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MELCOR Code Change History: Revision 11932 to 14959

Patch Release Addendum

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ABSTRACT

This document summarily provides brief descriptions of the MELCOR code enhancement made between code revision number 11932 and 14959. Revision 11932 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, 14959. Along with the newly updated MELCOR Users' Guide [2] and Reference Manual [3], users will be aware and able to assess the new capabilities for their modeling and analysis applications.

Following the official release an addendum section has been added to this report detailing modifications made to the official release which support the accompanying patch release. The addendums address user reported issues and previously known issues within the official code release which extends the original Quicklook document to also support the patch release. Furthermore, the addendums section documents the recent changes to input records in the Users' Guide applicable to the patch release and corrects a few issues in the revision 14959 release as well.

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ACRONYMS AND DEFINITIONS

Acronym	Definition
AC	Atmosphere Chemistry
BWR	Boiling Water Reactor
CCM3	CORCON-Mod. 3 (Software package integrated into MELCOR)
COR	Core (Package)
CV	Control Volume
CVH	Control Volume Hydrodynamic (Package)
EOS	Equations of State
FL	Flow Path (Package)
FLiBe	Lithium Fluoride Beryllium Fluoride, Molten Salt EOS (Filename: tpffi)
He	Helium, EOS (Filename: tpfhe)
HMX	Heavy Mixture Layer (Heavy oxides and metals mixed)
HP	Heat Pipe
HS	Heat Structure (Package)
LWR	Light Water Reactor
N2	Nitrogen, EOS (Filename: tpfn2)
Na	Sodium, EOS (Filename: tpfna)
NRC	U.S. Nuclear Regulatory Commission
Pb-Li	Lead Lithium, EOS (Filename: tpflipb)
PD	Particulate Debris
PWR	Pressurized Water Reactor
RN	RadioNuclide (Package)
SNL	Sandia National Laboratories
TMI	Three Mile Island

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ADDENDUMS FOR THE PATCH RELEASE

Following the release of the MELCOR code revision 14959, a set of known and reported issues from the severe accident analysis community have been addressed by the patch release which this document is meant to accompany. Summaries for each issue or modification are detailed within this section. Additionally, the main report has been adjusted to similarly reflect these changes as described below.

Default Behavior for Particulate Debris Heat Transfer to the Lower Head

An issue was report that the default 'MODEL' option for input fields 2, 3, and 4, on input record COR_LHF was incorrect and that the Users' Guide still provides default values of 1000.0. Additionally, the MELGEN output file supported this conclusion by also reporting values of 1000.0.

The model for heat transfer between the particulate debris and lower head was correctly enabled in the release version, but MELGEN did not correctly indicate this in output. This has been corrected in the patch. At this time, only particulate debris – lower head heat transfer model has been enabled by default. Section 2.1.1 has been modified to:

"For some time, an optional model has been available for calculating this heat transfer by using local particulate debris (PD) temperature to determine thermal conductivity and the height of the PD to determine the conduction path length. To standardize the use of this model, the default value on the COR_LHF record for heat transfer from PD to the lower head has been changed to 'MODEL'."

Eutectic Model Enabled by Default

A discrepancy between the Quicklook Report and the Users' Guide exists regarding the default behavior of the eutectic model. The Quicklook stated that the eutectic model was now on by default and the Users' Guide stated it was not enabled by default.

At the time of the official code release the Users' Guide was correct and the eutectic model was not enabled by default. However, following the release of the patch the eutectic model is now on by default. The following was appended to Section 2.1.2:

"The new model is activated using the COR_EUT record and specifying ON for the first field. Similarly, OFF will deactivate the eutectic model."

Additionally, if a user uses the UO2-INT or ZRO2-INT materials, the eutectic model will deactivate in for the patch release, and a diagnostic message will appear detailing this feature.

Eutectic Default Temperature for UO_2 and ZrO_2

Section 2.1.2 stated the default minimum melt temperature of a mixture of UO2 and ZrO2 as 2450 K at 0.5 mole fraction; however, the Users' Guide COR_EUT description states that the default is 2800 K.

The correct value is 2450 at 0.5 mole fraction. The MELGEN output file will report this correctly with the patch release.

Extension of Bubble Rise Model to Vertically Stacked Control Volumes

The bubble rise model extension is not documented in the Users' Guide.

This model is still undergoing testing and development and isn't available to users at this time. The section has been removed from this report.

Condensation/Evaporation Model Correction

The RN model discussion suggested a new default behavior associated with a new algorithm for better resolution of particle mass during condensation.

> An issue was discovered for this new feature and it is off by default at this time. The following sentence was removed from Section 3.1:
>
> *"The new algorithm is now activated by default whereas it was previously off by default but available to users."*

FeCrAl Oxide Thickness

Incorrect FeCrAl oxide mass due to array indexing led to an isolated error in the oxide thickness calculation.

> Error was corrected. No changes to any documentation.

New Cavity Defaults

In the absence of any user intervention via the CAV_U and/or the CAV_DFT input record, all phasic conductivity multipliers, boiling heat transfer multipliers, and inter-layer heat transfer coefficient enhancement multipliers are set to unity and the water ingression model is configured as active. The oxide, metal, and surroundings emissivity values are set to 0.9.

> The Users' Guide entries for CAV_DFT and CAV_U will be updated on the next official release. Their eventual updates can be observed in the New Input and Modified Records section within this Addendums section.

In the prior official code release, revision 11932, cavity heat transfer multipliers greater than 1.0 were used to enhance heat transfer to better approximate debris-water interaction. Section 2.1.3 includes the following text to direct users to this option.

> *"Additionally, a new keyword under the WATERINGRESSION model option on record CAV_U can be applied to impose the previous set of conduction heat transfer multipliers used to enhance heat transfer between debris and overlying water. This option permits backwards compatibility with Users' Guide r11932 CAV_U default values."*

Revised Energy Accounting for Cavity

Plot variables related to CAV and global energy error tracking, namely CAV-ENERGYERR and EXE-RELGEE, were recently corrected so that their respective values are exposed in the plot file. When water ingression modeling is inactive or when water ingression modeling is active and water ingress is not occurring, CAV-ENERGYERR and EXE-RELGEE are expected to reflect the true imbalance in CAV and global energy budget. There remains an issue with energy error tracking that manifests only when water ingression modeling is active and water ingress is occurring at the top surface of the CAV debris pool. Small energy discrepancies occurring at each time step tend to accumulate, thus leading to larger energy errors than would otherwise be observed in the absence of water ingress model action. The appearance of these errors is often coincident with first activation of the water ingression model physics. The magnitude of the observed error accumulation is directly proportional to the size of the problem, i.e. to the magnitude of the CAV energy inventory. Additionally, under the same conditions the integral energy counter reflected by the plot variable CAV-INTERN intermittently demonstrates poor behavior. Nevertheless, the physical response of the debris pool under influence of the water ingression model is typically reasonable as observed.

RF_MOD Functionality

RF_MOD record was reported to not function appropriate when users attempted to create reduced restart files.

This issue has been resolved in the patch release.

New Input and Modified Records: PROPRIETARY, MARKINGS, CAV_DFT, CAV_U, and COR_EUT

A new capability was added permitting the use of a pre-generated marking message for all text output, diagnostic, and html files as well as the binary plot file. The record is a global data record and will be documented in subsequent releases within the Users' Guide Exec Package as follows:

PROPRIETARY – Prepends a Proprietary Statement Marking to the Output Files

Optional

If this record is present, the following statement will appear in all diagnostic files, text output files and html files:

```
//////////////////////////// P R O P R I E T A R Y ////////////////////////////
  The input deck used in this calculation is marked as proprietary. Consequently,
  output files are also assumed to contain information that should be regarded
  as proprietary.
//////////////////////////// P R O P R I E T A R Y ////////////////////////////
```

Example

```
PROPRIETARY
```

MARKINGS – Prepends a Generic Statement Marking to the Output Files

Optional

If this record is present, a general statement will appear in all diagnostic files, text output files and html files. The user will specify the identification of the marking with a keyword on the first input field.

(1) MARKING

A user specifies a character string to be used to create a general marking statement. The statement is provided below, and "Marking" indicates the fields of the statement which will be replaced by the user specified string.

(type = character*256, default = Proprietary)

```
//////////////////////////////////// M A R K I N G ////////////////////////////////
  The input deck used in this calculation is marked as Marking.  Consequently,
  output files are also assumed to contain information that should be regarded
  as Marking.
//////////////////////////////////// M A R K I N G ////////////////////////////////
```

Example

```
MARKINGS "General Access"
```

The following records have been modified since the release and will be updated in future Users' Guide releases. CAV_DFT and CAV_U as documented here are correct for the official release and the patch release. The COR_EUT as documented here is correct only for the patch release.

CAV_DFT – CAV Package Default Scheme Record

Optional

This record modifies the default set of values in the CAV package to the "1.8.6 standards". Note that these values may not reflect current MELCOR best practice modeling parameters for the analysis of severe accidents. If the record is present, one floating point field must be present. This record can be specified once and is not needed for each cavity (i.e. the record is not associated with any particular cavity input accompanied by CAV_ID).

(1) DEFAULT

Mode of default scheme. Permitted values are '1.86' and '2.0'.

(type = real, default = 2.0, units = none)

Example

```
CAV_DFT  1.86
```

If the DEFAULT field is 2.0, no change is made to the existing default values. If the DEFAULT field is 1.86, the following CAV package default values will be modified, unless otherwise specified by the user input record

Record	DEFAULT = 1.86	DEFAULT = 2.0
EMISS.OX	0.6	0.9
EMISS.MET	0.6	0.9
EMISS.SUR	0.6	0.9
BOILING	None	1.0
COND.OX	1.0	1.0
COND.MET	1.0	1.0

A complete set of the following records (at least the required one) must be input for each cavity. They define:

(1) The initial cavity size, shape, concrete type, and contents (if any);
(2) The control volume that provides boundary conditions and the transfer process (if any) that will deposit material into the cavity;
(3) The method for calculating internal (decay) heating, (if not the default); and
(4) Miscellaneous control and model parameters;

although not necessarily in that order.

CAV_U – Miscellaneous Control and Model Parameters

Optional

Unique to the cavity package is the number of models or parameters that can be disabled/enabled or modified. These options have been gathered into one record, the CAV_U record. CAV_U is a table input record which permits numerous models and/or parameters to be adjusted.

For each table entry, the user will specify a unique model or parameter to be modified. The following input fields, which are specific to the model or parameter chosen, have been assembled below to be readily grouped with their respective model or parameter.

Note: Prior to the inclusion of the water ingression and melt eruption models, the default values for several heat transfer processes have been specified with multiples greater than 1.0. These multipliers were intended to represent the improved heat transfer between debris and overlying pools due to water ingression and melt eruption. Currently, the default treatment is that all such multipliers are set to unity, the water ingression model is active, and the melt eruption model is inactive by default. An option to revert to the multiplier treatment was added and – if selected – is echoed in MELGEN/MELCOR output.

(1) NUMMISC

Number of user-input miscellaneous control and model parameters, dimension of the table below.

(type = integer, default = 0, units = none)

The following fields define the table. The number of rows must be equal to NUMMISC. Each row consists of integer number N, character variable (keyword) and either a real or integer variable. The keyword identifies the parameter and the real or integer variable specifies the value of the parameter.

(1) N

User-input number of table's row

(type = integer, default = none, units = none)

(2) MODELOPTION

A keyword must be specified by the user which corresponds to the models listed below. Each model or parameter selected have unique input requirements any following fields.

(a) BOILING
(b) COKE
(c) CTOXYREA
(d) EMISS.OX
(e) EMISS.MET
(f) EMISS.SUR
(g) GFILMBOTT
(h) GFILMSIDE
(i) HTRBOT
(j) HTRINT
(k) HTRSIDE
(l) MIXING
(m) NONIDEAL
(n) RADLEN
(o) SHAPEPLOT
(p) TDEBUG
(q) IBUBX
(r) COND.OX
(s) COND.MET
(t) COND.CRUST
(u) WATINGR or WATERINGRESSION or INGRESS or INGRESSION

(v) ERUPT
(type = character, default = none, units = none)

… (removed records that weren't adjusted to save space)

If MODELOPTION is set on field two to EMISS.OX

Emissivity of the oxide phase

(3) EO
Value of emissivity of the oxide phase

(type = real, default = 0.9, units = none)

If MODELOPTION is set on field two to EMISS.MET

Emissivity of the metal phase

(3) EM
Value of emissivity of the metal phase

(type = real, default = 0.9, units = none)

If MODELOPTION is set on field two to EMISS.SUR

Emissivity of the surroundings

(3) ES
Value emissivity of the surroundings

(type = real, default = 0.9, units = none)

… (removed records that weren't adjusted to save space)

If MODELOPTION is set on field two to COND.OX

Optional thermal conductivity of oxidic mixtures, having one of the following meanings

(3) CONDOX
option having one of the following values

(a) 0 or MODEL
Use internal model

(b) 1 or TF
Use table function

(c) 2 or CONST
Constant conductivity

(d) 3 or MULT
Multiplier on conductivity

(type = integer / character, default = 3, units = none)

followed by:

(4) CONDVAL

Name of table if CONDOX = TF, value of conductivity if CONDOX = CONST, or value of multiplier if CONDOX = MULT.

(type = real, default = 1., units = none)

If MODELOPTION is set on field two to COND.MET

Optional thermal conductivity of metallic mixtures, having one of the following meanings.

(3) CONDMET

Option having one of the following values

(a) 0 or MODEL
Use internal model

(b) 1 or TF
Use table function

(c) 2 or CONST
Constant conductivity

(d) 3 or MULT
Multiplier on conductivity

(type = integer / character, default = 3, units = none)

followed by:

(4) CONDVAL

Name of table if CONDMET = TF, value of conductivity if CONDMET = CONST, or value of multiplier if CONDMET = MULT.

(type = real, default = 1., units = none)

If MODELOPTION is set on field two to COND.CRUST

Optional multiplier for the conductivity in a solid (crust) sublayer in contact with water

(3) CONDVAL

Direct multiplier on the thermal conductivity of the crust.

(type = real, default = 1., units = none)

… (removed records that weren't adjusted to save space)

COR_EUT – Eutectic Model Activation

Optional.

This record allows the modeling of eutectic formations between zirconium and stainless-steel, zirconium and inconel, and uranium oxide and zirconium oxide. By default, the eutectic models are enabled. The prior modeling practice where eutectic modeling was enabled on the COR_MS record along with providing the material property definitions for the interacting materials is no longer allowed. Should a user incorporate material UO2-INT or ZRO2-INT, the eutectic models will be deactivated.

(1) N

Specify an integer for the number table records to follow. Table entries are only permitted if an integer is specified.

Or

(1) IEUMOD

Enable eutectic models with default specifications or disable eutectic models.

(a) ON
Enable eutectic models

(b) OFF
Disable eutectic models

(type = integer/character*3, default = ON, units = none)

The following data are input as a table with length N:

(1) NPM

Table record index.

(type = integer, default = none, units = none)

(2) PairMelt

Model switch enabling eutectic model for paired material. Users may input:

(c) 1 or ZR/SS
Zirconium and stainless-steel

(d) 2 or ZR/INC
Zirconium and inconel

(e) 3 or UO2/ZRO2
Uranium oxide and zirconium oxide

(type = integer or character*16, default = none, units = none)

(3) TM

Solidus temperature for the eutectic pair. Default values are 1210.0, 1210.0, and 2450.0 for ZR/SS, ZR/INC, and UO2/ZRO2, respectively.

(type = real, default = see description, units = K)

(4) F1

Molar ratio of the first member in the pair at the eutectic temperature. Default values are 0.76, 0.76, and 0.5 for ZR/SS, ZR/INC, and UO2/ZRO2, respectively.

(type = real, default = see description, units = -)

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 Wash1400[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 is continuously being developed to meet the evolving regulatory needs for licensing and analyzing postulated accidents for nuclear power plants. This report provides the code users 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 11932 to rev 14959), and previews the validation results for the new official release of the code (rev 14959). The user is referred to the MELCOR User Guide[2] and Reference Manual[3] to provide clarification of existing code parameters or models.

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2. MELCOR CODE IMPROVEMENTS

2.1. New Defaults

2.1.1. Heat Transfer Model between Particulate Debris and the Lower Head

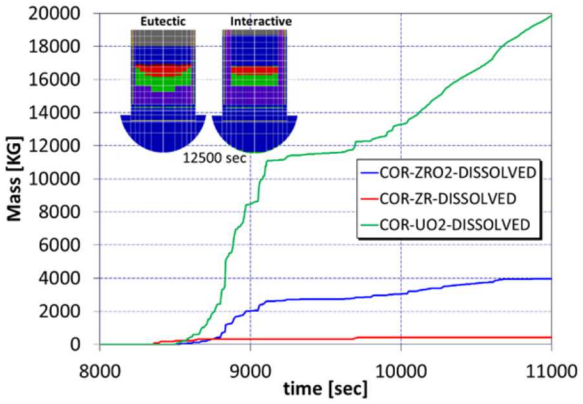
Heat transfer from particulate debris to the lower head is an important consideration for predicting the heat up and failure of the lower head. Even so, the default input describing this heat transfer was historically implemented as a single heat transfer coefficient, 1000 W/m^2, that may not always be reflective of temperatures or the conduction path through the particulate debris. Furthermore, the input for this parameter is optional (COR_LHF record). For some time, an optional model has been available for calculating this heat transfer by using local particulate debris (PD) temperature to determine thermal conductivity and the height of the PD to determine the conduction path length. To standardize the use of this model, the default value on the COR_LHF record for heat transfer from PD to the lower head has been changed to 'MODEL'.

Effective Heat Transfer Coefficient (W/m2-K) Using Thermal Conductivity of Materials at 1700 K

	Conduction Path Length (m)		
	0.5	0.25	0.1
UO2	4.4	8.8	22
ZR	83.6	167.2	418
ZRO2	4.88	9.76	24.4
SS	69	138	345
SSOX	40	80	200.

2.1.2. COR Eutectics Model

For users to simulate intermetallic formations and their effect on core degradation, users have been required to specify surrogate material with effective melt temperatures, UO2-INT and ZRO2-INT. However, introduction of these materials was often overlooked by experienced users. Improvements to the COR eutectics model were introduced since revision 11932 but were not activated by default until this release. With the new eutectic model materials in their intact form will melt at the molecular liquidus, i.e., UO2 melts at 3113 K and ZRO2 melts at 2990 K. However, when UO2 and ZRO2 are in a mixture, the melt temperature is dependent on the fractional content of UO2 and ZRO2 with a minimum melt temperature of 2450 K at 0.5 mole fraction. In addition, models for liquefaction of intact materials assumed in contact with a eutectic mixture are calculated using a parabolic rate limitation and dependent on the updated melt temperature of the conglomerate.

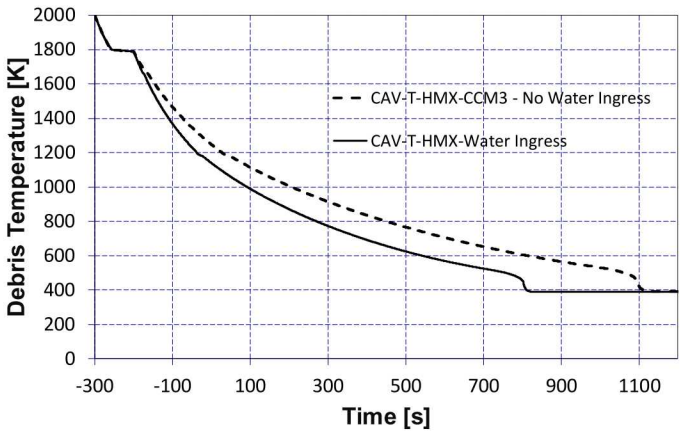


The new model is activated using the COR_EUT record and specifying ON for the first field. Similarly, OFF will deactivate the eutectic model.

2.1.3. CAV Water Ingression Model for Top-cooled Debris in Cavity

Experimental data[4] and the Fukushima accidents have supported revisiting the heat transfer modeling between the cavity debris bed and overlying water. By default, the code now utilizes the Epstein water ingression model[5] within the debris/pool solution algorithm, leveraging enhanced molten debris cooling effects between the overlying water pool and a permeable debris top crust. This model replaces the prior user-specified heat transfer coefficient multipliers used to enhance interfacial heat transfer. The water ingression is now enabled by default and is available to users on the CAV_U input record. The closely-related melt eruption model is still off by default due to perceived second order of importance based on current analyses.

For a simple one-to-one comparison of predicted cavity/debris thermal-hydraulic response, a wet cavity was initialized with debris (metal and oxide) at 2000.0 K with 1) water ingress and melt eruption active, and 2) water ingress and melt eruption inactive (CCM3-No Water Ingress). The same boiling heat transfer and slag film correlations were selected in both cases, and the two debris temperature responses were observed as a function of time. This comparison indicates the difference in debris cooling due solely to water ingress (melt eruption is inactive as, in this case, the sparging gas volumetric flux is insufficient to entrain molten material). The initially molten debris layer heavy mixture layer (HMX) reaches a partially frozen state (so-called "liquid-with-crusts" configuration) at approximately the same time in both cases, but the enhanced cooling due to water ingression is evident from the eventual divergence in values of HMX layer average temperature. The cooling trends are the same throughout the transient, but the water ingression acts to accelerate the debris cooling – a physically reasonable and expected result.



Additionally, a new keyword under the WATERINGRESSION model option on record CAV_U can be applied to impose the previous set of conduction heat transfer multipliers used to enhance heat transfer between debris and overlying water. This option permits backwards compatibility with Users' Guide r11932 CAV_U default values.

2.2. Significant Code Corrections since Revision 11932

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 (https://melzilla.sandia.gov/) as well as the changelist that is provided with the code release.

2.2.1. Corrections to the Water Ingression Models

Using formerly implemented mathematical models of water ingression and melt eruption, numerical implementation in MELCOR was revised for better performance within the iterative debris pool layer solution.

In a wet cavity, a water pool atop the debris pool may infiltrate a cracked (permeable) top crust and establish a dry-out front at depth. This can partially negate the insulating effect that an intact top crust might otherwise have on interior molten debris. This results in a more deeply cooled convective melt. A concomitant mode of enhanced debris cooling is melt eruption or the upward entrainment of molten inventory through a permeable top crust by sparging gas flow (e.g. due to release of gaseous concrete decomposition products to the bottom of the debris pool). Molten debris inventory erupts directly to the overlying water pool and is subsequently quenched in a coolable geometry.

Two new debris pool layers were introduced into the overall scheme to account for 1) a wet or "ingressed" top crust thickness, assumed quenched by water pool, and 2) quenched debris rubble atop the whole debris pool that results from melt eruption.

Early results with the revised implementation demonstrate the presence of enhanced cooling effects.

2.2.2. Corrections to the Oxidation Modeling

An error in the COR oxidation routines was uncovered that would affect BWR calculations where blocking occurs, possibly leading to an overprediction of oxidation rate during late phase core degradation. For a PWR, the situation can lead to an underprediction of hydrogen generation during late phase core degradation.

2.2.3. Sequential Ordering of Component Numbers in the CVH and HS Output Edits

For an input model with a large number of control volumes, flow paths, and heat structures, the MELCOR output edits can be difficult to use. The text outputs have been improved by writing both the name and the number of control volumes, flow paths, and heat structures. For example, the heat structure number is added under its name for output of HEAT TRANSFER DATA. Furthermore, MELCOR output of control volumes and heat structures are now sorted by sequential number and should be easier to navigate.

2.2.4. Class Specific Filter Removal

The input option permitting user to specify the RadioNuclide class decontamination factors, DFCTFA, on input record RN2_FLC was not functioning correctly. This model option has been corrected and will now function as intended.

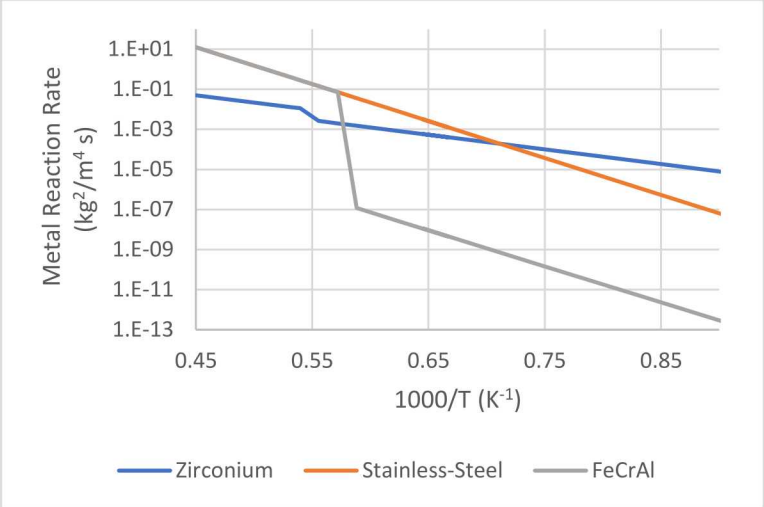
2.3. New or Extended Modeling

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. Accident Tolerant Fuels – FeCrAl Model

A new default core material, FeCrAl, has been introduced allowing users to perform accident tolerant fuel analyses within MELCOR. The material can be initialized as cladding and will undergo melt relocation, refreezing, and oxidation. Control function and plot file arguments support the material shortname 'FCA' and 'FCAO'.

As the FeCrAl material is still developmental, the final composition applied in nuclear applications remains uncertain at this time. The assumed composition is currently hardcoded as 21/5 for Cr/Al, which may change in the future. A comparison of the default parabolic rate constant for FeCrAl oxidation is made to the other default materials. The reduced reaction prior to breakaway oxidation shows potential advantage in reaction rates, in addition to reducing exothermic energy generation.

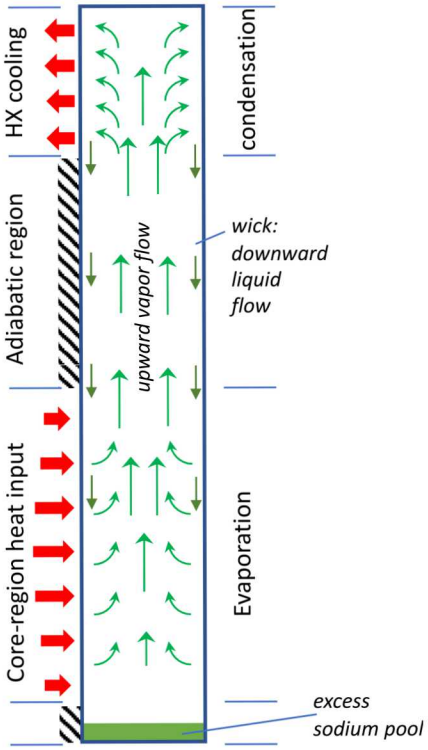


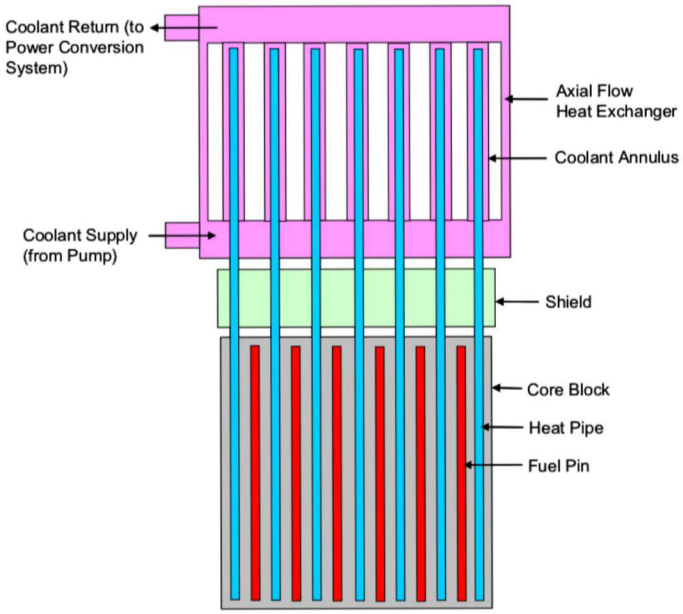
2.3.2. Heat Pipe Model

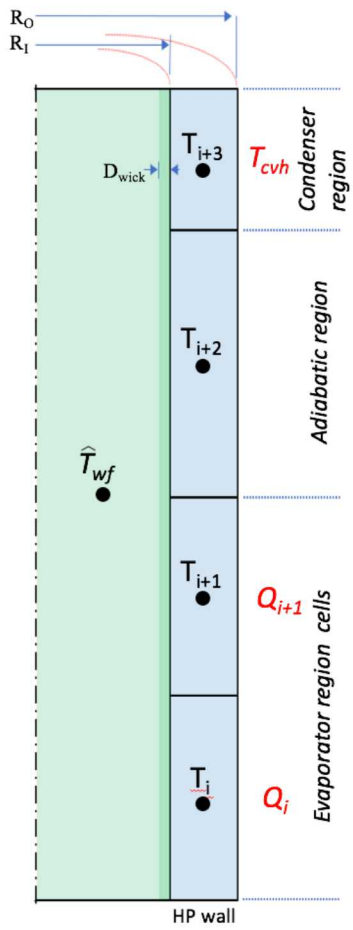
Heat pipes (HPs) are self-contained transport systems that use the large latent heat associated with phase transition together with the very high heat transfer coefficients for boiling and condensation to enable remarkably efficient heat transfer. Several recent reactor development efforts have included HPs for heat removal from the core, effectively replacing the functionality of the primary cooling loop that typically exists in a more traditional reactor design. Various innovative designs with different geometric configurations are being explored that suggest new modeling challenges for safety analysis codes such as MELCOR. One example, described by McClure et. al. [6], at Los Alamos, is a vertically oriented concept illustrated schematically in the second figure below.

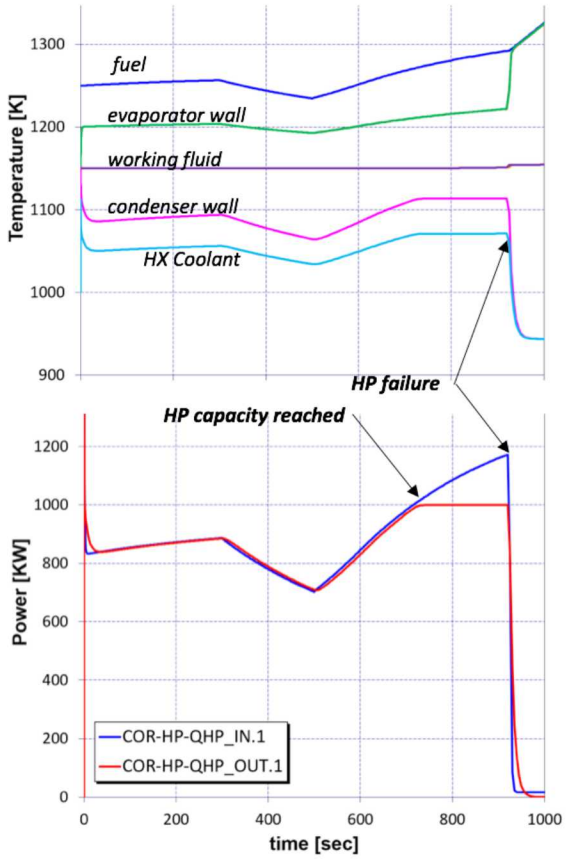
To enable modeling such reactors, a generalized approach has been developed and implemented for modeling HPs in MELCOR. Internally, the approach defines software interfaces to MELCOR packages that are independent of the details of the HP internal model so that models of different fidelity and applicability can be written and made available as needs arise. Use of an HP model replaces the conventional convective heat transfer between the fuel and coolant channel with the energy transfer from the fuel to the evaporative region of the HP. Heat rejection from the HP model at the condensation interface is then transferred to the CVH package.

A simple, functional HP model that meets the interface requirements has been written and used to test the approach and the associated interfaces with other MELCOR models and packages. The model qualitatively simulates various transient behaviors and limitations of a functional heat pipe (see illustration and plots below). As HP design details become available during reactors design licensing, additional development work will occur to improve the internal heat pipe modeling and better address issues such as heat-transfer between HP regions (lateral "heat paths"), HP degradation and failure (conversion to melt or rubble material), fission product release and transport, etc.









Illustrative output (temperatures and in/out power) from a slow transient of a simple HP test problem

2.3.3. Atmospheric Chemistry Model for Sodium Fire Modeling

The atmospheric chemistry (AC) model from CONTAIN-LMR has been implemented in MELCOR. The AC model will account for atmospheric (or gas-phase) chemical reactions of sodium by-products (such as Na_2O_2 and Na_2O aerosols) and sodium coolant with moisture and oxygen in the air. The sodium by-products are those generated from sodium pool and spray fires implemented in the previous MELCOR official release, revision 11932.

Oxygen in the atmosphere is assumed to react with sodium to form the monoxide and peroxide, respectively as follow:

$$\mathbf{2\ Na + \frac{1}{2} O_2 \rightarrow Na_2O}$$

$$\mathbf{2\ Na + O_2 \rightarrow Na_2O_2}$$

Two subsequent reactions may take place. The first subsequent reaction is for peroxide reacting with sodium:

$$\mathbf{Na_2O_2 + 2\ Na \rightarrow 2\ Na_2O}$$

This reaction is always assumed to occur if the peroxide and condensed sodium are in contact due to being present within an aerosol particle. The second subsequent reaction is between aerosol deposits and condensate film on surfaces.

Sodium monoxide and peroxide can react with water vapor (moisture) to form sodium hydroxide:

$$\mathbf{Na_2O + H_2O\ (g)\ \rightarrow 2\ NaOH}$$

$$\mathbf{Na_2O_2 + H_2O\ (g)\ \rightarrow 2\ NaOH + \frac{1}{2}O_2}$$

Currently, water vapor is treated as an ideal gas; therefore, no water condensate will be present. Additionally, the user should note that while the hydroxide is expected to be the principal reaction product with water at low temperatures or with excess water, the possible subsequent conversion of the hydroxide to the monoxide is not modeled if conditions change. The chemical reaction models presented here assume that all reaction heat is retained only by the gases present or by the structures; the models ignore the increase in the heat content of the aerosols or aerosol deposits due to an increase in temperature above the temperature of formation. The heat generated by the surface reactions is assumed to be deposited to the surface node of the structure. This treatment is regarded as conservative.

2.3.4. Radiant Heat Transfer to Aerosols

MELCOR allows for radiation from surfaces to a participating gas within the atmosphere of a control volume. Both heat structures and pool surfaces are permitted to radiate to the intermediate gas. Furthermore, a radiation enclosure model was recently added to MELCOR to allow the user to define an enclosure network. However, until now, aerosols could not interact with radiant heat transfer. For sodium fires, the emission of smoke aerosol would suggest the need for including aerosols for radiation heat transfer. A model for aerosol radiation developed by Pilat and Ensor[7] was recently added to the code. Aerosol cloud emissivity derived per Pilat and Ensor:

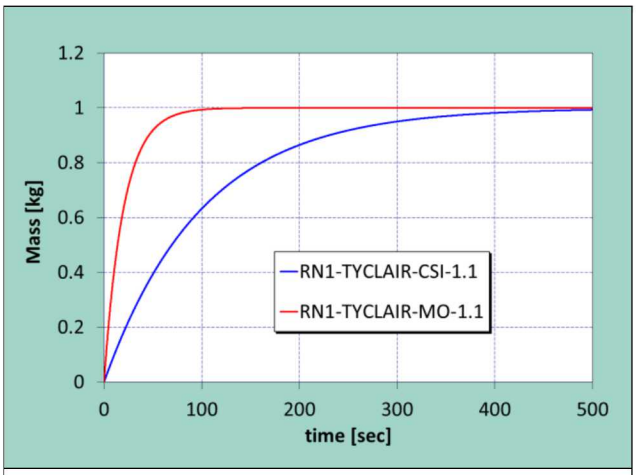
$$\mathbf{\alpha_{\lambda m} = 4000 C_{\lambda m} f_m}$$

Where $C_{\lambda m}$ is a user-defined parameter for radiation enclosure model and f_m is the total aerosol mass concentration (kg/m^3) calculated by the code.

$C_{\lambda m}$ in this equation is provided to allow the user to account for the effects of wavelength, index of refraction, particle size distribution, and aerosol particle material density. $C_{\lambda m} = 1$, corresponds to soot-like particles with a density of 2000 kg/m^3

2.3.5. Radionuclide Transfer from Pool to Atmosphere

When radionuclides are deposited within a pool they remain there until the pool evaporates. Upon evaporation, the aerosols are distributed between the floor, heat structures, and flow-through areas. Processes for evaporation or other means of release to the atmosphere are not considered significant in light water reactor (LWR) applications. However, as part of our development for non-LWR applications, a simple means for transferring radionuclides to the atmosphere by use of a control function has been developed. This option will be exercised in developing codified models to account for these processes.



Example case:

1 kg of CSI specified in pool at t=0 sec

1 kg of MO specified in pool at t=0 sec

Input specifies a constant CF of 0.01 sec^{-1} for CsI

Input specifies a constant CF of 0.05 sec^{-1} for MO

Plot shows release to atmosphere over time.

The user will specify a table for a given control volume (CV), identifying the RadioNuclide (RN) classes and their corresponding fractional release rate.

$$\frac{dC_{RN,ICV}}{dt} = C_{RN,ICV} \cdot CF\left(t, C_{RN,ICV}, \ldots\right)$$

Where C_{RN} is the concentration of RN class in volume, ICV, and CF defines the fractional transfer rate.

Aerosols that are transferred into the atmosphere are done so by placing them into the smallest aerosol section.

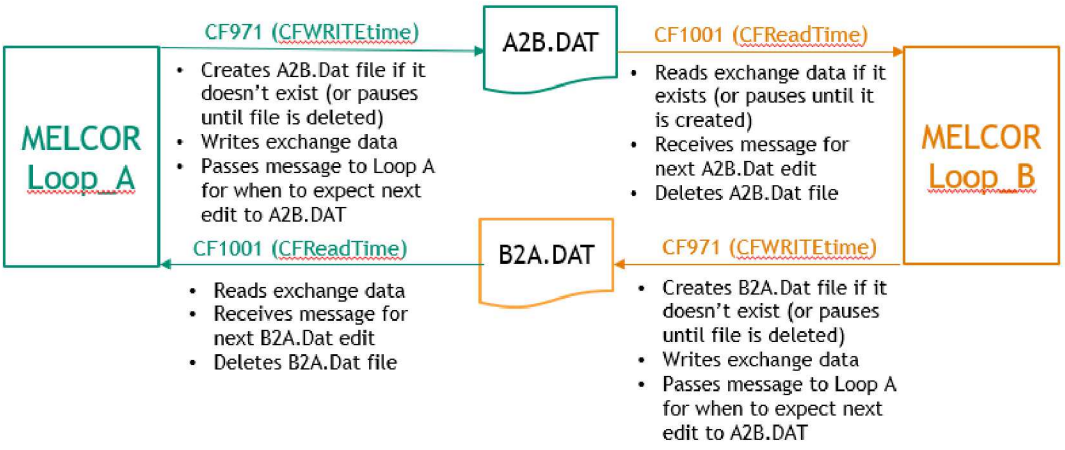
2.3.6. Coupling to Codes Using MELCOR's Control Function Capability

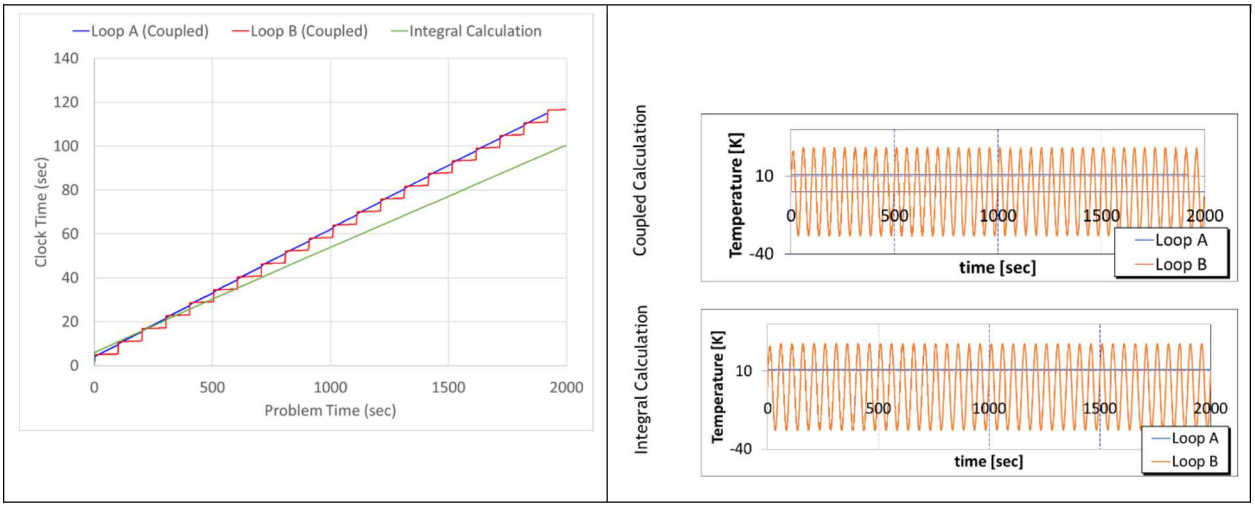
MELCOR is a fully integrated, system-level computer code. The integrated architecture is necessary for source term analysis as it allows the capture of complex coupling between a myriad of phenomena involving movement of fission products, core materials, and safety systems. Early analyses of severe accidents were performed with the Source Term Code Package (STCP) which involved a number of separate effects codes that were run separately without being able to simulate feedback mechanisms. Such analyses were plagued by challenges associated with transferring data, consistency in data and properties among codes, and in capturing the coupling of physics.

Even so, there are occasions when code users need to couple MELCOR with other codes. As an example, a reactor system having two working fluids might be coupled across a heat transfer surface. The level of coupling is small and poses few problems. Coupling also provides a framework for testing models by first coupling them to a MELCOR simulation prior to be integrated into MELCOR.

Coupling to a MELCOR simulation can be accommodated through the use of the CFREAD and CFWRITE control function types. As an example, two instances of MELCOR can pass message files between each other to transfer data as well as to agree on synchronization times. This methodology was originally developed in a branch version of MELCOR 1.8.6 and was implemented into this release of the code. Two MELCOR input decks that demonstrate this capability are

provided with this release. The test case shows two input decks, Loop A and Loop B which exchange data for a common heat structure interface. The same calculation was performed with an analogous simulation where the two calculations were integrated into a single run and gave nearly identical output.





2.3.7. HTML Charting Capability

The text output generated by a MELCOR run contains an exhaustive summary of the state of the simulation at a user-defined frequency. The data are organized by package and individual snapshots in time are concatenated into a potentially very large file. Because of the file length, navigating such information is difficult for users. This may result in the file being ignored by all but the very experienced MELCOR user. To make navigation of this file easier, an HTML version of the output was generated in revision 732 (2008). This improvement separated the individual snapshots in time into separate HTML files and links were added to jump from one file to the next as well as links to various bookmarks in the output. In 2015, the routines for drawing bitmaps showing the core degradation were added to place an image of the core degradation state into the HTML files.

Current code improvements add the capability to embed Google charts directly into the HTML files. This allows a rich representation of data at snapshots of time throughout the accident scenario by providing graphical plots of temperature profiles, power density profiles, material masses, component volumes and surfaces, heat structure temperature profiles, and radionuclide distribution

plots. At the end of the calculation or at termination of a calculation due to a detective code issue, a final HTML file output will be made that also contains time trends from the plot file. Several routines in the calculation will generate error conditions and appropriate plots showing variables related to the error condition.

2.4. Minor Code Improvements

2.4.1. Enhancements for Vectorized Control Functions and Miscellaneous Corrections

The following control function arguments can now be used by vector control functions: RN1-ADEP, RN1-VDEP, RN1-CVCLT, and RN1-DEPHS. Additionally, the Formula type control function can now be vectorized. Corrections were made to the following control function arguments which were not functioning properly: HS-DEGAS-ENERGY, HS-DEGAS-MASS, and HS-DEGAS-RATE.

3. VALIDATION CASES

MELCOR 2.2.14959 contains many enhancements and error corrections throughout key portions of the accident progression modeling. This section presents code comparisons with data from important experiments and the TMI-2 accident. While code corrections have been made that impact key models such as the quench behavior, the core material eutectics, the oxidation modeling, and the debris heat transfer, the following section show several validation tests continue to be predicted with reasonable agreement.

3.1. Hygroscopic Model

Several changes have been made to the hygroscopic model over the years. Revisions 9445 and 9446 changed the precision of the 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. A new algorithm for remapping particle sizes after condensation (or evaporation) was introduced in revision 11908 to improve resolution of the aerosol mass within a section (particle size bin).

The AHMED tests were designed to provide data for hygroscopic and non-hygroscopic aerosol behavior under controlled temperature and humidity conditions. Due to the simplicity of the facility and the relatively low-aerosol concentration, the AHMED tests provided a wealth of hygroscopic aerosol data, free of integral effects. The results of two AHMED test comparisons are shown in Figure 3.1 and Figure 3.2. The new MELCOR 2.2 results showed good comparison with the data and relatively little change from the previous results.

The LACE LA-4 experiments included both hygroscopic (CsOH) and non-hygroscopic (MnO) aerosols. The purpose of the experiment was to determine the disposition of aerosols in the containment building under conditions of high steam concentrations. The experiments highlighted differences in aerosol settling between hygroscopic (i.e., water-soluble) aerosols such as CsOH and non-hygroscopic aerosols such as MnO in a high-steam concentration. CsOH is a highly hygroscopic material, while MnO is insoluble and essential non-hygroscopic. The results of the CsOH and MnO behavior in LA-4 test are shown in Figure 3.3 and Figure 3.4, respectively. The new comparisons are shown with and without the new MAEROS numerics model and with 20 and 30 aerosol sections. The results of the old and new numerics have similar responses during the aerosol build-up phase and initial deposition phase. The new coding has a slightly better prediction of the long-term, low concentration aerosol deposition rate. There is an improvement in the hygroscopic aerosol deposition rate with 30 aerosol sections but not an excessive settling rate for the non-hygroscopic aerosols.

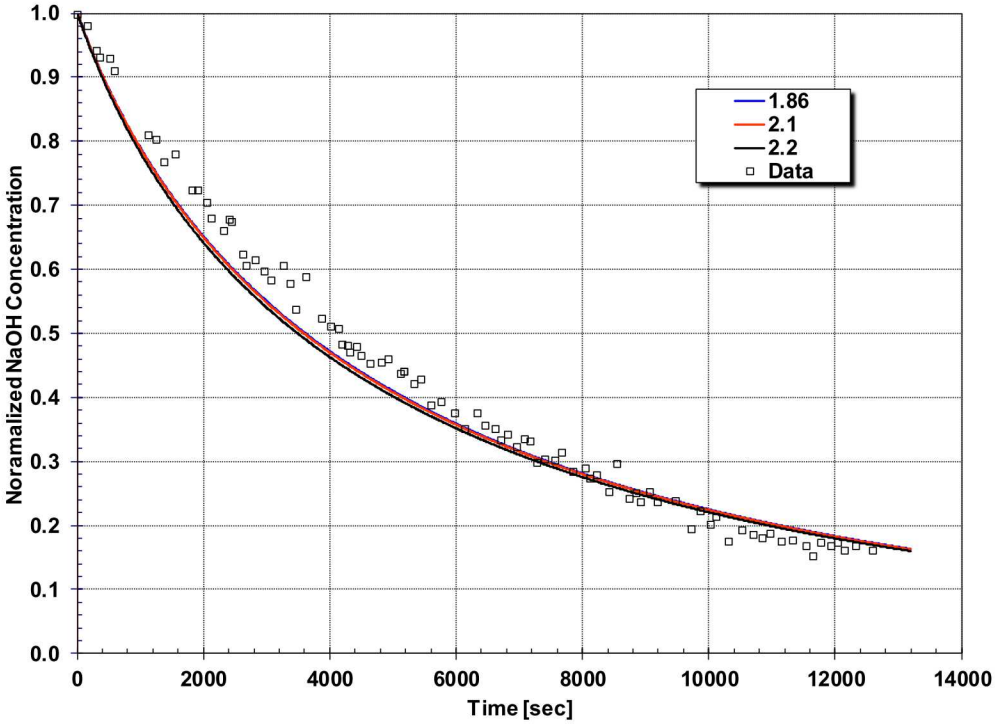


Figure 3.1 AHMED Experiments (22% Relative Humidity)

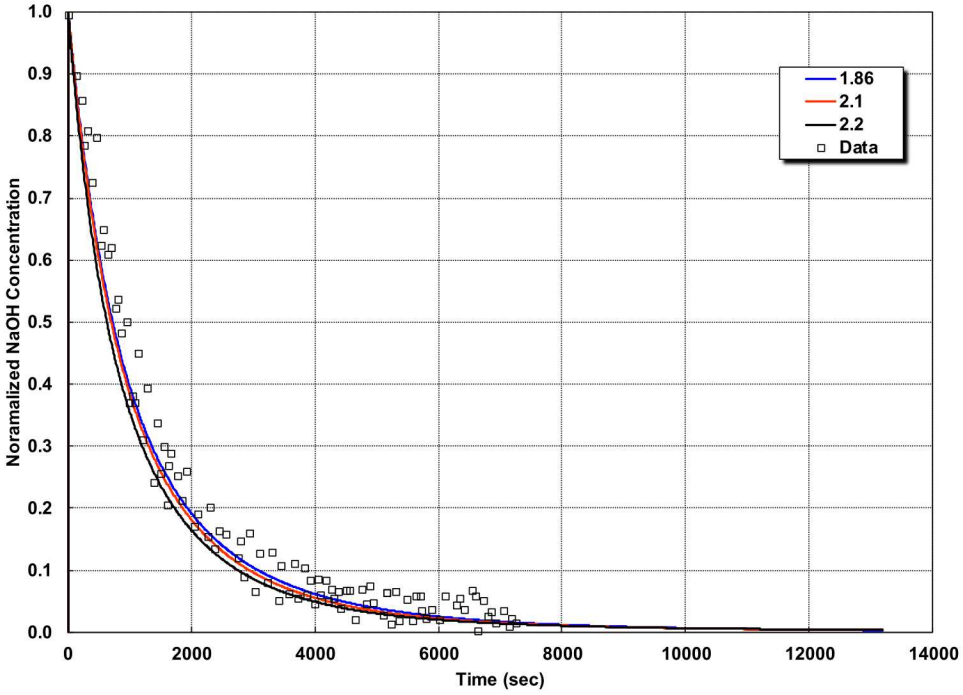


Figure 3.2 AHMED Experiments (96% Relative Humidity)

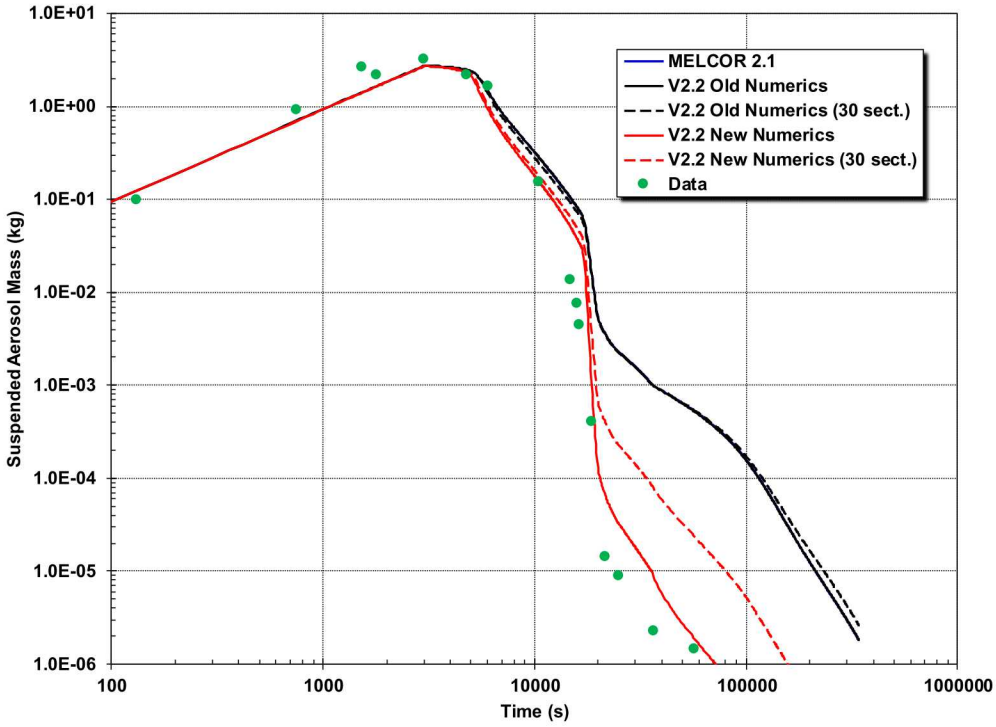


Figure 3.3 LACE LA-4 Experiment (Hygroscopic CsOH Aerosol Response)

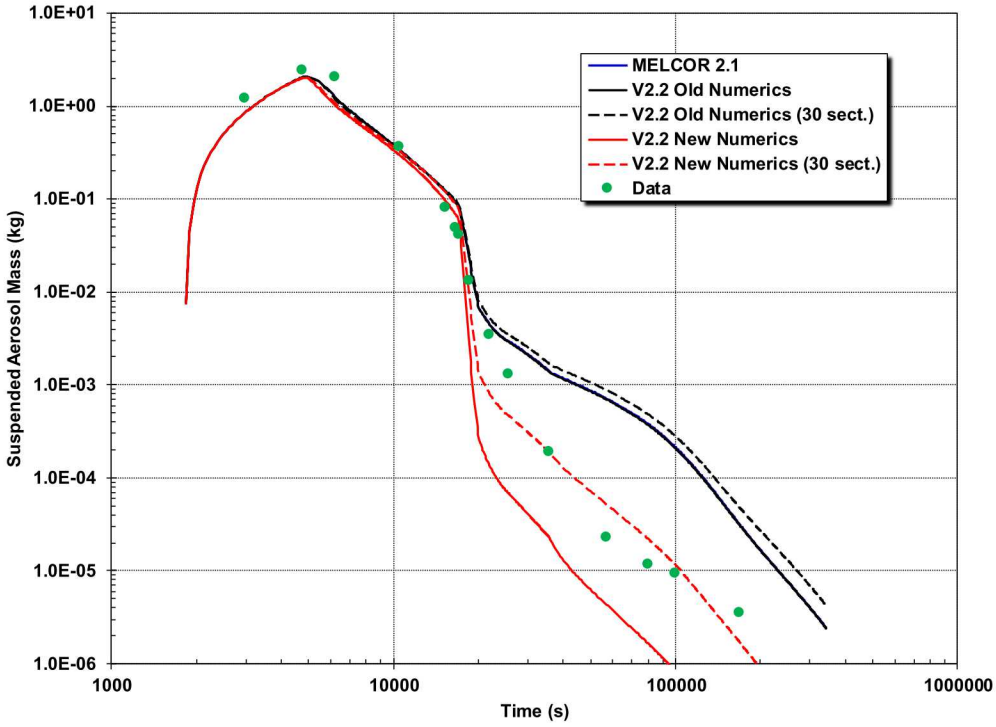


Figure 3.4 LACE LA-4 Experiment (Non-hygroscopic MnO Aerosol Response)

3.2. Oxidation Models

A significant code correction was made to the oxidation routines (i.e., see Section 2.2.2). The code correction was expected to impact the total oxidation, but its impact varied showing a dependency on model nodalization, the transient, and the reactor type (i.e., BWR versus PWR). Figure 3.5 shows the results of the Phebus FPT1 test using the new oxidation correction. The FPT1 test included severe degradation of an irradiated bundle in a steam rich environment, which allowed for significant oxidation. Overall, the corrections to the oxidation routine did not change the relatively good results observed in the Phebus FPT1 comparisons. The new MELCOR 2.2 FPT1 calculation also included the new eutectics model, which impacts the fuel degradation and subsequent behavior.

The results of the CORA-13 and QUENCH-6 tests are also presented. Both experiments included electrically heated fuel elements with a rapid quench capability. Figure 3.6 shows the results from the CORA-13 test. Interestingly, MELCOR 2.2 shows a spike in hydrogen production during the quench phase. In addition to corrections to the oxidation routines, MELCOR 2.2 includes corrections to the quench model, which might explain the spike in oxidation during the quench phase versus the older code versions. Finally, Figure 3.7 shows no significant impact to the total hydrogen production in the Quench-6 test. The MELCOR 2.2 calculated hydrogen production is higher than measured but not significantly different compared to MELCOR 2.1. The calculated rapid oxidation phase continued slightly longer than measured during the quench phase, which accounts for the higher calculated hydrogen production.

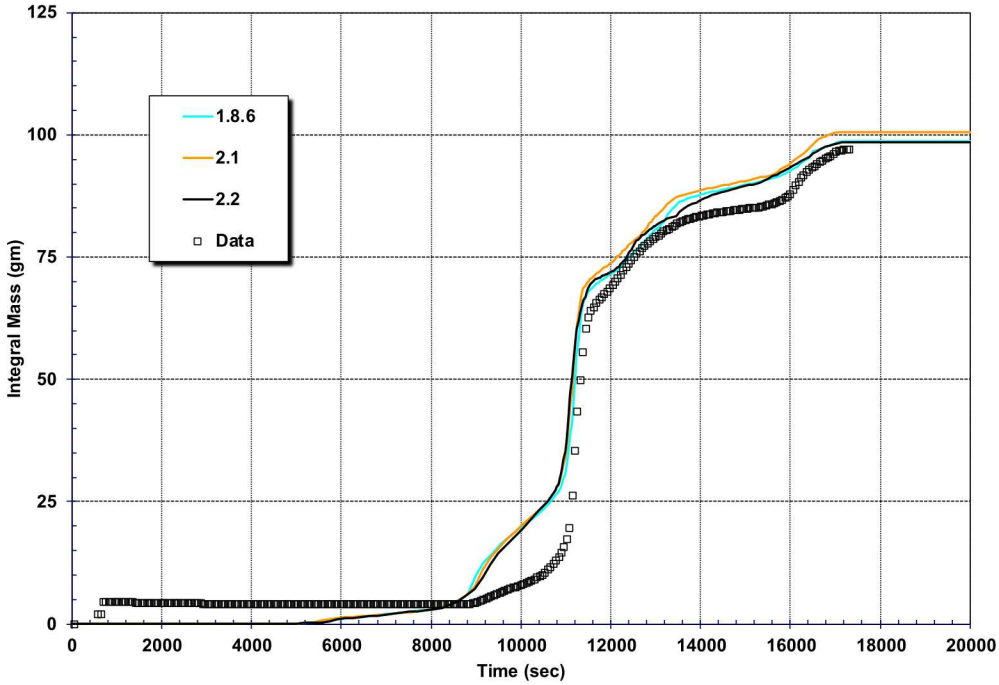


Figure 3.5 FPT-1 Hydrogen Generation from Oxidation

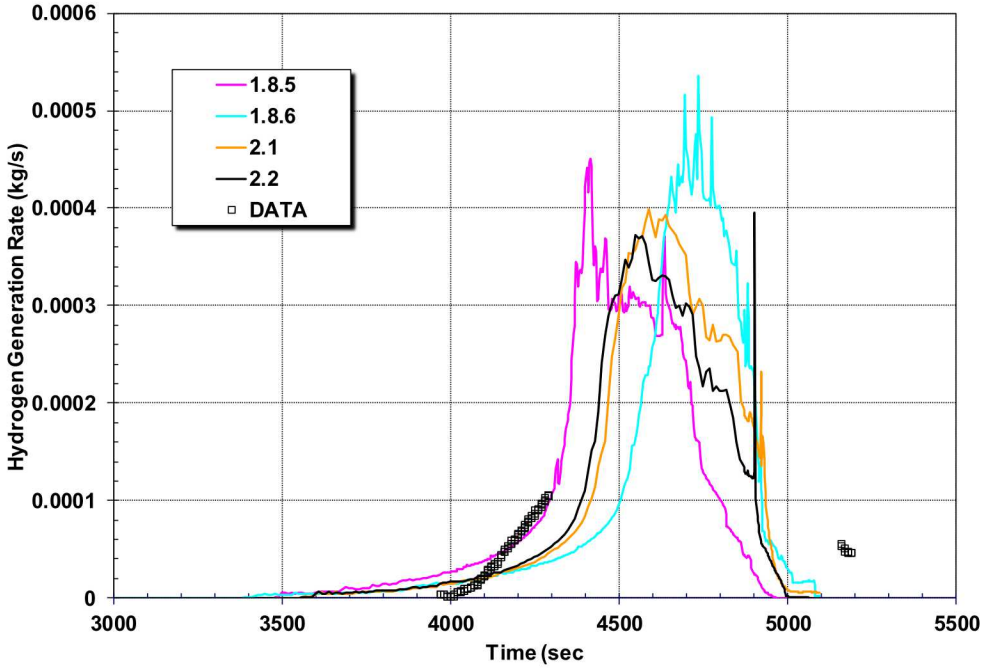


Figure 3.6 CORA-13 Hydrogen Generation from Oxidation

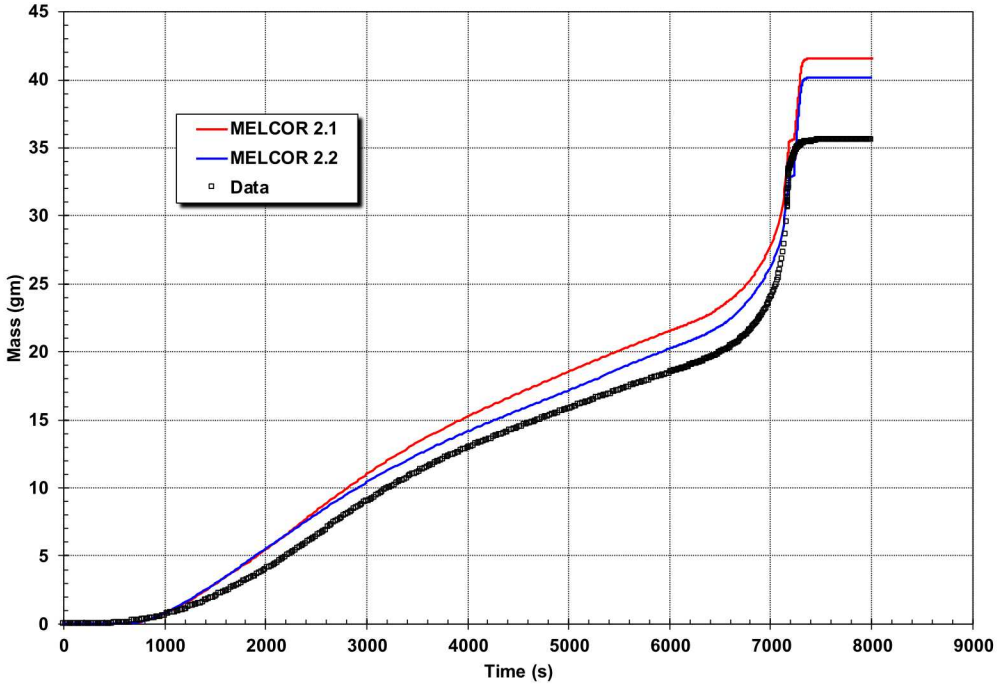


Figure 3.7 Quench-6 Hydrogen Generation from Oxidation

3.3. Condensation Improvements

The DEMONA B3 test emphasized phenomena associated with steam condensation effects on aerosol settling in a scaled containment facility. The tests characterized the depletion rate of non-

hygroscopic and hygroscopic aerosols under varying humidity and thermal-hydraulic conditions. The DEMONA B3 test was computed using the old and the new MAEROS numerical models with and without the hygroscopic model active. Since the DEMONA B3 test used non-hygroscopic aerosols, the results might not be expected to be sensitive to activation of the hygroscopic model. However, the MELCOR hygroscopic model is a complete reformulation of the water aerosol, fog, behavior as well as treating water-solubility of aerosols, the Kelvin effect, and near-field energy transfer. Additionally, activating the hygroscopic model results in water aerosol calculations being performed solely within the RN aerosol package versus the non-hygroscopic approach that is handled more simply in the CVH package.

As shown in Figure 3.8, the latest MELCOR 2.2 DEMONA B3 results give identical results when the hygroscopic model is off, which is expected. The agreement with the data is good, especially at low aerosol concentrations. When the hygroscopic model is active, there is a change in the results. The new MAEROS numerics shows a faster settling rate with better agreement with higher aerosol concentrations. In contrast, the old numerical solution has better agreement with the data at low aerosol concentrations but worse initially with a higher aerosol concentration.

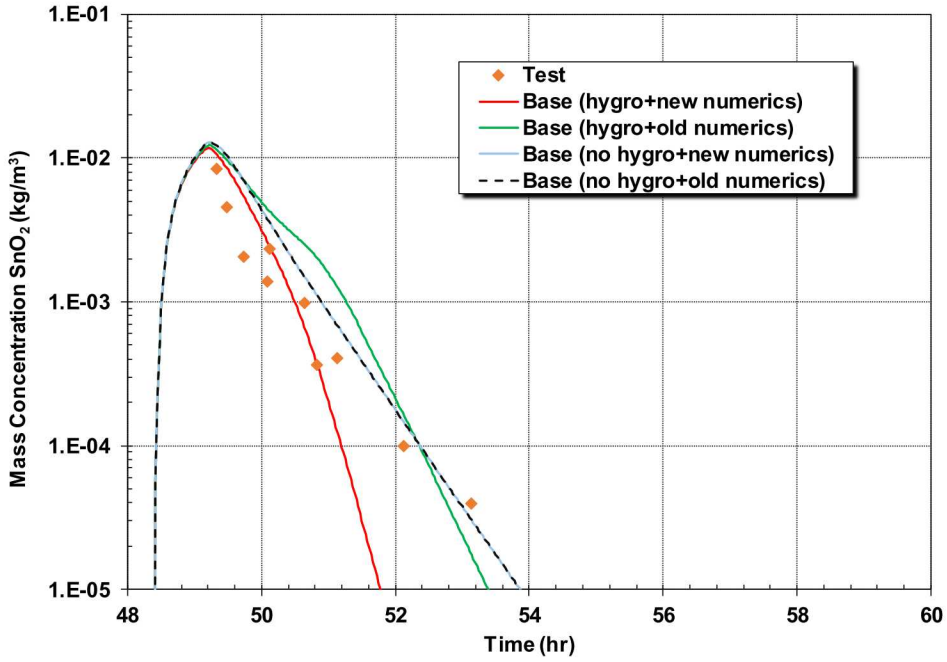


Figure 3.8 DEMONA Test B3 (Non-hygroscopic Aerosols)

3.4. New CORSOR-Booth Release Model

The original CORSOR-Booth model calculated the diffusion release fraction for all classes by scaling the diffusion release rate of cesium. A new modified version of the CORSOR-Booth is now available in MELCOR that instead scales the diffusion coefficient for each RN Class based on the diffusion coefficient for cesium. This new model make the release fractions for all non RN Class 2 Classes independent of the cesium inventory. For the analyses with especially long durations, such as spent fuel pools, depletion of RN Class 2 will no longer prevent other RN Classes from releasing.

The new release model, available through ICRLSE on the RN1_FP00 record, was enabled by specifying ICRLSE=-7 and compared against the default release model, ICRLSE=-5, using the latest Phebus FTP1 (see Section 3.6). The computed Phebus results use the updated eutectics model. The fuel failure time-at-temperature and sensitivity coefficient 1132(1) have been disabled, to impose failure using only the eutectics model. Figure 3.9 through Figure 3.12 show a comparison of the two models with the Phebus FPT1 experiment. The volatile releases (xenon, cesium, iodine, tellurium, and ruthenium) are low relative to the data but in good agreement with one another. The lower volatile releases are believed to be attributed to a lower fuel collapse temperature than FPT1 (i.e., difficult to determine due to failing thermocouples). The barium release is different with the new model but has better agreement with the data.

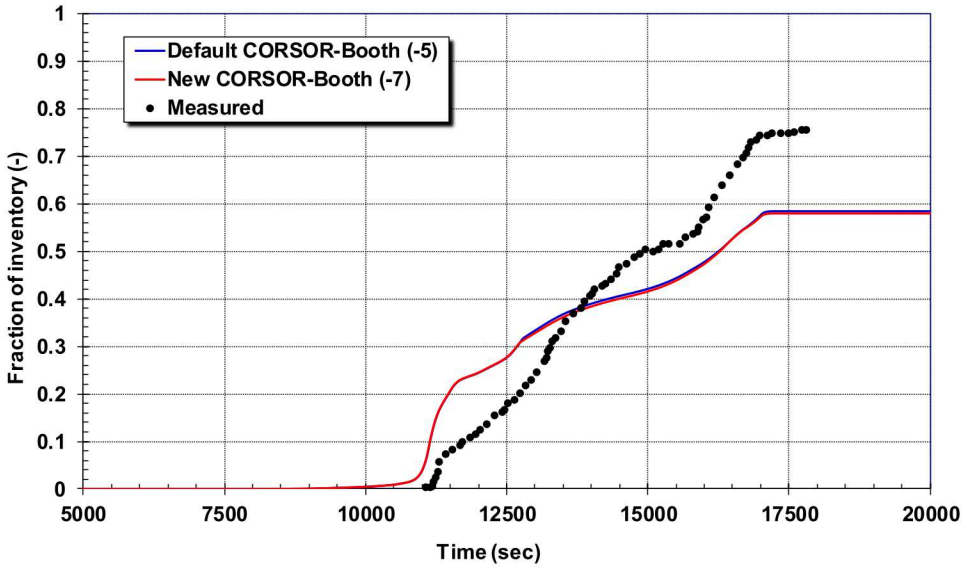


Figure 3.9 Phebus FPT1 Xenon Release from the Fuel

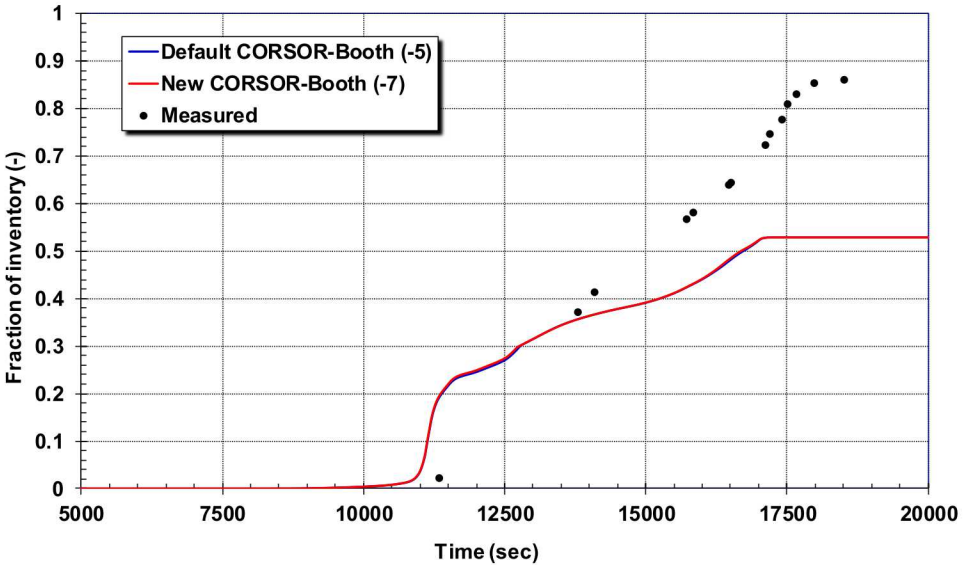


Figure 3.10 Phebus FPT1 Cesium Release from the Fuel

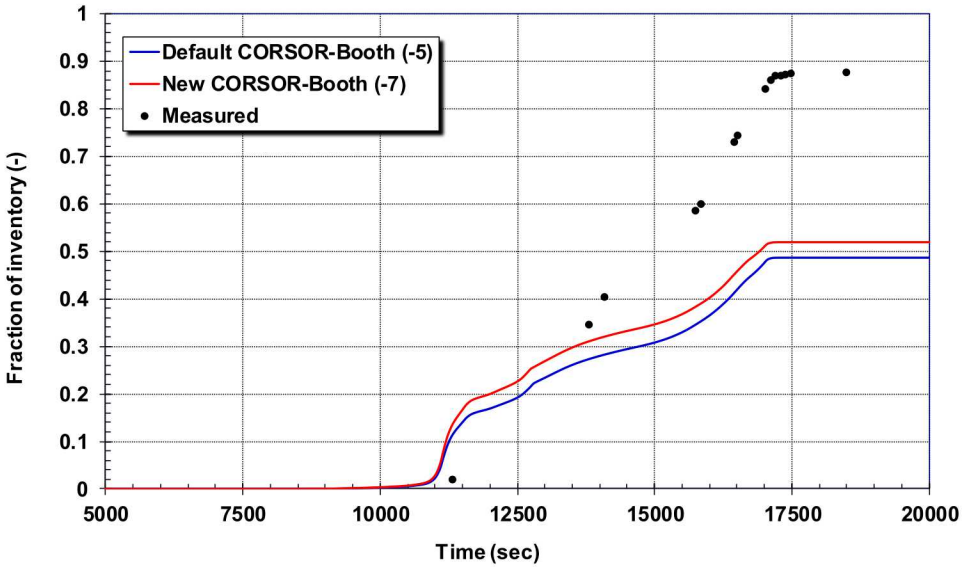


Figure 3.11 Phebus FPT1 Iodine Release from the Fuel

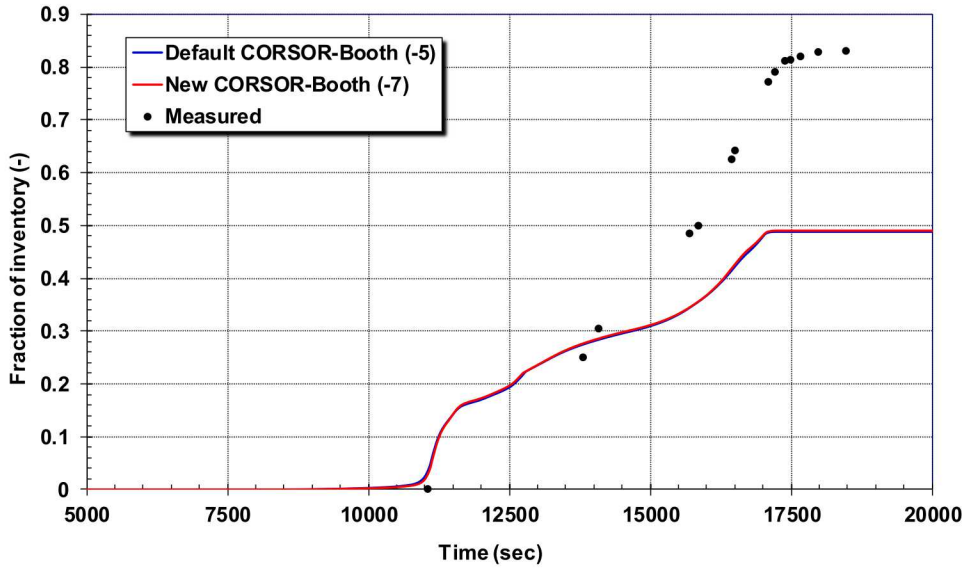


Figure 3.12 Phebus FPT1 Tellerium Release from the Fuel

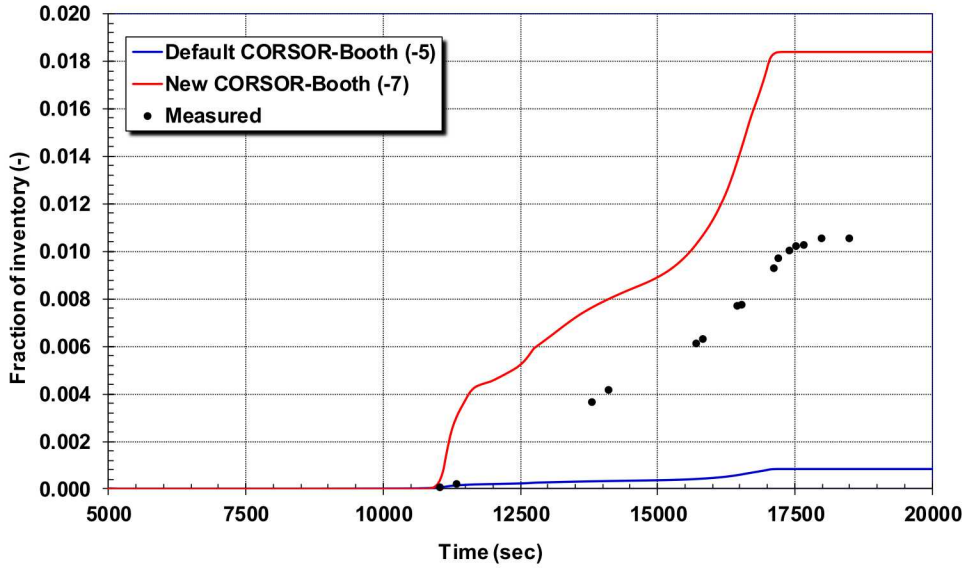


Figure 3.13 Phebus FPT1 Barium Release from the Fuel

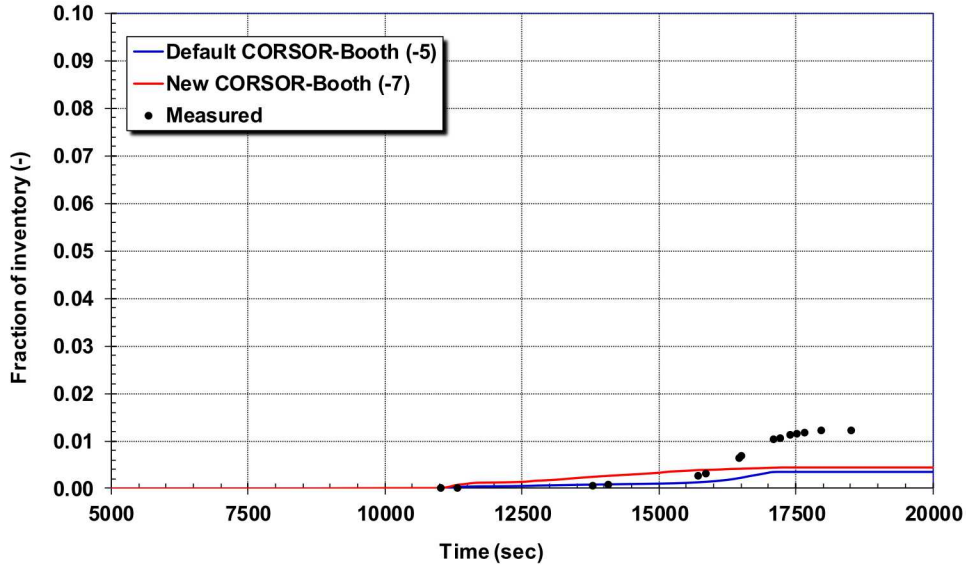


Figure 3.14 Phebus FPT1 Ruthenium Release from the Fuel

3.5. Resuspension Improvements

The STORM aerosol behavior tests simulate the behavior of the relief lines of a pressurized water reactor during a station blackout sequence. The test facility included a 5 m straight pipe section for aerosol deposition and resuspension. The SR-11 test included two distinct phases: (1) the aerosol deposition by thermophoresis and eddy impaction and (2) the aerosol resuspension phase. During the deposition phase, a plasma torch was used to generate aerosols that settled primarily due thermophoresis on to the cool walls relative to the gas stream. The resuspension phase was simulated using stepwise increases to the gas flows to measure the impact of the pipe gas velocity on the aerosol liftoff.

The resuspension model in MELCOR is dependent on the surface roughness when calculating the wall shear for aerosol liftoff. The effective pipe roughness for resuspension can be adjusted through user input to model increased roughness due to aerosol settling. The results of the initial thermophoretic deposition phase is shown in Figure 3.15. The results from MELCOR 2.2 are slightly better than MELCOR 2.1 due to some corrections in the specifications for the control volume velocity used in the heat transfer correlations. Following the deposition phase, the resuspension phase increased the gas velocity in a step-wise manner until almost all the settled aerosols were resuspended. At each resuspension velocity, the surface shear force could lift a range of aerosol sizes. The large aerosols lifted first followed by increasingly smaller aerosol sizes. The results from the STORM assessment show good agreement with the resuspension model using a specified surface roughness of 2.3x10-5 m.

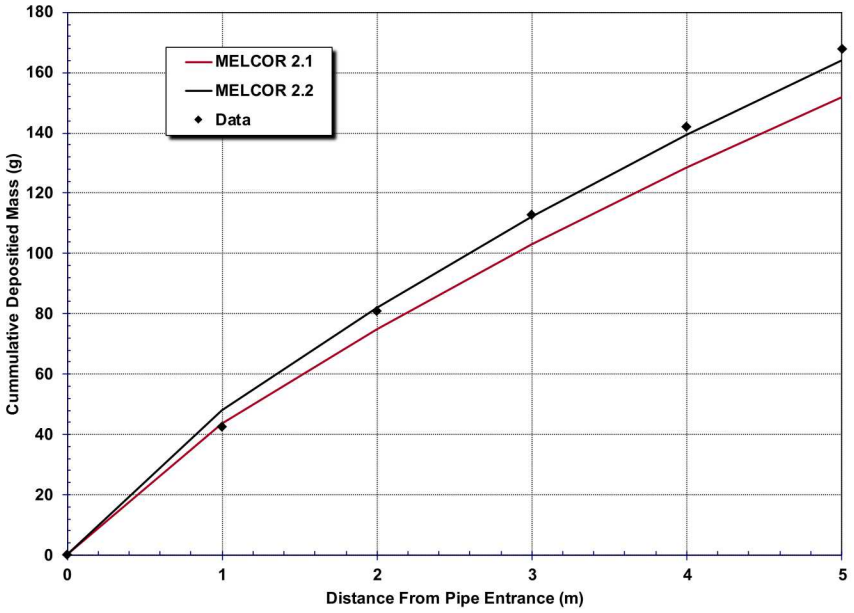


Figure 3.15 STORM SR-11 Test Section Cumulative Aerosol Mass Distribution at the Deposition Phase

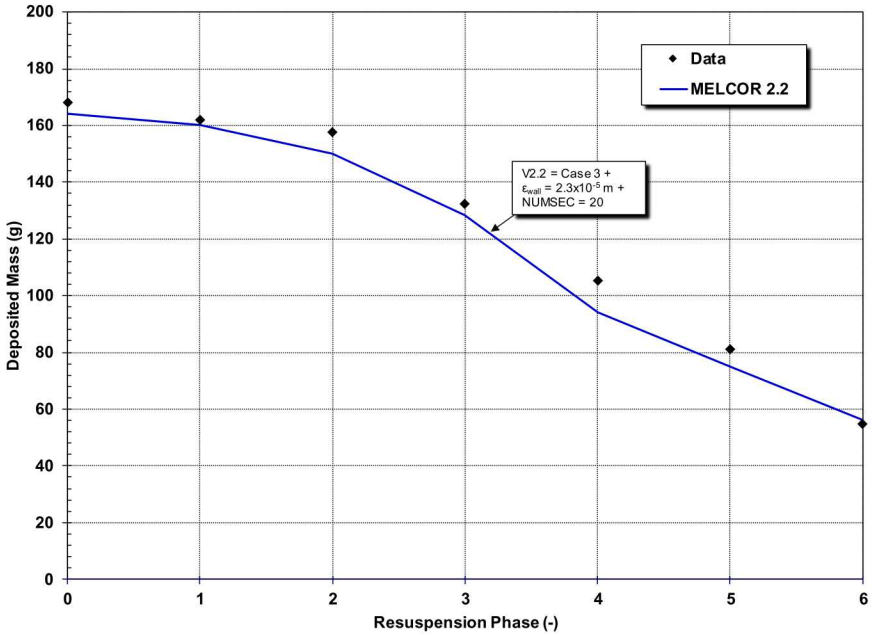


Figure 3.16 STORM TR-11 Deposited Mass After Each of the 6 Resuspension Phases.

3.6. COR Eutectics Model

The COR eutectics model, which has been disabled due to functionality issues, is now the recommended default approach for core material property evaluations (see Section 2.1.2). The updated eutectics model is used for all validation calculations with fuel degradation (e.g., 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 (see Figure 3.17).

Considerable work has been done to fully integrate all internal COR Package energy balances into the eutectics model. Figure 3.18 shows the total energy in the COR Package and the energy error. The maximum energy error is <0.1%. The total COR Package energy rises over two orders of magnitude during the heat-up and degradation phases. The more complex thermophysical properties of the eutectics model required substantial updates to achieve such a low energy error. Although the energy error is very low, there are ongoing efforts to identify and eliminate all sources of energy error.

Phebus also shows good comparisons with data (see Figure 3.19). Like the Material Properties (MP) Package adjustments on the effective eutectic melting temperature, the eutectics model allows adjustments to the UO2-ZRO2 solidus phase diagram. The Phebus model included modifications to disable other fuel failure mechanisms including the time at temperature model and sensitivity coefficient 1132(1), which is the limiting temperature where a fuel rod can stand. Consequently, the fuel collapse occurs due to the formation of a eutectic rather than a prescribed method. Similar to TMI-2, the energy error was <0.1%.

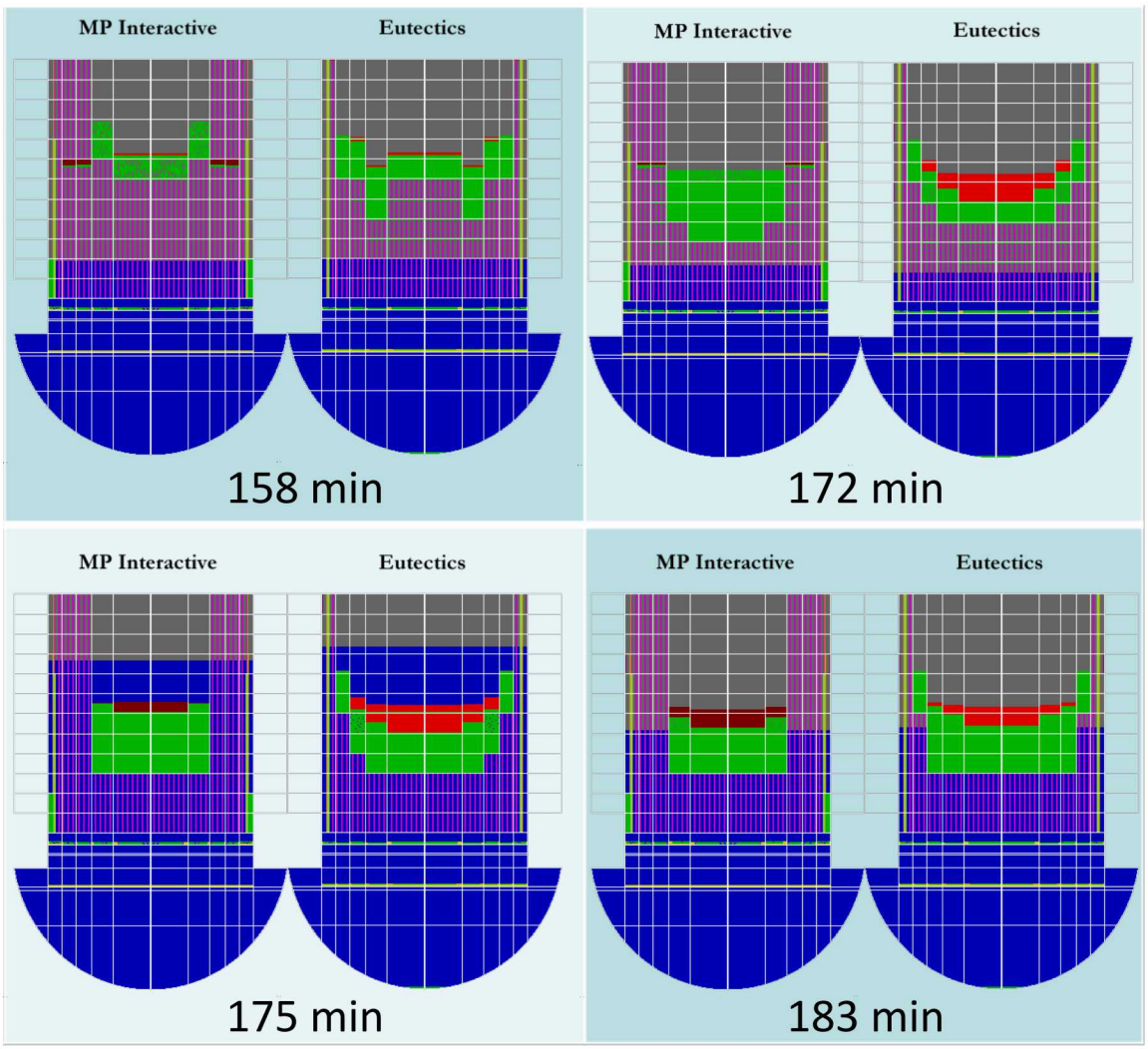


Figure 3.17 Comparison of the TMI-2 Response with and without the Eutectics Model

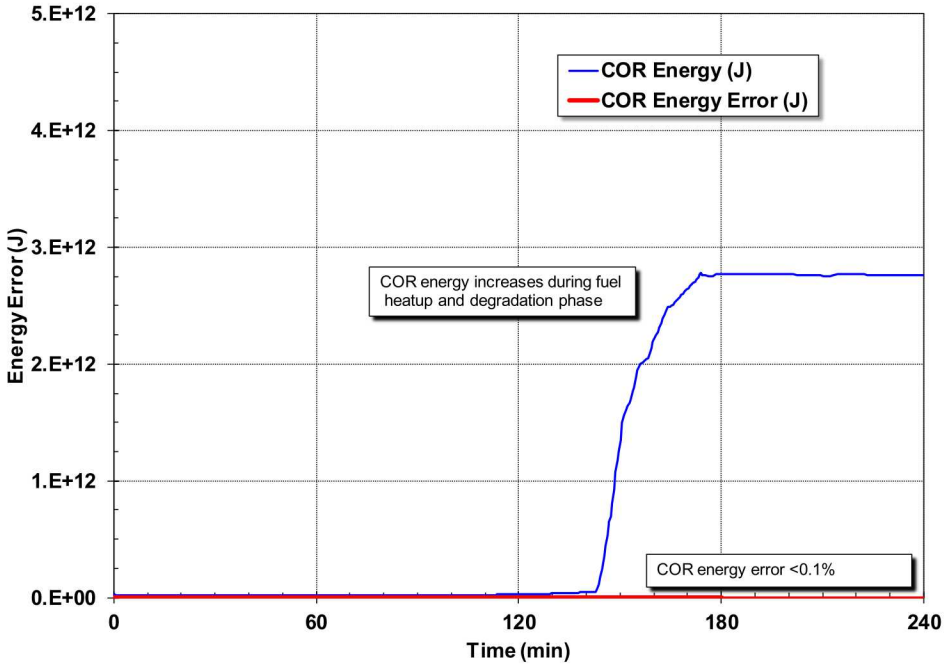


Figure 3.18 COR Package Energy and Energy Error with the Eutectics Model

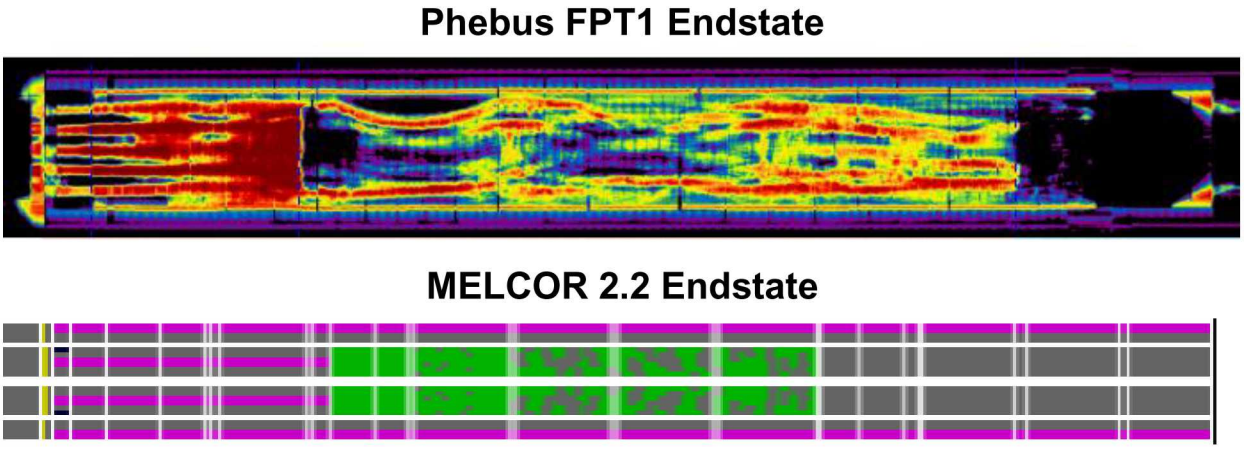


Figure 3.19 Comparison of Phebus and MELCOR 2.2 FPT1 Final States using the Eutectics Model

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