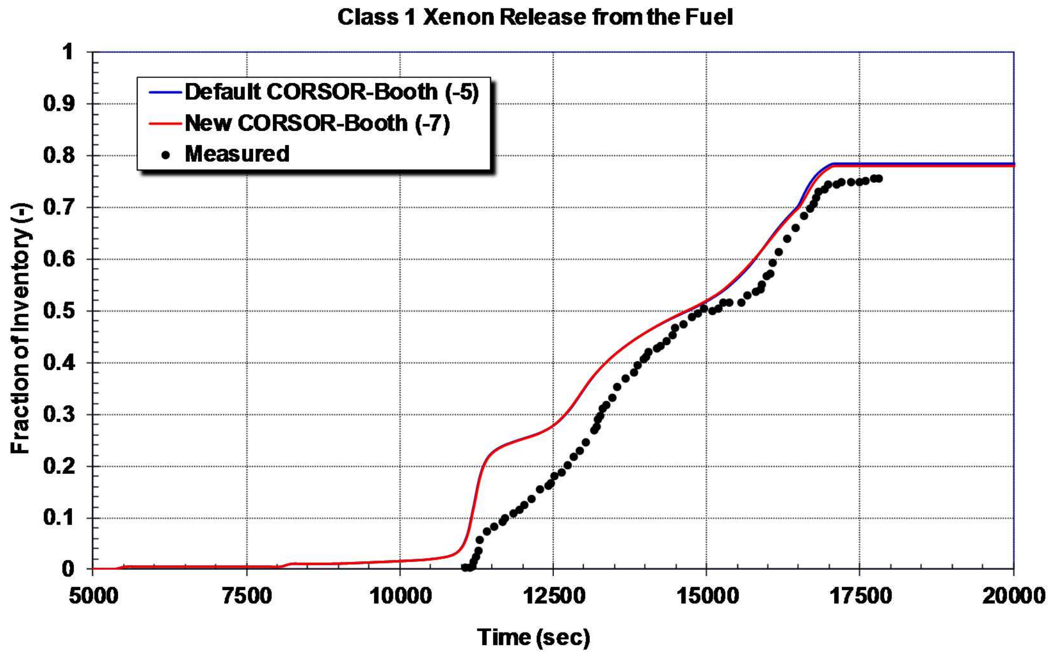


**Figure 3-8 Phebus FPT1 Xenon release from the fuel**

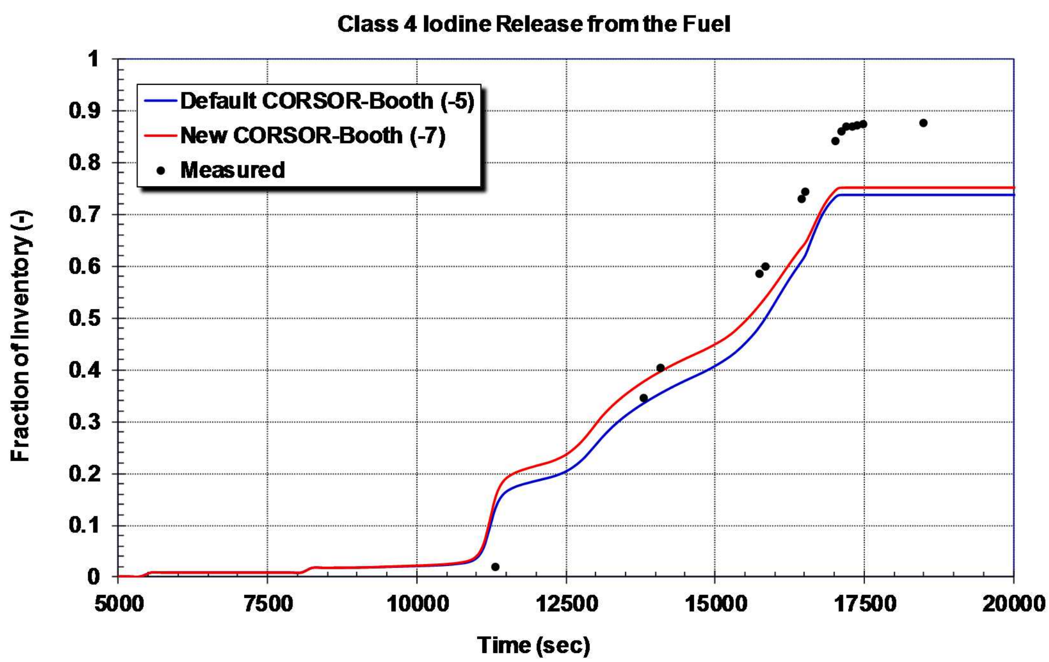


**Figure 3-9 Phebus FPT1 Iodine release from the fuel**

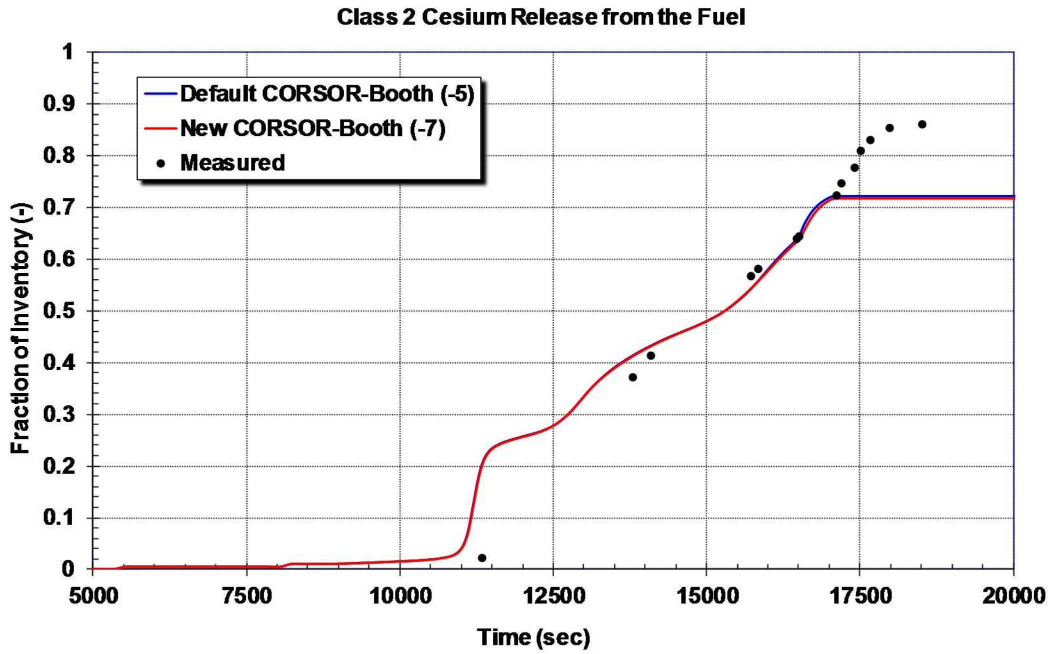


**Figure 3-10 Phebus FPT1 Cesium release from the fuel**

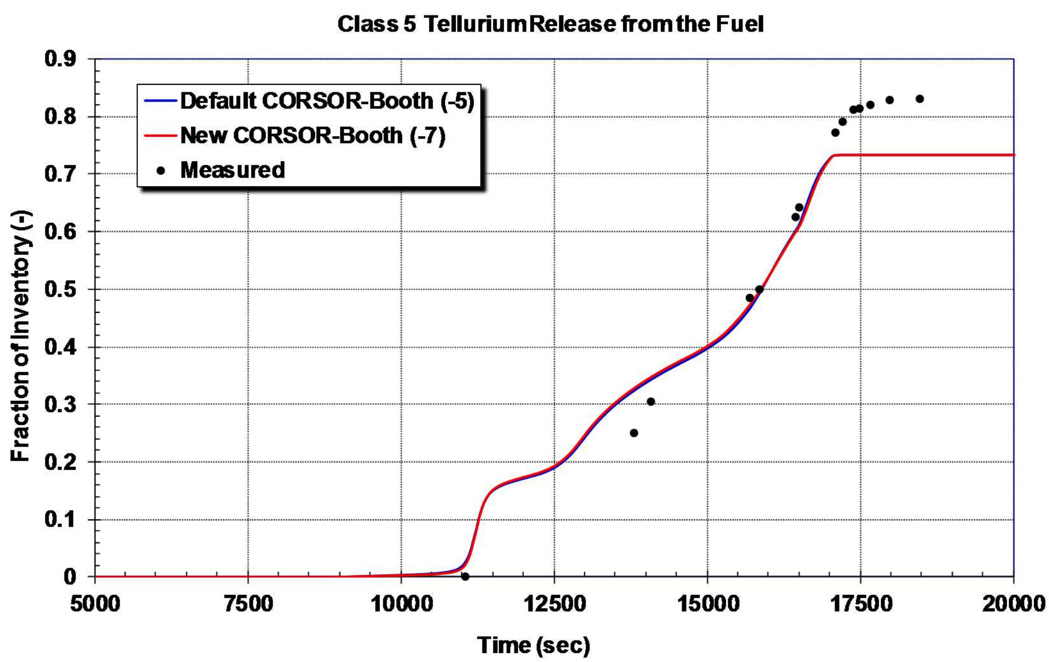


**Figure 3-11 Phebus FPT1 Tellurium release from the fuel**

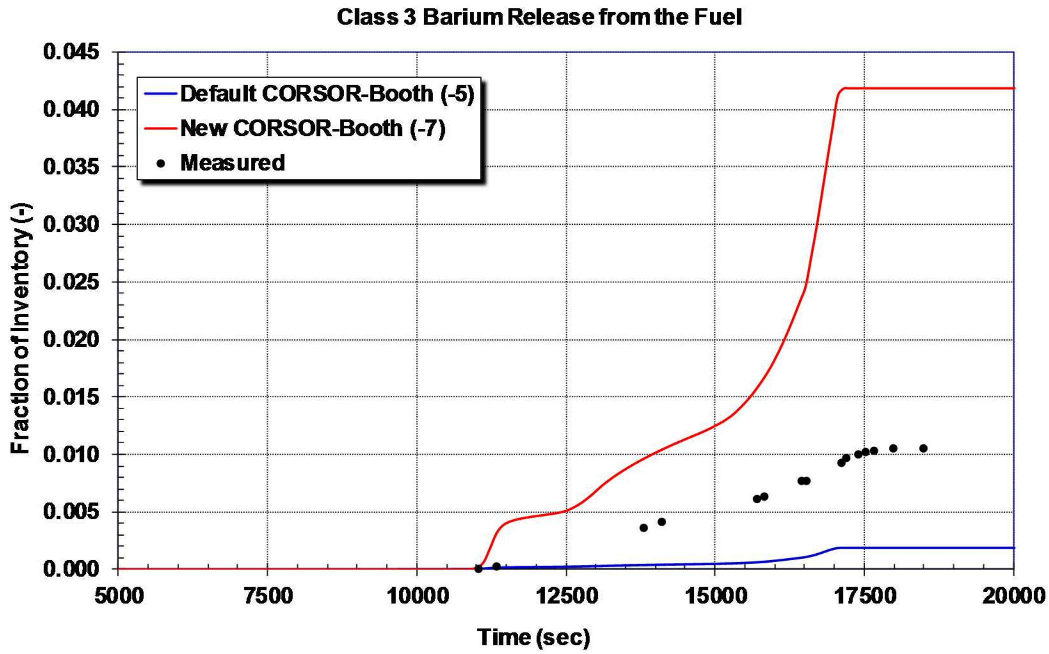


**Figure 3-12 Phebus FPT1 Barium release from the fuel**

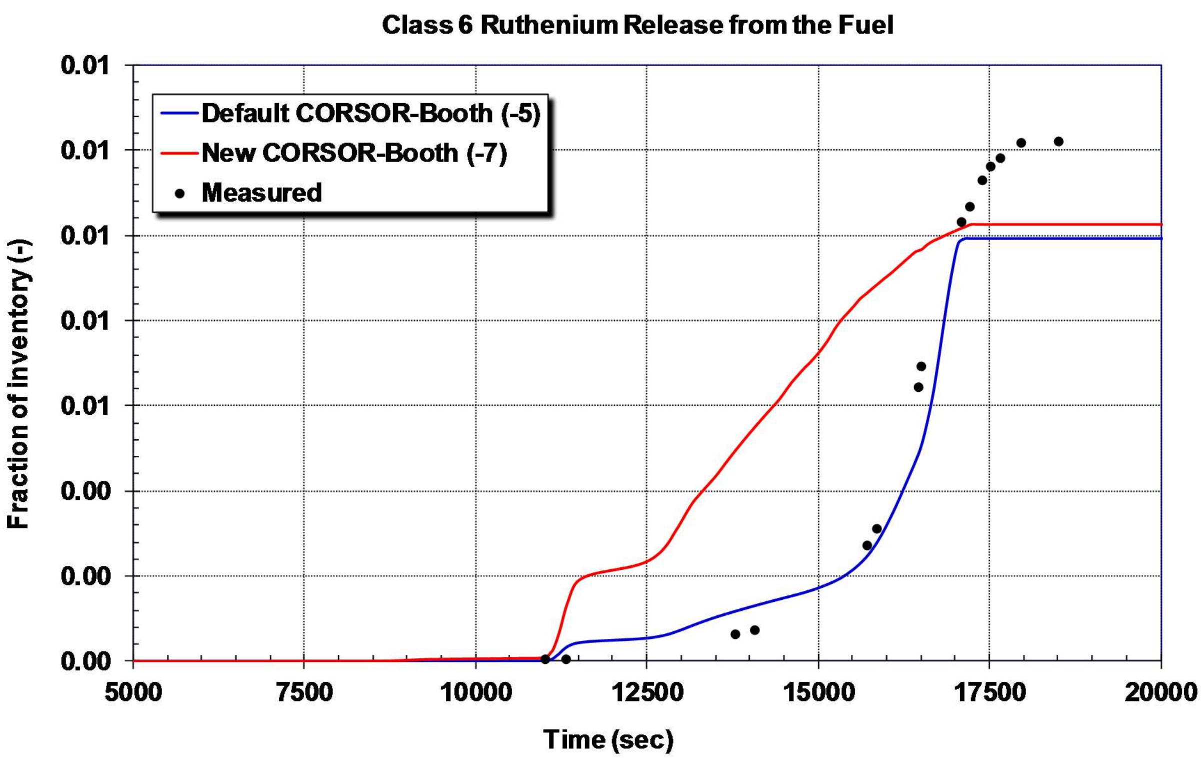


**Figure 3-13 Phebus FPT1 Ruthenium release from the fuel**

## 3.5. Resuspension Improvements

Previously, the resuspension (or liftoff) model used a hard-coded value for the surface roughness (i.e., 1.5e-5 m) to calculate the wall shear. The effective roughness at the surface can now be input by the user, which increases the flexibility of the modeling. The results from the STORM assessment show good agreement with the resuspension model using a user specified surface roughness.

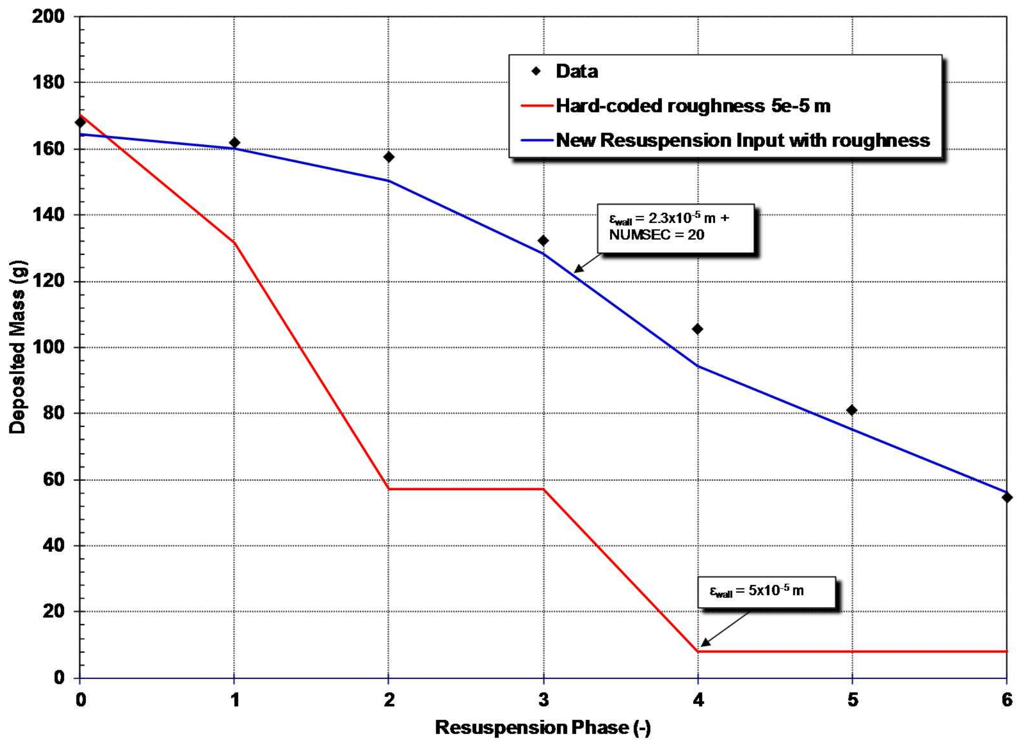


**Figure 3-14 STORM Deposited Mass during after each of the 6 resuspension phases.**

## 3.6. New Sodium Fire Model

Two sodium fire models have been implemented into MELCOR, a spray fire model (NACOM) and a pool fire model (SOFIRE II). These models were based on models found in the CONTAIN/LMR code. Figure 3-15 and Figure 3-16 shows a comparison of the calculated and measured airborne concentration of sodium aerosols for the ABCOVE AB1 and AB5 pool and spray fire experiments, respectively.

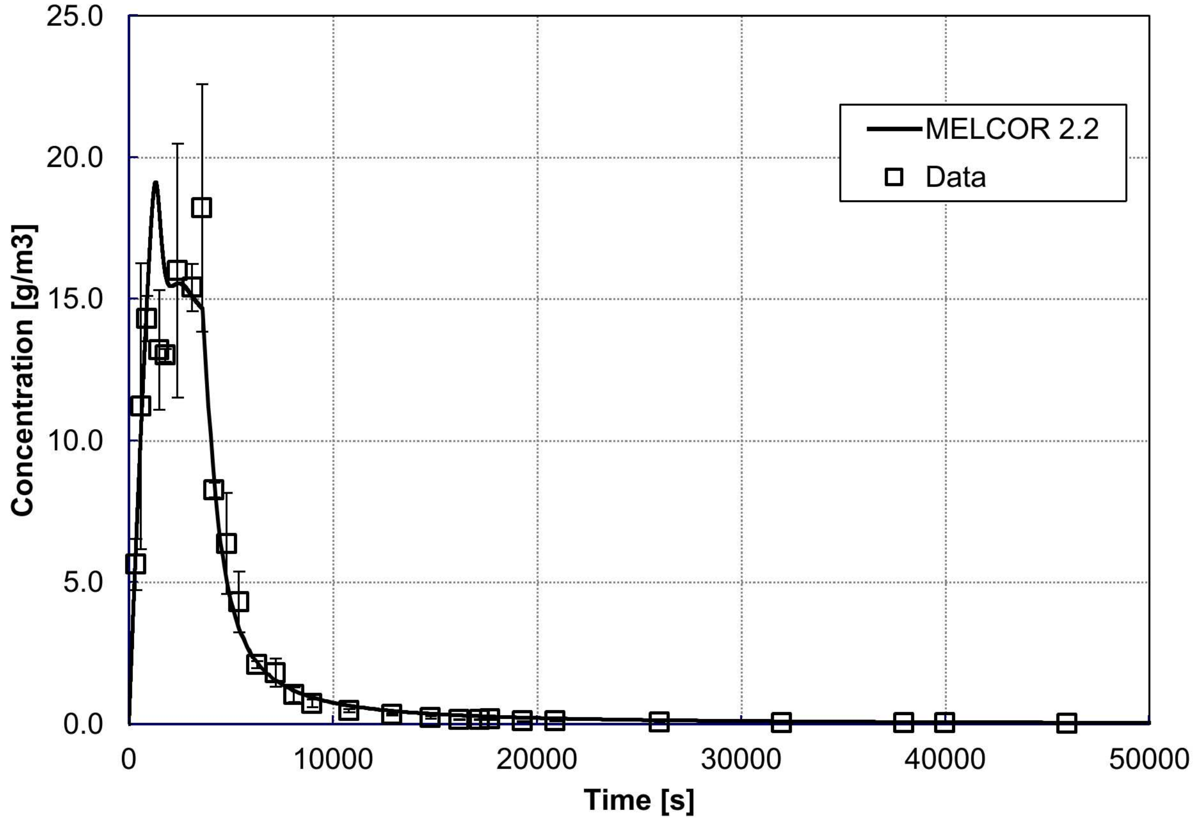


**Figure 3-15 Comparison of AB1 and MELCOR CSTF Na Airborne Concentrations.**

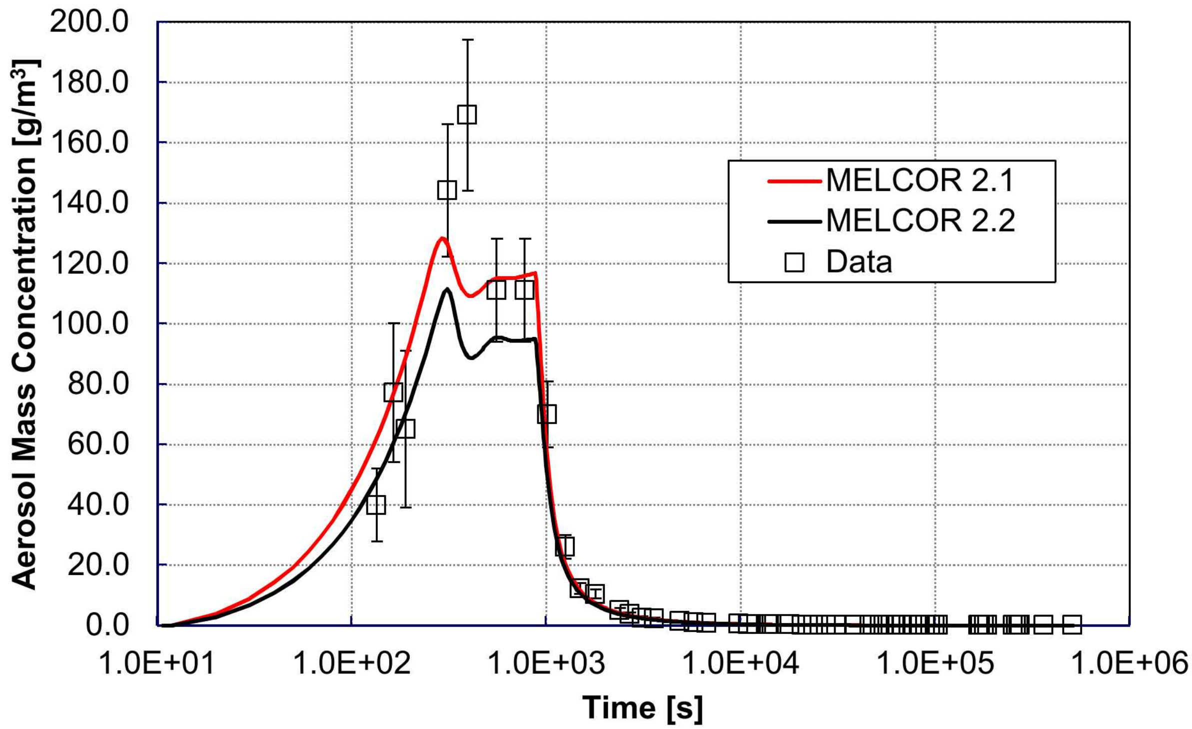


**Figure 3-16 Comparison of AB5 and MELCOR Na Airborne Concentrations.**

### 3.7. COR Eutectics Model

The COR eutectics model, which has been disabled due to functionality issues, has been updated to now run properly. It has been routinely used for current TMI-2 and Phebus validation calculations. The most extensive comparisons have been made using the TMI-2, which showed improvements in the size of the molten pool in the center of the core prior to the Pump B restart at 174 min. Phebus also shows good comparisons with data. No significant error occurs using the new model. Like the MP adjustments on the effective eutectic melting temperature, the eutectics model allows adjustments to the UO2-ZRO2 solidus phase diagram.

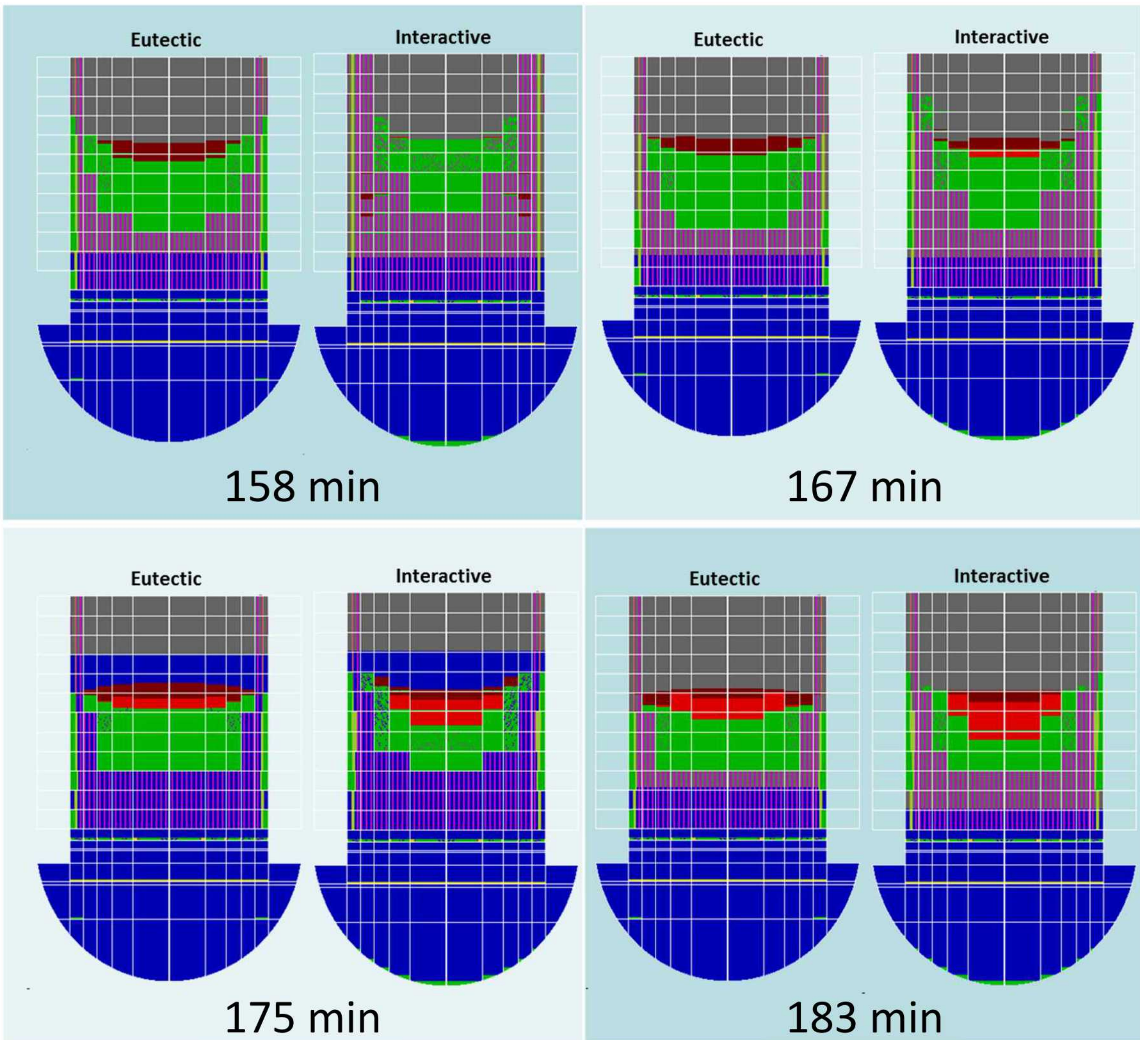


**Figure 3-17 Comparison of TMI-2 responses with and without the eutectics model.**

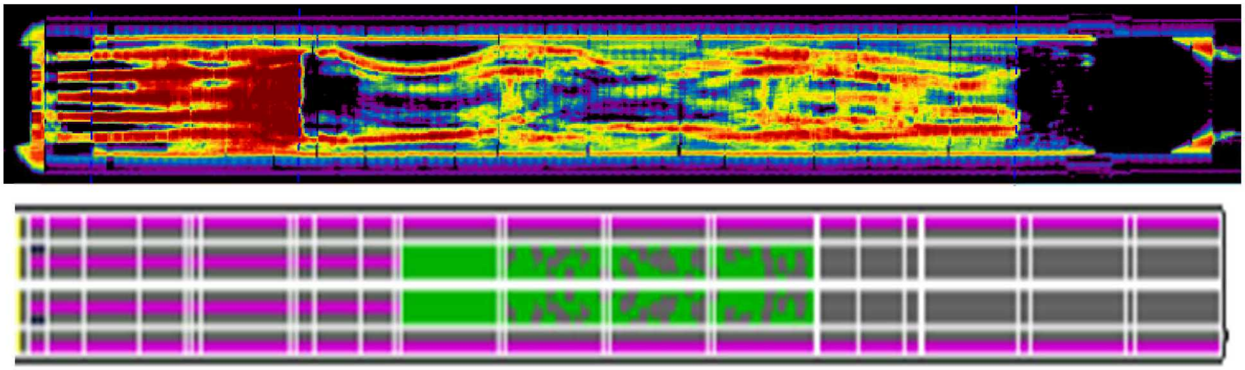

**Figure 3-18 Comparison of Phebus and MELCOR FPT1 final states using the eutectics model.**

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