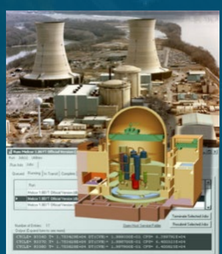
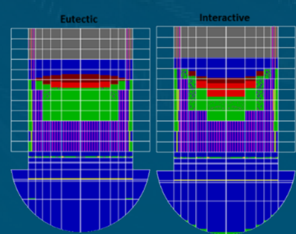
MELCOR Code Development Status EMUG 2022

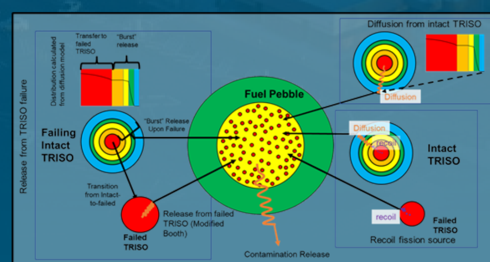
SAND2022-5473 PE

MELCOR

- New Modeling
- SQA
- Utilities





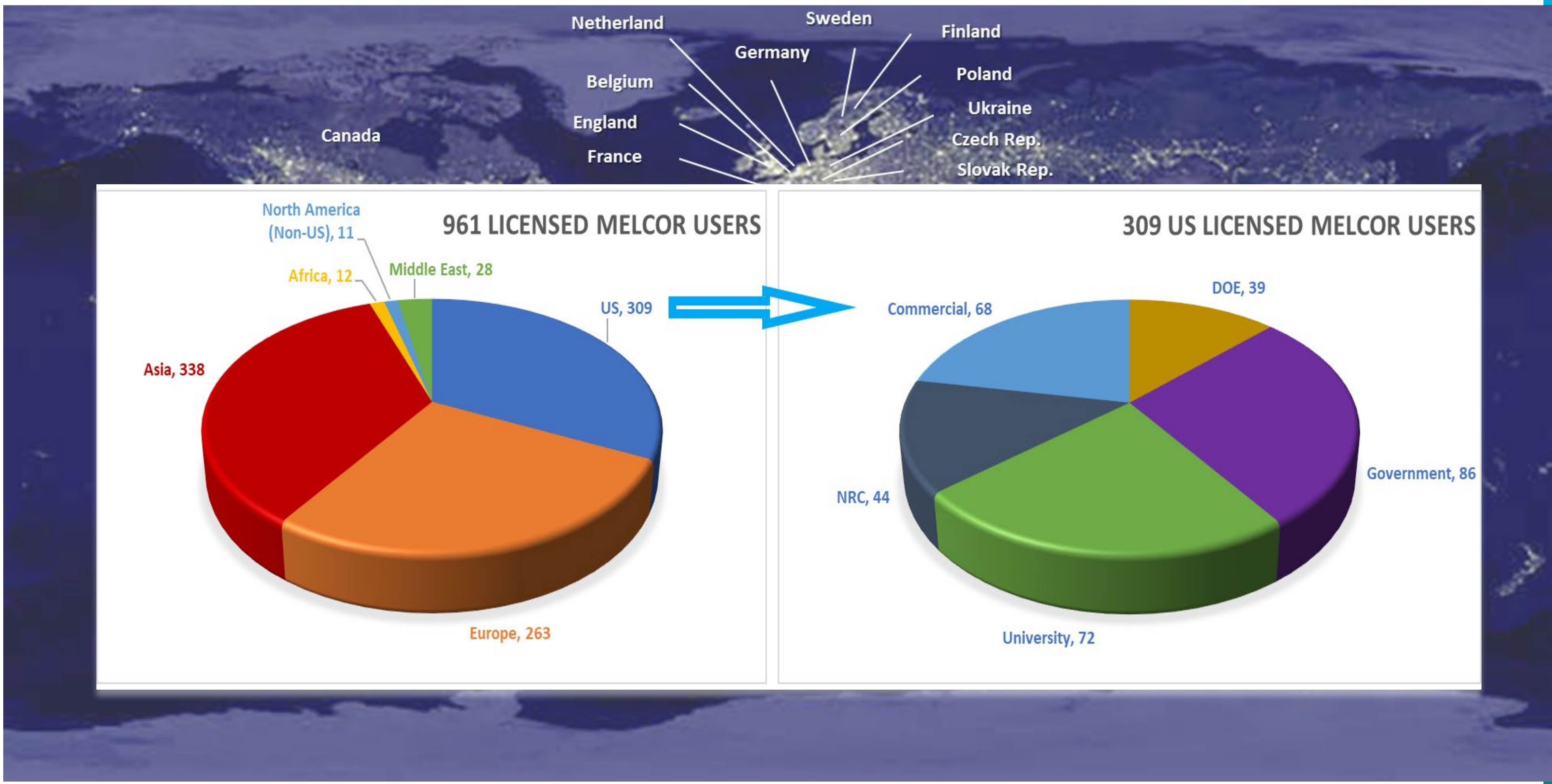


MELCOR Team, Sandia National Laboratories

PRESENTED BY

Larry Humphries, Sandia National Laboratories

International Use of MELCOR



Recent MELCOR Workshops & Meetings

2021 Non-Nuclear facilities workshop
- One-week in-person
- May, New Mexico
- Another 1-week, in-person workshop scheduled for April 2022
- Funded by participants

2021 European MELCOR User Group (EMUG)
- Virtual – Hosted by NUBIKi, Budapest, Hungary
- April 14-16
- Two ½ day MELCOR workshop on MELCOR visualization

2021 CSARP/MCAP
- Virtual – U.S. Nuclear Regulatory Commission
- June 7-11, 2021

2021 Asian MELCOR User Group (AMUG)
- Hosted by Singapore Nuclear Research and Safety Initiative - National University of Singapore
- November 2021
- Two ½ day MELCOR workshop on HTGR application

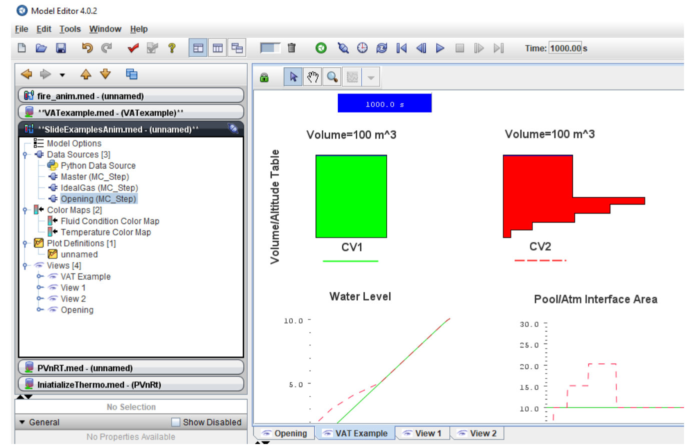
2022 Non-Nuclear facilities workshop
- 4-day in-person
- April, New Mexico
- Funded by participants

Upcoming MELCOR Workshops

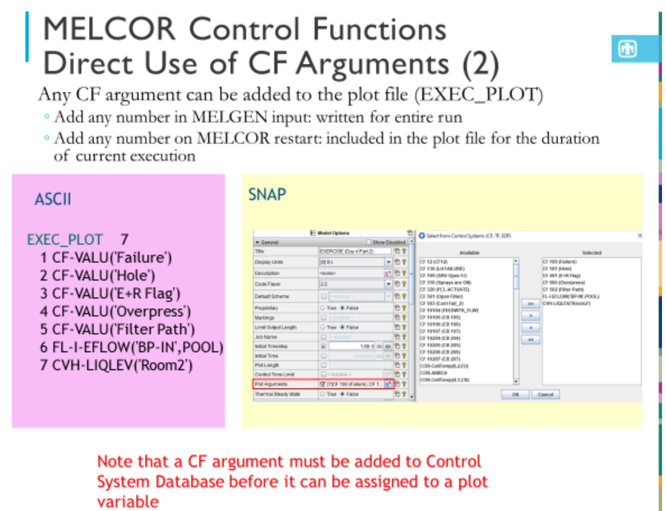
June 2022 in-person, week-long workshop in Bethesda, MD, USA

- 3 ½ days introductory material
  - Updated content
    - MELCOR Overview
      - More discussion on validation
    - CF Package
      - Side-by-side comparison between SNAP & ASCII input
      - New CF exercises
        - integration, trips, Formula type CFs, Range, Vector CF
      - Updated for new features (ranges, vector CFs)
    - CVH Package
      - Simple 'SNAPlette' examples scattered throughout the presentation demonstrating basic concepts
        - VAT, Opening Heights, initializing thermodynamic conditions, static head
- 1 ½ days reactor applications
  - HTGRs, Spent Fuel Pools, Sodium Fire Modeling, possibly Heat Pipe Reactors

June 2023 in-person, week-long workshop in Bethesda, MD, USA



Volume-Altitude SNAPlette



Side-by-side SNAP/ASCII Input

Requirements of an Integrated Severe Accident Code

Fully Integrated, multi-physics engineering-level code

Model a wide range of coupled phenomena at a level commensurate with the application to source term analysis, data availability for model parameters under severe accident conditions, and validation experiments for the modeled phenomena

- Thermal-hydraulic response in the reactor coolant system, reactor cavity, containment, and confinement buildings;
- Core heat-up, degradation, and relocation;
- Core-concrete attack;
- Hydrogen production, transport, and combustion;
- Fission product release and transport behavior

Diverse Application

- Multiple 'CORE' designs
- User constructs models from basic constructs
- Adaptability to new or non-traditional reactor designs
  - HPR, HTGR, SMR, MSR, ATR, VVER, SFP,…

Validated physical models

- ISPs, benchmarks, analytic results, experiments, accidents

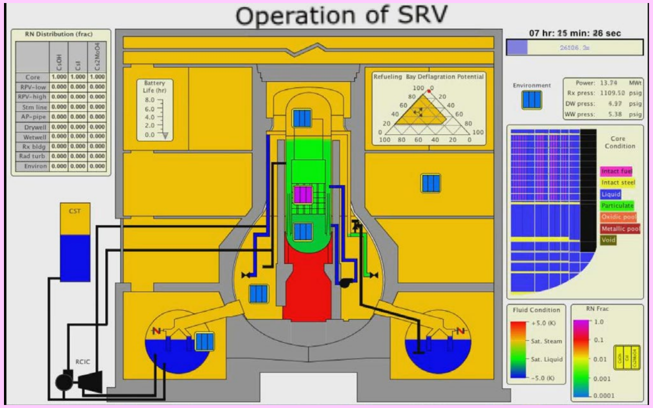
Uncertainty Analysis

- Relatively fast-running
- Reliable code
- Access to modeling parameters
  - Properties of materials, coefficients in correlations, numerical controls and tolerances, etc

User Convenience

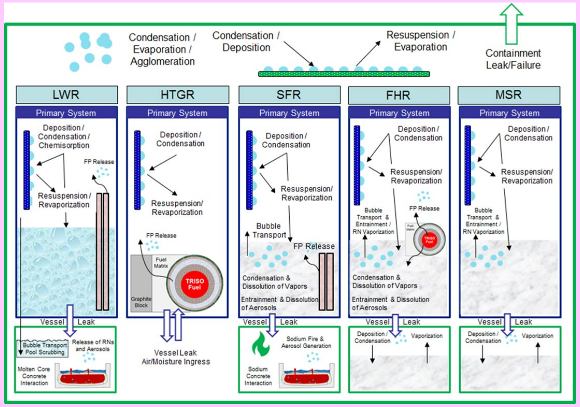
- Windows/Linux versions
- Utilities for constructing input decks (GUI)
- Capabilities for post-processing, visualization
- HTML Output
- Extensive documentation

Multi- Physics



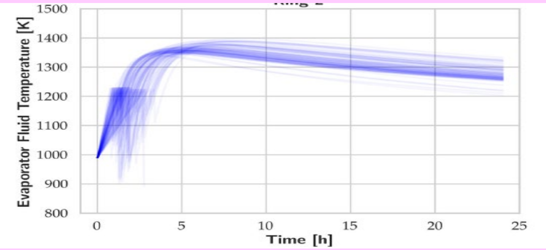
SOARCA LTSBO

Diverse Application



Advanced Reactors

Uncertainty Analysis



Uncertainty Analysis

Significance of a fully-integrated source term tool

MELCOR is a fully-integrated, system-level computer code

- Prior to the development of MELCOR, separate effects codes within the Source Term Code Package (STCP) were run independently
  - Results were manually transferred between codes leading to a number of challenges
    - transferring data
    - ensuring consistency in data and properties
    - capturing the coupling of physics

Advantages of using a fully-integrated tool for source term analysis

- Integrated accident analysis is necessary to capture the complex coupling between a myriad of interacting phenomena involving movement of fission products, core materials, and safety systems.
- A calculation performed with a single, integrated code as opposed to a distributed system of codes reduces errors associated with transferring data downstream from one calculational tool to the next.
- Performing an analysis with a single integrated code assures that the results are repeatable.
- Methods for performing uncertainty analysis with an integrated tool such as MELCOR are well established.
- Time step issues are internally resolved within the integral code

MELCOR "Systems-level" Modeling Approach

Modeling is as mechanistic as possible, consistent with a reasonable run time.

- Examples: Zonal diffusion release in TRISO particles, Lagrangian droplet combustion models for sodium spray fires, multi-component/multi-particle size aerosol physics models, etc.
- Advances in computer run-time over the past few decades led to increased mechanistic modeling in MELCOR.

Simplified models where appropriate consistent with available supporting experimental data

- Example: Simple force balance model vs kinetic "rock'n' roll" model for resuspension
  - Kinetic model based on data that are unavailable, difficult/impossible to characterize under accident conditions
  - Simple model performs as well on fundamental validation experiments

Some parametric models, where appropriate

- Example: Data for large scale core degradation are sparse or non-existent.
  - Validation limited to small-scale bundle experiments or post-accident conditions for Fukushima and TMI-2 and indirect temperature/pressure measurements
  - Use of Cross-walk comparisons to other codes
- Parametric models are general enough that they do not force a particular outcome (i.e., TMI-2)
- Core degradation for non-LWRs generally do not have such uncertainties

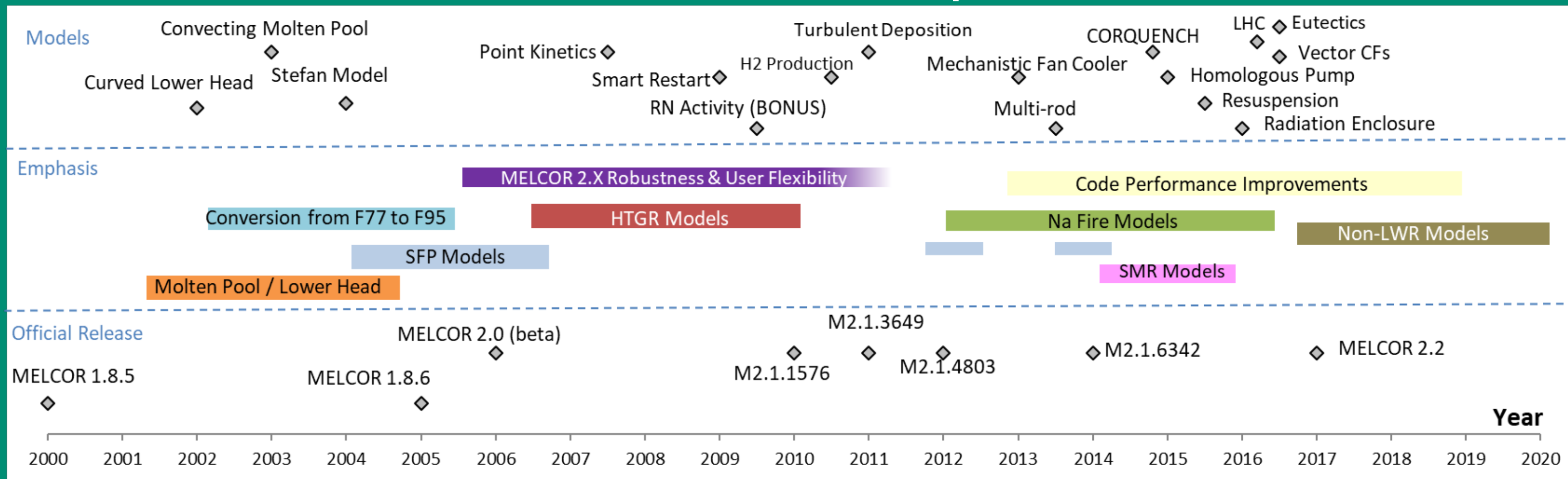
Modeling is consistent with current state of practice in modeling phenomena

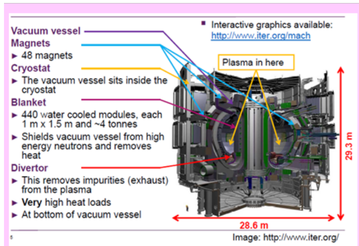
Applies to LWRs and non-LWRs

- Uses general, flexible models rather than models for specific system components (no LWR steam generator models or PWR pressurizer models)
  - Relatively easy to model novel designs
  - Puts greater burden on analyst to develop input that well-represents the problem

MELCOR Model Development

MELCOR Code Development





Fusion

- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

Spent Fuel

Spent f... risk studi...

Multi... area ... (n)

Dry S...

HTGR Reactors

Sodium Reactors

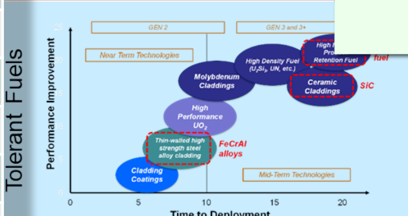
...odium Properties
- Sodium Equation of State
- Sodium Thermo-mechanical properties

...ontainment Modeling
- Sodium pool fire model
- Sodium spray fire model
- Atmospheric chemistry model
- Sodium-concrete interaction

Molten Salt Reactors

- Properties for LiF-BeF2 have been added
  - Equation of State
  - Thermal-mechanical properties

Tolerant Fuels



M2x Official Code Releases

Version	Date
2.2.18019	December 2020
2.2.14959	October 2019
2.2.11932	November 2018
2.2.9541	February 2017
2.1.6342	October 2014
2.1.4803	September 2012
2.1.3649	November 2011
2.1.3096	August 2011
2.1.YT	August 2008
2.0 (beta)	Sept 2006

Non-Reactor Applications

Advanced Reactor Applications

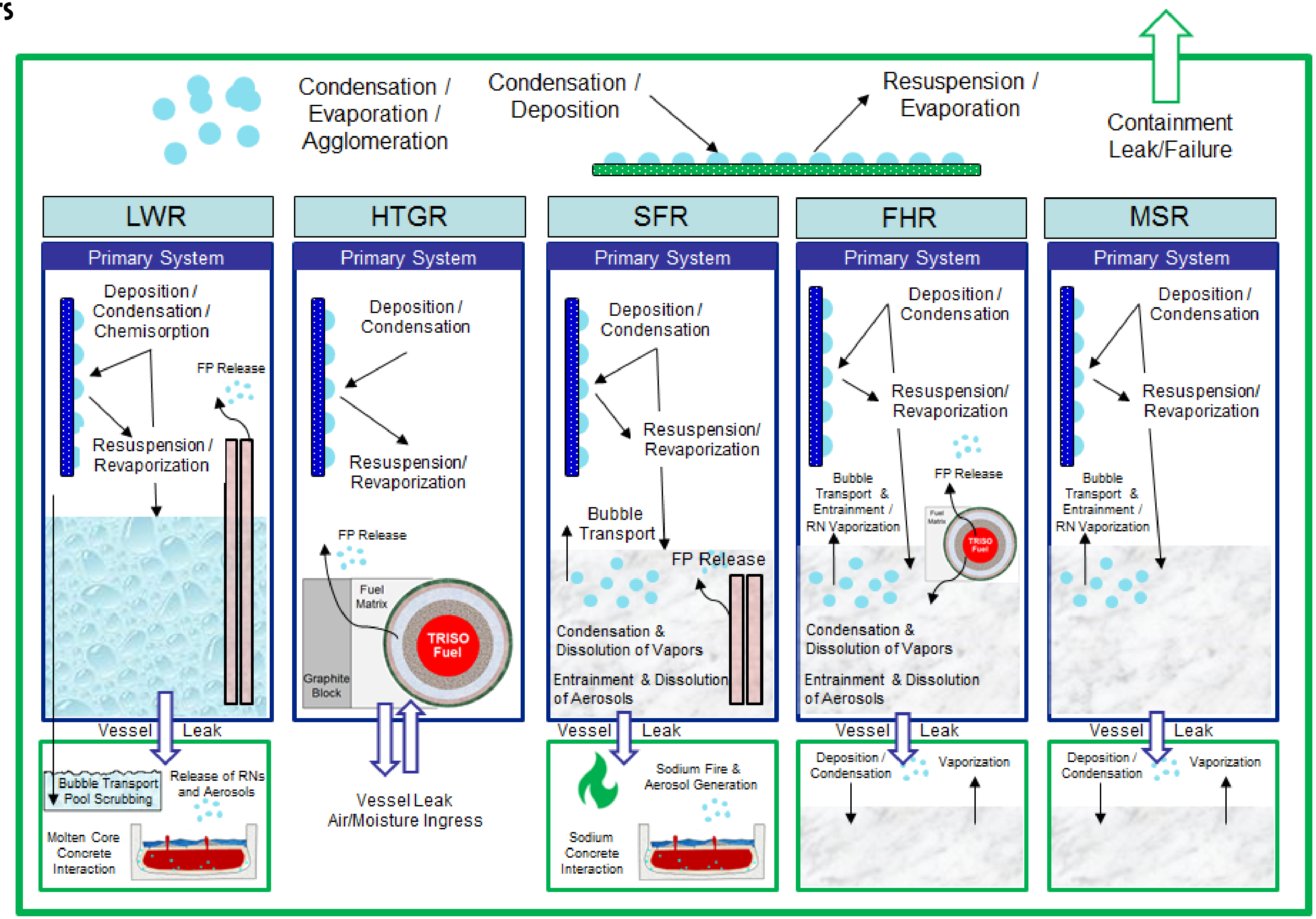
LWR/Non-LWR/ATF Fuels Development

LWR and General MELCOR development

Advanced Technology Fuels (ATF)

Non-LWR Reactors
- HTGR
- Sodium
- Molten Salts

Spent Fuel Pools



MELCOR HTGR modeling

Overall goals of the HTGR fission product release model include:

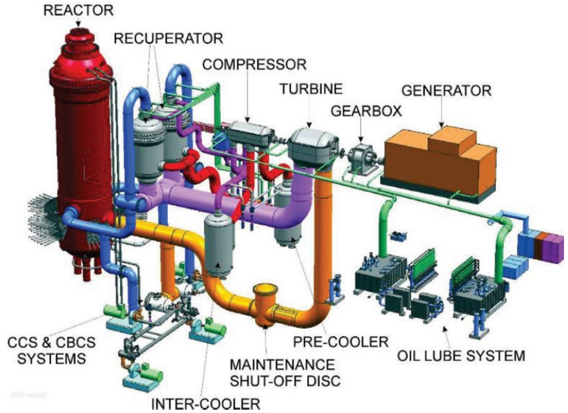
- Predict radionuclide distributions within fuel
- Predict radionuclide release from fuel elements to coolant

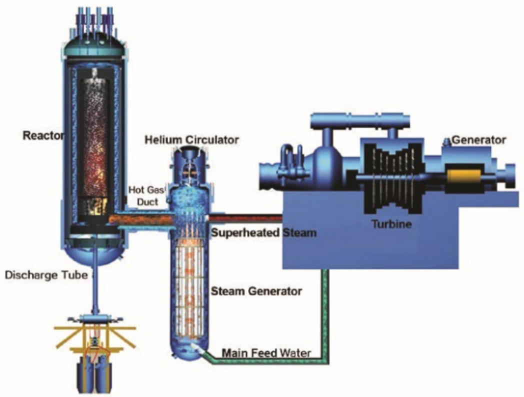
Radionuclide release and transport model

- Diffusion transport of fission product species
- MELCOR transient/accident solution methodology
  - Steady-state diffusion
  - Steady-state transport
  - Transient diffusion/transport

HTGR Specific models

- Analytic release
- Energy/temperature for temperature-dependent diffusion
- Graphite oxidation
- Intercell and intracell conduction
- Convection & flow
- Point kinetics
- Dust generation and resuspension

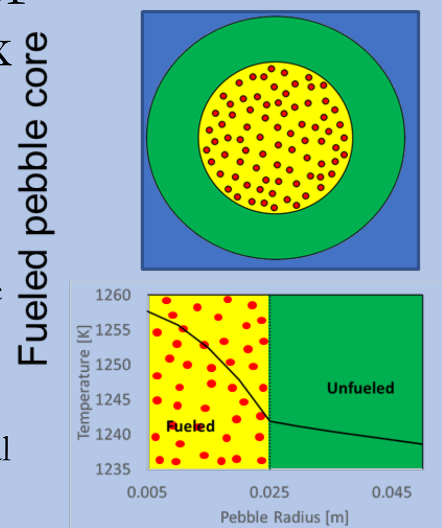


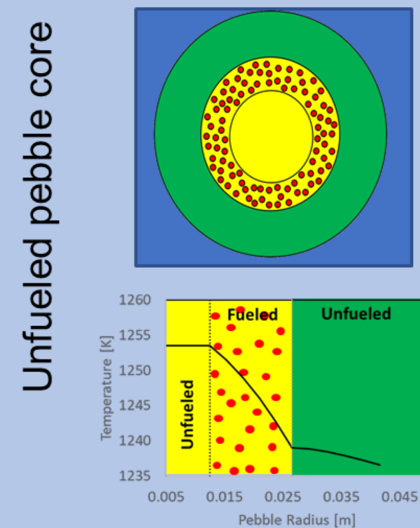


HTGR Components

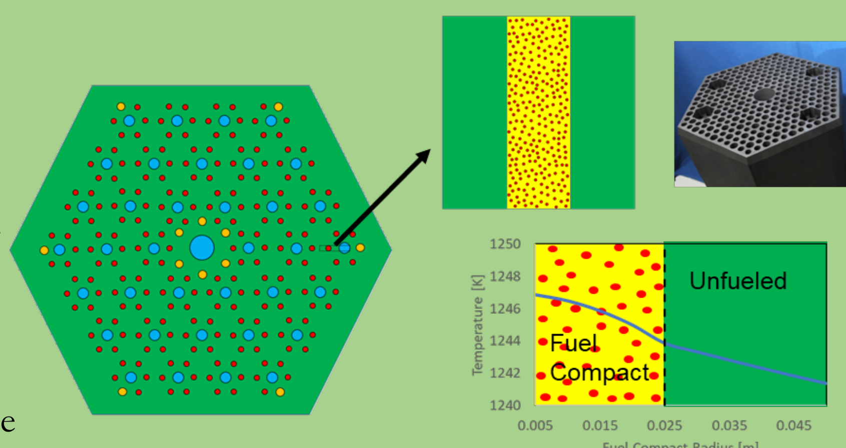
High Temperature Gas Reactors

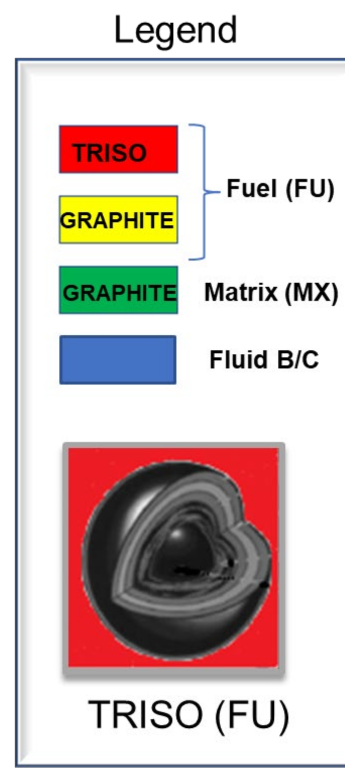
- Pebble Bed Reactor (PBR) Fuel/Matrix Components
  - Fueled part of pebble
  - Unfueled shell is modeled as separate component (Matrix)
  - Fuel radial temperature profile for sphere
    - Provides peak and surface pebble temperature
    - Modified for unfueled central core





- Prismatic Modular Reactor (PMR) Fuel/Matrix Components
  - More "rod-like" geometry
  - Fuel compacts represented as fuel component
  - Part of hex block associated with a fuel channel is matrix component
  - Fuel radial temperature profile for cylinder



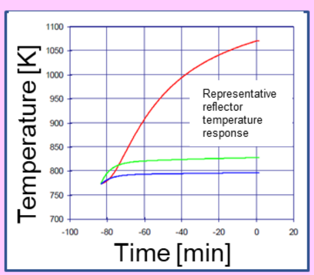


Sub-component model for zonal diffusion of radionuclides through TRISO particle

Transient/Accident Solution Methodology

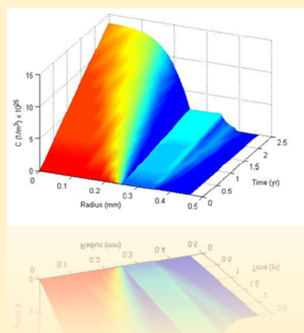
Stage 0:
Normal Operation
Establish thermal state

- *Time constant in HTGR graphite structures is very large*
  - *>24 hours for reflector to reach steady state*
- *Reduce heat capacities for structures to reach steady state thermal conditions.*
- *Reset heat capacities after steady state is achieved.*



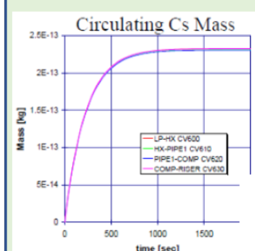
Stage 1:
Normal Operation
Diffusion Calculation

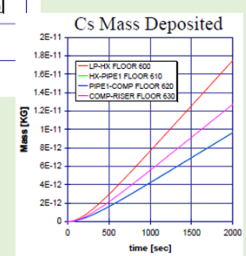
Establish steady state distribution of radionuclides <u>in TRISO particles (and matrix)</u> for normal operation



Stage 2:
Normal Operation
Transport Calculation

Calculate steady state distribution of radionuclides <u>throughout system</u> during normal operation (deposition on surfaces, convection through flow paths, etc.)

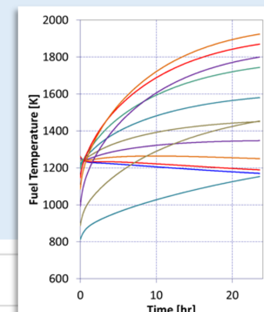


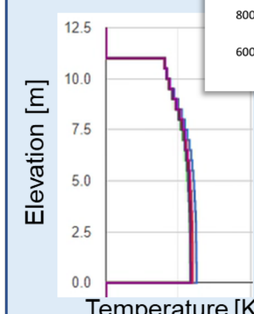


Example:
PBMR400 Cs Distribution in Primary System

Stage 3:
Accident
Diffusion & Transport calculation

Calculate accident progression and radionuclide release





All steps performed in one run with data passed transparently between stages

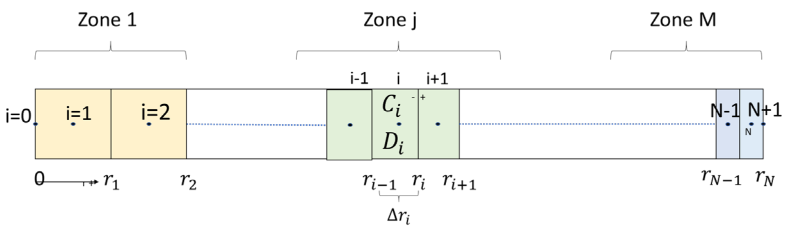
HTGR Radionuclide Diffusion Release Model

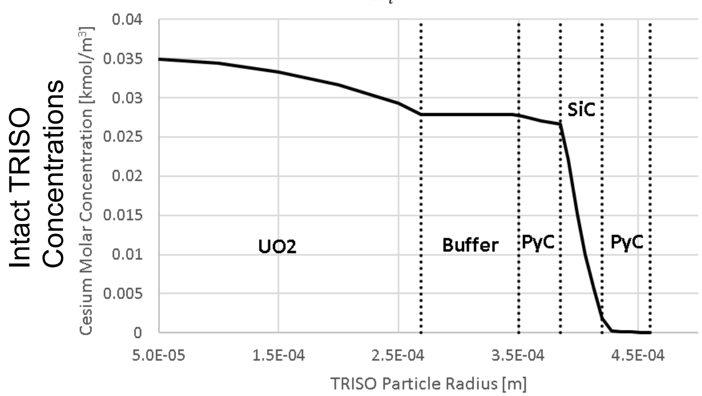
Intact TRISO Particles

- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

$$\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \boldsymbol{D}\frac{\partial C}{\partial r}\right) - \lambda C + \beta$$

$$D(T) = D_0 e^{-\frac{Q}{RT}}$$





Diffusivity Data

Radio-nuclide	UO_2	UCO	PyC	Porous Carbon	SiC	Matrix Graphite	TRISO Overall
Ag	Some	unknown	Some	unknown	Extensive	Some	Extensive
Cs	Some	unknown	Some	unknown	Extensive	Some	Some
I	Some	unknown	Some	unknown	Some	unknown	unknown
Kr	Some	unknown	Some	unknown	unknown	Some	Some
Sr	Some	unknown	Some	unknown	Extensive	Some	Some
Xe	Some	unknown	Some	unknown	Some	Some	unknown

$$A = \pi r^2$$

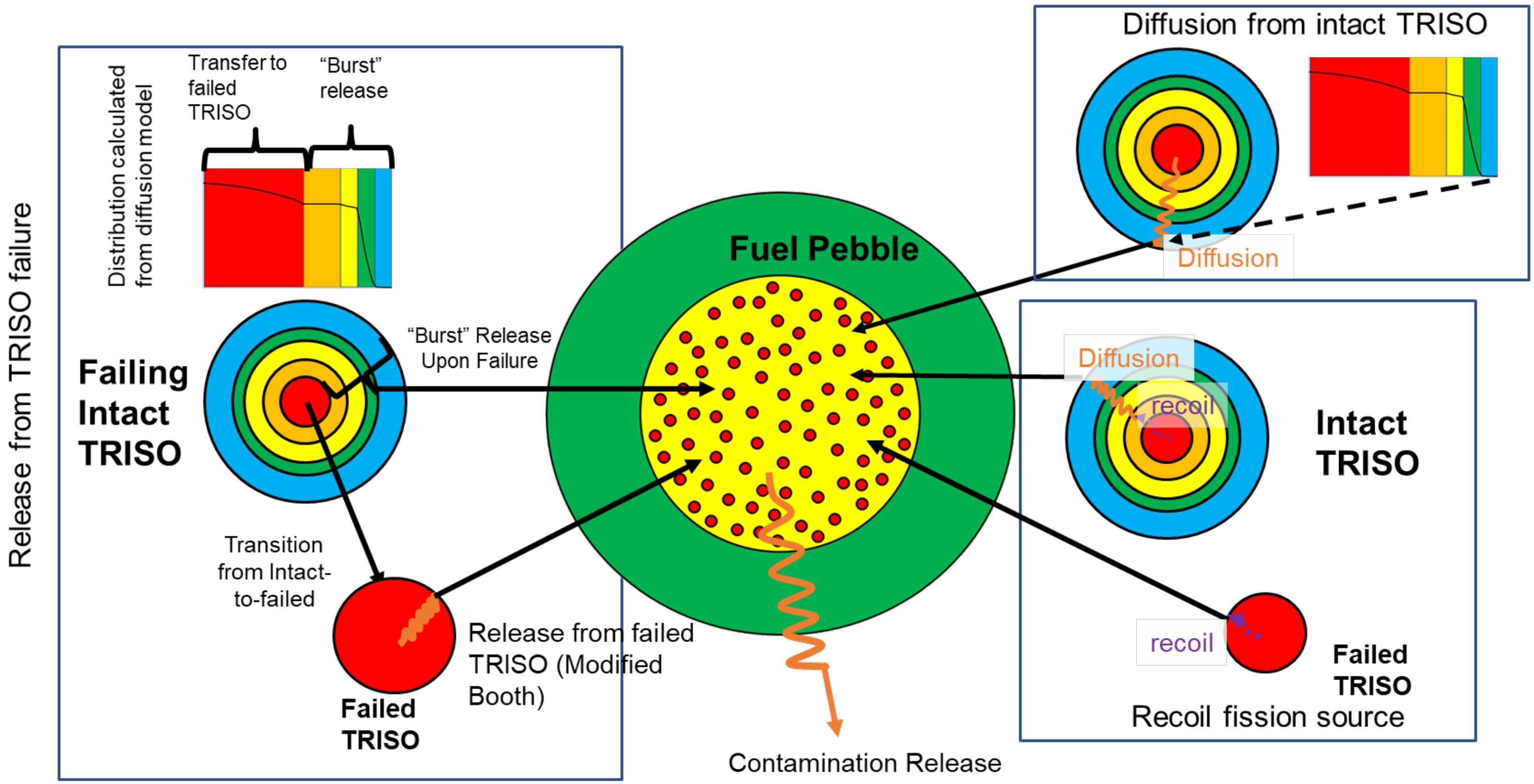
Availability

Layer	FP Species							
	Kr		Cs		Sr		Ag	
	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m2/s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6-8	209000.0	2.2E-3	488000.0	6.75E-9	165000.0
Buffer	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0
PyC	2.9E-8	291000.0	6.3E-8	222000.0	2.3E-6	197000.0	5.3E-9	154000.0
SiC	3.7E+1	657000.0	7.2E-14	125000.0	1.25E-9	205000.0	3.6E-9	215000.0
Matrix Carbon	6.0E-6	0.0	3.6E-4	189000.0	1.0E-2	303000.0	1.6E00	258000.0
Structural Carbon	6.0E-6	0.0	1.7E-6	149000.0	1.7E-2	268000.0	1.6E00	258000.0

Data used [IAEA TECDOC-0978]

HTGR Radionuclide Release Models

- Recent failures – particles failing within latest time-step (burst release, diffusion release in time-step)
- Previous failures – particles failing on a previous time-step (time history of diffusion release)



Graphite Oxidation

Steam oxidation

$$R_{OX,steam} = \frac{k_4 P_{H_2O}}{1 + k_5 P_{H_2}^{0.5} + k_6 P_{H_2O}}$$

Reaction + Energy

$C + H_2O(g) \rightarrow CO(g) + H_2(g)$
$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$

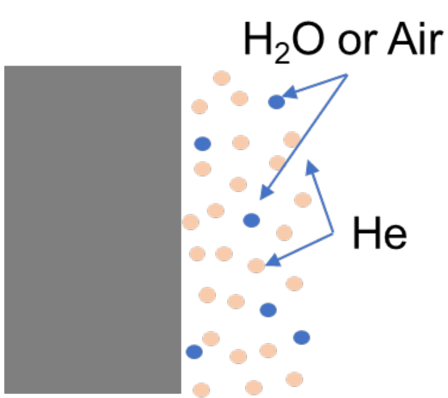
Air oxidation

$$R_{OX} = 1.7804x10^4 \exp\left(-\frac{20129}{T}\right)\left(\frac{P}{0.21228x10^5}\right)^{0.5}$$

Reaction

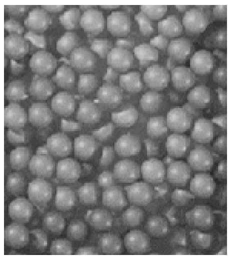
1. $C + O_2 \rightarrow CO_2(g)$
2. $C + \frac{1}{2}O_2 \rightarrow CO(g)$
3. $CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g)$
4. $C + CO_2(g) \rightarrow 2CO(g)$

Both steam and air include rate limit due to steam/air diffusion towards active oxidation surface



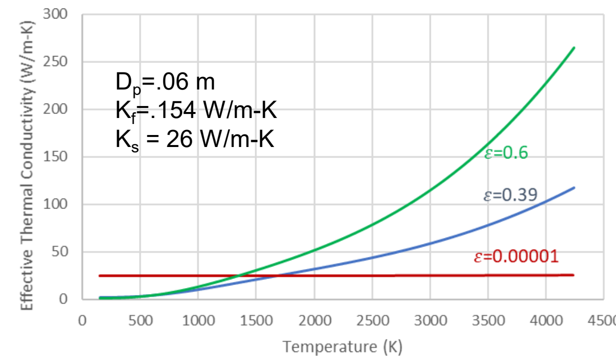
COR Intercell Conduction

Effective conductivity prescription for PBR (bed conductance)

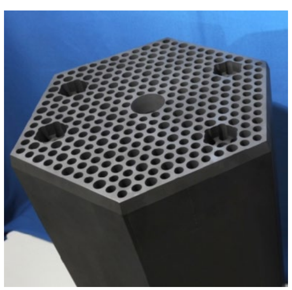


- Zehner-Schlunder-Bauer with Breitbach-Barthels modification to the radiation term

$$k_{eff} = \left(1-\sqrt{1-\varepsilon}\right)\varepsilon 4\sigma T^{3} D_{p} + \left(1-\sqrt{1-\varepsilon}\right)k_{f} + \sqrt{1-\varepsilon}\, k_{c}(T, D_p, \varepsilon, k_f, k_s, k_r)$$



Effective conductivity prescription for PMR (continuous solid with pores)



- Tanaka and Chisaka expression for effective radial conductivity (of a single PMR hex block)

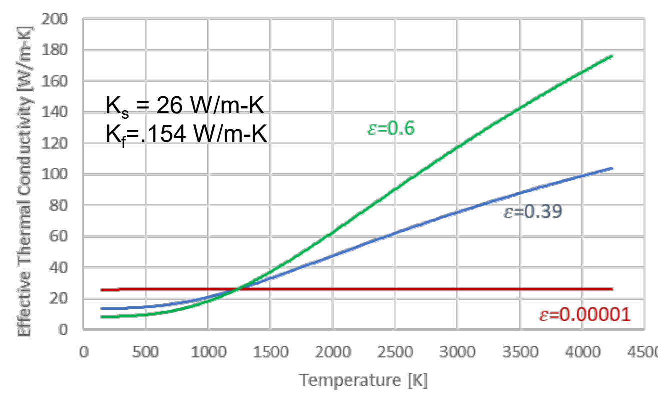
$$k_{eff} = k_s\left[A + (1-A)\frac{\ln\left(1+2B\left(k_{por}/k_s - 1\right)\right)}{2B\left(1-k_s/k_{por}\right)}\right]$$

- A radiation term is incorporated in parallel with the pore conductivity

$$k_{rad} = 4\varepsilon_{r}\sigma T^{3} D$$

- Thermal resistance of helium gaps between hex block fuel elements is added in parallel via a gap conductance term

$$k_{er} = \left({}^{1}/_{h_{gap}D_{blk}} + {}^{1}/_{k_{eff}}\right)^{-1}$$



Interface Between Thermal-hydraulics and PBR Core Structures

Heat transfer coefficient (Nusselt number) correlations for PBR convection:

- Isolated, spherical particles
- Use Tfilm to evaluate non-dimensional numbers, use maximum of forced and free Nu

$$Nu = 2.0 + 0.6\ Re_f^{1/2}\ Pr_f^{1/3} \qquad Nu = 2.0 + 0.6\ Gr_f^{1/4}\ Pr_f^{1/3}$$

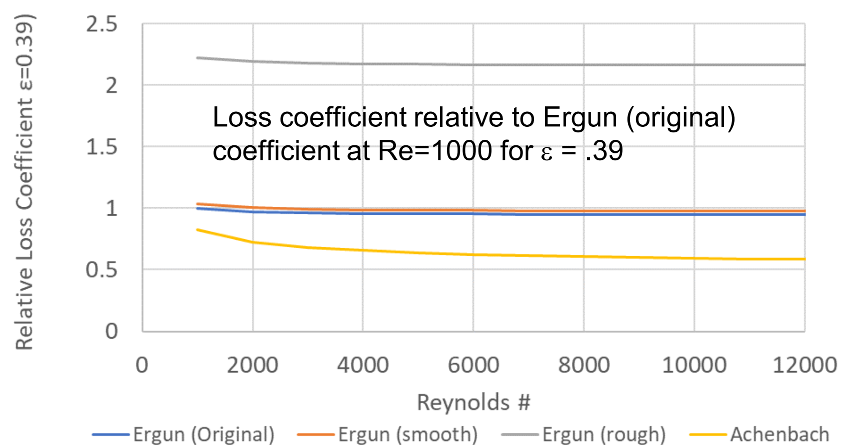
- Constants and exponents accessible by sensitivity coefficient

Flow resistance

- Packed bed pressure drop

$$K_L(\varepsilon, Re) = \left[C_1 + C_2\frac{1-\varepsilon}{Re} + C_3\left(\frac{1-\varepsilon}{Re}\right)^{C_4}\right]\frac{(1-\varepsilon)}{\varepsilon D_p}L$$

Correlation	C_1	C_2	C_3	C_4
Ergun (original)	3.5	300.	0.0	-
Modified Ergun (smooth)	3.6	360.	0.0	-
Modified Ergun (rough)	8.0	360.	0.0	-
Achenbach	1.75	320.	20.0	0.4



$$Relative\ Loss(.39, Re) = \frac{K_L(.39, Re)}{K_{L\ Ergun(original)}(.39, 1000)} = \frac{\left[C_1 + C_2\frac{.61}{Re} + C_3\left(\frac{.61}{Re}\right)^{C_4}\right]}{\left[C_1 + C_2\frac{.61}{Re} + C_3\left(\frac{.61}{Re}\right)^{C_4}\right]}$$

Point Reactor Kinetics

Standard delayed-group treatment

$$\frac{dP}{dt} = \left(\frac{\rho - \beta}{\Lambda}\right) P + \sum_{i=1}^{6} \lambda_i Y_i + S_0$$

$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P - \lambda_i C_i, \qquad for\ i = 1 \ldots 6$$

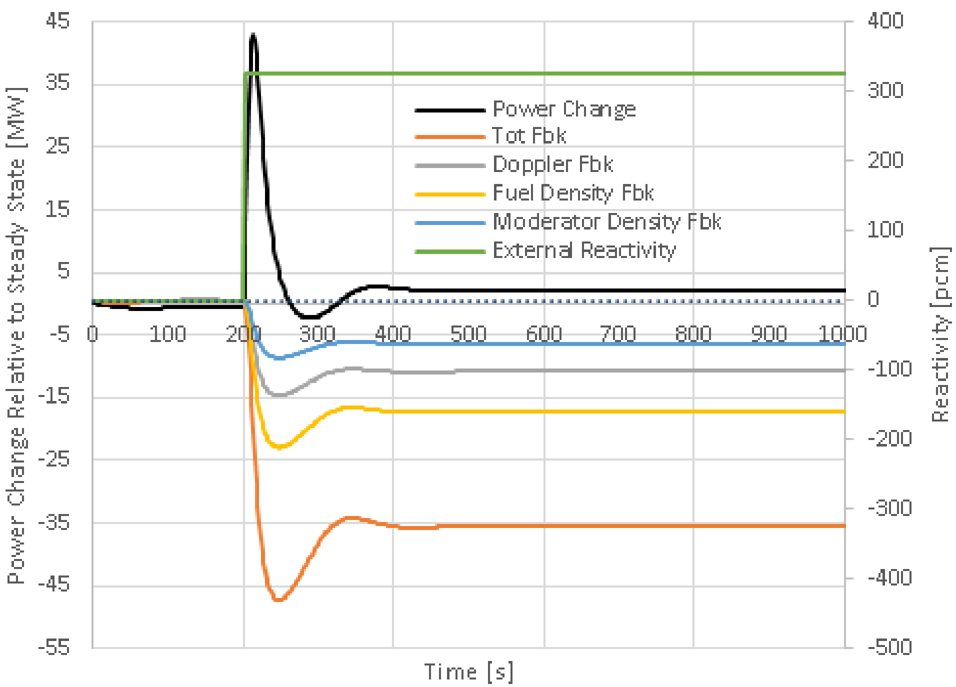
Kinetics data accessible by coefficients

Feedback models

- Control function-specified external component
- Doppler
- Fuel and moderator density

Define core cell ranges as regions over which averages are taken to inform feedback models

Useful capability for Anticipated Transient Without Scram (ATWS) scenarios



MELCOR/CONTAIN-LMR Implementation

Implement sodium as replacement to the working fluid for a MELCOR calculation

- Implement properties & Equations Of State (EOS) from the fusion safety database
  - Na (tpfna), FLiBe (tpffi), Pb-Li (tpflipb), He (tpfhe), N2(tpfn2)
- Implement properties & EOS based on SIMMER-III

Implementation and Validation of:

- Sodium spray fires
  - Based on NACOM spray model from BNL
  - Input requirement: fall height, mean diameter and source
    - Droplet acceleration model
  - Internal droplet size distribution (11 bins) from Nukiyama-Tanasama correlation
  - Reactions considered:
    - (S1) $2\,Na + {}^1/_2\,O_2 \rightarrow Na_2O$,
    - (S2) $2\,Na + O_2 \rightarrow Na_2O_2$
- Sodium pool fires
  - Based on SOFIRE II code from ANL
    - Reactions considered:
      - $2\,Na + O_2 \rightarrow Na_2O_2$, 10.97 MJ/kg
      - $4\,Na + O_2 \rightarrow 2\,Na_2O$, 9.05 MJ/kg

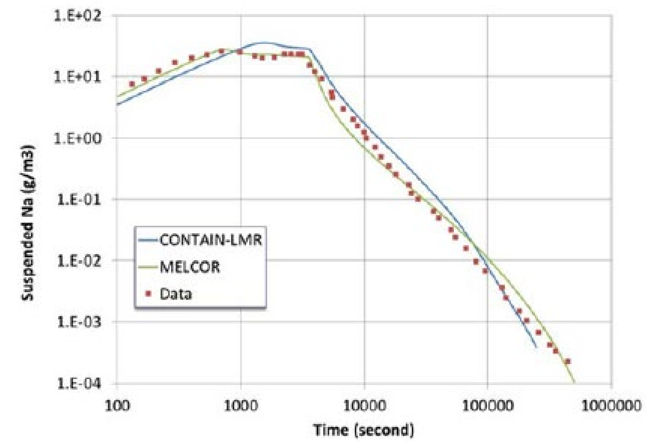


Figure 33. Suspended Na Aerosol Mass - AB1

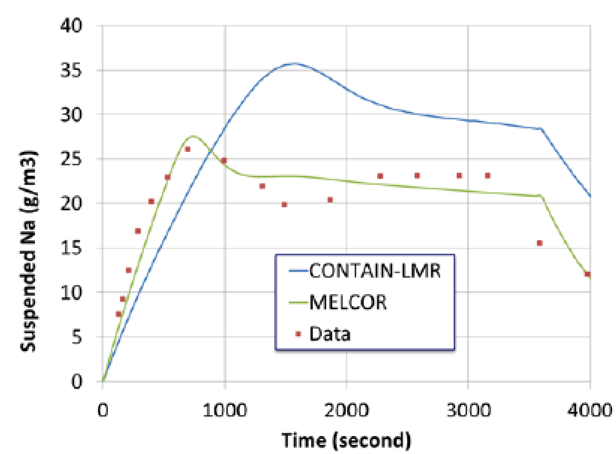


Figure 34. Suspended Na Aerosol Mass-AB1

Atmospheric Chemistry New in 2019 Code Release

A number of reactions have been considered:

- $Na(l) + H_2O\ (l) \rightarrow NaOH(a) + \frac{1}{2} H_2$
- $2\ Na(g,l) + H_2O\ (g,l) \rightarrow Na_2O(a) + H_2$
- $2\ Na(g,l,a) + \frac{1}{2} O_2$ or $O_2 \rightarrow Na_2O(a)$ or $Na_2O_2(a)$
- $Na_2O_2(a) + 2\ Na(g,l) \rightarrow 2\ Na_2O(a)$
- $Na_2O(a) + H_2O\ (g,l) \rightarrow 2NaOH(a)$
- $Na_2O_2(a) + H_2O\ (g,l) \rightarrow 2NaOH(a) + 0.5O_2$

Kinetics of atmosphere gases are not explicitly modeled.

All these reactions are assumed to occur in hierarchal order:

- In the order listed above
- By location of reactions
  - Atmosphere(g), aerosol, surfaces (i.e., HS)

Outputs

- Reaction number, reaction energy, byproducts (Na classes, H_2), gas and liquid consumed (Na, H_2O, O_2)

MELCOR Heat Pipe Reactor Modeling

HPs replace 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 transferred to the CVH package.

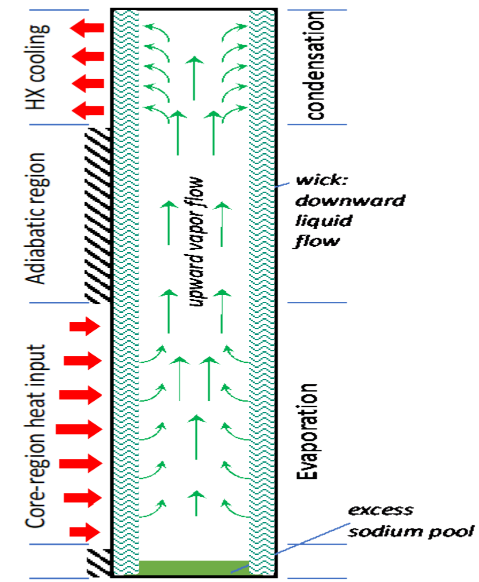
Distinct wall and working fluid region nodalization. MELCOR accommodates HP models of different fidelity through a common interface.

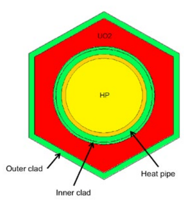
- Model 1: working fluid region modeled as high thermal conductivity material
- Model 2 (new in 2020 release): thermodynamic equilibrium approximation of working fluid (sodium or potassium EOS). P, T and liq/vap fraction evolve in time. Sonic, capillary and boiling limits enforced.
- If needed, higher fidelity models straight-forward to implement to interface.

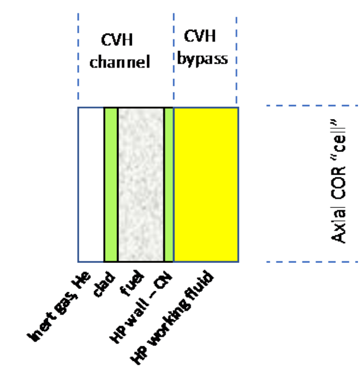
MELCOR heat transfer paths enable radial (lateral) heat transfer in the core among multiple HP regions and to other MELCOR structures.

- Thermal resistance network approximation across heterogeneous domain

At failure, HP materials and regions transition to COR and CVH modeling.







Molten Salt Reactors

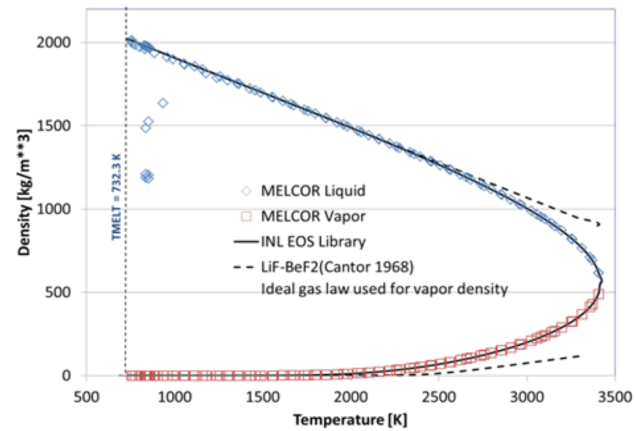
Properties for LiF-BeF2 have been added
- Equation of State (current capability)
- Thermal-mechanical properties (current capability)
- EOS for other molten salt fluids would need to be developed

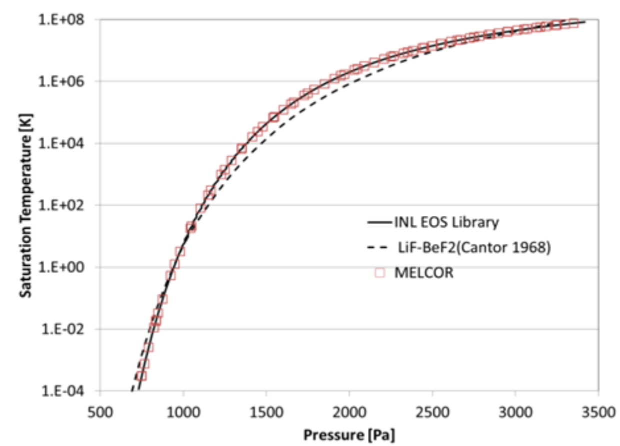
Two reactor types envisioned
- Fixed fuel geometry
  - TRISO fuel models (current capability)
- Liquid fuel geometry
  - MELCOR CVH/RN package can model flow of coolant and advection of internal heat source with minimal changes (current capability)
  - Framework for fission thermal power generation without COR package (current capability)
    - Control volumes defined as "vessel" type or "loop" type
    - Specify axial/radial power profile shape and magnitude (over "vessel" type CV's)
    - Specify flow paths constituting transitions between vessel and loop
    - Preserve decay heat deposition capabilities (CVH/RN1 tracks decay heat from aerosol/vapor already)
  - COR package representation no longer applicable, but structures can be represented by HS package (current capability)
  - Calculation of neutronics kinetics for flowing fuel (under development)

Radionuclide Transport

Molten salt fission product release models (under development)

Thermochemistry modeling using Thermochimica (under development)



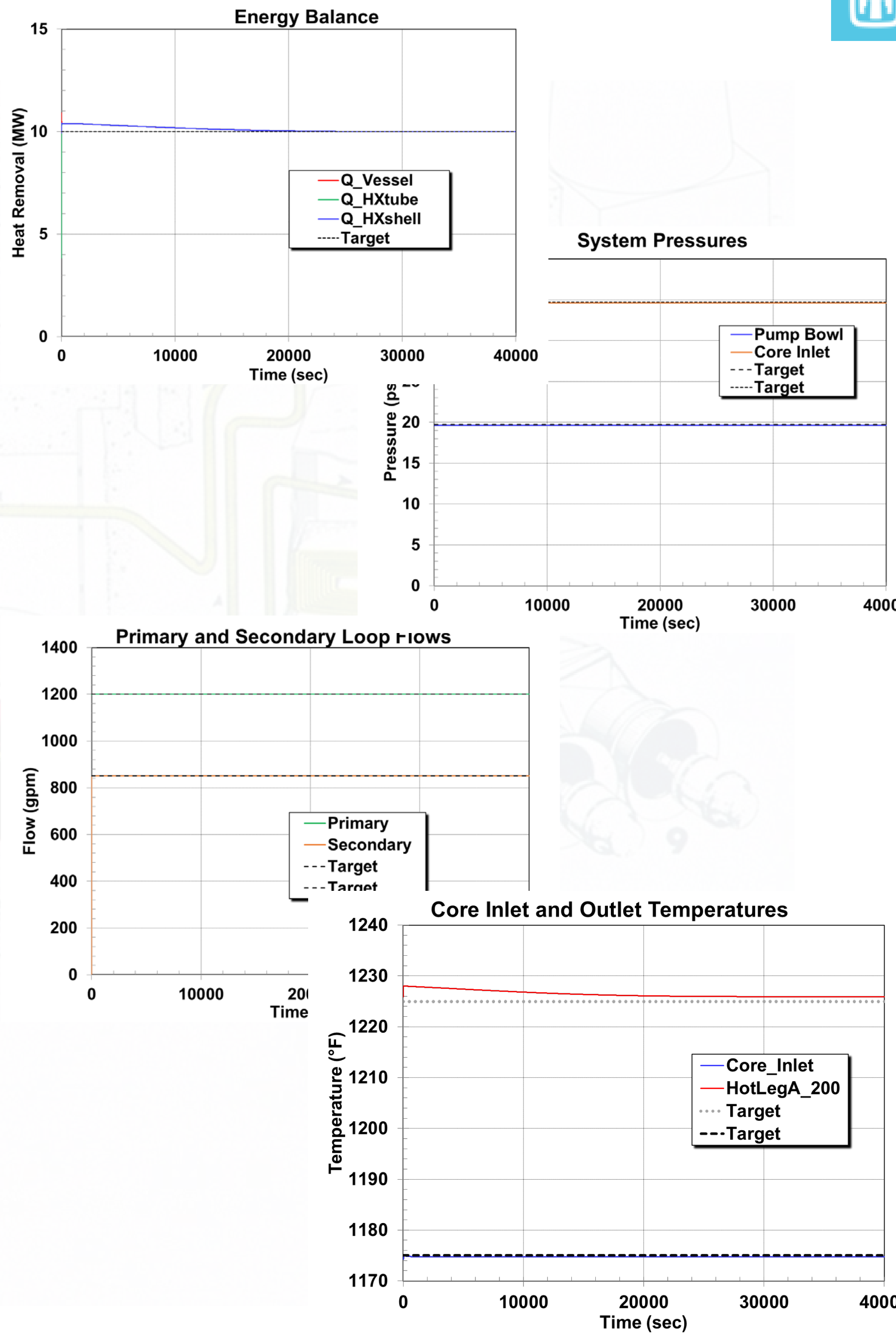


MSRE MELCOR V2.2 Model 2019 Benchmark

Steady state operating conditions

The MELCOR MSRE model includes the following features

- **One-dimensional core**
  - 8 control volumes (2-dimensional enhancement straight-forward)
  - Graphite blocks
  - Connected diversion & drain tank
  - Core-bypass leakage flow
- **Primary system recirculation loop**
  - Schedule 40 INOR-8 piping – a high Nickel alloy (16% Ni, 7% Mo, 5% Cr, 0.05% Fe, 0.05% C)
- **Fuel pump and pump bowl** (aka pressurizer)
  - Connected overflow tank
  - Pump spray with He gas offtake (Xe & Kr removal)
- **Mechanistic horizontal U-tube heat exchanger**
  - 2-dimensional primary system shell-side
  - Secondary coolant flow in U-tube



Molten Salt Reactor Accident Fission Product Transport (Under Development)

Attractive safety features

1. Molten Salt is an unpressurized coolant.
2. Fluoride salts have broad liquid range (e.g. FLiBe, 459 C – 1430 C).
3. Actinides and most fission products are soluble in molten salt.

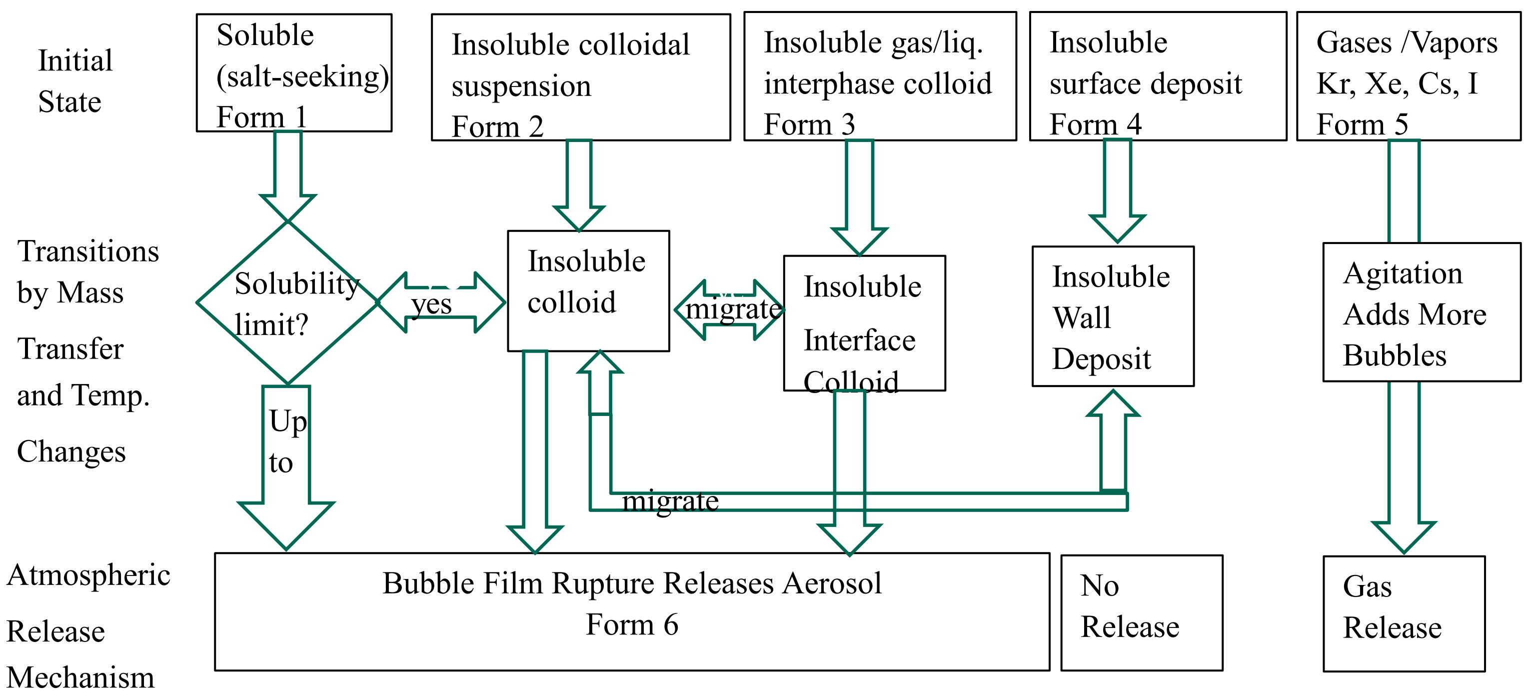
Solubility ≠ Immobility

Release processes

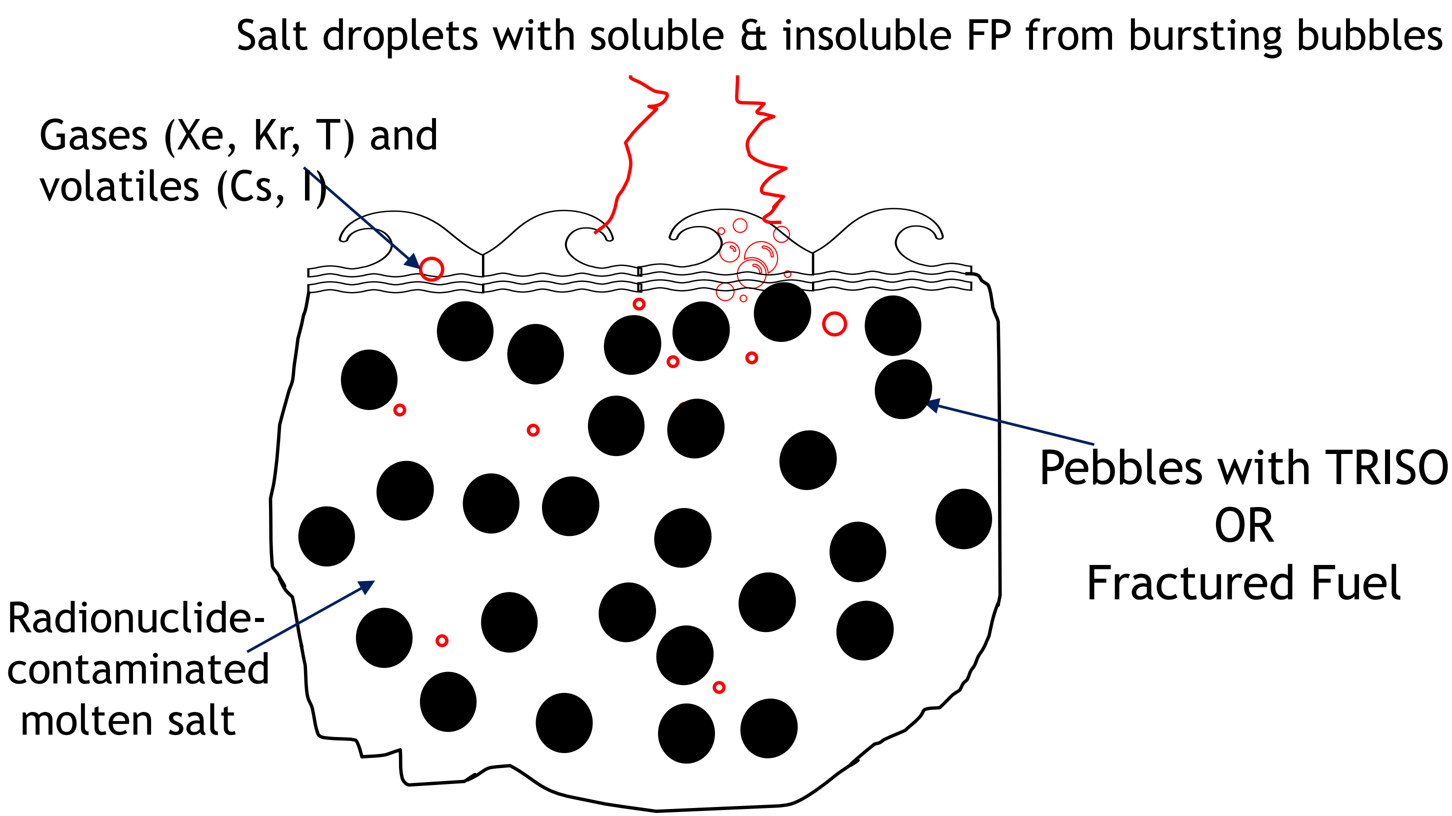
1. MELCOR provides the conditions and species released into salt, and MSM determines how much of that is released to the atmosphere as gas and aerosol particles.
2. Fission products tracked in six areas as observed in MSRE at ORNL.
3. Gases (e.g. Kr, Xe) bubble up through molten salt.
4. Volatile species (e.g. Cs, I) vaporize into bubbles and released at salt top surface, and later condense into particles.
5. Bursting bubbles create aerosol particles of salt droplets containing soluble and insoluble radionuclides.

Schematic of GRTR (Generalized Radionuclide Transport and Retention)

Radionuclides grouped into 6 areas as found in the Molten Salt Reactor Experiments at ORNL



Schematic of Phenomena (accident not expected to be quiescent)



Fluid-Fuel Point Reactor Kinetics (FFPRK) Model

Circulating fuel point kinetics model

$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \bar{\beta}(t)}{\Lambda}\right) P(t) + \sum_{i}^{6} \lambda_i C_i^C + S_0$$

$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P(t) - \left(\lambda_i + {}^2/_{\tau_C}\right) C_i^C(t) + \left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^2/_{\tau_L}\right) C_i^L(t), \qquad i = 1 \ldots 6$$

$$\frac{dC_i^L(t)}{dt} = \left(\frac{V_C}{\tau_C V_L}\right) C_i^C(t) - \left(\lambda_i + {}^1/_{\tau_L}\right) C_i^L(t), \qquad i = 1 \ldots 6$$

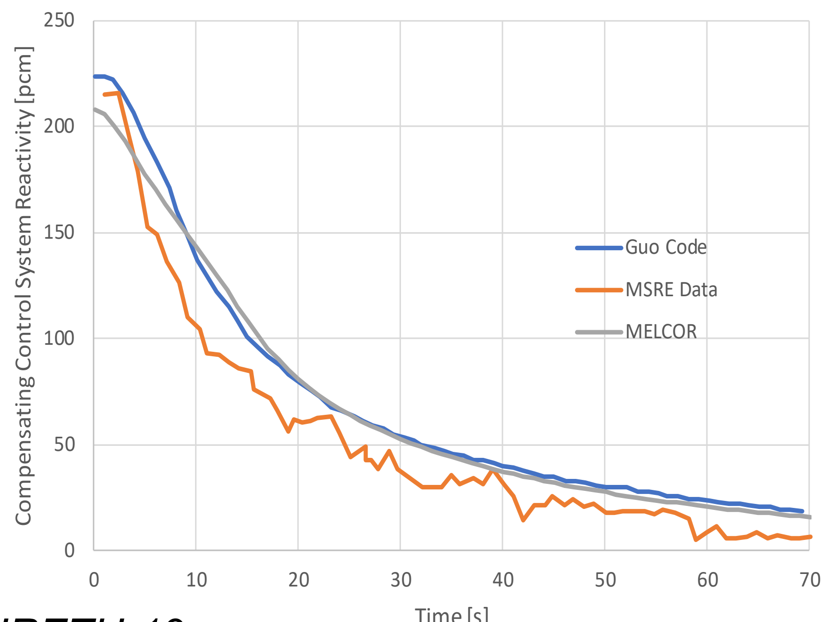
$$\bar{\beta}(t) = \beta - \beta(t)_{lost} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum_{i=1}^{6} \lambda_i C_i^L(t)$$

Show Legend

MSRE Pump Coast-down Compensating reactivity.

Benchmark to MSRE pump coast-down

- Critical at "zero-power" (10 W) and full flow, then initiate a coast-down to zero flow
- Control system intervenes to preserve criticality, thus the control reactivity trace maps flow reactivity
- Pump flow data and control system reactivity response documented in ORNL-4233



Documented in forthcoming NURETH-19 paper

Non-LWR Demonstrations Calculations

Develop an understanding of non-LWR beyond-design-basis-accident behavior

- Provide insights for enhancing source-term regulatory guidance
- Provide NRC staff with an understanding of non-LWR beyond-design-basis-accident behavior
  - Identify key accident characteristics influencing source terms
  - Highlight important uncertainties influencing accident progression and source terms

Demonstrate MELCOR for non-LWR beyond-design-basis accidents

- Distribution of non-LWR input models with MELCOR executable
- Shakedown the MELCOR modeling and identify missing models or data needs

Non-LWR Demonstrations Calculations

Demo Case Selection

- Demonstrate/exercise breadth of non-LWR physics modeled by MELCOR
- Consider NRC priority relative to timing of licensing submittal
- Utilize non-proprietary designs
- Build on existing decks where possible

Demo Cases

PBMR-400

- Pebble bed HTGR
  - Maturity of plant input deck
  - Modeling of pebble bed supports subsequent modeling of FHR accident progression and source term

Megapower Heat Pipe Reactor

- Heat pipe reactor
  - 1st priority due to imminent submittal of Oklo application
  - Insights into accident progression and source term will support NRC review of Oklo

Flouride Salt Cooled High Temperature Reactor

- Pebble bed FHR
  - Builds on work to evaluate pebble bed HTGR
  - Additional modeling capability evaluated related to molten salt working fluid

Extensions to the CF Package

Ranges
- User defined construct that generates an ordered list of objects to be used by vectorized CFs

Vectorized CF arguments
- Control Function arguments can now be specified as a vector of values by specifying and index with a range

Vector Control Functions
- Certain control functions now permit vector operations such as add, multiply, divide, equals, L-GT, L-GE, etc.

Package input support of vector CFs
- Some input records have been modified to allow vector fields in place of scalar fields

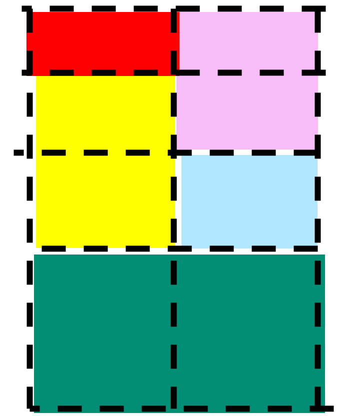
Analytic Control Functions
- Ultimate flexibility allowing users to pass vectors to a user specified FORTRAN function.

Vectorized Formula type CF (NEW in 2019 release)
- Integrates ranges into the 'Formula' type CF

Dependent Ranges for Vector CFs (New in 2020 Release)

A new keyword for constructing a range was added to facilitate the use of vectors in analytic functions. This new keyword references another range (i.e., #Range1) since it is entirely dependent on the other range for definition. As an example,

- A range was constructed for all COR cells of interest in the calculation
- For each COR cell in this range, a range consisting of the control volume associated with each cell is desired.
- This new construction keyword generates that range automatically and guarantees a one-to-one correspondence.



- COR cells indicated by dashed lines
- CV volumes indicated by colors

```
CF_RANGE CORCELLS2 CELLS 10
CONSTRUCT 1
  1 ALL
CF_RANGE CVCELLS CVOLUMES 20
CONSTRUCT 1
  1 #CORCELLS2
```

CORCELLS2	CVCELLS
Cell101	CV_GREEN
Cell102	CV_Yellow
Cell 103	CV_Yellow
Cell 104	CV_Red
Cell 201	CV_GREEN
Cell 202	CV_Blue
Cell 203	CV_Pink
Cell 204	CV_Pink

Improvements to Lower Head Model (New in 2020 Release)

Spheroidal Lower Head

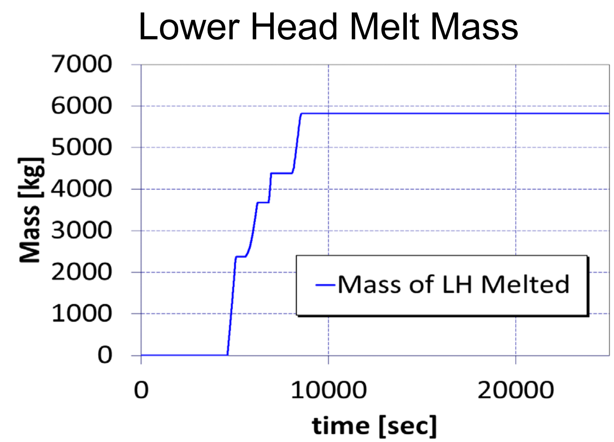
- Generalization of hemisphere model to allow for an oblated lower cap
- Users specify two dimensions: a horizontal radius and a vertical radius

Spheroidal Lower Head

```
!       RCOR  RVESS  ILHTRN  DZRV  DZLH  ILHTYP      ELLIPA  ELLIPC
COR_VP  1.8   2.2    RVESS   0.24  0.24  SPHEROIDAL  2.5     1.25
```

Melting Lower Head

- Debris relocating to the lower head contains sufficient decay heat to lead to melting of the interior surface of the lower head.
- Though MELCOR already accounts for the reduction in load-bearing material as the lower head melts, it does not allow the melted material to become part of the COR package where it
  - can affect heat transfer (focusing effect) of molten materials,
  - can be oxidized (contributing to hydrogen production),
  - can be transferred to the CAV package for MCCI.
- This code modification will source steel into the calculation along with the associated thermal energy where the COR package then takes control for further relocation



Limitations:

Currently only accounts for melting carbon steel

Mass, energy, and available volume sourced into the COR package

Currently only SS can receive the melting carbon steel

Mechanical Properties of Lower Head

SC 1602 – Vessel Steel Elastic Modulus Parameters

The elastic modulus of vessel steel is given as a function of temperature, T, by

$$E(T) = C1602(1) \cdot \left(\left\{ 1 + [T / C1602(3)]^{C1602(4)} \right\}^{-1} - \left\{ 1 + [C1602(2) / C1602(3)]^{C1602(4)} \right\}^{-1} \right)$$

(1) Leading multiplicative constant.
(default = 2.E11, units = Pa, equiv = none)
(2) Temperature at which elastic modulus vanishes.
(default = 1800.0, units = K, equiv = none)
(3) Temperature at which elastic modulus is approx halved.
(default = 900.0, units = K, equiv = none)
(4) Exponent of scaled temperatures.
(default = 6.0, units = none, equiv = none)

SC1603 – Vessel Steel Yield Stress Parameters

The yield stress of vessel steel is given as a function of temperature, T, by

$$\sigma_Y(T) = C1603(1) \cdot \left(\left\{ 1 + [T / C1603(3)]^{C1603(4)} \right\}^{-1} - \left\{ 1 + [C1603(2) / C1603(3)]^{C1603(4)} \right\}^{-1} \right)$$

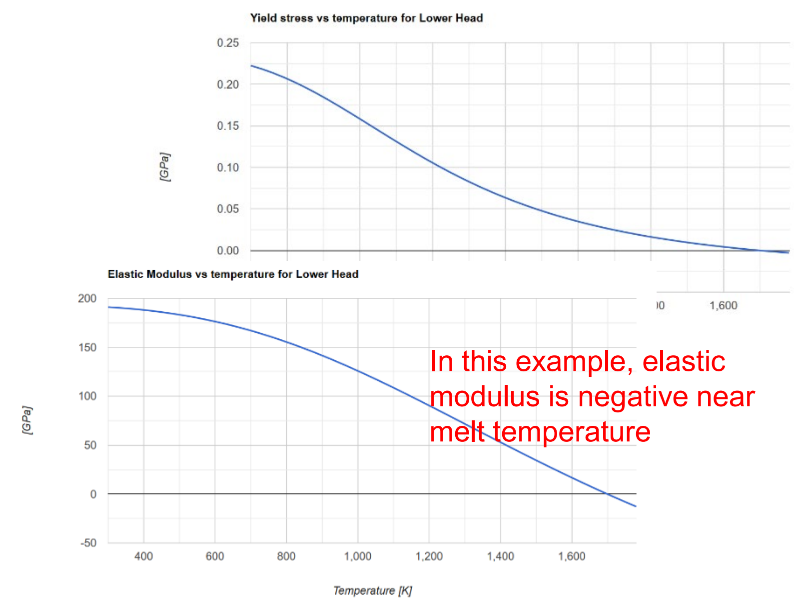
(1) Leading multiplicative constant.
(default = 4.E8, units = Pa, equiv = none)
(2) Temperature at which yield stress vanishes.
(default = 1700.0, units = K, equiv = none)
(3) Temperature at which yield stress is approx halved.
(default = 900.0, units = K, equiv = none)
(4) Exponent of scaled temperatures.
(default = 6.0, units = none, equiv = none)

New in 2020 Release

- Lower Head Yield Stress & Elastic Modulus can now also be specified by a Tabular Function with optional fields on COR_LH

```
COR_LH    8   0  ElasticModulus YieldStress

TF_ID 'ElasticModulus'    1.0 !(
TF_TAB   2
          1      273.15     0.15E9
          2      1.0E+5     0.15E9
```

- Lower Head Yield Stress & Elastic Modulus plotted in HTML during MELGEN



Material Property Development (New in 2020 Release)

User-defined Materials

- Default material properties can be templated onto new materials
- Can be defined for COR with extra input
  - Emissivity, Viscosity, Thermal expansion coefficient, Oxidation behavior

- COR User-Defined Material

```
MP_ID       NewZirc  COR-USER-METAL  NUZR
MP_BHVR     Zircaloy  METAL   OXIDATION-MODEL
EXEMPT
MP_BETMU    1.65E-5   3313.0  1.076E-3
MP_COREMIS CF  'NewEmissivity'  0.0001  0.9999
```

- Initialize Mass in component

```
COR_NMAT 1 ! IA    IR   IC   USRM1   USRM2   USRM3
USRM4
         1   ALL   ALL CL   0.0     0.0     64.2    0.0
```

- Associate with metal pool

```
COR_LAY 1 ! LAYMAT   MPLAY
        1   NUZR     UPPER   ! Associate with MP2
```

Generalized Oxidation Model (New in 2020 Release)

Historically, MELCOR had a specific set of oxidizable material:

- Zirconium, Stainless-steel, Graphite, B_4C, Aluminum
- Now extended to use the user-defined materials (UDMs)

General Oxidation Model makes use of the new UDMs to create a new oxidizable material.

- Define a reactant core material, COR-USER-METAL, and its oxide product, COR-USER-OXIDE.User permitted to fully specify material properties
- May use templating or be wholly user-defined

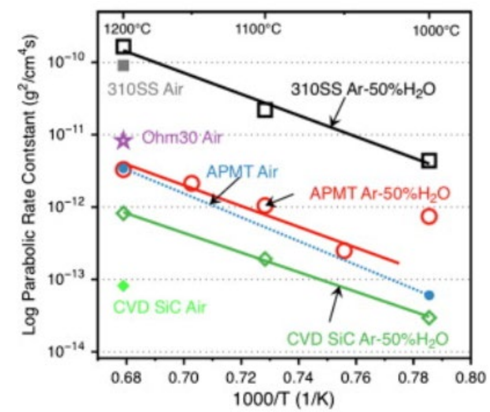
```
MP_ID FeCrAl COR-USER-METAL UFCA
MP_BHVR    Itself  METAL   OXIDATION-MODEL
EXEMPT
MP_BETMU   3.1e-5 7.7 3313. 1.076e-3
MP_COREMIS linear - 0.0001 0.9999
0.042003702 0.0003474
MP_PRTF 4 ! NPAR PROPERTY DEFAULT/TF/CF(may
be only for THC)
        1 ENH FCA-IntEn
        2 CPS FCA-SpHeat
        3 THC FCA-Conduct TF
        4 RHO FCA-Density

MP_ID FeCrAl-Oxide COR-USER-OXIDE UFCAO
MP_BHVR ITSELF
MP_PRC 5180.0 1901.0 687463.0 193.4102395
MP_COREMIS linear - 0.0 1.0 0.7 0.0
MP_BETMU 3.1e-5 7.7 3313. 1.076e-3
MP_PRTF 4 ! NPAR PROPERTY DEFAULT/TF/CF(may
be only for THC)
        1 ENH FCAO-IntEn
        2 CPS FCAO-SpHeat
        3 THC FCAO-Conduct TF
        4 RHO FCAO-Density
```

ATF – Oxidation Simple Reaction Assumptions

While it is recognized that an alumina layer initially forms, MELCOR materials do not presently track oxidation of constituents individually.

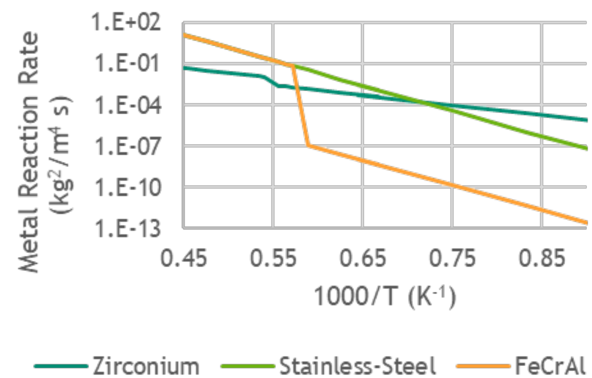
Stoichiometric reactions of the following equations are simply applied producing an assumed FeCrAl-Oxide, similar to the default stainless-steel treatment:

$$Fe + \frac{4}{3}H_2O \rightarrow \frac{1}{3}Fe_3O_4 + \frac{4}{3}H_2 + Q_{ox}$$
$$Cr + \frac{3}{2}H_2O \rightarrow \frac{1}{2}Cr_2O_3 + \frac{3}{2}H_2 + Q_{ox}$$
$$Al + \frac{3}{2}H_2O \rightarrow \frac{1}{2}Al_2O_3 + \frac{3}{2}H_2 + Q_{ox}$$



Reaction Rates (based on prior work by INL/ORNL)

- Pre-Breakaway
  - Reaction rates apply data from Pint, et.al
- Post-breakaway
  - Rates are taken from Stainless-steel as a surrogate until additional data are available
- Breakaway
  - Based on ORNL experiments, the breakaway transition was set to 1425-1450C by default
    - available as sensitivity coefficients



FeCrAl clad oxidation modeled using new Generalized Oxidation Model cladding

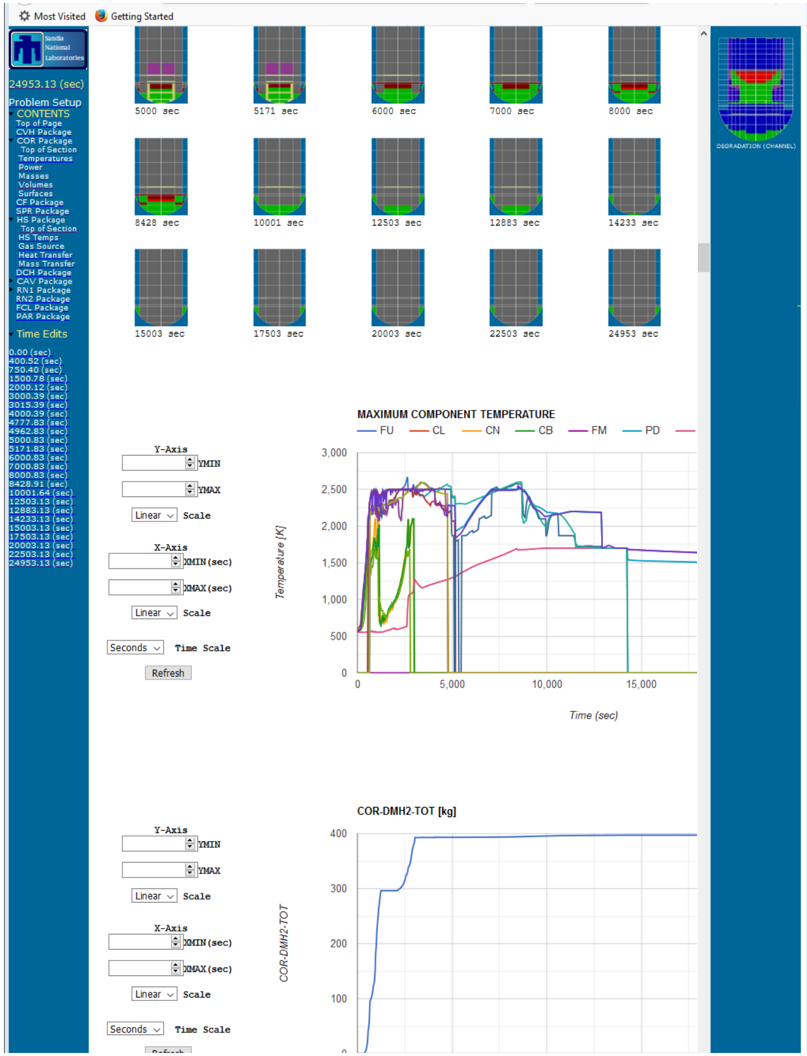
Merrill, B.J., Bragg-Sitton, S.M., Humrickhouse, P.W., Modification of MELCOR for Severe Accident Analysis of Candidate Accident Tolerant Cladding Materials, Nuclear Engineering and Design 315 170-178, 2017

K.R. Robb, H. Howell, and L.J. Ott, "Design and Analysis of Oxidation Tests to Inform FeCrAl ATF Severe Accident Models", Oak Ridge National Laboratory, ORNL/SPR-2018/893 (July 2018).

B.A. Pint, et al., "High Temperature Oxidation of Fuel Cladding Candidate Materials in Steam-Hydrogen Environments," Journal of Nuclear Materials 440, pp. 420-427, 2013.

HTML Output

- Lightning fast hyper-linked navigation to MELCOR output
- Graphical depiction of core degradation
- Automatic plot generation for enhanced user efficiency
- Trend plots, profile plots, animated plots
- Plots of material property functions, EOS functions, and fluid properties automatically generated for user verification/QA
- Animated temperature profile for greater insight into accident progression
- User customized plots and model specific plots for ultimate flexibility
- Embed user customized HTML input for problem description
- Access to more data: Energy balances, energy/mass error plots, aerosol size distribution plots, CPU, distribution of aerosol sectional mass, core degradation, candled material distributions, …

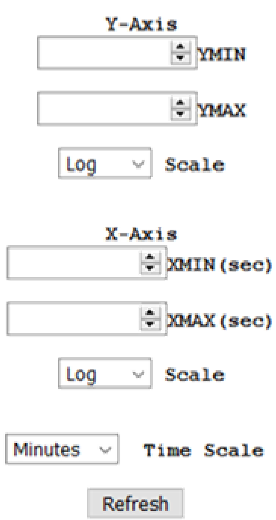


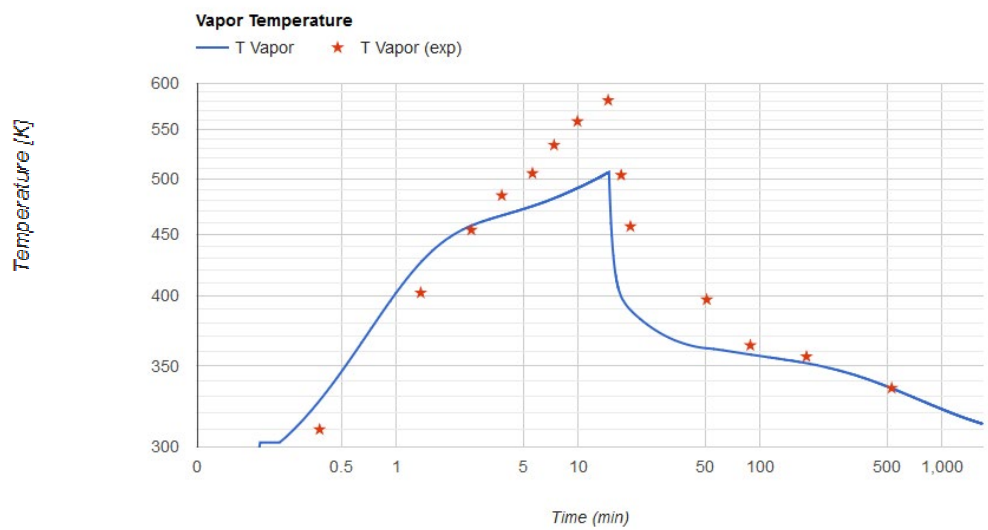
User Customized Plots

- User can easily add plots of control functions or any plot variable to HTML output.
- Controls
  - Time units can be changed in HTML plot
  - Log/Linear scale for x or y axis
- Maximum and minimum values can be selected by user

Minimal input required

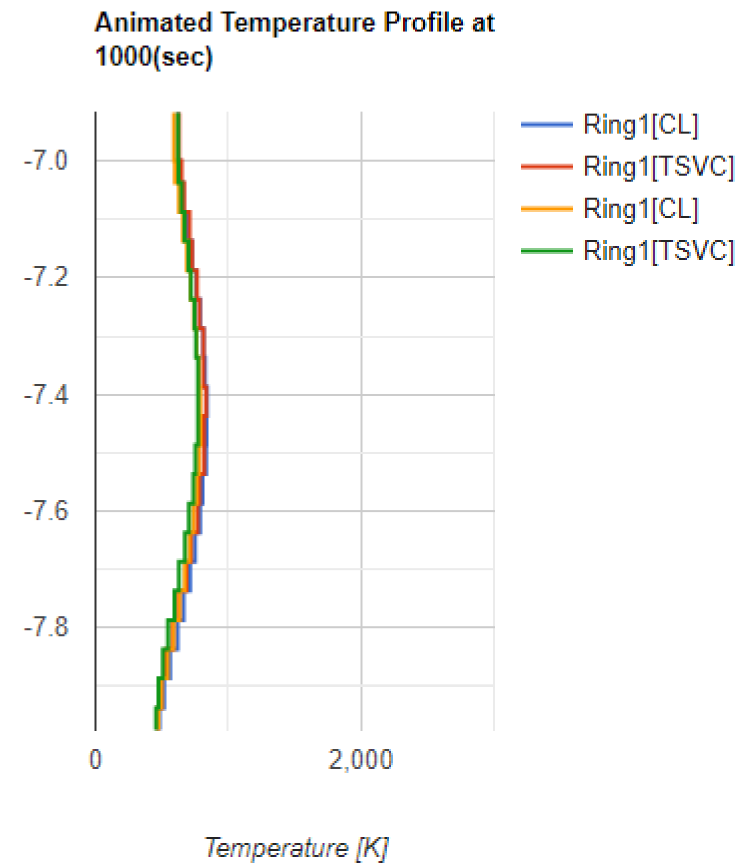
```
CF_HTML  4
 1 'Integral Hydrogen Mass'  'Int H2'   'Int H2 (Exp)'
 2 'Vapor Temperature SG-HL-313' 'CVH-TVAP.313'   'TEPF717'
 3 'Vapor Temperature SG-HL-316' 'CVH-TVAP.316'   'TEPF719'
 4 'Vapor Temperature SG-HL-319' 'CVH-TVAP.319'   'TEPF721'
```

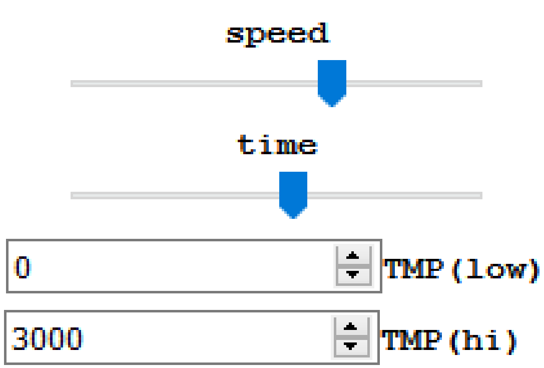




Static and Animated Profiles

- Temperatures, mass, power, surface area, volumes
- Static plots generated automatically at each time edit
  - MELGEN plots provide graphical means for verifying input
- User can create animations of component temperature profile
  - Local COR atmosphere fluid temperature and lower head temperature also supported
  - Controls
    - Playback speed
    - Scroll to time frame
    - Maximum and minimum temperature scale





Minimal Input Required

```
COR_AXPLT 2
 1  RING1   3  CL  1  FU 1 NS 1 20.0  0
 2  RING1b   4  CL  1 TSVC 1 CL  2 TSVC 2 20.0  0
```

Material Property Plots Generated at MELGEN

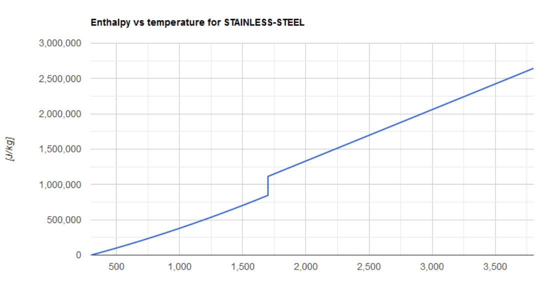
MATERIAL PROPERTIES PACKAGE

Show Properties for fiberglass

Show Properties for STAINLESS-STEEL

Show Properties for ZIRCALOY

- Materials
  - User-defined materials
  - Default Materials
- Properties
  - Thermal conductivity
  - Enthalpy
  - Heat capacity

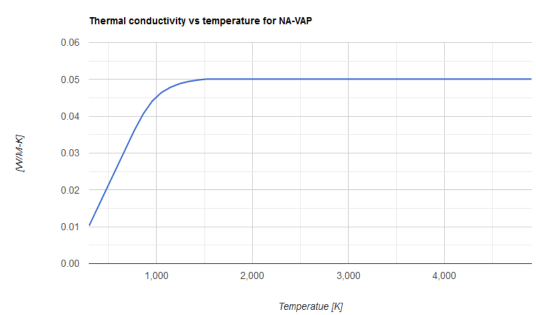


NON CONDENSIBLE GAS PACKAGE

Show Properties for POOL

Show Properties for NA-VAP

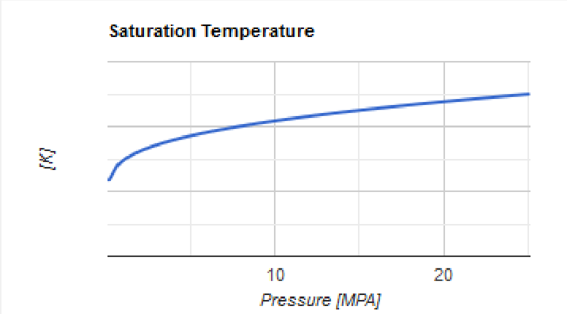
- Viscosity
- Thermal conductivity



Equation of State PACKAGE

EOS Properties for Na

- Saturation Pressure
- Saturation Temperature
- Liquid Density at saturation
- Vapor density at saturation
- Liquid specific enthalpy at saturation pressure
- Vapor specific enthalpy at saturation pressure
- Liquid specific heat
- Vapor specific heat

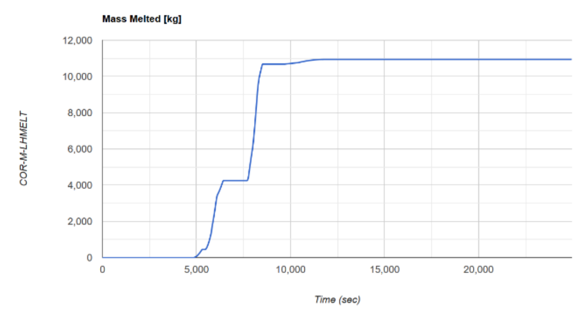


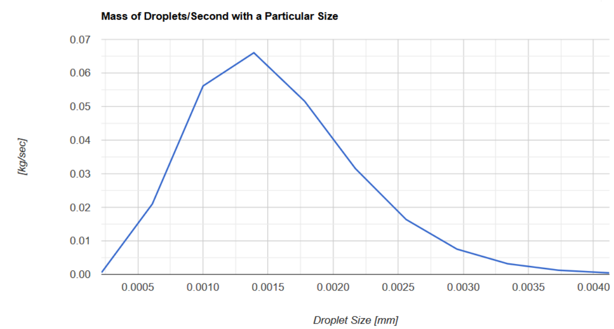
Additions to HTML in MELCOR 2020 Release

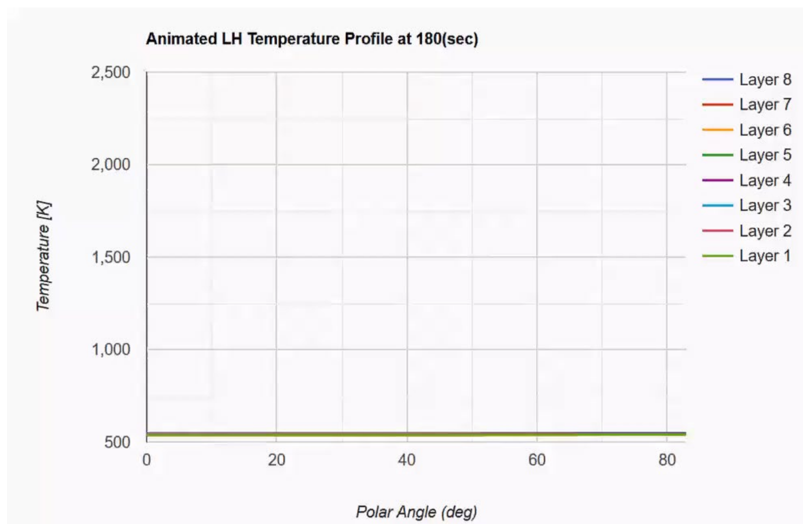
New plots generated at each write to text output

- Mass of melt from lower head
- Lower head energy balance
- Polar plot of temperature profile in lower head
- Heat of mixture (eutectics) added to energy balance
- Added plots for sodium spray fire
  - Number (or mass) of droplet of a particular size
  - Droplet velocity with time (by size)
  - Mass fraction burned with time(by droplet size)
  - Droplet temperature with time (by size)
  - Droplet diameter with time (by size)

Animation of lower head temperatures

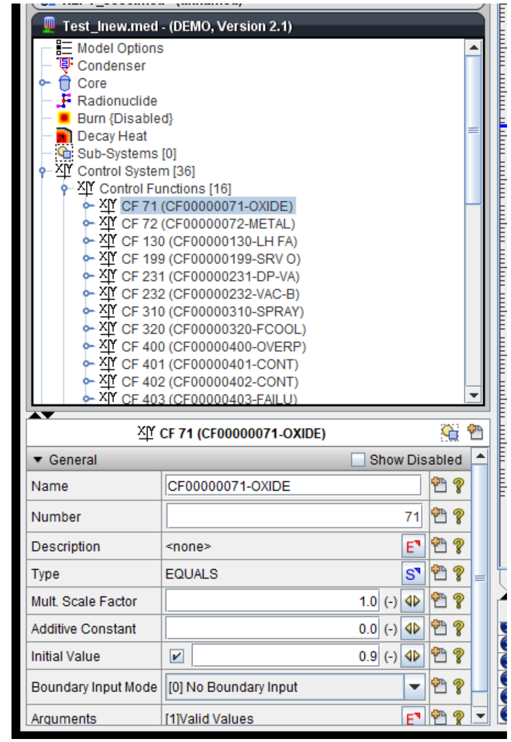


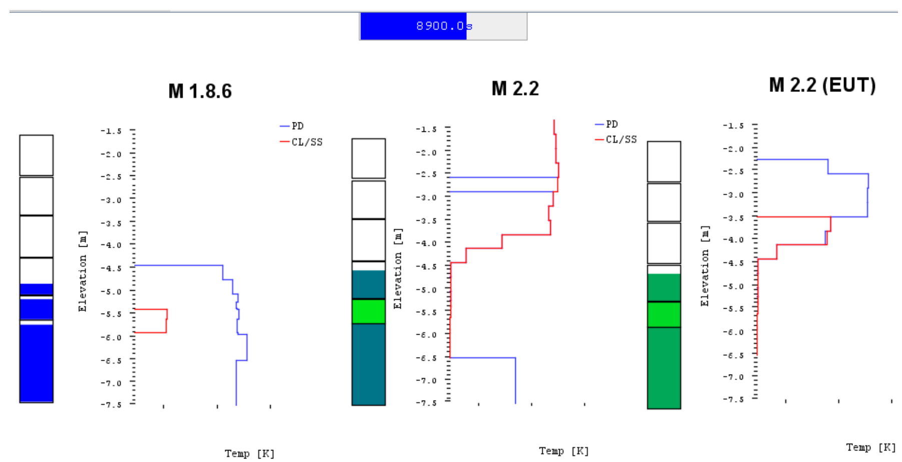




SNAP Upgrade

- MELCOR 2.2 plugin update
  - Support input for new models
    - Vector Control Functions
    - LHC Package
    - Radiation enclosure model
    - New MCCI Models
    - Support for named comment blocks
    - Support for Variable input.
  - Most features have been implemented
    - Testing phase
  - Post-processing Improvements?





MELCOR 2.2.18019 Code Release (December 23, 2020)

SAND2021-0726 O

MELCOR Computer Code Manuals

Vol. 1: Primer and Users' Guide
Version 2.2.18019

Date Published: January 2021

Prepared by
L.L. Humphries, B.A. Beeny, F. Gelbard, D.L. Louie, J. Phillips, R.C. Schmidt, N.E. Bixler

Sandia National Laboratories
Albuquerque, NM 87185-0748

Operated for the U.S. Department of Energy

H. Esmaili, Nuclear Regulatory Commission Project Manager

Prepared for Division of Systems Analysis
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

SAND2021-0241 O

MELCOR Computer Code Manuals

Vol. 2: Reference Manual
Version 2.2.18019

Date Published: January 2021

Prepared by
L.L. Humphries, B.A. Beeny, F. Gelbard, T. Haskin, D.L. Louie, J. Phillips, R.C. Schmidt, N.E. Bixler

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U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

SAND2015-6693 R

MELCOR Computer Code Manuals

Vol. 3: MELCOR Assessment Problems
Version 2.1.7347 2015

Date Published: August 2015

Prepared by: L. L. Humphries, D. L. Y. Louie, V. G. Figueroa, M. F. Young, S. Weber, K. Ross, J. Phillips, and R. J. Jun*

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Volume I: User Guide — SAND2021-0726 O

Volume II: Reference Manual — SAND2021-0241 O

Volume III: Assessments — SAND2015-6693 R

Volume III to be updated by September 2022

2.2.18019 Quicklook: New defaults, significant code corrections, new models, validation cases, single parameter variant study, code performance.

MELCOR Modeling Guide (Volume IV)

- User Guidance
  - MELCOR has a steep learning curve and guidance is needed to help new users learn how to develop input decks.
    - Generate non-proprietary plant decks
      - BWR, PWR, SFP
    - Volume IV references these sample plant decks
  - Provide meaningful insights, recommendations, demonstrations of modeling methodology in a formal report for many commonly asked questions across much of the model space
  - Describe pitfalls and methods for troubleshooting and assessing results.
    - How to address code execution problems
    - How to review results to know the code is giving reasonable results
- Best Practices
  - Provide guidelines for appropriate use of the code in modeling severe accidents.
    - Recommended models and model options

Topics

- COR/CVH Nodalization
- HTGR Modeling
- Heat Pipe Modeling
- Molten Salt Modeling
- Sodium Reactor Modeling
- Spent Fuel Pool Modeling
- Containment DBA
- Numerical Variance
- Uncertainty Analysis
- FL/CVH Modeling
- Steady State Initialization
- Radionuclide Class Modeling
- MELCOR/MACCS Integration
- Troubleshooting MELCOR runtime issues
- Lower Head Modeling
- Heat Structure Modeling
- Cavity Related Modeling
- Fusion Applications

MELCOR Code Stress Testing and Debugging

LWR Applications

Plant Deck	Number of Variants
PWR	36
BWR	48

- Surry and Sequoyah decks updated to latest best practices. SBO, Large break, Small break, pump seal failure, etc.
- Peach Bottom and Grand Gulf decks updated to latest best practices, STSBO, LTSBO, small break, ATWS

Non-LWR Applications

Reactor Type	Number of Variants
Heat Pipe	Reference Calcs: 9 TOP references Uncertainty Variants: > 1000 TOP
HTGR	Model Testing: 10 TRISO Reference Calcs: 20 DLOFCs, Uncertainty Variants >1000 DLOFC variants planned
FHR	Reference Calcs: 5 LOCAs & 5 LOPAs, Uncertainty Variants: >100 planned for each
MSR	Pending

MELCOR Modernization Plan (5 years)

Modernization

- Improvements in code structure designed to strengthen
  - Performance – shorter run times and more robust calculation
  - Numerics – reduced numerical variance, improved accuracy, and improved characterization of uncertainty
  - Capability – Removal of limitations that hinder modeling of some effects
  - Maintainability – more extensible framework to allow code to adapt to new reactor designs., flexibility in future code/model development
- Maintain currently validated physics
  - Objective is not to add new physics models
  - This is not a re-write of the code (still FORTRAN though incorporating new FORTRAN features and possible other languages in new modules/routines)
- Incremental benefits in the existing code base

Five Year Plan

- Generalized Numerical Solution Engine Module
- MELCOR hydrodynamic modeling
- MELCOR In-Vessel Core Damage Progression
- Ex-Vessel Damage Progression
- Fission Product Release and Transport Modeling
- Rationalization of Current MELCOR Code Base with Modernized MELCOR Code Base / Finalization of the Modernized Code

Generalized Numerical Solution Methods

Implementation of a generalized numerical solution framework that can integrate a range of numerical algorithms required by MELCOR to advance the state of the plant to the next point in simulation time.

- Stateless, Testable, Defined interface

This does not apply to a specific area of phenomenological modeling.

The functionality implemented during this phase enables the modernization of the MELCOR code architecture, separating numerical solution functionality from functionality that implements the representation of physical models in software.

MELCOR hydrodynamic modeling

Reformulation of the hydrodynamic equation set and numerical solution scheme to utilize an enhanced solver. This will enhance overall robustness of the numerical solution, adopting state-of-the-art numerical solution methods.

This effort is necessary to enhance the capabilities of the hydrodynamics numerical solution strategy to reflect new strategies developed to handle known issues where the hydrodynamic equations are particularly difficult to solve.

MELCOR In-Vessel Core Damage Progression

Generalization of the code architecture to simplify the addition of new components, improve numerics, and restructure the lower head model to improve treatment of melting and interactions with the lower head.

COR component objects

The COR database will be restructured to allow creation of component objects with properties such as oxidation, hold-up, number of surfaces in contact with CVH, etc. to allow templating for new components. This should allow more flexibility for users in defining COR component attributes for specific design needs.

Candling Model

Currently MELCOR will move melting material down a component surface (candle) in a single time step. Such modeling overlooks the oxidation that may occur during the transition and would affects the heat transfer.

Material interactions

Enhancements will enable the code to more adequately reflect new types of material interactions in advanced reactors and for ATF, and more generally treat fission product speciation.

Lower Head Structure

- The lower head model will be rewritten to improve the numerical solution of the equations to better account for melting at the interior boundary.

MELCOR In-Vessel Core Damage Progression

Original code conversion

cor%cell(i,j)%new
- cor%cell(i,j)%new%volu{...}
  - cor%cell(i,j)%new%volu(1:kcmp)
  - cor%cell(I,j)%new%volu(LVHSST)
  - cor%cell(I,j)%new%volu(LVHP)
  - cor%cell(i,j)%new%volu(LVFLUB)
  - cor%cell(i,j)%new%volu(LVFRE)
  - cor%cell(i,j)%new%volu(LVFREB)
  - cor%cell(i,j)%new%volu(LVTOT)
  - cor%cell(i,j)%new%volu(LVTOTB)
- cor%cell(i,j)%new%xmdp
- cor%cell(i,j)%new%xmdb
- cor%cell(i,j)%new%xm1p
- cor%cell(i,j)%new%xm1b
- cor%cell(i,j)%new%xm2p
- cor%cell(i,j)%new%xm2b
- cor%cell(i,j)%new%xmcs
- cor%cell(i,j)%new%xmns
- cor%cell(i,j)%new%xmss
- cor%cell(i,j)%new%xmcb
- cor%cell(i,j)%new%xmcn
- cor%cell(i,j)%new%xmcl
- cor%cell(i,j)%new%xmfl

- cor%cell(i,j)%old{...}
  - cor%cell(i,j)%new%volu
  - cor%cell(i,j)%new%xmdp
  - cor%cell(i,j)%new% ...
- cor%cell(i,j)%cellcomp(:)%new{...}
  - cor%cell(i,j)%cellcomp(:)%new%xmdc
  - cor%cell(i,j)%cellcomp(:)%new%voly
  - cor%cell(i,j)%cellcomp(:)%new%volt
- cor%cell(i,j)%cellsurf(:) {...}
  - cor%cell(i,j)%cellsurf(:)%ASURI
  - cor%cell(i,j)%cellsurf(:)%ASURY
  - ...

After Modernization

cor%cellcomp(ic) {...}
- cor%cellcomp(ic)%voluIntact(inew,i,j)
- cor%cellcomp(ic)%volConglomerate(inew,i,j)
- cor%cellcomp(ic)%volEff(inew,i,j)
- cor%cellcomp(ic)%**MassIntact**(inew,i,j)
- cor%cellcomp(ic)%MassConglomerate(inew,i,j)
- cor%cellcomp(ic)%NSURF
- cor%cellcomp(ic)%Surfaces{...}
  - cor%cellcomp(ic)%Surfaces(inew,isurf,i,j)
    - cor%cellcomp(ic)%Surfaces(inew,isurf,i,j)%ASURI
    - cor%cellcomp(ic)%Surfaces(inew,isurf,i,j)%ASURY
    - …

- cor%cel(i,j)%VOLU(:)
- cor%cell(i,j)%new%volu{...}
  - cor%voluNonComp(inew,LVHSST,i,j)
  - cor%voluNonComp(inew,LVHP ,i,j)
  - cor%voluNonComp(inew, LVFLUB ,i,j)
  - cor%voluNonComp(inew, LVFRE ,i,j)
  - cor%voluNonComp(inew, LVFREB ,i,j)
  - cor%voluNonComp(inew, LVTOT ,i,j)
  - cor%voluNonComp(inew, LVTOTB ,i,j)

- Structure changes
  - Components are objects at highest level
  - COR cell is just a dimension on an array at the deepest level
  - Remove old/new structure and use inew as an index that is used to swap new and old at end of timestep
- Motivation
  - Simplifies Coding
  - Easier to add new components
  - Easier to add properties to all components
  - Facilitate debugging
  - Performance improvements due to localization, stride reduction
  - Achieving identical results from restarts
  - Finding/reducing cliff-edge effects

Ex-Vessel Damage Progression

Code Numerics

- The numerical solution and physical modeling functionality will be separated. Introduction of a state-of-the-art numerical solution methodology will be performed.

Generalized Geometry

- A key component of this effort also involves generalization of how ex-vessel geometries (i.e., the cavity beneath reactor vessels) are represented. This will facilitate significantly enhanced functionality in support of greater severe accident modeling realism, critical to evaluating efforts to credit insights from Fukushima Daiichi accident.

Replace Vanessa with a generalized Gibbs free energy minimizer

Fission Product Release and Transport Modeling

Improvements to numerics

- The numerical solution and physical modeling functionality will be separated. Introduction of a state-of-the-art numerical solution methodology will be performed. A result of this effort will be a modernization of the underlying radionuclide transport equations (in the MAEROS model).

Improvements to RN class representations

- Generalized to facilitate more flexible addition of new classes.
- The ability to template radionuclide classes from an existing class.
- Generalization of chemical interactions to enable modeling radionuclides undergoing chemical reactions and transformations between classes.

Questions

- MELCOR Code Development
  - New Modeling
    - Non-LWR Models
      - HTGR
      - Heat Pipe Reactors
      - Molten Salt Reactors
    - LWRs
      - Melting Lower Head
      - New Defaults (MCCI, eutectics, etc.)
  - SQA
    - Documentation
    - Validation
  - Utilities
    - SNAP
      - Upgrade for new models
    - HTML
  - Modernization