

**SANDIA REPORT**

SAND2020-0114

Printed December 2021

**Sandia  
National  
Laboratories**

# **MELCOR Code Change History: Revision 18019 to 21440**

Larry Humphries, Lucas Albright, Brad Beeny, and Fred Gelbard

Prepared by  
Sandia National Laboratories  
Albuquerque, New Mexico  
87185 and Livermore,  
California 94550

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology & Engineering Solutions of Sandia, LLC.

**NOTICE:** This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from

U.S. Department of Energy  
Office of Scientific and Technical Information  
P.O. Box 62  
Oak Ridge, TN 37831

Telephone: (865) 576-8401  
Facsimile: (865) 576-5728  
E-Mail: [reports@osti.gov](mailto:reports@osti.gov)  
Online ordering: <http://www.osti.gov/scitech>

Available to the public from

U.S. Department of Commerce  
National Technical Information Service  
5301 Shawnee Rd  
Alexandria, VA 22312

Telephone: (800) 553-6847  
Facsimile: (703) 605-6900  
E-Mail: [orders@ntis.gov](mailto:orders@ntis.gov)  
Online order: <https://classic.ntis.gov/help/order-methods/>



## Abstract

This document summarily provides brief descriptions of the MELCOR code enhancement made between code revision number 18019 and 21440. Revision 18019 represents the previous 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, 21440. Along with the newly updated MELCOR Users' Guide [2] and Reference Manual [3], users are aware and able to assess the new capabilities for their modeling and analysis applications.

This page left blank.

## CONTENTS

1. Introduction.....	9
2. MELCOR Code Improvements.....	11
2.1. New Defaults .....	11
2.2. Significant Code Corrections since Revision 14959.....	11
2.2.1. RN Audit Tables .....	11
2.2.2. Corrections to the Eutectics Model.....	11
2.3. Updates and New Features.....	11
2.3.1. MP Package Updates and New Features .....	11
2.3.2. Control Functions.....	12
2.3.3. COR Improvements.....	12
2.3.4. Melting Lower Head.....	13
2.3.5. Heat Pipe Models.....	14
2.3.6. High-Temperature Gas Cooled Reactor Modeling .....	15
2.3.7. ATF Modeling with User-defined Materials.....	16
2.3.8. New Plot Variables .....	17
3. Validation Cases .....	19
3.1. Lower Head Melting .....	19
3.2. Revision Comparison.....	23
3.2.1. Hygroscopic Model .....	23
3.2.2. Oxidation Models .....	26
3.2.3. Condensation Improvements .....	28
3.2.4. New CORSOR-Booth Release Model .....	29
3.2.5. Resuspension Improvements.....	33
3.2.6. COR Eutectics Model.....	34
3.3. Single Parameter Variant Study.....	38
3.3.1. Hydrogen Generation Results .....	38
3.3.2. Code Performance Results .....	40
References.....	41

## LIST OF FIGURES

Figure 2.1. Diagram of the two distances $d_1$ and $d_2$ to create a spheroidal cap.....	12
Figure 2.2. Some key heat pipe regions modeled in MELCOR.....	14
Figure 3.1 Simple BWR Lower head Node temperature Comparison.....	19
Figure 3.2 Simple BWR Molten Pool Mass Size Comparison.....	19
Figure 3.3 Simple BWR Lower head Melting Mass for LHM model active.....	20

Figure 3.4 Simple BWR Fission Product Mass Comparison .....	20
Figure 3.5 Simple PWR Lower Head Node Temperature Comparison .....	21
Figure 3.6 Simple PWR Molten Pool Mass Size Comparison .....	21
Figure 3.7 Simple PWR Lower head Melting Mass for LHM active .....	22
Figure 3.8 Simple PWR Fission Product Mass Comparison .....	22
Figure 3.9 AHMED Experiments (22% Relative Humidity).....	23
Figure 3.10 AHMED Experiments (96% Relative Humidity) .....	24
Figure 3.11 LACE LA-4 Experiment (Hygroscopic CsOH Aerosol Response) .....	24
Figure 3.12 LACE LA-4 Experiment (Non-hygroscopic MnO Aerosol Response) .....	25
Figure 3.13 FPT-1 Hydrogen Generation from Oxidation.....	26
Figure 3.14 CORA-13 Hydrogen Generation from Oxidation.....	26
Figure 3.15 Quench-6 Hydrogen Generation from Oxidation .....	27
Figure 3.16 DEMONA Test B3 (Non-hygroscopic Aerosols) .....	28
Figure 3.17 Phebus FPT1 Xenon Release from the Fuel.....	29
Figure 3.18 Phebus FPT1 Cesium Release from the Fuel.....	29
Figure 3.19 Phebus FPT1 Iodine Release from the Fuel .....	30
Figure 3.20 Phebus FPT1 Tellurium Release from the Fuel.....	30
Figure 3.21 Phebus FPT1 Barium Release from the Fuel.....	31
Figure 3.22 Phebus FPT1 Ruthenium Release from the Fuel.....	31
Figure 3.23 STORM SR-11 Test Section Cumulative Aerosol Mass Distribution at the Deposition Phase .....	32
Figure 3.24 STORM TR-11 Deposited Mass After Each of the 6 Resuspension Phases.....	33
Figure 3.25 Comparison of the TMI-2 Response with and without the Eutectics Model.....	34
Figure 3.26 COR Package Energy and Energy Error with the Eutectics Model.....	35
Figure 3.27 Temperatures and Pressures for TMI-2.....	36
Figure 3.28 Hydrogen generation mass beyond 14807 revision for PWR.....	38
Figure 3.29 Hydrogen generation mass beyond 14807 revisions for BWR.....	38
Figure 3.30 Code Performance in CPU for Several Plant Decks (from 3803 to 17260 revisions comparison) .....	39

## 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

This page left blank.



## **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 has been to model the progression of accidents in light water reactor nuclear power plants though models for non-LWR have been added, opening a new scope of application. 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 18019 to rev 21440), and previews the validation results for the new official release of the code (rev 21440). The user is referred to the MELCOR User Guide [2] and Reference Manual [3] to provide a detailed description of existing code parameters and models.

This page left blank.

## 2. MELCOR CODE IMPROVEMENTS

Though few new models have been implemented during this development cycle, important code corrections have been made, leading to an improved user interface to non-LWR models and resolution of significant code issues resulting in a more robust code. Support of two major NRC sponsored application programs which assessed a wide range of reactor types and accident scenarios have provided the opportunities to address many of these code fixes and improvements.

### 2.1. Non-LWR Source Term Demonstration Project

A multi-year project for the NRC is underway to assess various NRC tools (notably MELCOR and SCALE) for application to non-LWR severe accident modeling and calculation of source term. This project has numerous objectives in assessing these tools in terms of providing a meaningful shakedown of the existing, though often relatively new, modeling capabilities, and to identify any missing models, model weaknesses, or data needs. Such an activity enhances the maturity of these models and guides future code development or potential experimental activities. The input decks are often based on existing, public, plant design data (i.e., PBMR-400, Megapower Heat Pipe Reactor, and a Pebble bed FHR) with the intention of providing a starting template for modeling more specific or proprietary designs by vendors. In many cases, multiple accident scenarios were investigated, and, in some instances, uncertainty analyses were performed. Such stress testing of the existing models has led to improvements to the existing models, improved flexibility for user specification of data, and enhanced diagnostic output.

#### 2.1.1. Public Workshops

Public workshops for the non-LWR source term demonstration project are being provided by Sandia National Labs, Oak Ridge National Labs, and US Nuclear Regulatory Commission staff. These workshops cover the application of SCALE and MELCOR to non-LWR accident analysis, including simulating system thermal hydraulic response, fuel heat-up, heat transfer through the reactor to the surroundings, and radionuclide release for five classes of non-LWRs. Presentations for those workshops already conducted can be found on the NRC website (<https://www.nrc.gov/reactors/new-reactors/advanced/details.html#non-lwr-ana-code-dev>) and the schedule is as follows:

Heat Pipe Reactor .....	Jun 29, 2021
High-Temperature Gas-Cooled Reactor.....	Jul 20, 2021
Fluoride-Salt-Cooled High-Temperature Reactor (FHR).....	Sep 14, 2021
Molten-Salt-Fueled Reactor .....	TBD
Sodium-Cooled Fast Reactor.....	TBD

### 2.2. Advanced LWR Fuel Technology Assessments

The U.S nuclear power industry intends to introduce advanced fuels into operating reactors to enhance safety, operational efficiency, and economics. To support licensing efforts related to advanced fuel technologies, the USNRC has undertaken a campaign to evaluate the impact of advanced fuel technologies on in-containment source terms. This activity includes MELCOR modeling and simulation of both boiling water reactors (BWRs) and pressurized water reactors (PWRs) with different containments across a spectrum of accident scenarios including short-term station blackout (STSBO), long-term station blackout (LTSBO), small-break loss of coolant accident

(SBLOCA), large-break loss of coolant accident (LBLOCA), and anticipated transient without scram (ATWS). Simulation and analysis of this broad range of light water reactor technologies and accident scenarios has not been performed with MELCOR in over a decade. This advanced LWR fuel technology assessment has prompted a number of MELCOR code improvements relevant to LWR modeling capabilities. These code improvements are expected to lead to enhanced robustness of MELCOR for its users.

### **2.3. New Defaults**

No modifications to defaults of existing models were made in this code release.

### **2.4. Significant Code Corrections since Revision 18019**

#### **2.4.1. *Improvements to the Stefan Model***

Heat transfer from the molten pool to the underlying substrate in the Stefan model is not calculated implicitly as is the case for conduction. As a result, large heat transfer rates from the overlying molten pool can lead to large temperature rises in the substrate such that the substrate may completely melt and heat up to temperatures higher than the overlying molten pool (exceeding the driving potential of the heat transfer). Performing an implicit calculation for the Stefan model is complicated by the fact that there is a phase change. However, a simple fix was implemented to limit the heat transfer from the freezing molten pool to the enthalpy required to completely melt the underlying substrate.

While implementing this improvement to the Stefan model, it was observed that the composition for a contiguous pool could vary by cell, meaning that heat transfer limitations that were added to account for freezing of a small amount of pool in a cell were not adequate, since heat transfer is based on homogeneous properties and not local properties. This was unexpected since it was thought that CORMIX would leave each convecting molten pool in a homogeneous composition. This discrepancy was corrected by moving the procedure CORMIX before the call to CORPMX which mixes debris between bypass and channel when the channel box loses integrity.

#### **2.4.2. *Correction to DTDZ model for Packed COR Cell***

When the atmosphere temperature calculated by the dtdz model exceeds an error threshold the calculation terminates in an error condition. The COR cell is completely packed with molten pool material and the upper surface lies in a cell above. There is no fluid volume available in the COR package. The associated CV spans several COR cells and decay heat associated with the CV continues to generate heat in the gas but there is no surface contact with COR components for heat rejection since the cell is fully blocked. The minimum porosity C4413(5) will be applied to the molten pool component to calculate a surface area for heat transfer as it is for PD.

#### **2.4.3. *Inconsistency in AG-IN-CD structural tin release model documentation***

A user reported an unexpected absence of release from the AG-IN-CD control rod structural release model. It turned out to be an inconsistency between documentation and coding for the parameter IAICON on record COR\_CR. The coding was modified to be consistent with the manual.

#### **2.4.4. *B4C Oxidation energy issue***

A modification was made to the simplified B4C oxidation model to place the heat of reaction in the COR component and not directly in the atmosphere. This resolves a serious problem when the fluid volume is small as the heat of reaction overwhelms the heat capacity of the fluid. Depositing this energy in the component mass, as is done for Zr and Fe oxidation, resolves the problem.

#### **2.4.5. *Component Quench temperatures***

When the atmosphere fraction is small in a COR cell, the unquenched temperature that is calculated becomes suspect. New coding tests for a small liquid volume in a cell and if it is below 0.001, the average component temperature is used in dtdz rather than the unquenched component temperature.

#### **2.4.6. *DTDZ issues with large coherent molten pool***

Problems with the dtdz model were observed when a coherent molten pool completely blocks a COR cell and the upper surface of that pool is in another control volume (and COR cell) where there are no other COR components. For this particular case, heat generation continues due to decay heat in the atmosphere though the atmosphere becomes completely thermally decoupled from any COR components. The modification that was made is similar to what is in effect for PD where C4413(5) provides a minimum porosity for the atmosphere in the molten pool component. Several other changes were made that essentially zeroed the heat transfer coefficient for molten pool when that molten pool is part of a coherent pool. A test in CORTSV was also modified which now issues an error condition and forces a time step reduction when the calculated dtdz temperature exceeds c1030(6). This modification allows the calculation to continue as long as the calculated temperature is less than the incoming flow temperature and the local gas temperature.

#### **2.4.7. *Minimum contact surface area for molten pool***

The minimum contact surface area for MP and fluid is now calculated as  $SVRX(IC)*C4413(5)*VOLTOT$ , where the surface to volume ratio defined in SC1151, C4413(5) is the minimum porosity, and VOLTOT is the cell volume. Previous this minimum contact surface area was calculated as  $C4413(5)*VOLTOT$  which did not account for the surface to volume ratio.

#### **2.4.8. *COR volume Consistency errors***

Several calculations in the repository failed due to a volume consistency error. Began investigating this issue and added a plot to the HTML output showing the maximum volume consistency error plotted (from all COR cells) to aid in diagnostics. An error in the candling routine was uncovered that resulted when candled molten material was unable to completely relocate downwards due to blockage. Material that did not successfully drain downward due to blockage was correctly placed back in the original cell, but proper corrections were not made to the fluid volume in the original cell. This correction eliminated some of the volume inconsistency errors observed but not all. Debugging will continue in the next reporting period.

#### **2.4.9. *RN Mass Errors***

An issue was observed in a calculation that resulted in an error message indicating that RN mass remaining in a COR component was negative. The problem occurred when the remaining mass was near roundoff, though positive with a calculated remaining fraction  $>1$ . Such a condition is non-

physical and led to removing more mass than was available. A correction was made to account for roundoff.

#### 2.4.10. ***Molten Pool Convective Heat Transfer Coefficient***

The convective heat transfer coefficient calculated in corhtc for molten pool was zero at the bottom of the pool when the bottom of the pool was above the lowest cell in contact with the lower head structure. Several code changes were required to address this issue. A correction was made to the bottom of the molten pool to recognize the top of the intact debris in the bottom cell. In addition, the call to CORHTC was extended to allow different modeling of the heat transfer coefficient when crust is present. Also, the angular range for each segment is now used rather than the angle subtended by molten pool in direct contact with lower head. Finally, the stefan model is always invoked, regardless of pool interface.

#### 2.4.11. ***Particulate Debris Slumping***

An issue was observed in a test deck associated with the slumping of particulate debris. The debris originated in the channel but was observed to move into the bypass due to failure of the canister. In this particular case, there was also particulate debris originating in the bypass that also relocated into that bypass cell. If PD → PB and PB → PB are both possible, then the summation of the eutectic mass and energy should be initialized only once at the top of this block of code.

#### 2.4.12. ***MACCS Flowpaths for multi-batch spent fuel pool calculations***

A number of corrections were made to the spent fuel pool multi-batch calculation variables. These variables are not used in performing any calculation but are merely output variables that estimate releases of various batches (rings) to the environment based on the total radionuclide releases to the environment. Unless new classes are defined for each batch (a prohibitive option in many cases due to increased run time) there is no marker to distinguish radionuclides released to the environment that originated from different batches and which have different burnups and residence time in the spent fuel pool. As an estimate, the total release of a radionuclide to the environment is ‘partitioned’ among the various rings based on the partitioning of the release from the fuel in the core. The previous model performed this partitioning using time integral releases which can lead to negative releases to the environment late in the calculation as new rings begin to release material. The current model partitions the current release to the environment using the current release distributions calculated for the fuel,

$$dMrelease_{env,i,r} = dMrelease_{env,i} \cdot \frac{dMrelease_{fuel,i,r}}{\sum_{all\ batches\ r} dMrelease_{fuel,i,r}}$$

Where i is the radionuclide class, r is the batch number and fuel and environment indicates whether the release is calculated for the fuel or as a release to the environment.

Previously this estimate was performed using cumulative values.

### 2.5. **Updates and New Features**

#### 2.5.1. ***Molten Salt Model***

The molten salt model (MSM) package is an addition to MELCOR so that accidental releases of radioactive vapors and/or aerosol particles from the salt into the headspace, and deposition on to

surfaces in contact with the salt may be modeled. As shown schematically in Figure 1, this is accomplished in three steps given the state of fission products in five forms in the salt, and the state of the atmosphere in a cell. This is the first application in which the thermodynamic state was calculated within MELCOR to dynamically determine the vapor pressure of a fission product for each cell.

At the beginning of a time step, the fission products can be in forms 1 to 5 as: (1) salt-soluble, (2) salt-insoluble, (3) residing at the interface layer between the liquid salt and the atmosphere, (4) deposited on structures, and (5) in vapor form either in the atmosphere or in small bubbles in the liquid salt. Some species may be in more than one form. The first step is to calculate the equilibrium conditions to determine the masses that are soluble, insoluble, and gaseous. This step may be accomplished using Thermochemica, a Gibbs Energy Minimization (GEM) code, which has been integrated into MELCOR. With the appropriate thermochemical database, Thermochemica provides the solubility and vapor pressure of species as a function of temperature and composition. The Gibbs energy of the system includes nonideal solution effects. Thus, the activity coefficient is not set at one which is the case for ideal solutions. Molten salt Thermochemical databases are under development, and currently the only fission product and salt of interest that can be included in MSM is cesium in FLiBe. The second step as shown in Figure 1 is to perform a transport calculation within the Molten Salt Model. In this step, the insoluble fission products in the salt are modeled as colloidal particles that migrate to and deposit on surfaces. These particles may contain not just the fission products, but also corrosion products and abraded graphite particles. The particles may migrate to surfaces such as heat structures or pebbles in the reactor core. Particles on the core may be released into the salt, but as found experimentally, particles that attach to heat structures are modeled as permanently adhering to the heat structure surface. Particles may also migrate to the surface layer that is an interface between the salt pool and the atmosphere. All transport rates are currently user-specified with control functions, but we are developing mechanistic models as an alternative. Finally, the third step is release to the headspace as either vapors or particles. Noncondensable gases such as Xe and Kr bubbles are released to the headspace when the bubbles reach the pool surface. Soluble and insoluble species with a significant vapor pressure can be released as vapor in the headspace. Clearly, if the atmosphere is much colder than the salt pool, such vapors may recondense or nucleate to form aerosol particles. Some of these particles may settle back into the pool. Aerosol particles may also be released by bubbles that rupture. The bubble film may result in aerosol particles of the salt which contains soluble fission products. These transfer rates are currently also specified with control functions that are to be replaced by mechanistic models. MELCOR takes this information, accounts for decay heating, and transports aerosol and vapor from the salt control volume to other control volumes.

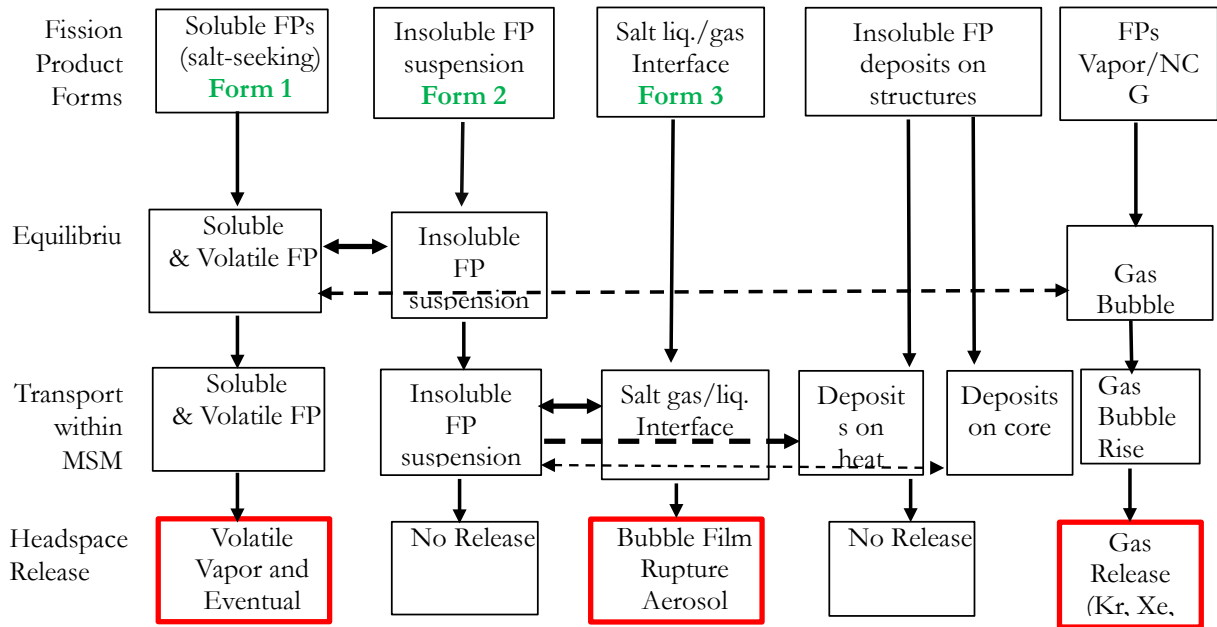


Figure 1. Schematic of Molten Salt Model (MSM) package logic flow. The horizontal arrows correspond to mass transfer processes between forms. Only the forms pointed to by an arrowhead indicate mass transfer. Masses of released species are given in the bottom row in red-bordered boxes.

### 2.5.2. Fluid Fuel Point Reactor Kinetics Modeling

A capability to compute point reactor behavior in the presence of delayed neutron precursor drift has been added to MELCOR to facilitate fluid fuel reactor (e.g. MSR) modeling. This is the fluid fuel point reactor kinetics equations (FFPRKEs) model and it is affected through the control volume hydrodynamics (CVH) code physics package.

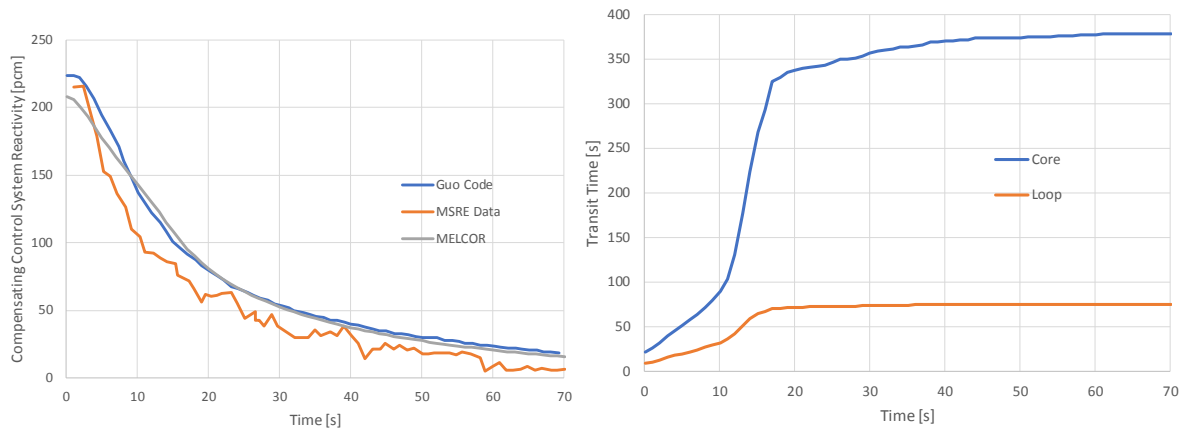
Building upon previous work on standard fixed-fuel point kinetics (PRKEs), the equation set was extended according to a grouping of delayed neutron precursors into “cohorts” to include in-core and ex-core. The in-core cohort of delayed neutron precursors accounts for inventory within the user-defined core region, whereas the ex-core cohort of delayed neutron precursors accounts for inventory within the user-defined flow loop (the primary loop excluding the core). The expanded set of equations includes source and sink terms that transfer delayed neutron precursor inventory between cohorts to predict the flow effects on reactivity and core power.

MELCOR text outputs and a series of plot variables have been added. The new plot variables allow a user to monitor reactivity and its components plus core power and core/loop flow transit times.

The FFPRKE model has been validated against Molten Salt Reactor Experiment (MSRE) zero-power flow reactivity experimental data for pump ramp-up and coast-down. The validation demonstrates:



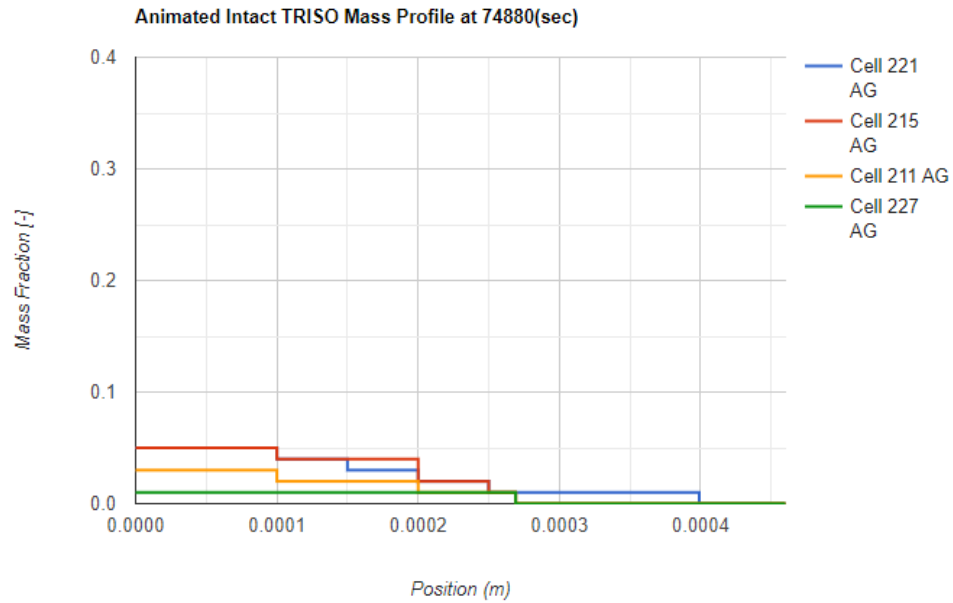
- The initial steady-state solution to the FFPRKE's,
- The null transient (criticality is preserved if flow is steady),
- The ability to predict reactivity effects and power changes due solely to flow change,
- Good agreement with experiments in terms of required control system intervention to maintain criticality during pump flow coast-down



**Figure 1. MELCOR -to-MSRE comparison for MSRE pump coast-down (left), MELCOR core and loop flow transit time predictions for MSRE pump coast-down (right)**

### 2.5.3. *Additions to HTML Output*

Several new standard plots and animations were added to provide improved visualization of calculated results. Animations of temperature profiles and stress profiles in the lower head are provided to observe local behavior of the heated vessel head. Finally, in order to make the results of the TRISO diffusion calculations more transparent to users, animations of the TRISO temperatures and distributions of radionuclide masses in both the TRISO particles as well as the graphite matrix was made available. The user must specify the cell of interest and, when animating the RN mass distributions, the radionuclide class of interest.



#### 2.5.4. **New Control Function Arguments**

HS-Q-FILM(NameHS, Side, Type)	<p>Description</p> <ul style="list-style-type: none"> <li>• NameHS shall be a valid heat structure name</li> <li>• Side in {LHS, RHS}</li> <li>• Type in {Rate, Int, Flux}</li> </ul>
HS-Q-SOLID(NameHS, Type)	<p>Description</p> <ul style="list-style-type: none"> <li>• NameHS shall be a valid heat structure name</li> <li>• Type in {Rate, Int}</li> </ul>

#### 2.5.5. **New Plot Variables**

COR-ROD-DAM.n	Monitors the rod damage function in cell n. (units = kg, default = OFF, Reference = 'COR-ROD-DAM')
COR-PKM-REACT-TOTAL	Total reactivity (units = pcm, default = ON)
COR-PKM-REACT- FEEDBACK	Total feedback reactivity (units = pcm, default = ON)
COR-PKM-REACT- DOPP	Total Doppler feedback reactivity (units = pcm, default = ON)

COR-PKM-REACT- FUELRHO	Fuel density feedback reactivity (units = pcm, default = ON)
COR-PKM-REACT- MODRHO	Moderator density feedback reactivity (units = pcm, default = ON)
COR-PKM-REACT- CONTROL	Reactor control reactivity (units = pcm, default = ON)
COR-PKM-QTOTAL	Total point kinetics power (units = W, default = ON)
COR-PKM-PRECURSOR	Total precursor power (units = W, default = ON)
COR-PKM-TEMP-DOPP	Temperature used for doppler feedback (units = K, default = ON)
COR-PKM-TEMP-FUELRHO	Temperature used for fuel-density feedback (units = K, default = ON)
COR-PKM-TEMP-MODRHO	Temperature used for moderator-density feedback (units = K, default = ON)
COR-DMO2-GRAPH	Total cumulative oxygen consumption in PBR or PMR core due to graphite oxidation (units = kg, default = ON)
CVH-FFPKM-REACT-FLOW	Flow reactivity according to the fluid fuel point kinetics model (units = pcm, default = ON)
CVH-FFPKM-REACT-FEEDBACK	Total temperature feedback reactivity according to the fluid fuel point kinetics model (units = pcm, default = ON)
CVH-FFPKM-REACT-CONTROL	Flow reactivity according to the fluid fuel point kinetics model (units = pcm, default = ON)
CVH-FFPKM-REACT-TOTAL	Total reactivity according to the fluid fuel point kinetics model

	(units = pcm, default = ON)
CVH-FFPKM-REACT-BIAS	Bias reactivity according to the fluid fuel point kinetics model (units = pcm, default = ON)
CVH-FFPKM-CORTTRANS	Transit time for delayed neutron precursors drifting across core according to the fluid fuel point kinetics model (units = s, default = ON)
CVH-FFPKM-LOOPTRANS	Transit time for delayed neutron precursors drifting across loop according to the fluid fuel point kinetics model (units = s, default = ON)
CVH-FFPKM-BETAEFF	Effective delayed neutron fraction according to the fluid fuel point kinetics model (units = -, default = ON)
CVH-FFPKM-BETALOST	Lost delayed neutron fraction according to the fluid fuel point kinetics model (units = s, default = ON)
RN1-CVCLSOL-x-y.cv	Liquid-phased soluble form mass (MSM) of class x in control volume cv. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2) (units = KG, default = ON)
RN1- CVCLCOL-x-y.cv	Liquid-phased colloid form mass (MSM) of class x in control volume cv. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2) (units = KG, default = ON)
RN1- CVCLFCOL-x-y.cv	Liquid-phased floating colloid form mass (MSM) of class x in control volume cv. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2) (units = KG, default = ON)
RN1- CVCLCOLHSDEP-x-y.cv	Deposited mass of colloid form (MSM) deposited on HS, class x in control volume cv, including aerosols and vapors. The parameter y

	<p>specifies either total mass (y=1) or just the radioactive mass (y=2).</p> <p>(units = KG, default = ON)</p>
RN1- CVCLCOLCORDEP-x-y.cv	<p>Deposited mass of colloid form (MSM) on COR MX, class x in control volume cv, including <b>XXX</b>. The parameter y specifies either total mass (y=1) or just the radioactive mass (y=2).</p> <p>(units = KG, default = ON)</p>
RN1- MSMDT	<p>Total radioactive and non-radioactive MSM mass deposited on heat structures.</p> <p>(units = KG, default = ON)</p>
RN1- MSMDR	<p>Total MSM radioactive mass deposited on heat structures.</p> <p>(units = KG, default = ON)</p>
RN1- MSMCORDT	<p>Total radioactive and non-radioactive MSM mass deposited on COR MX surfaces.</p> <p>(units = KG, default = ON)</p>
RN1- MSMCORDR	<p>Total radioactive MSM mass deposited on COR MX surfaces.</p> <p>(units = KG, default = ON)</p>
RN1- MSMCORDR	<p>Total radioactive MSM mass deposited on COR MX surfaces.</p> <p>(units = KG, default = ON)</p>

### 3. VALIDATION CASES

Since the last 2020 Quick Look release, the only new physics model that has been implemented is the molten salt model, for which development and validation are ongoing efforts and thus will not be discussed in this document. However major improvement to existing models and code corrections have been completed in 2021. Other major improvement involves user friendliness of inputs for specific models, such as:

- Heat Pipe reactor models
- TRISO fuel modeling
- Core degradation modeling for LWRs
- B4C Oxidation modeling as well as surface areas for oxidation

In this release, variances in results for various validation cases related to these changes are shown.

#### 3.1.1. *Oxidation Models*

No changes were made directly to the zirconium or stainless-steel oxidation models. However, as observed later in the TMI-2 validation and in the simple PWR/BWR demonstration input decks, variations in the total mass of hydrogen generated are observed. Such changes can be due to other physics models such as core degradation and heat transfer models which can change the contact areas, contact times, and temperatures of reactants. In particular, it is expected these changes are responsible for the variances observed.

The results of the CORA-13 and QUENCH-6 tests are presented to demonstrate that the oxidation models are invariant over this development cycle. Both experiments include electrically heated fuel elements with a rapid quench capability. Figure 3.1 shows the results from the CORA-13 test while QUENCH-6 results are shown in Figure 3.2. No variation in hydrogen generation and hence no variance in the oxidation modeling is observed for these validation cases.

For the case of oxidation of B4C control rods, a slight modification was made to the code to partition the reaction energy between the solid component mass and the atmosphere. The effect of this modification is observed in the validation of PHEBUS FPT-3 as shown in Figure 3.3. The placement of some of the reaction energy in the component leads to faster degradation of the control rods leading to relocation of material downwards into cooler zones leading to less oxidation.

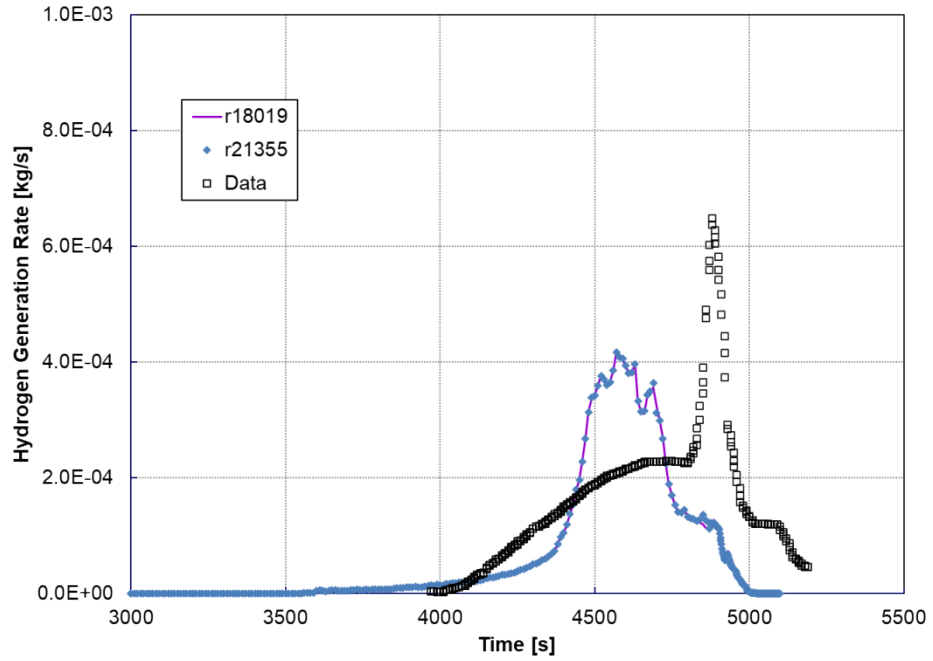


Figure 3.1 CORA-13 Hydrogen generation rate from oxidation

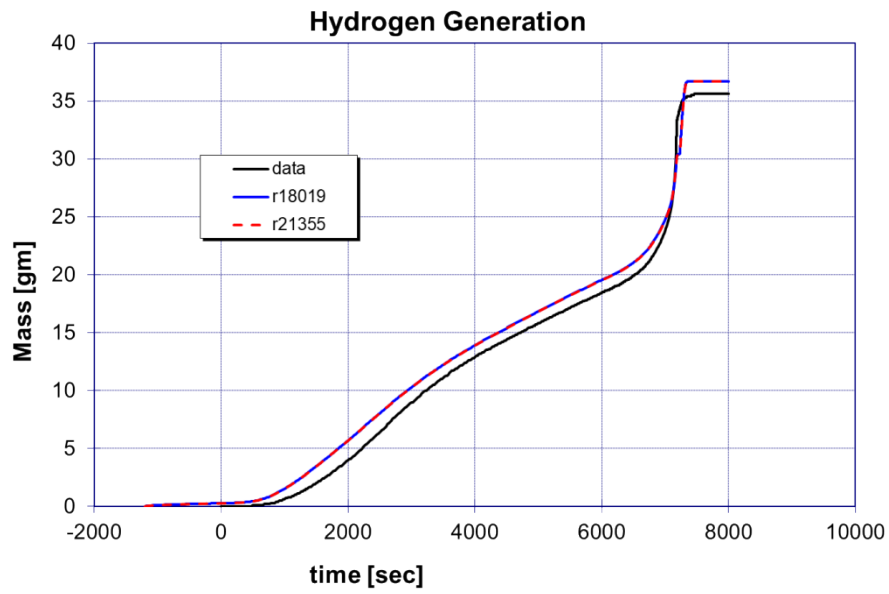
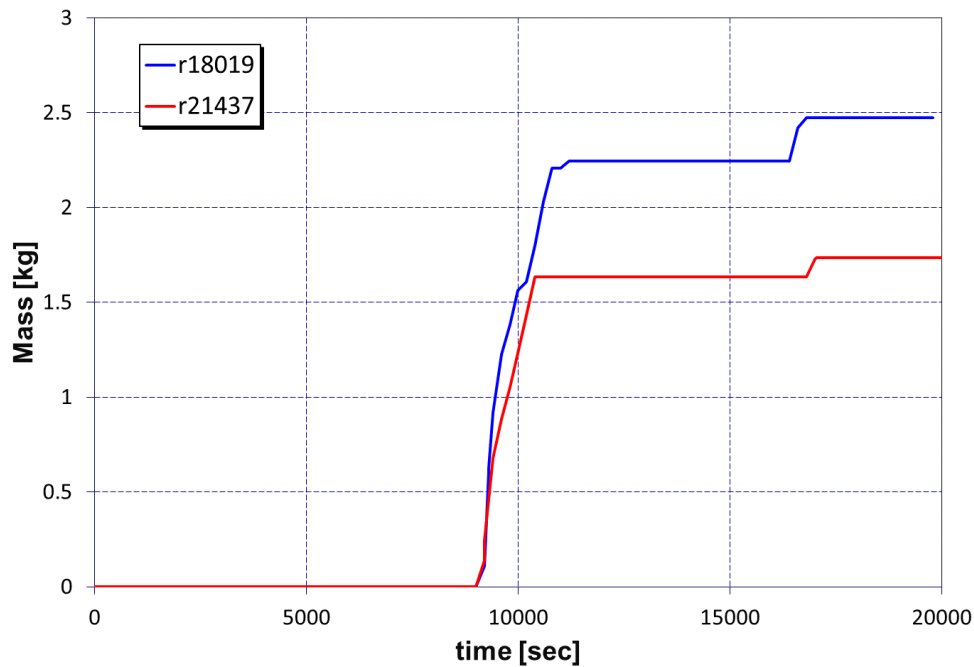


Figure 3.2 Quench-6 Hydrogen generation from oxidation



**Figure 3.3 Comparison of hydrogen generation from B4C in PHEBUS FPT-3 (revision 18019 and revision 21440)**

### 3.1.2. **COR Degradation Modeling**

The COR eutectics model, was enabled for the TMI-2 model and results associated with degradation were compared. Figure 3.4 compares the core degradation maps at four snapshots in time, near the onset of core degradation, just prior to reflood, just after reflood, and late in time when debris cooling is anticipated. The comparison shows reasonable agreement between the two code versions. The notable exception is that the oxidic convecting molten pool in r18019 is larger than it is for r21335. However, overall, the total mass of degraded core appears to be about the same. This is confirmed in Figure 3.5 where core damage is compared for the two code revisions. The damage fraction in r21335 is somewhat smaller than it is for r18019 until late in the calculation where damage appears to stop in r18019 but continues slowly in r21335. This appears to indicate a decrease in heat removal from the degraded configuration predicted for r21335. This difference in configuration seems to be a result of where the molten material resides. In Figure 3.6 the total molten mass is compared between the two revisions. Not that generally the two revisions predict the same maximum molten mass, though this molten mass decreases in r18019 when the debris begins to cool. Since the convecting molten pool in r21335 is smaller than it is in r18019, this means that more of that molten mass resides in the interstitials of the debris component which suggests that blockages may occur lower in the debris, the debris may be more compact with less fluid volume and less access for cooling the debris.

Finally, hydrogen generation is compared in Figure 3.7 which shows a reduction in H<sub>2</sub> generation of about 10% in r21335. This is consistent with a more compacted debris bed with reduced contact with the fluid.



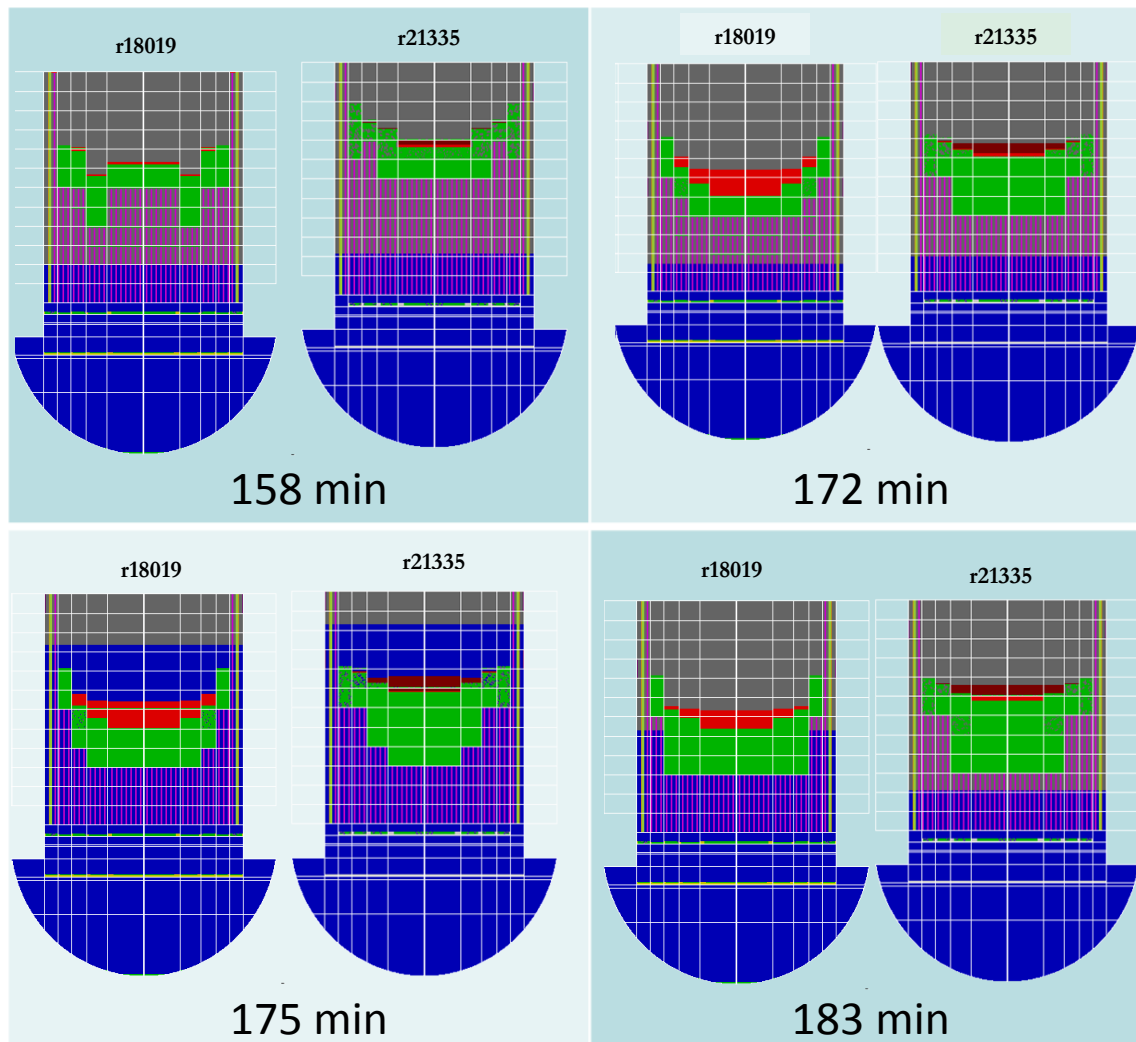


Figure 3.4 Comparison of the TMI-2 Response with and without the Eutectics Model for r21335

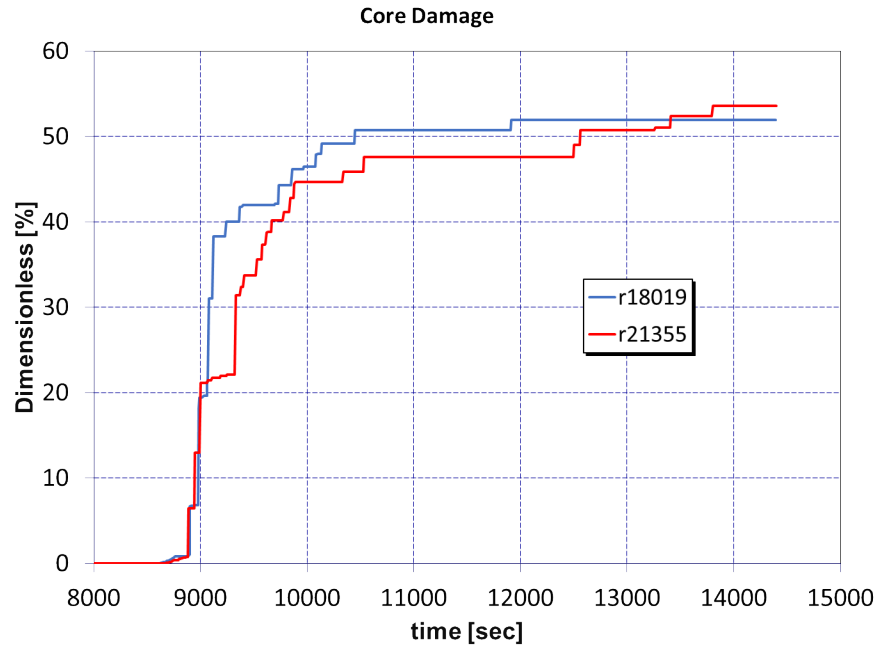


Figure 3.5 Comparison of core damage over development cycle (TMI)

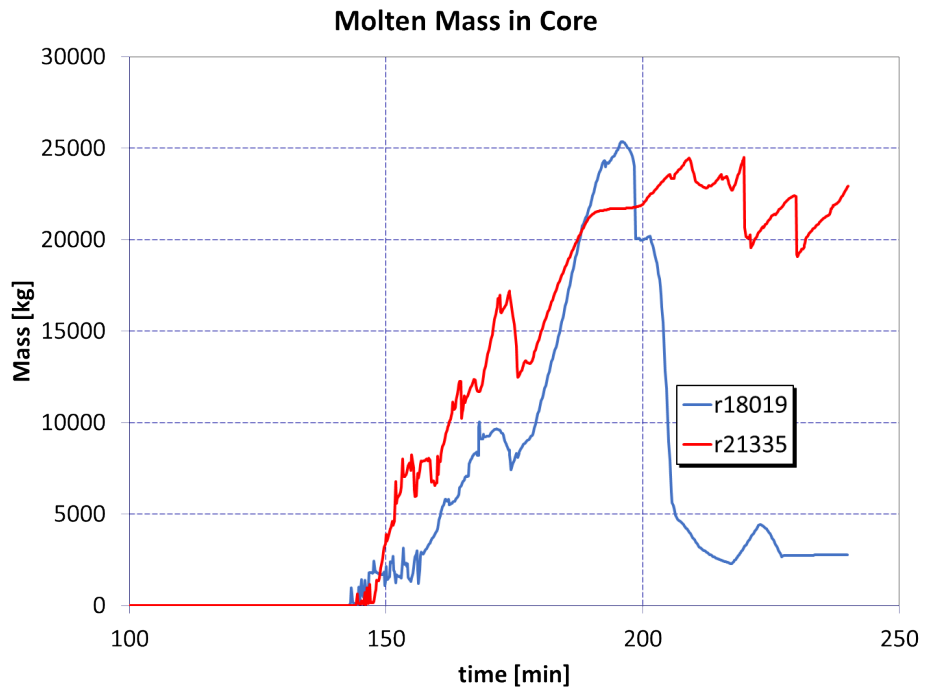


Figure 3.6 Comparison of core molten mass over development cycle (TMI)

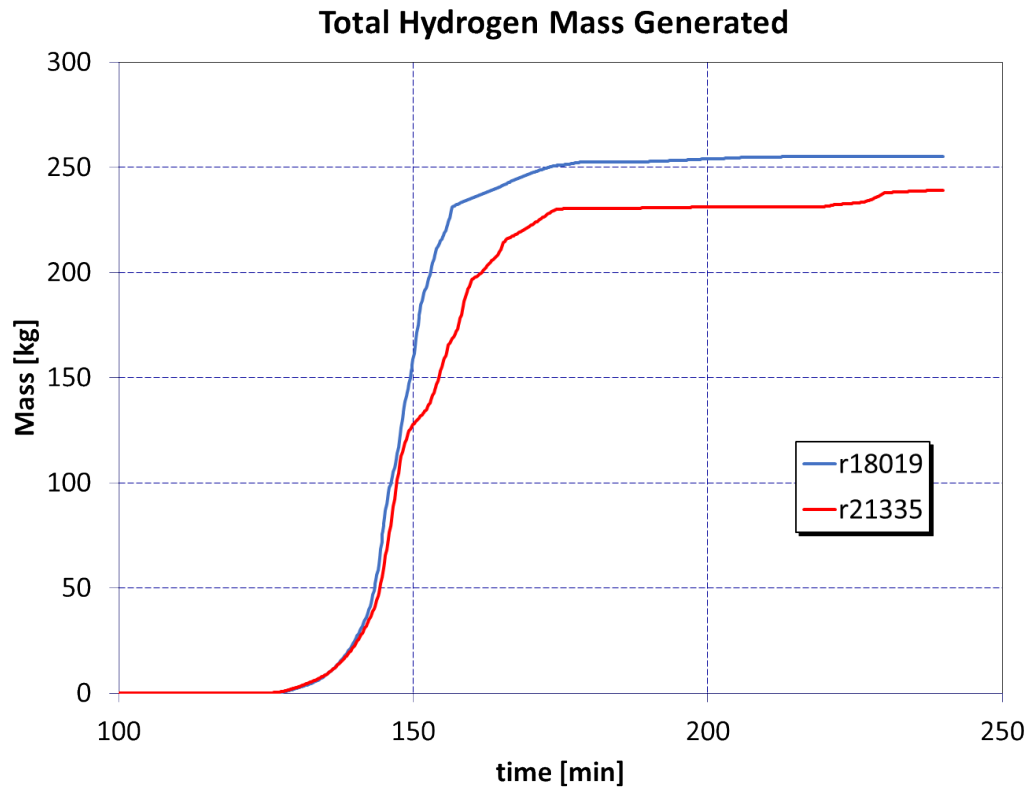


Figure 3.7 Comparison of total hydrogen generation over development cycle (TMI)

### 3.2. Single Parameter Variant Study

This section describes a single parameter variant study to review the impact of recent code changes. Section **Error! Reference source not found.** discusses the impact of the code changes affecting hydrogen generation compared with the last official code release, Revision 18019, based on the simple, demonstration, input decks. Section 3.2.2 illustrates the changes in code performance since Revision 18019.

#### 3.2.1. Hydrogen Generation Results

The simple demonstration input decks (PWR and BWR) that are provided with MELCOR were run with various code revisions to assess changes for important calculated metrics. In particular, the hydrogen mass generated for each case is reported here. This metric is affected by in-vessel phenomena resulting from core heat up, relocation, oxidation, and boil-off. Consequently, it provides an important indication of differences in calculation results. Since these are very simple input decks with extremely coarse nodalization, the sensitivity of this parameter may be larger than it would be for a detailed plant deck; however, it does provide a metric on the sensitivity of hydrogen production to code modifications.

Figure 3.8 shows the predicted hydrogen mass by revision starting with revision 18019, which corresponds to the 2020 Quicklook Report. The plot shows a gaping hole in missing data between r18736 and r19708, not because tests were not conducted, but because the testing procedures were changed making the generation of trend plots during this span impossible. Overall, there is a 2% change in hydrogen mass for the PWR case and a 17% increase in the hydrogen production for the BWR case. As shown in the plots, several revisions led to transient changes in the PWR hydrogen mass but most of these were due to new numerical issues arising from code corrections that were later resolved in a subsequent revision. For the BWR case, the substantial increase occurs during the span of missing data and are likely due to the changes to the minimum contact surface area in the molten pool which is a legitimate modeling change and not a numerical issue.

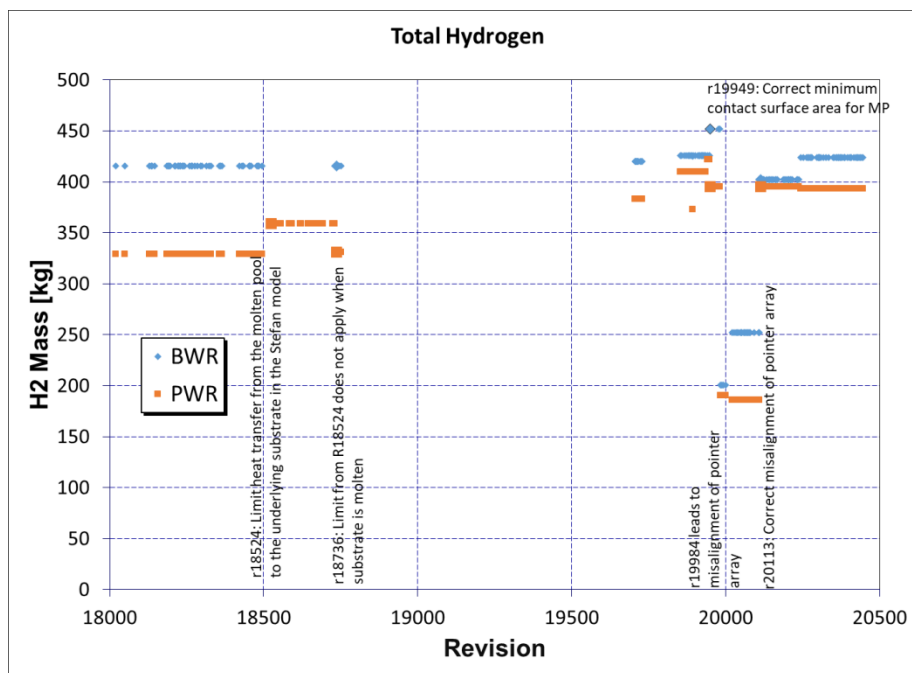


Figure 3.8 Hydrogen generation mass beyond revision 18019 revision

### 3.2.2. Code Performance Results

Several plant models were run to compare the central processing unit (CPU) time required for several revisions from MELCOR 2.1 to current MELCOR 2.2. Figure 3.9 compares the code performance for these plant decks. In general, code performance has improved since MELCOR 2.1.

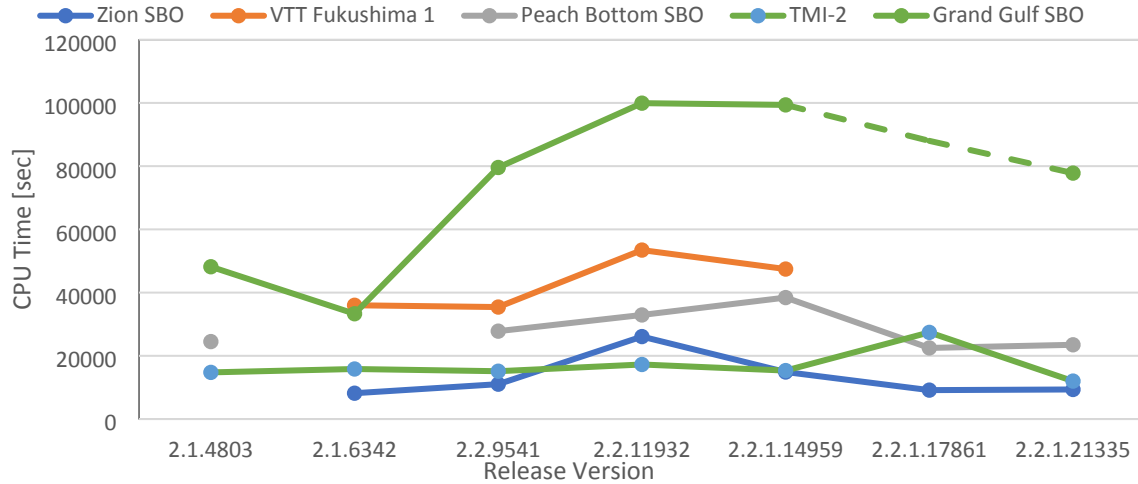


Figure 3.9 Code Performance in CPU for Several Plant Decks (from 3803 to 17260 revisions comparison)

## REFERENCES

- [1] Bartel, R, “WASH-1400 – The Reactor Safety Study – The Introduction of Risk Assessment to the Regulation of Nuclear Reactors,” NUREG/KM-0010, Office of Nuclear Regulatory Research, USNRC, August 2016.
- [2] Humphries, L.L., et.al., “MELCOR Computer Code Manuals Vol. 1: Primer and Users’ Guide Version 2.2.14959”, Sandia National Laboratories, October 2019.
- [3] Humphries, L.L., et.al. “MELCOR Computer Code Manuals Vol. 2: Reference Manual Version 2.2.14959”, Sandia National Laboratories, October 2019.



## DISTRIBUTION

### Email—Internal

Name	Org.	Sandia Email Address
Humphries, Larry	8852	llhumph@sandia.gov
Phillips, Jesse	8852	jphill@sandia.gov
Technical Library	9536	<a href="mailto:libref@sandia.gov">libref@sandia.gov</a>





Sandia  
National  
Laboratories

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.