SAND2022-7755D

MELCOR Posters

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.

MELCOR Emerging Applications

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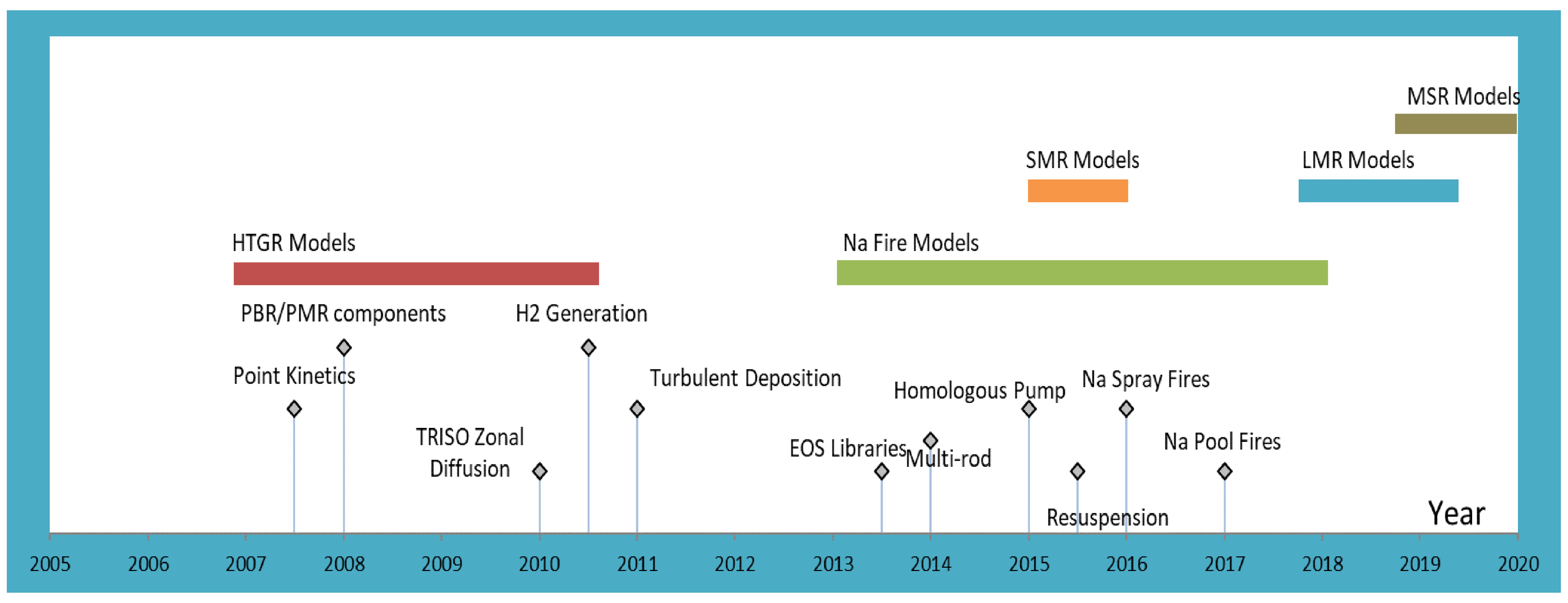
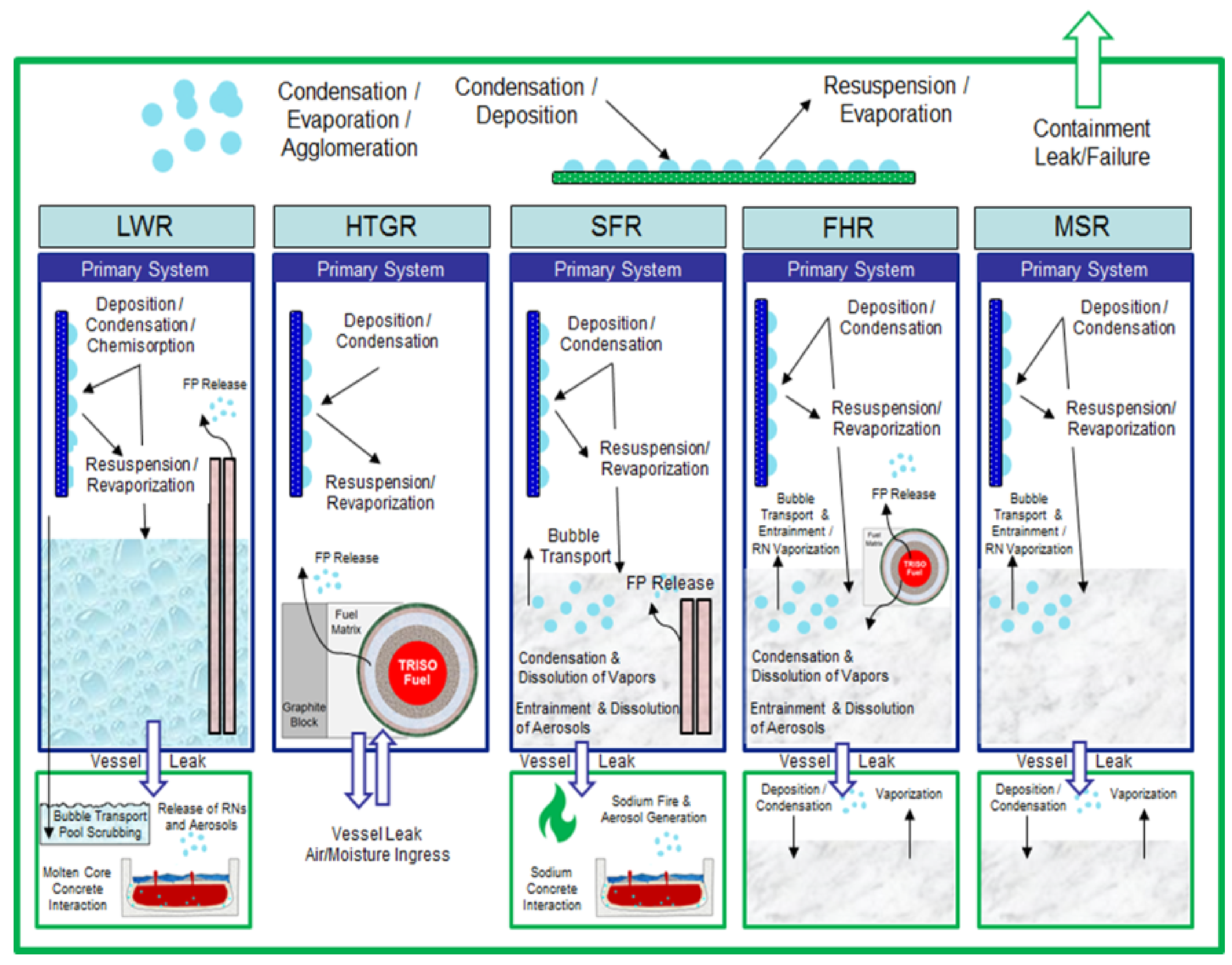
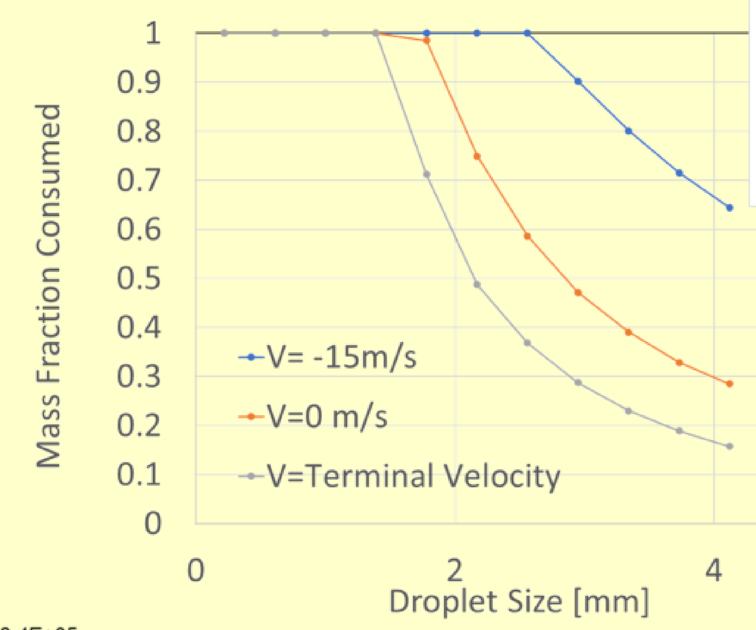
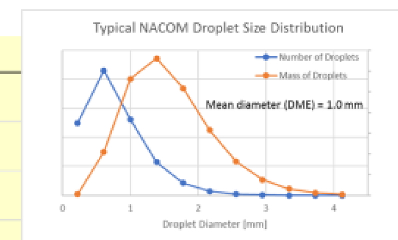


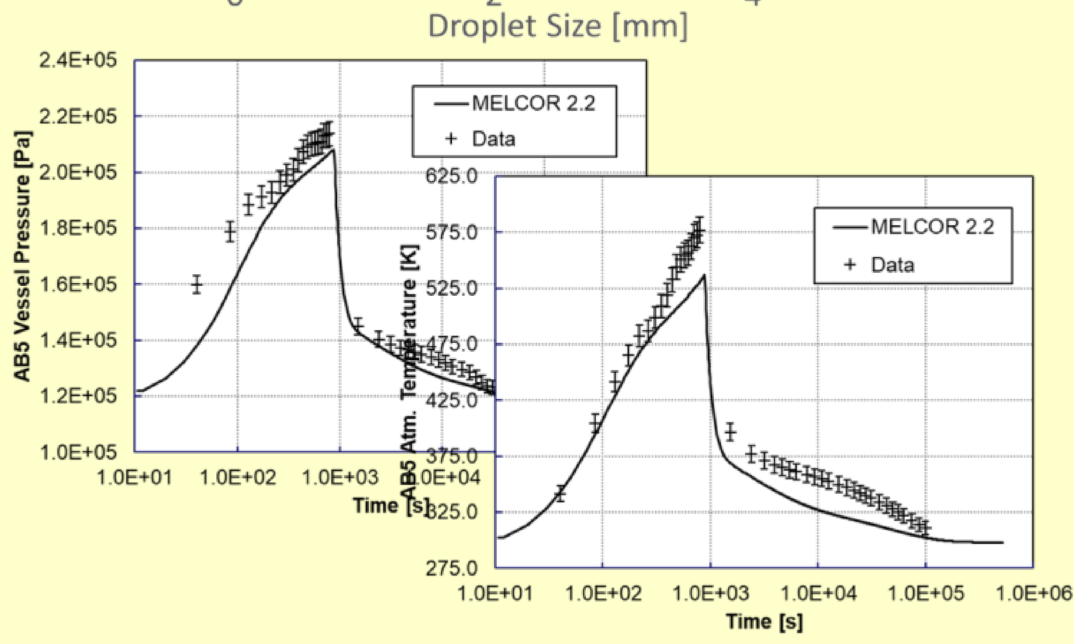


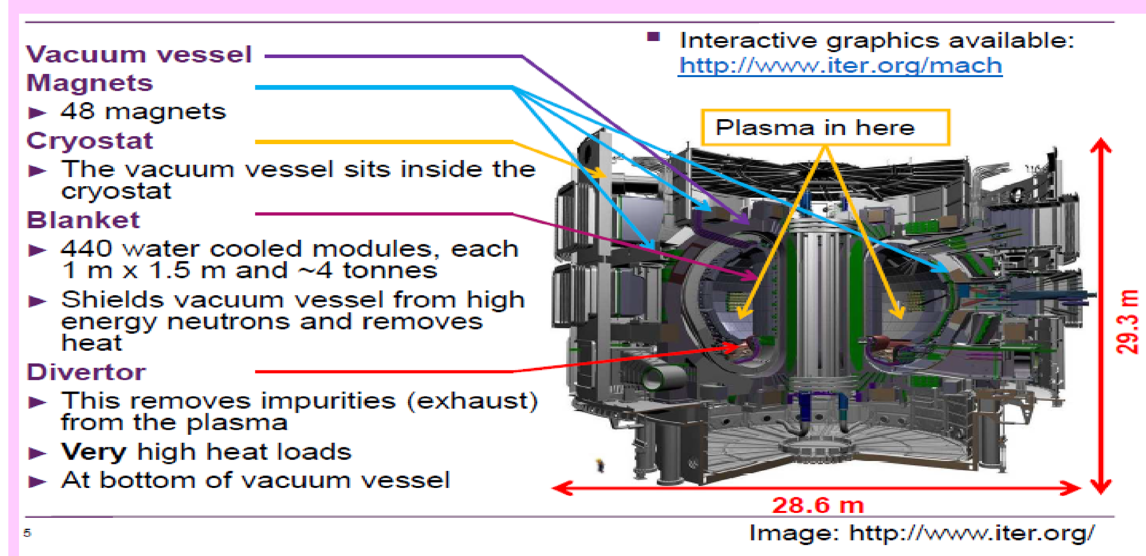
Sodium Reactors

- Sodium Properties
  - Sodium Equation of State
  - Sodium Thermo-mechanical properties
- Containment Modeling
  - Sodium pool fire model
  - Sodium spray fire model
  - Atmospheric chemistry model
  - Sodium-concrete interaction







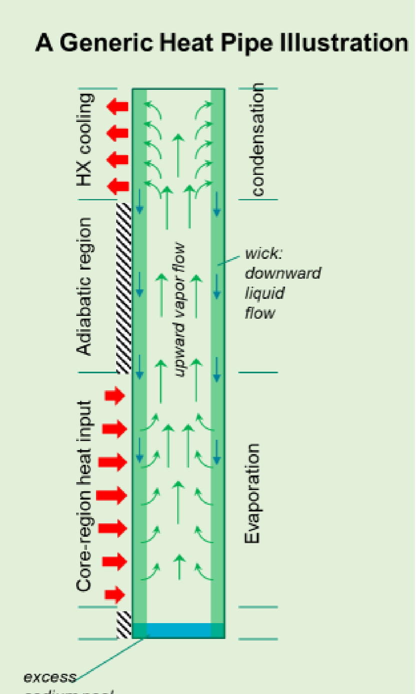


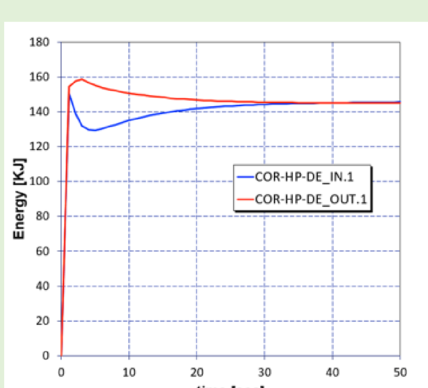
Fusion

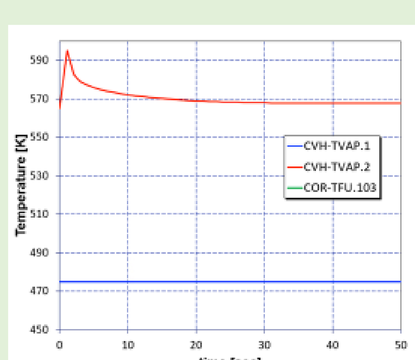
- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

Micro Reactors

- MELCOR 2 model for simulation of Heat Pipes (HP) to transfer heat from the fuel to the secondary coolant flow.





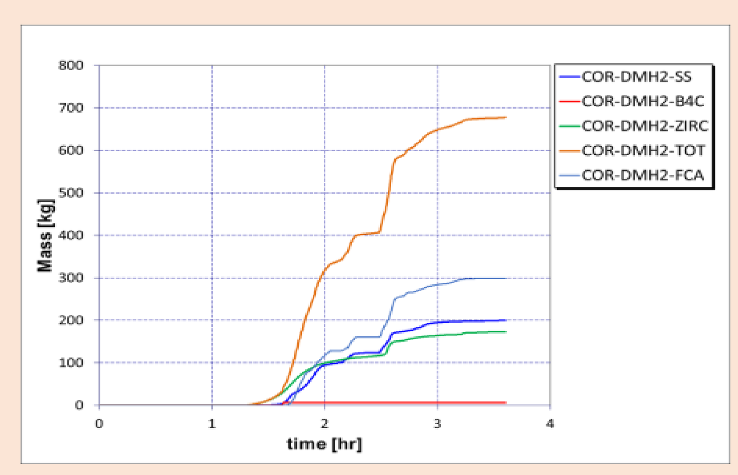


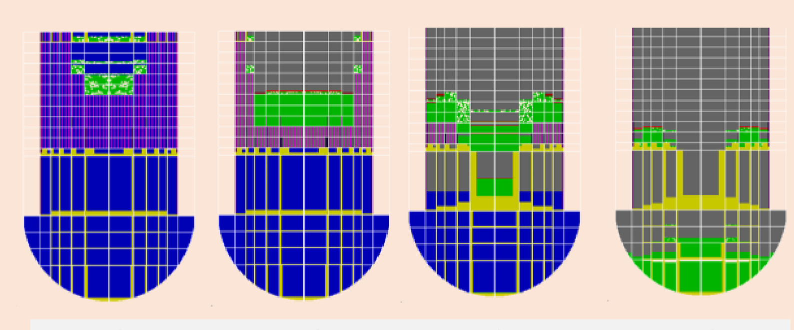
Accident Tolerant Fuels

FeCrAl has been added as a new cladding material has been added to MELCOR
- New thermal properties
  - Kanthal-APMT material and the ORNL material handbook.
- Oxidation Model
  - Pre breakaway - Pint, et.al
  - Post breakaway – Stainless-steel for now

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

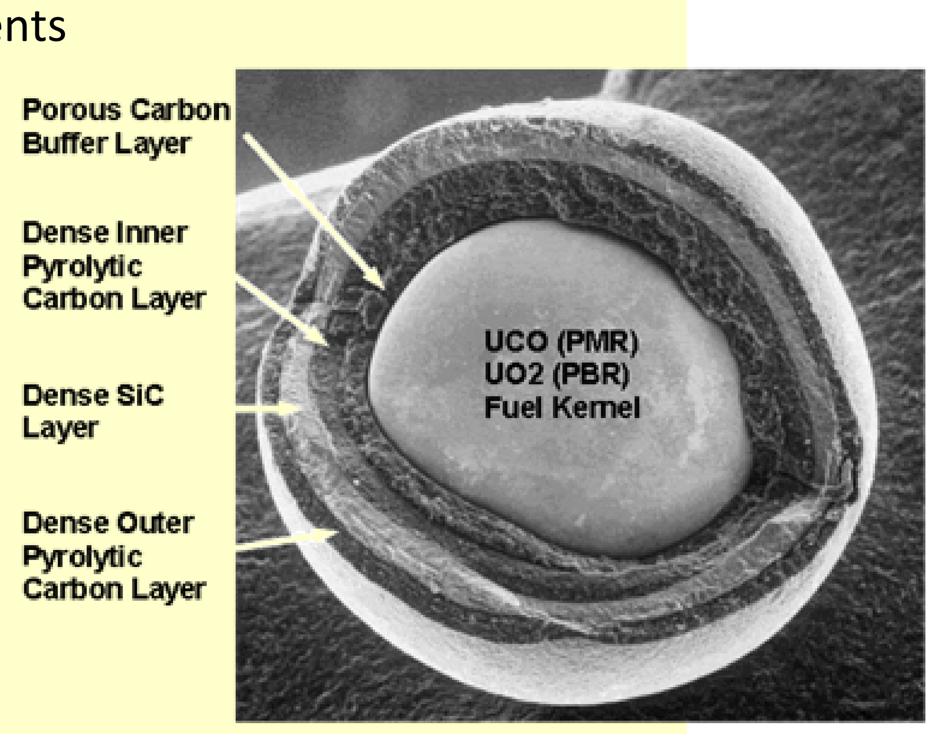
$$Fe + \frac{4}{3}H_2O \rightarrow \frac{1}{3}Fe_3O_4 + \frac{4}{3}H_2 + Q_{ox}$$
$$Cr + \frac{3}{2}H_2O \rightarrow \frac{1}{2}Cr_2O_3 + \frac{3}{2}H_2 + Q_{ox}$$
$$Al + \frac{3}{2}H_2O \rightarrow \frac{1}{2}Al_2O_3 + \frac{3}{2}H_2 + Q_{ox}$$

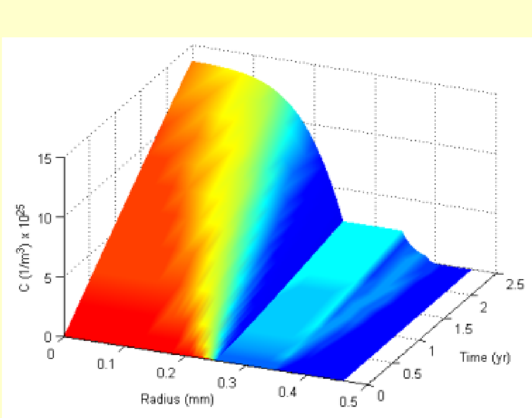


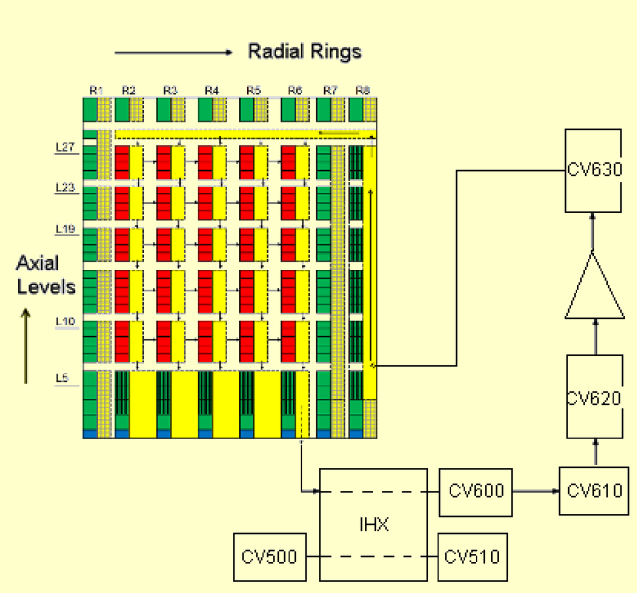


High Temperature Gas Reactors

- Reactor Components
  - Pebble Bed Reactor components
  - Prismatic Reactor Components
- Materials
  - TRISO Fuel Modeling
    - Fission product release modeling
  - Helium Treatment
  - Graphite modeling
    - Oxidation Models
- Graphite Dust Modeling
  - Aerosol physics models
    - Turbulent Deposition
    - Resuspension
- Point Kinetics Model
- Steady state initialization and transient solution strategy

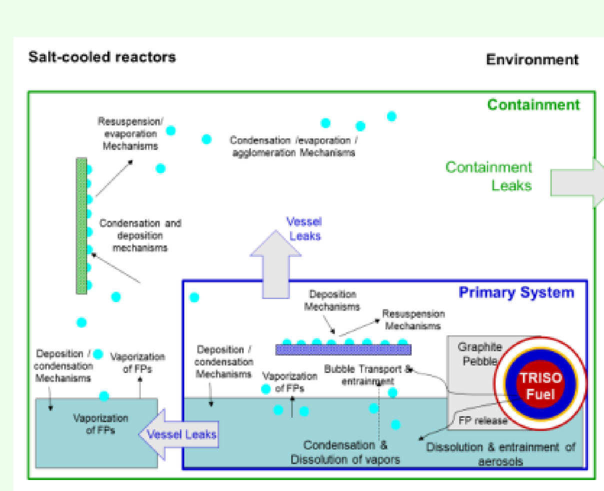


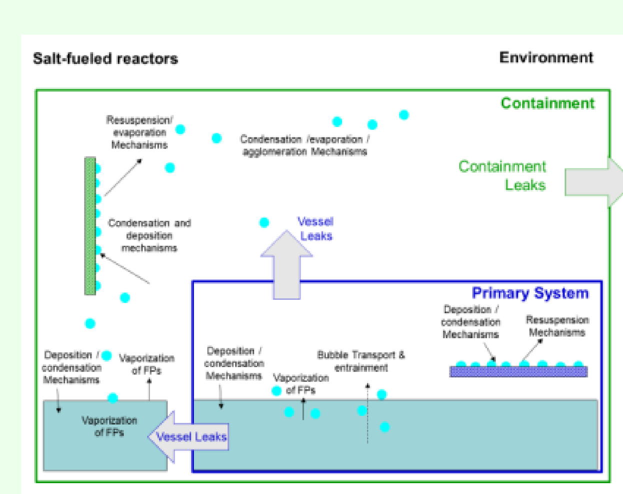


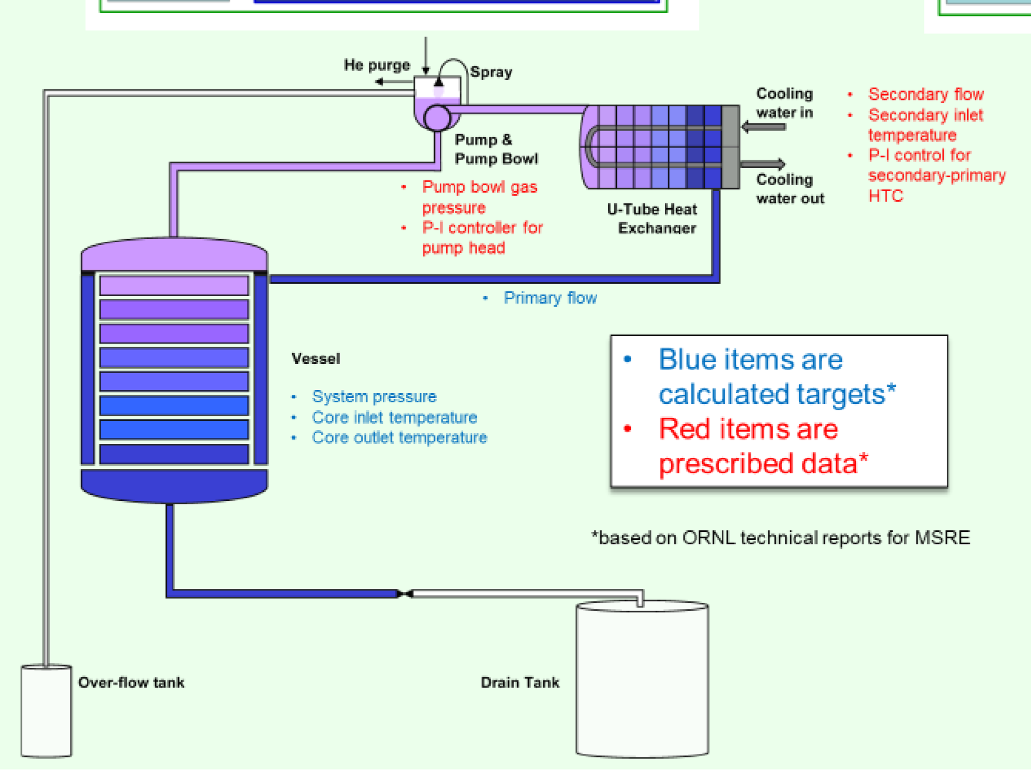


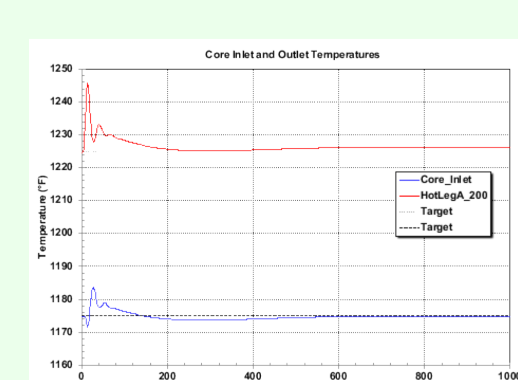
Molten Salt Reactors

- Leverage previous work and existing capabilities for salt-fueled and salt-cooled MSRs:
  - General EOS library read-in utility - developed for sodium/SFRs - enabled FLiBe (among others) as working fluid
  - TRISO fuel and pebble bed models – developed for HTGRs
  - Miscellaneous physics (see below) and flexible code architecture

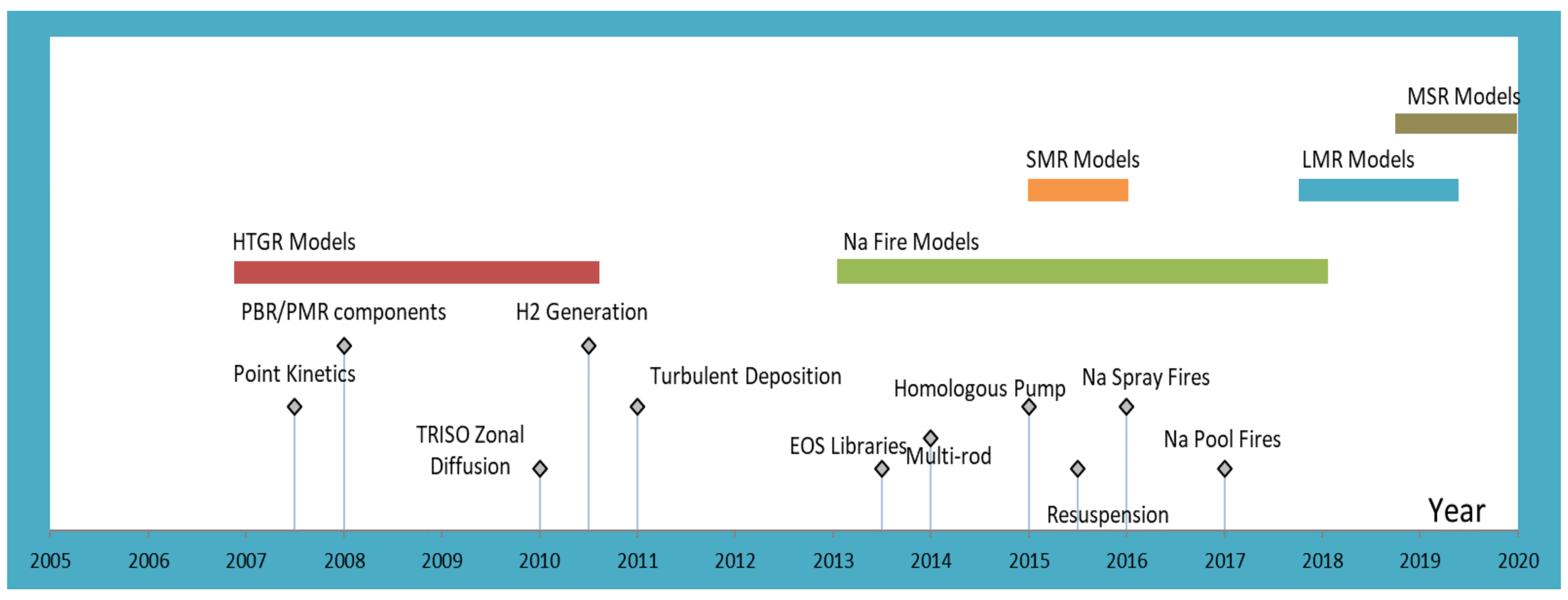








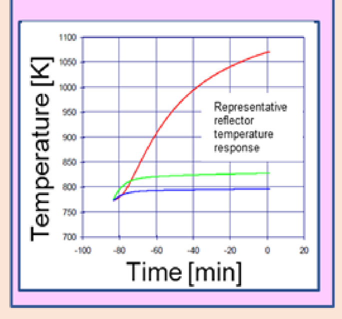
HTGR Reactor Modeling



Transient Accident Methodology

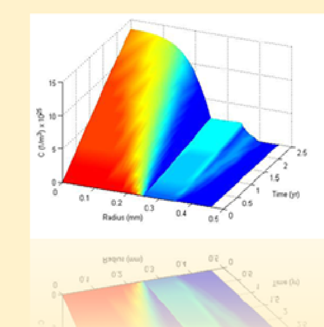
Stage 0: Normal Operation — Establish thermal state

- *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.*



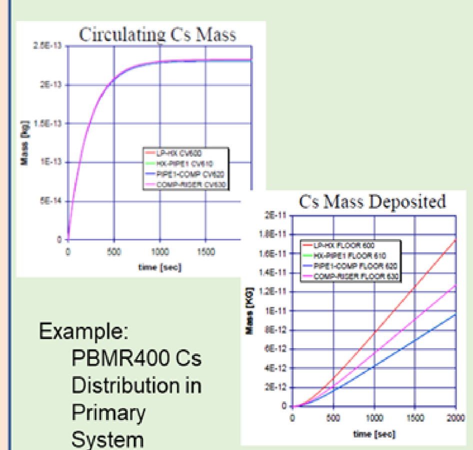
Stage 1: Normal Operation — Diffusion Calculation

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



Stage 2: Normal Operation — Transport Calculation

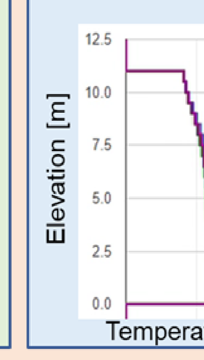
Calculate steady state distribution of radionuclides throughout system during normal operation (deposition on surfaces, convection through flow paths, etc.)

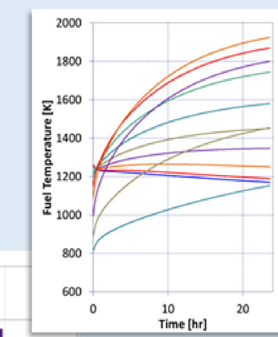


Example: PBMR400 Cs Distribution in Primary System

Stage 3: Accident — Diffusion & Transport calculation

Calculate accident progression and radionuclide release





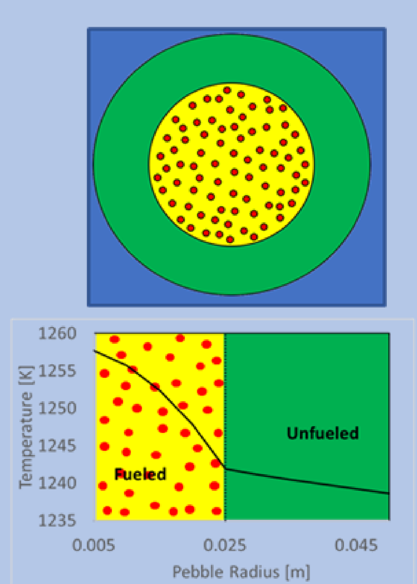
All steps performed in one run with data passed transparently between stages

HTGR Components

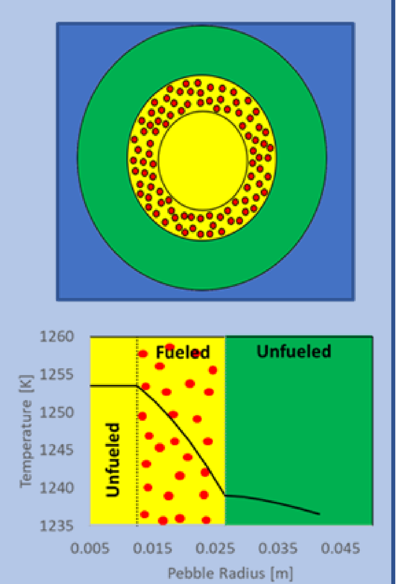
Pebble Bed Reactor (PBR) Fuel/Matrix Components

- 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

Fueled pebble core

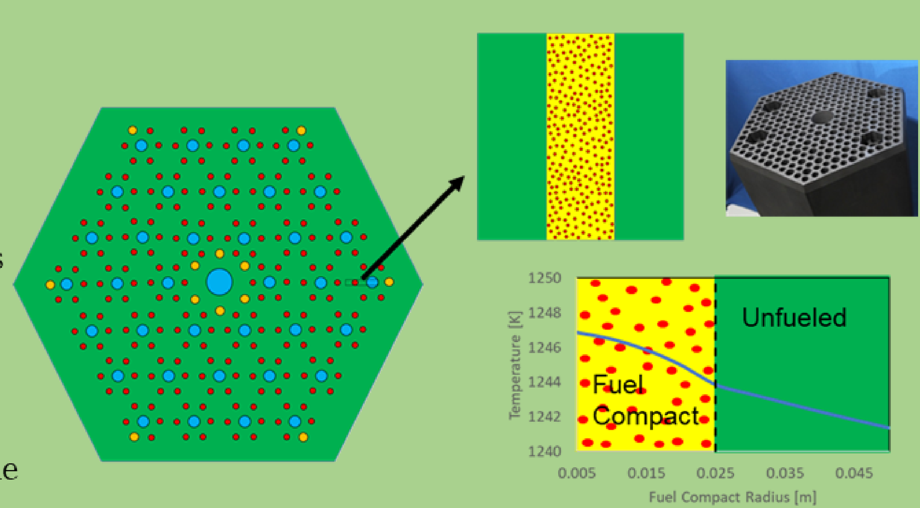


Unfueled pebble core

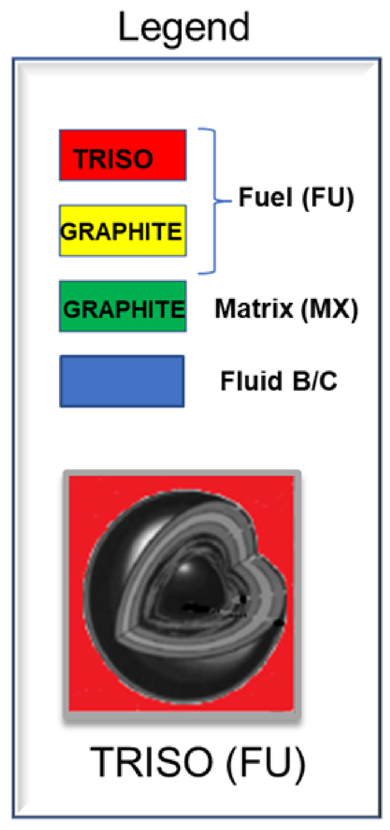


Prismatic Modular Reactor (PMR) Fuel/Matrix Components

- 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



Legend



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

Point Reactor Kinetics

Standard delayed-group treatment

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

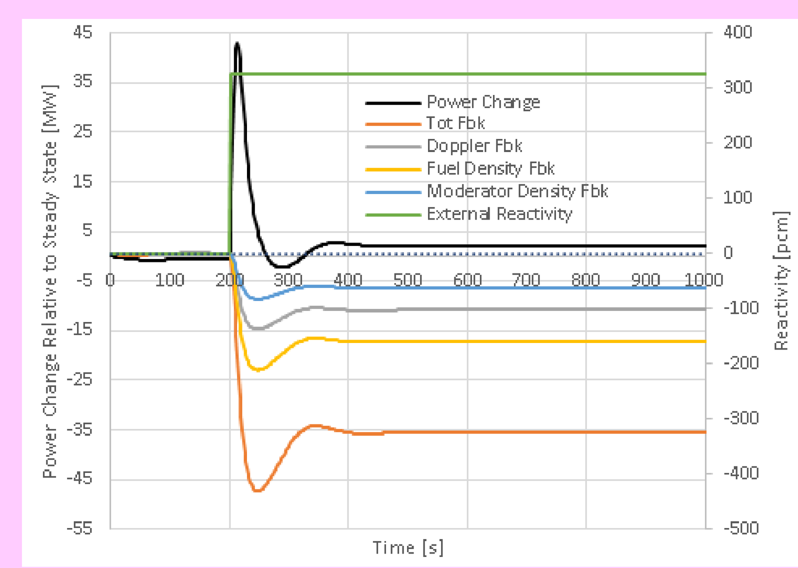
$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right)P - \lambda_i C_i, \qquad for\ i = 1 \dots 6$$

Kinetics data accessible by sensitivity coefficients

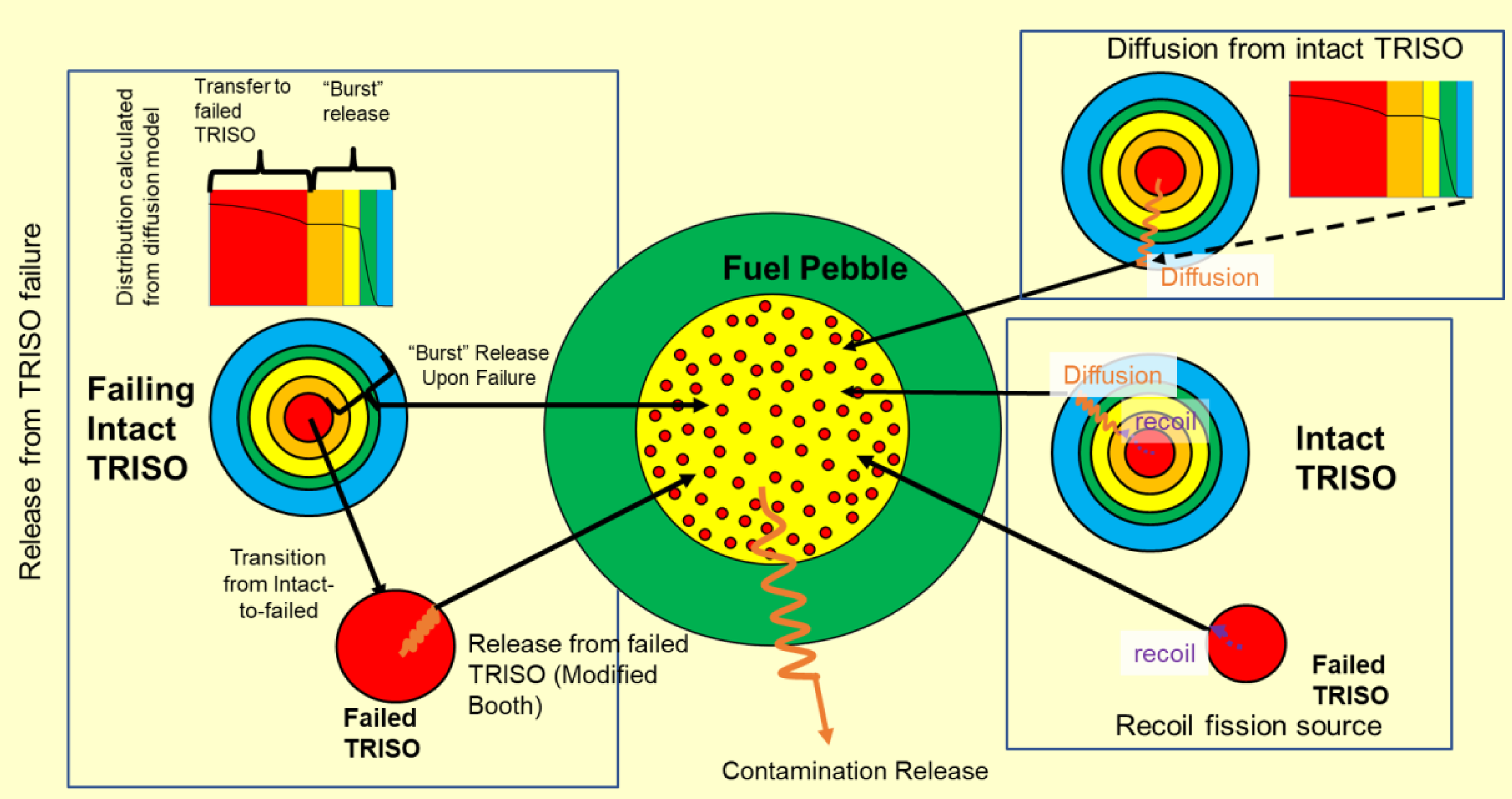
Feedback models

- Control function-specified externalcomponent
- Doppler
- Fuel and moderator density

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

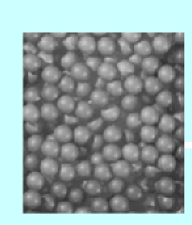


Release Models



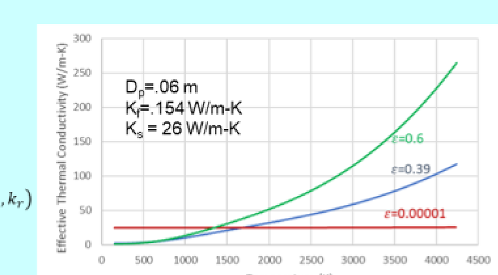
COR Intercell Conduction

Effective conductivity prescription for PBR (bed conductance)

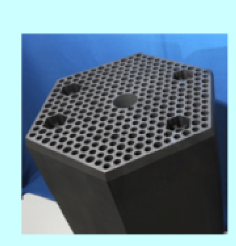


- Zehner-Schlunder-Bauer with Breitbach-Barthels modification to the radiation term

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



Effective conductivity prescription for PMR (continuous solid with pores)



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

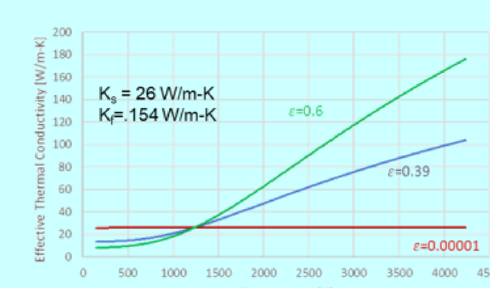
$$k_{eff} = k_s\left[A + (1-A)\frac{\ln\left(1 + 2B\left(k_{por}/k_s - 1\right)\right)}{2B\left(1 - k_s/k_{por}\right)}\right]$$

- 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

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



Graphite Oxidation

Steam oxidation

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

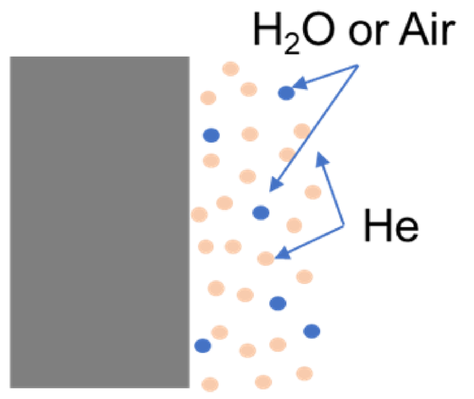
Reaction	+ Energy
$C + H_2O(g) \rightarrow CO(g) + H_2(g)$	
$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$	

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

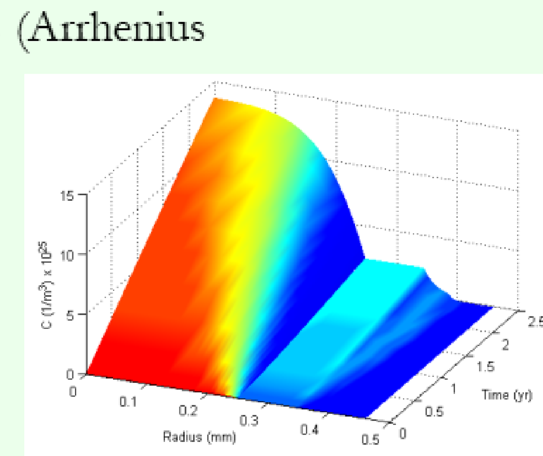


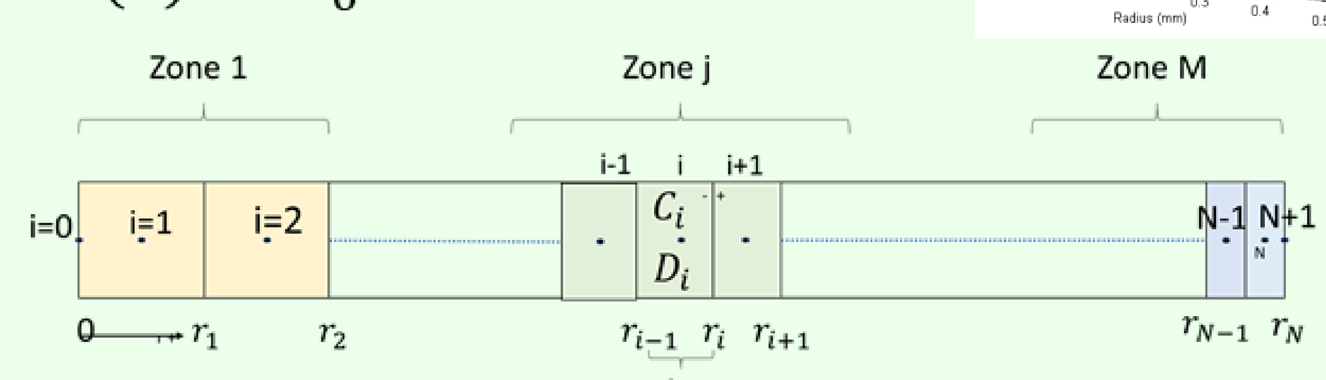
Intact TRISO Particles

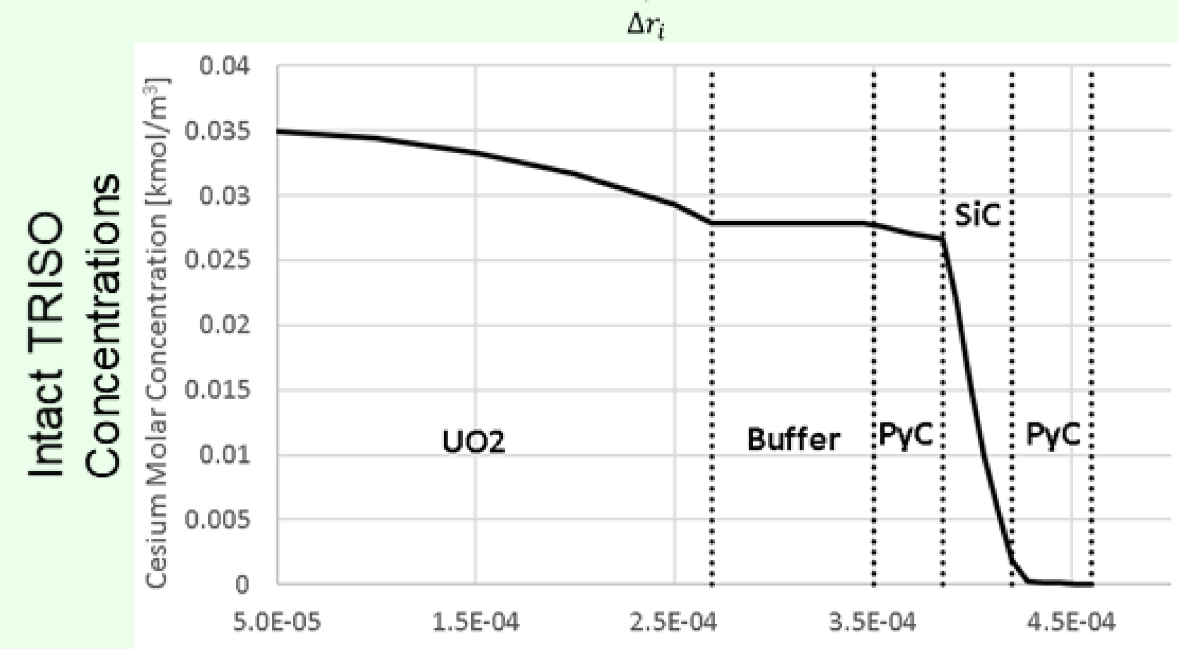
- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

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

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







MELCOR LWR Advancements

Top-Quenched Debris in Cavity

New Modeling based on CORQUENCH Model

Water-Ingression Model

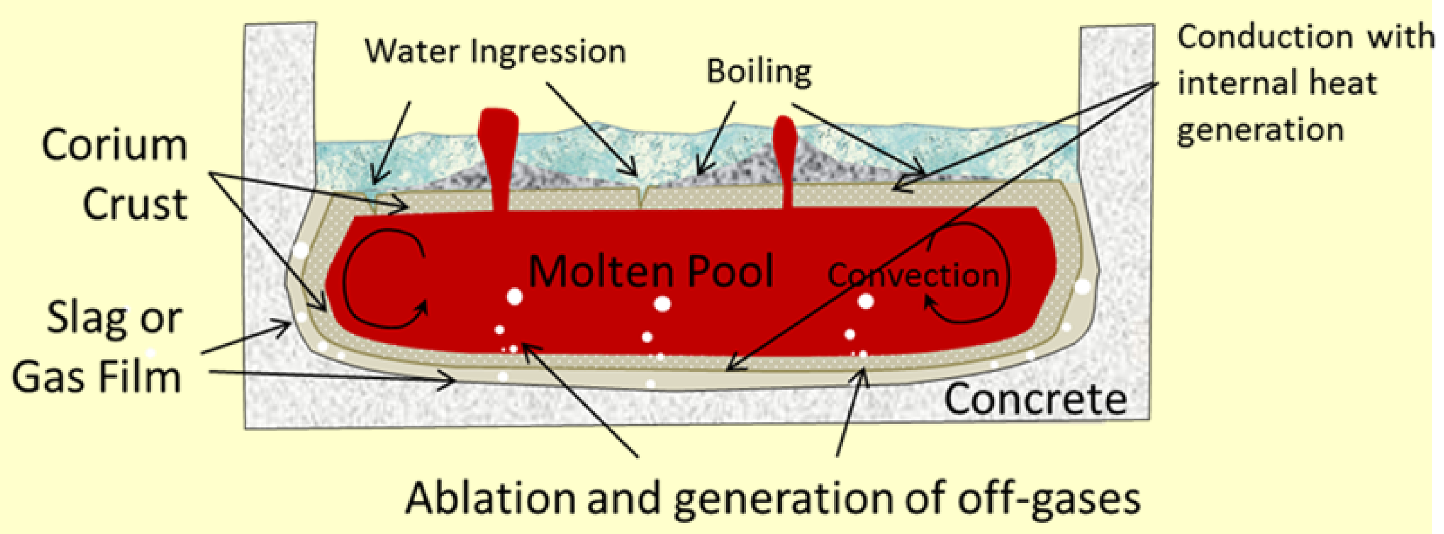
Quenching of the upper crust at the top of the corium debris can lead to a considerable density change (~18%volume) leading to cracking and formation of voids

- Water ingression reduces conduction path to molten pool and increases surface area of contact

Melt Eruption Model

Molten corium extruded through crust by entrainment from decomposition gases as they escape through fissures and defects in the crust.

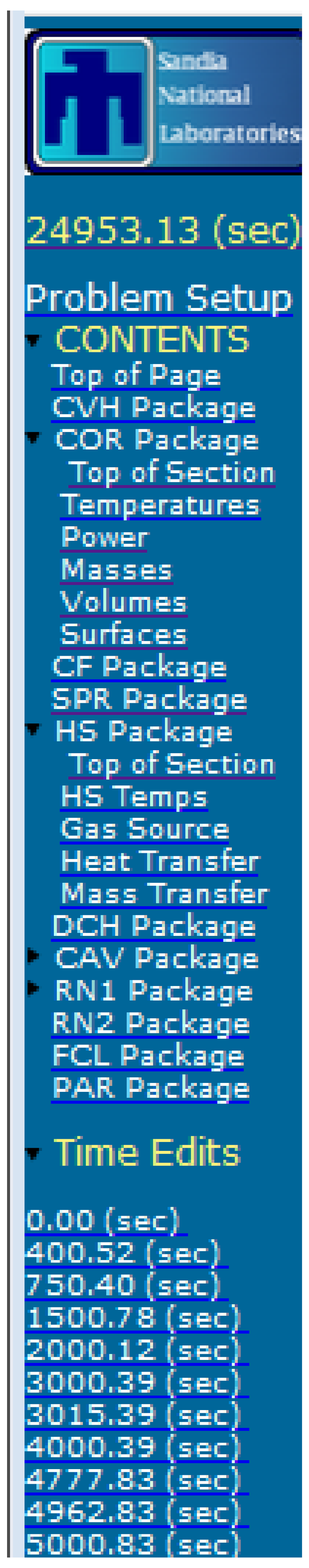
- Enhances the coolability of the molten corium by relocating enthalpy from the internal melt through the crust more coolable geometry that is more porous and permeable to water



Fully implemented

Validated

HTML Output

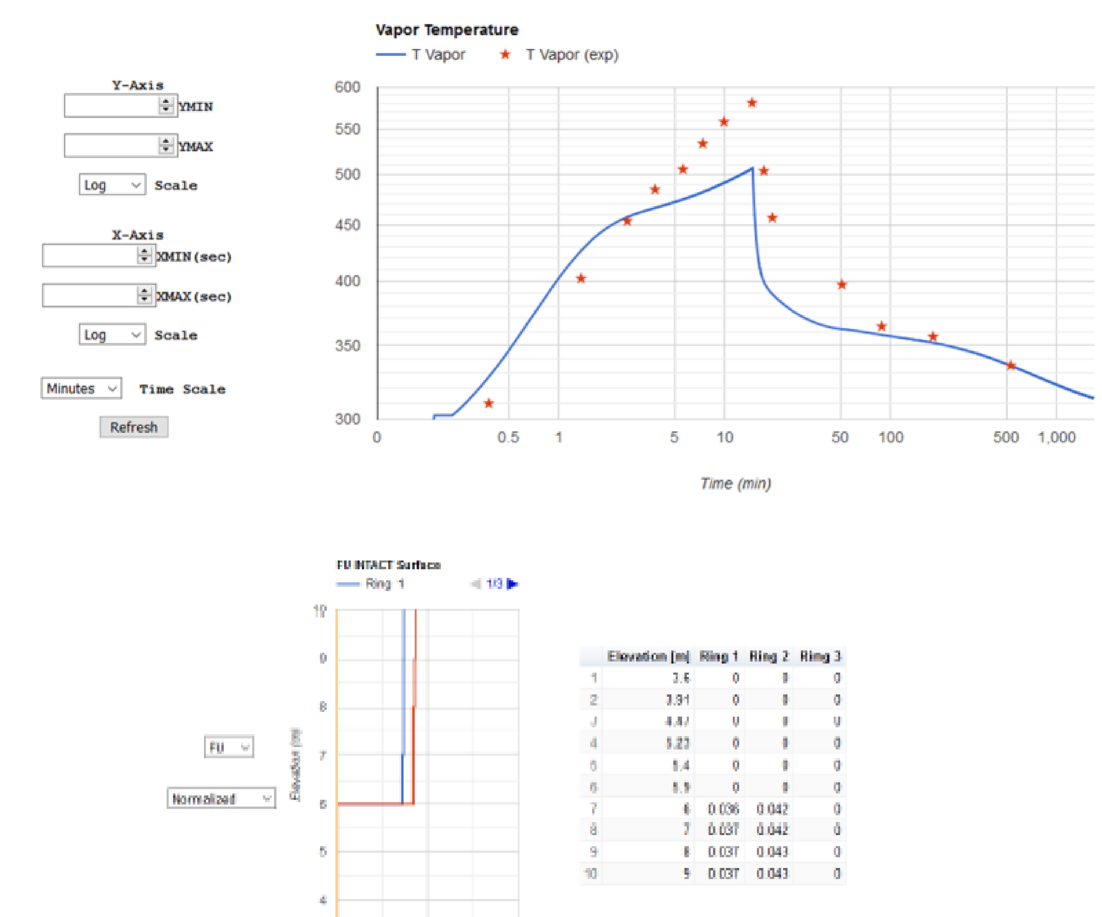


Automatic plot generation for enhanced user efficiency

- *Trend plots, profile plots, animated plots*

User customized plots and model specific plots for ultimate flexibility

Quick access to more data: Material properties, energy balances, energy/mass error plots, aerosol size distribution plots, CPU, distribution of aerosol sectional mass, core degradation, candled material distributions, …



Miscellaneous Improvements

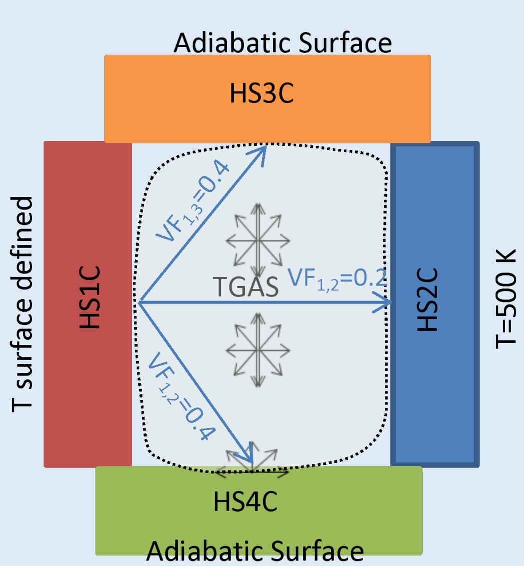
Radiation Enclosure Model

$\tau_{j,i}$ is the transmissivity through gas

$$J_i = (1-\varepsilon_i)\cdot \sum_j^N \left[F_{ij}\cdot \tau_{j,i}\cdot J_j\right] + \varepsilon_i \cdot \sigma \cdot T_i^4 + \rho_i \varepsilon_m E_{bm}$$

$$G_i = \sum_j^N \left[A_j \cdot F_{j,i}\cdot \tau_{j,i}\cdot J_j\right] / A_i + \varepsilon_m E_{bm}$$

$$q_i = A_i (J_i - G_i)$$




```
HS_RAD  4  NET3 !EM   BeamL    VF
  1 HS1C  LEFT     EM1  0.5       0.0  0.2  0.4  0.4
  2 HS2C  LEFT     EM2  0.5       0.2  0.0  0.3  0.5
  3 HS3C  LEFT      -   0.5       0.4  0.3  0.2  0.1
  5 HS4C  LEFT      -   0.5       0.4  0.5  0.1  0.0

TF_ID TEMP    1.0    0.0  !T Surface Defined
TF_TAB 4
       1 0.0        500.0
       2 500.0      1500.0
       3 1000.0     1500.0
       4 30000.0    1500.0
```

COR 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

Generalized Oxidation Model

Historically, MELCOR had a specific set of oxidizable material:

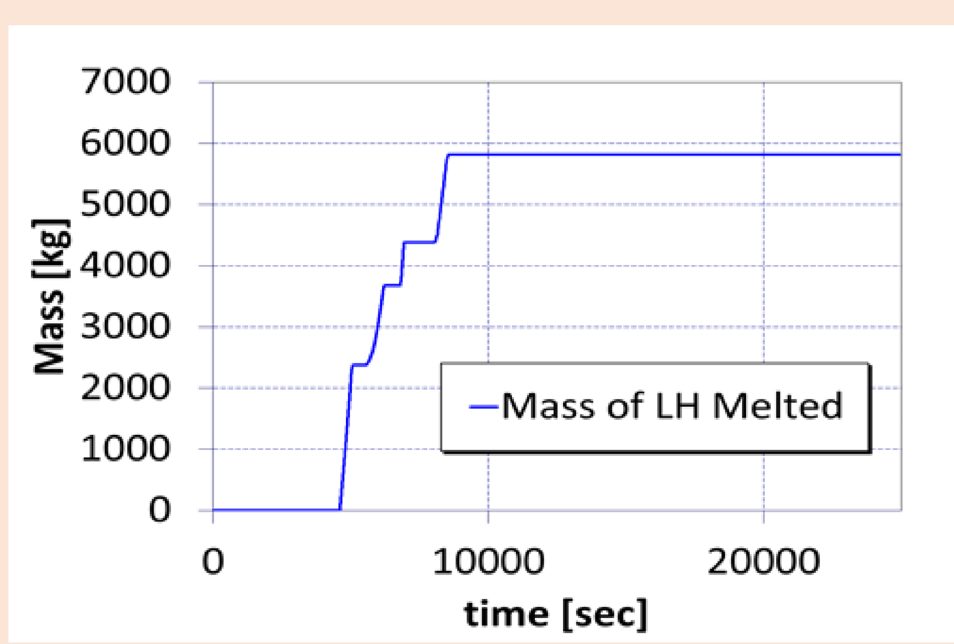
- Zirconium, Stainless-steel, Graphite, B_4C, Aluminum
- Now extended to use the user-defined materials (UDMs)

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

Melting Lower Head

- 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



Multi-rod Model

Implement additional fuel rod components to capture temperature gradient

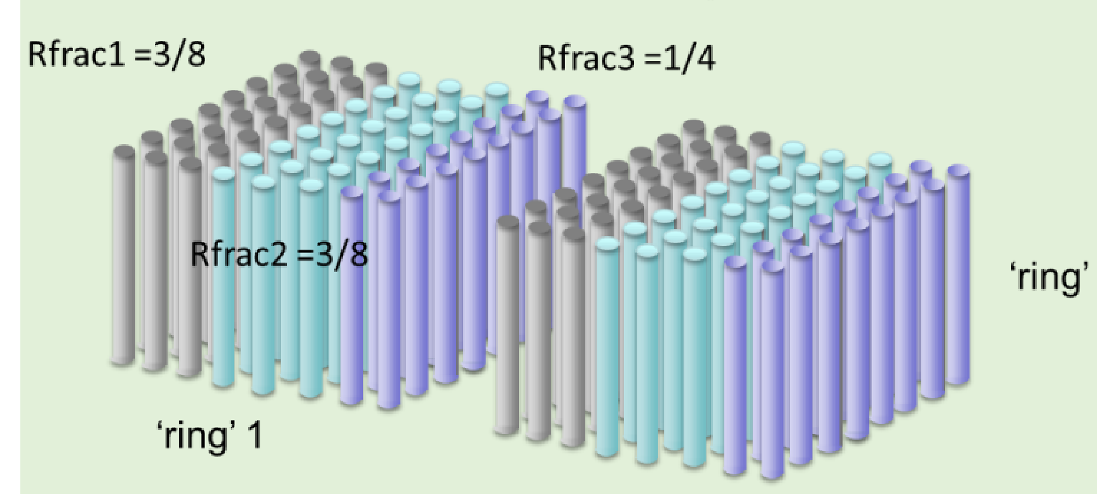
- Temperature in edge region simulated
- Oxidation and ignition captured

Minimal User Input

- Specify ring geometry as usual
- Specify fraction associated with each rod type
- Specify view factors connecting types

Implement sub-grid radiation model

- User provides view factors between rows of rods
  - Geometric view factor now meaningful

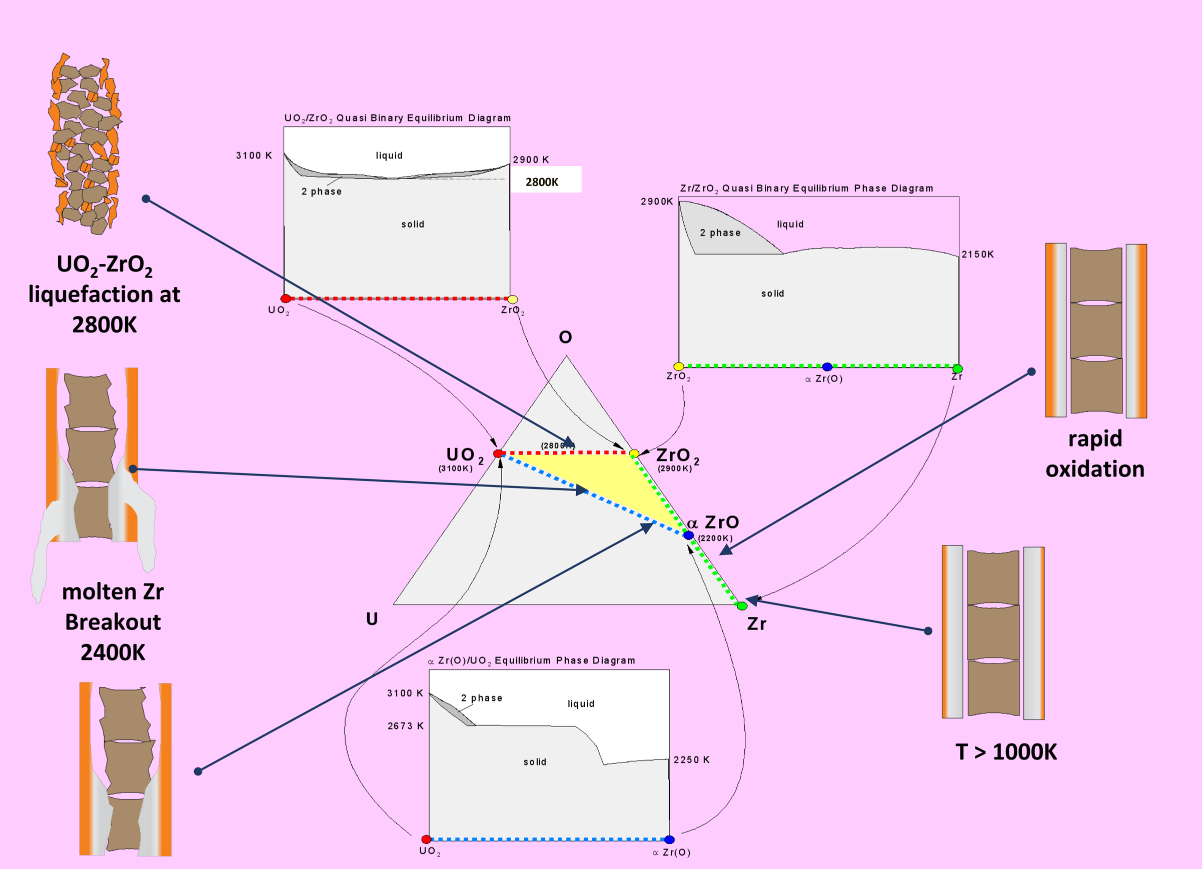


Eutectic Model

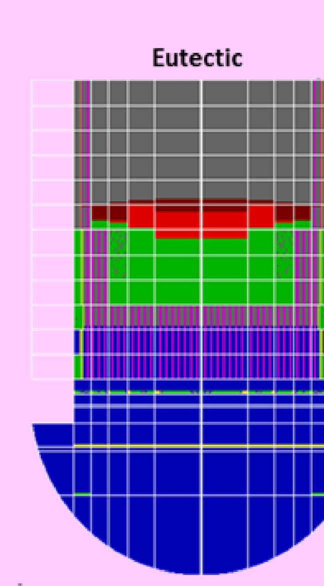
- Composition dependence of melting temperatures
- User specifies eutectic temperature and composition for material pairs
  - Zr/SS, Zr/INC, UO2/ZRO2
- Materials Interactions model
  - Parabolic rate of dissolution reaction accounting for changes to liquidus
  - Liquefaction of ZrO2 in BWR canisters
  - Liquefaction of UO2 from intact fuel

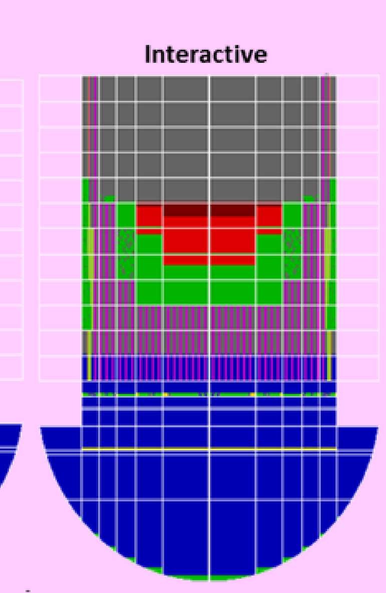
```
COR_EUT  1  !  PairMelt       T         f1
             1  'UO2/ZRO2'  2550.0    0.5
```

COR_EUT ON enables the model & uses defaults
COR_EUT OFF disables the eutectics model



Comparison of Eutectics Model and older interactive materials model



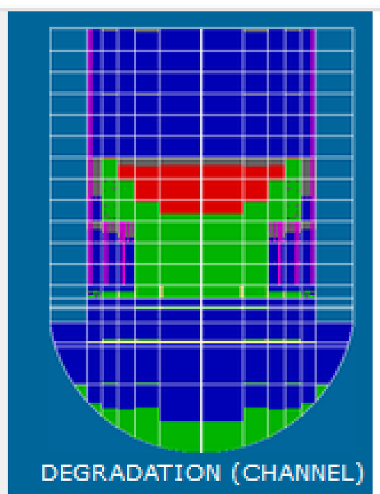


MELCOR HTML Output

24953.13 (sec)

Problem Setup

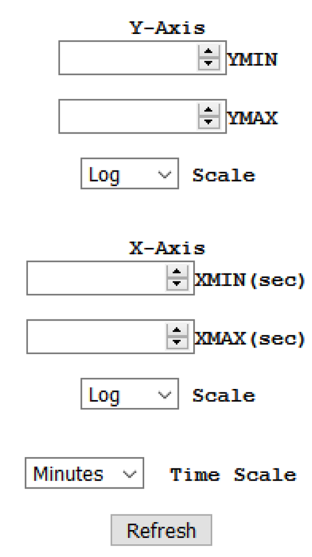
- *Lightning fast hyper-linked navigation to the MELCOR output you're looking for.*
- *Graphical depiction of core degradation*
- *Automatic plot generation for enhanced user efficiency*
  - *Trend plots, profile plots, animated plots*
- *Plots of material property functions, EOS functions, and fluid 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, …*

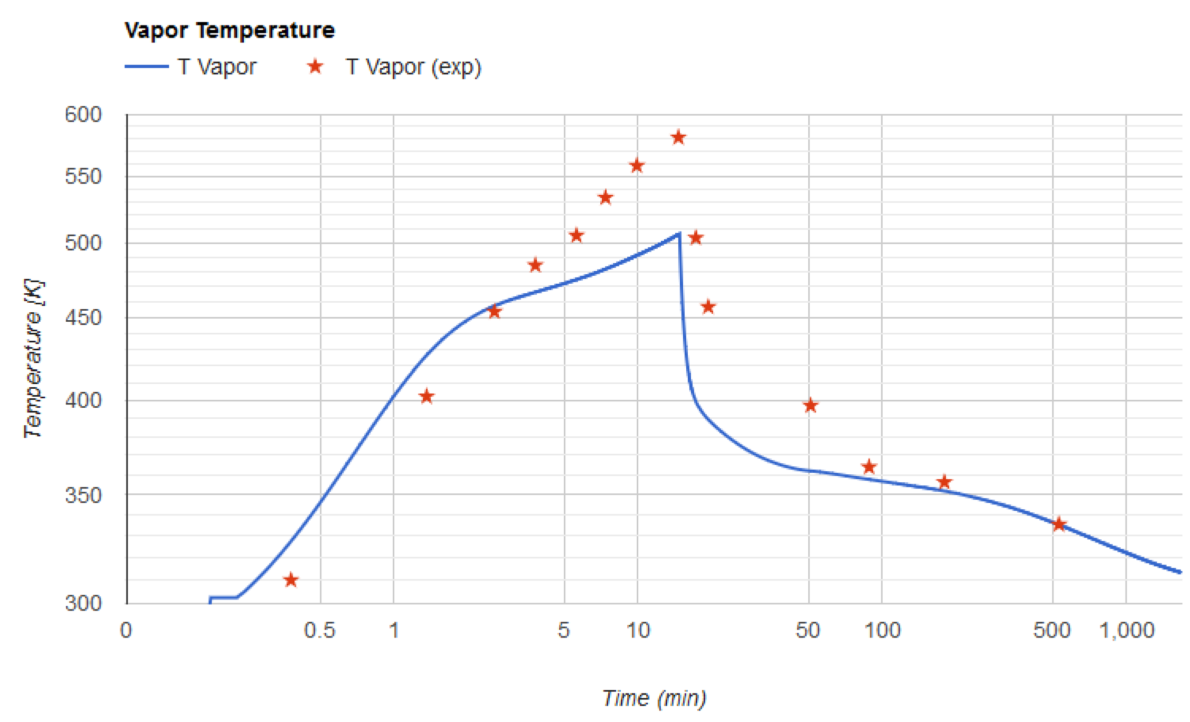


User Customized Plots

- 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 acis
  - 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'
```

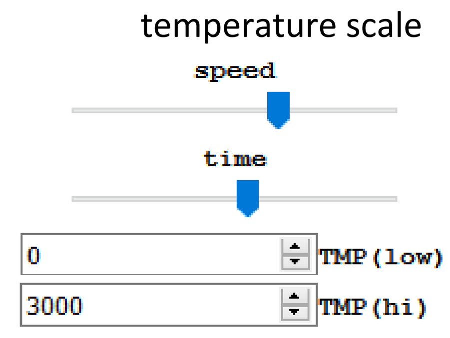




Static and Animated Profiles

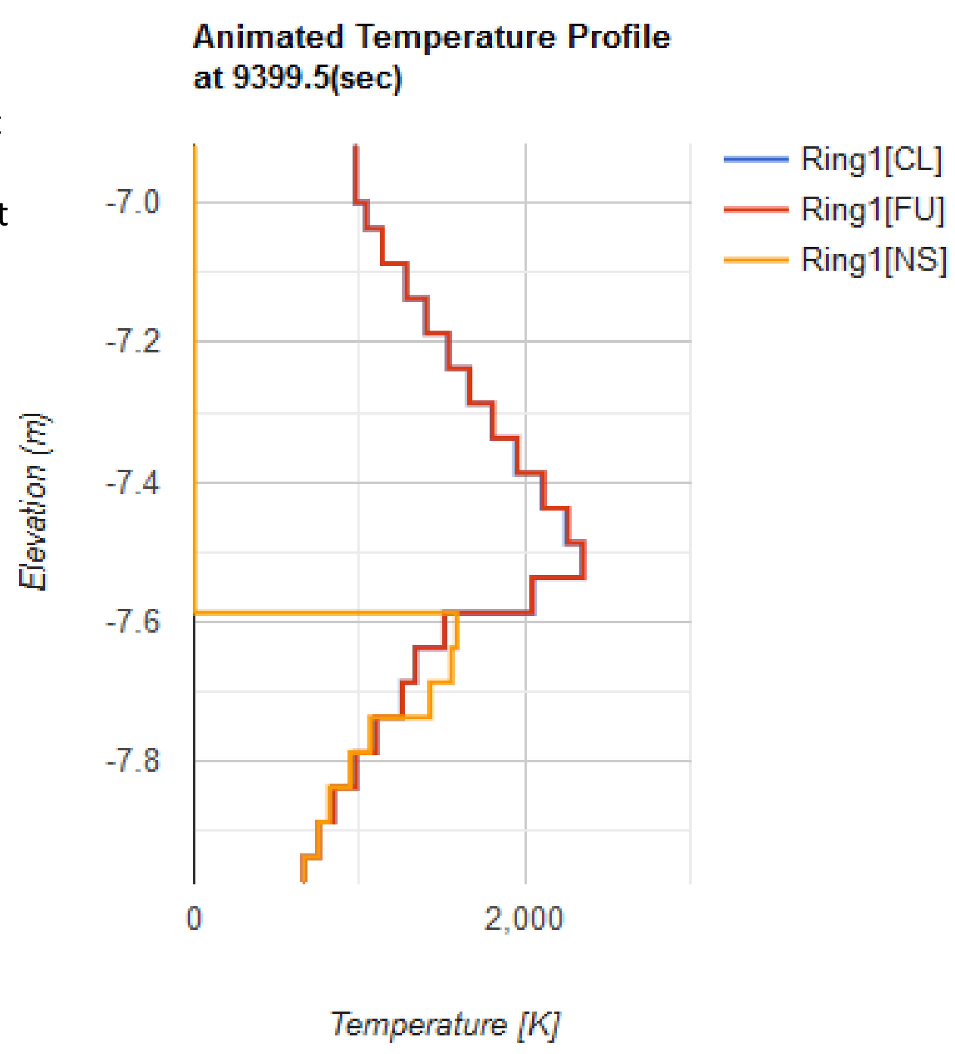
Temperatures, mass, power, surface area, volumes

- Static plots generated automatically at each time edit
  - MELGEN plots provide graphical plot for verifying input
- User can create animations of component temperature profile
  - Local COR atmosphere fluid 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
```



User HTML Description

Background

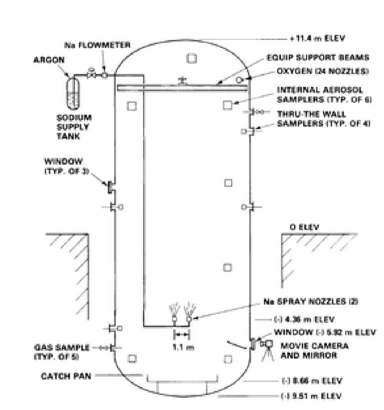
The Aerosol Behavior Code Validation and Evaluation (ABCOVE) experiments investigat breeder reactors (LMFBRs). The experiments provide a basis for judging the adequacy aerosol attenuation in containment buildings during postulated accidents. The ABCOVE Systems Test Facility (CSTF) located at the Hanford Engineering Development Laborato

This MELCOR assessment uses the MELCOR sodium chemistry (NAC) package, based o sodium atmospheric chemistry.

Key models exercised in the MELCOR analysis of this test include:

- Agglomeration behavior of hygroscopic and non-hygroscopic aerosol species
- Condensation of water vapor.
- Settling of aerosols.
- Sodium spray fires
- Radiant heat transfer in an enclosure
- Radiant heat transfer to an intermediate gas

Depiction of AB-5 Experimental Apparatus



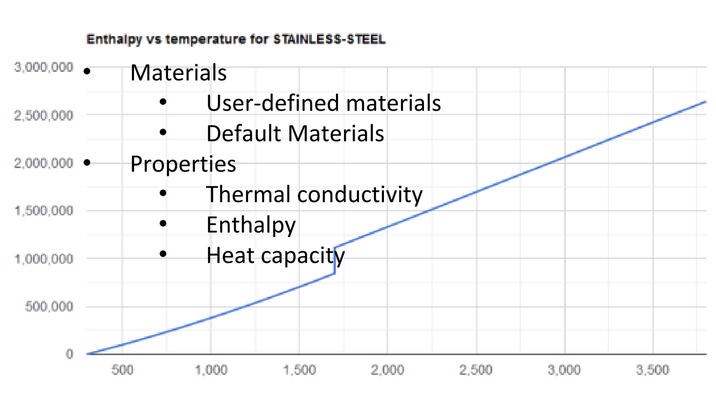
Material Property Plots Generated at MELGEN

MATERIAL PROPERTIES PACKAGE

Show Properties for fiberglass

Show Properties for STAINLESS-STEEL

Show Properties for ZIRCALOY



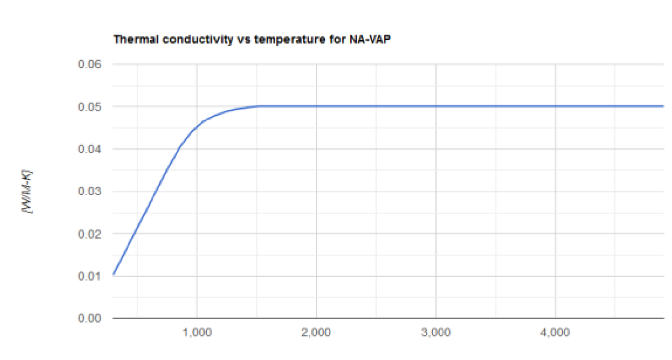
- Materials
  - User-defined materials
  - Default Materials
- Properties
  - Thermal conductivity
  - Enthalpy
  - Heat capacity

NON CONDENSIBLE GAS PACKAGE

Show Properties for POOL

Show Properties for NA-VAP

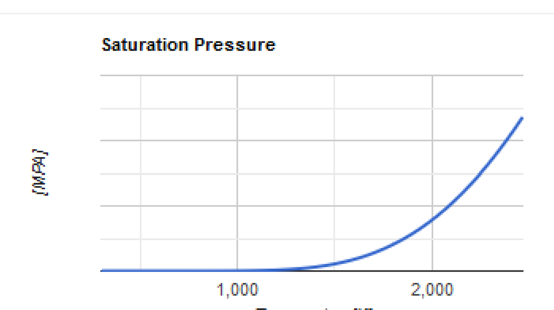
- Viscosity
- Thermal conductivity

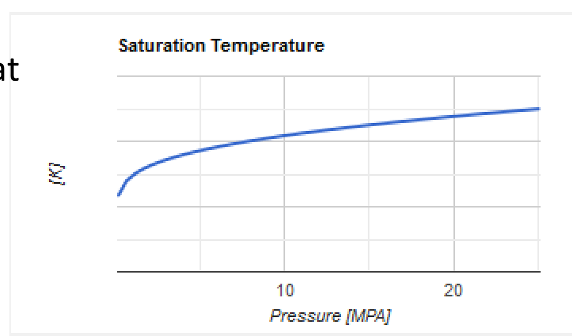


EOS PACKAGE

EOS Properties for Na

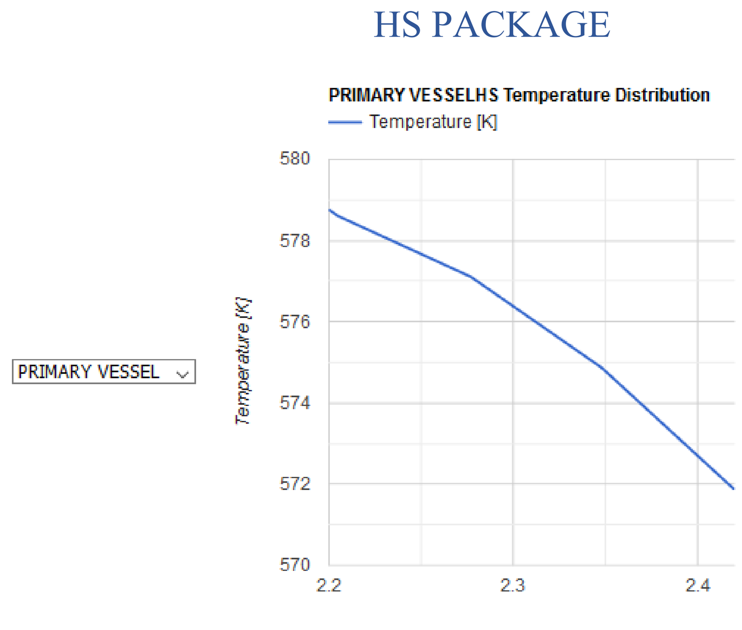
- Saturation Pressure
- Saturation Temperature
- Liquid Density at saturation
- Vapor density at saturation
- Liquid specific enthalpy at saturation pressure
- Vapor specific enthalpy at saturation pressure
- Liquid specific heat
- Vapor specific heat



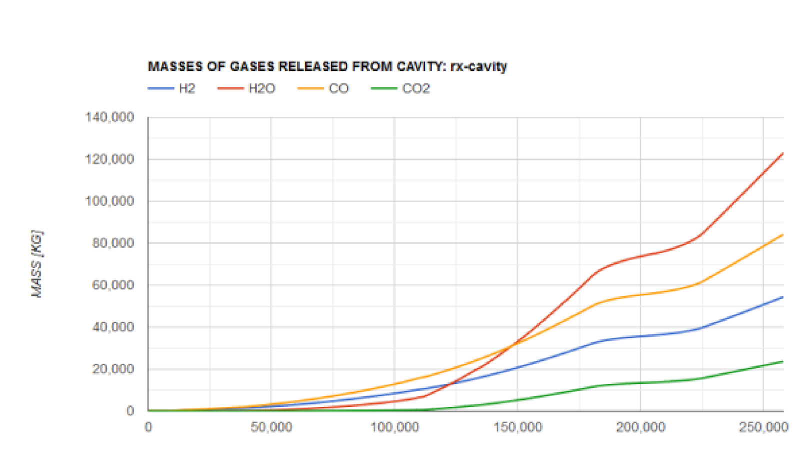


Automatically Generated Model-Dependent Plots

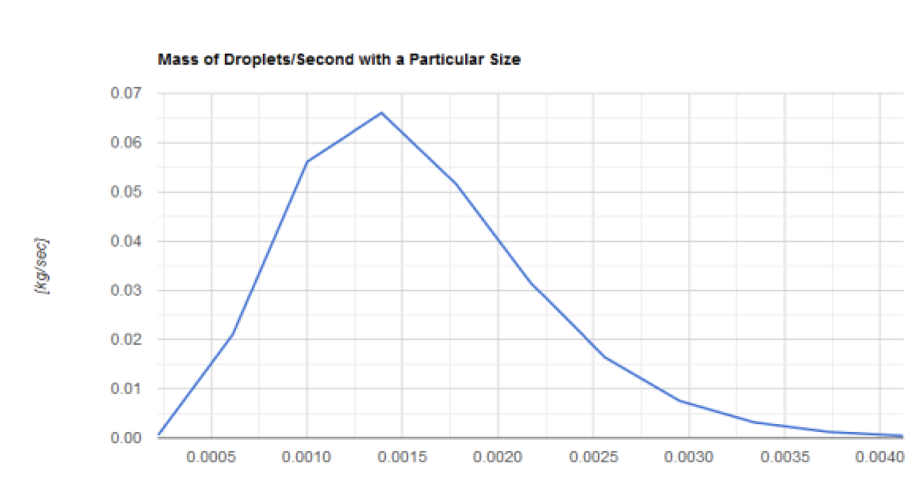
HS PACKAGE



MCCI MODELS



NA SPRAY FIRE MODEL

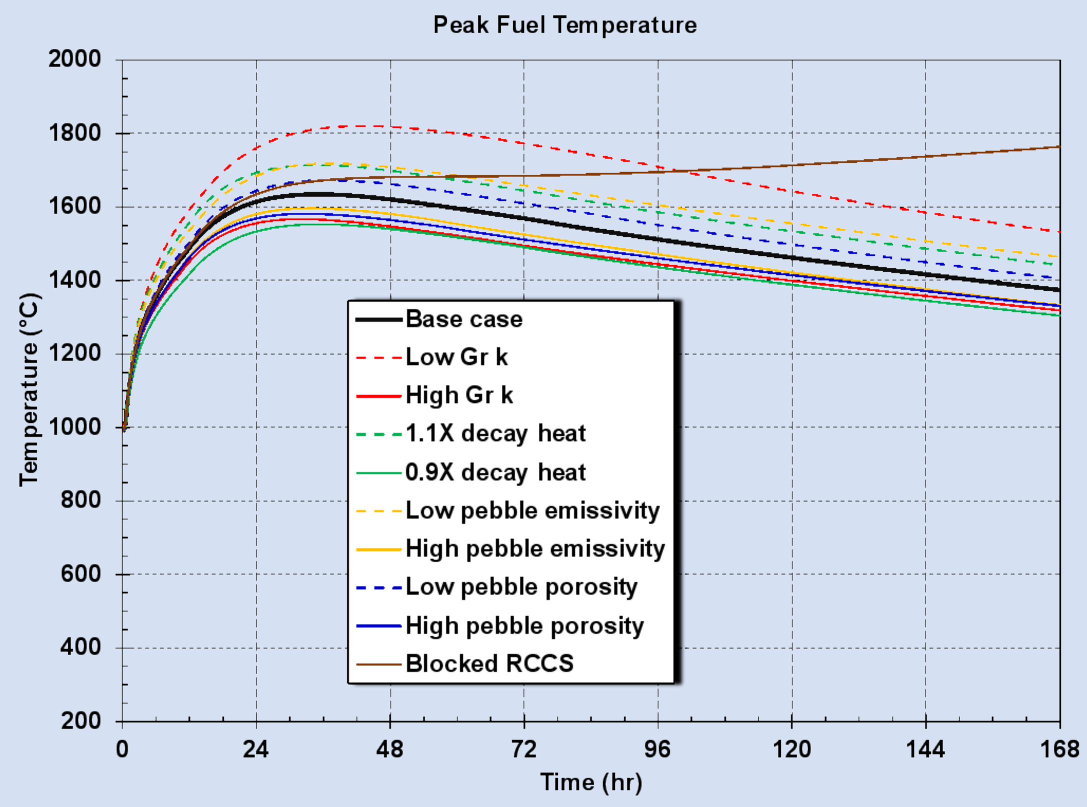


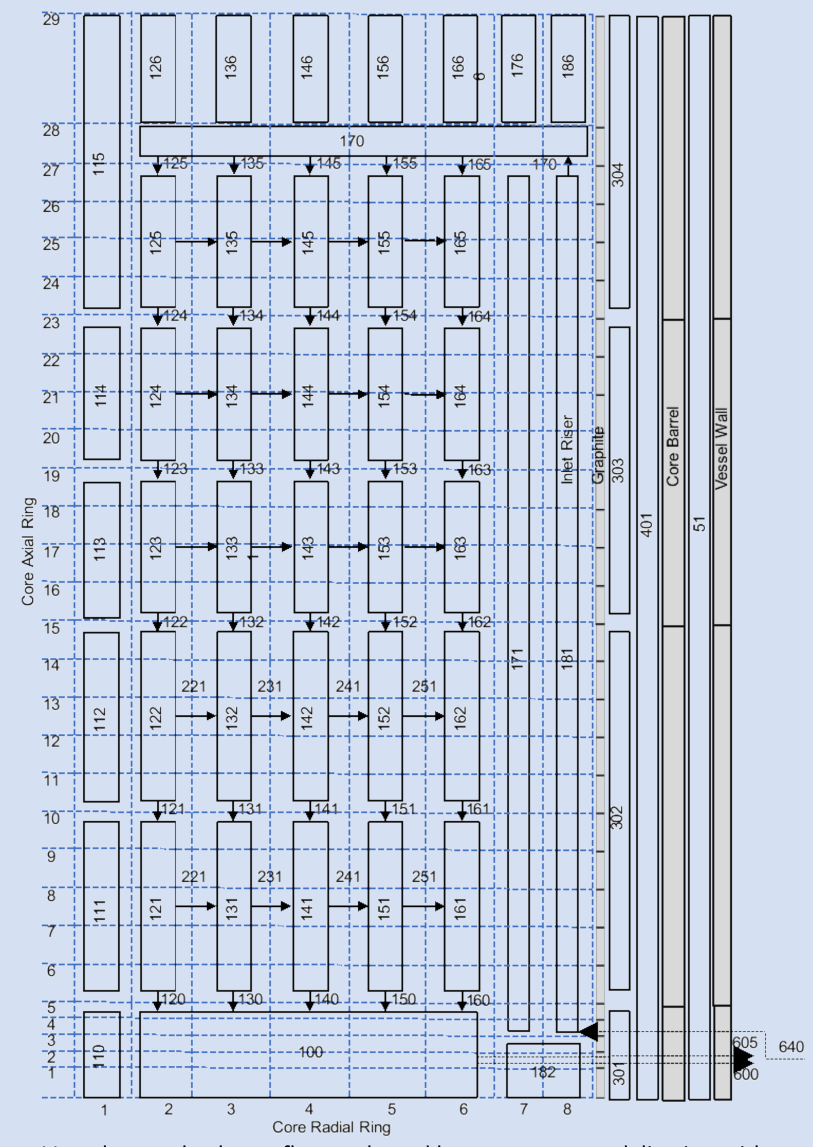
Now Available in MELCOR 2.2.14770 or Later

Non-LWR Demo Calculations

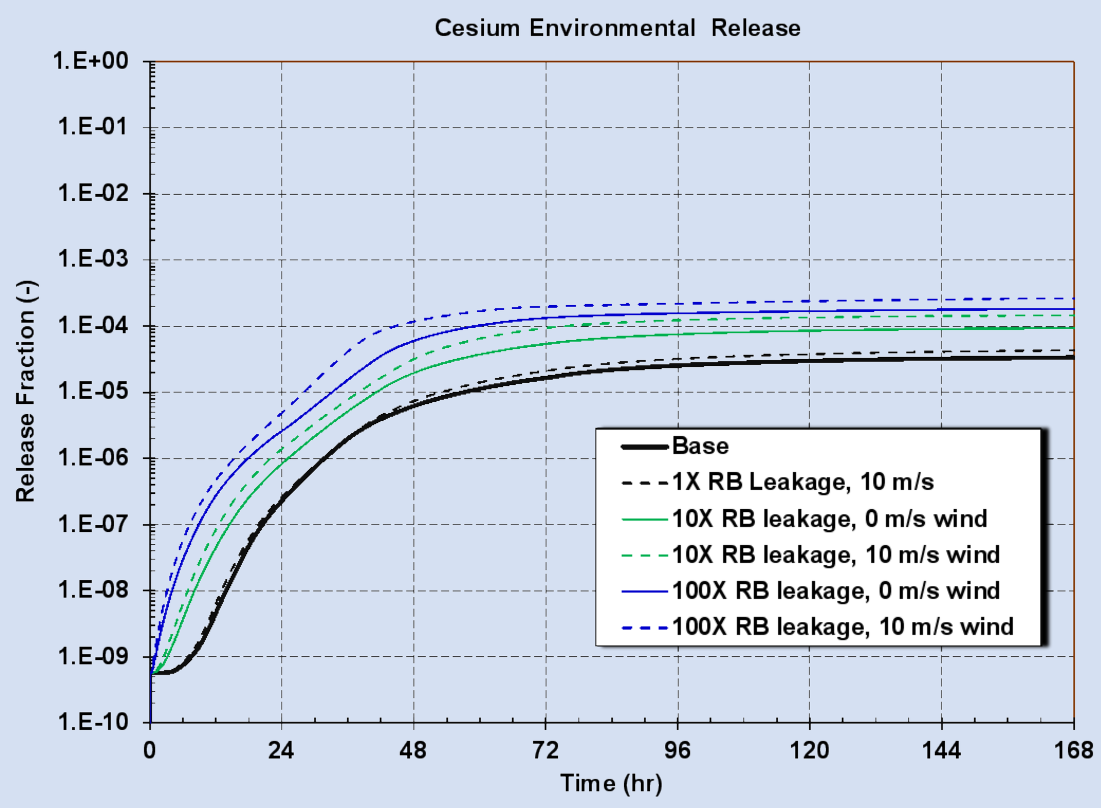
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

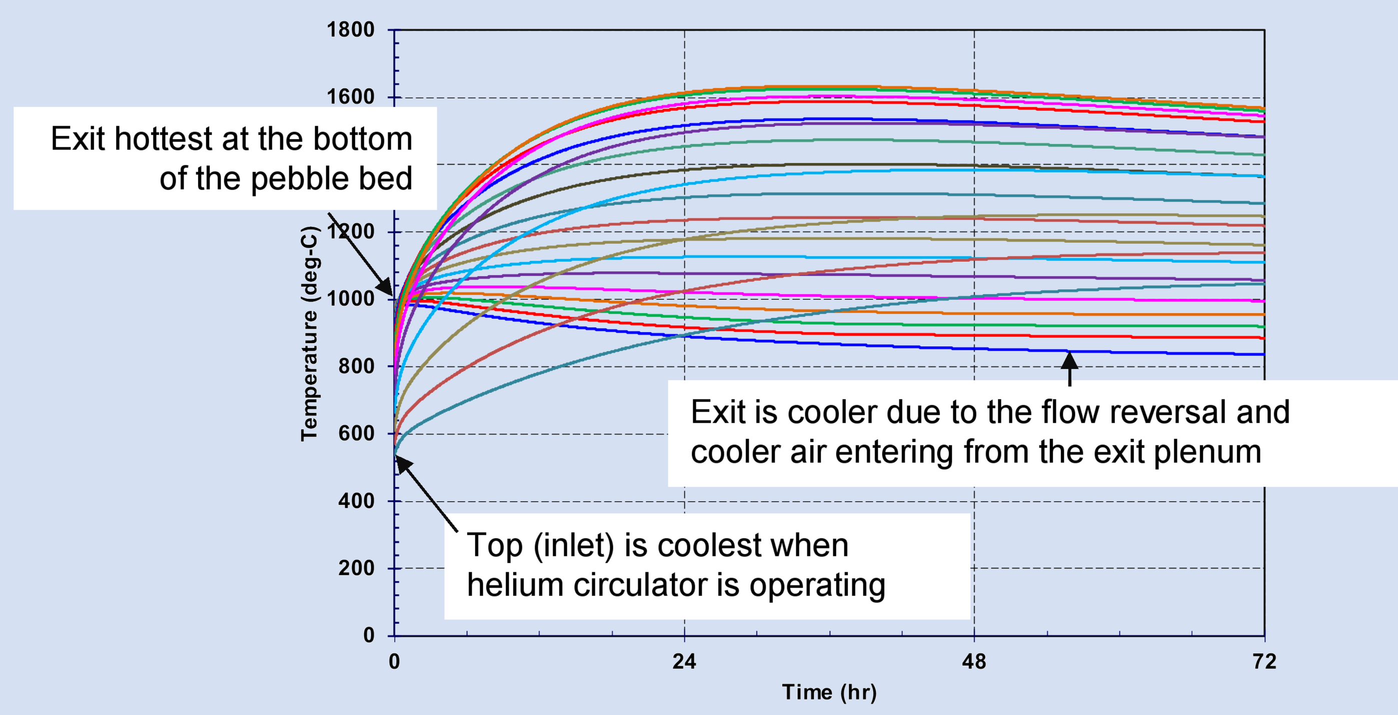
High Temperature Gas Cooled Reactor



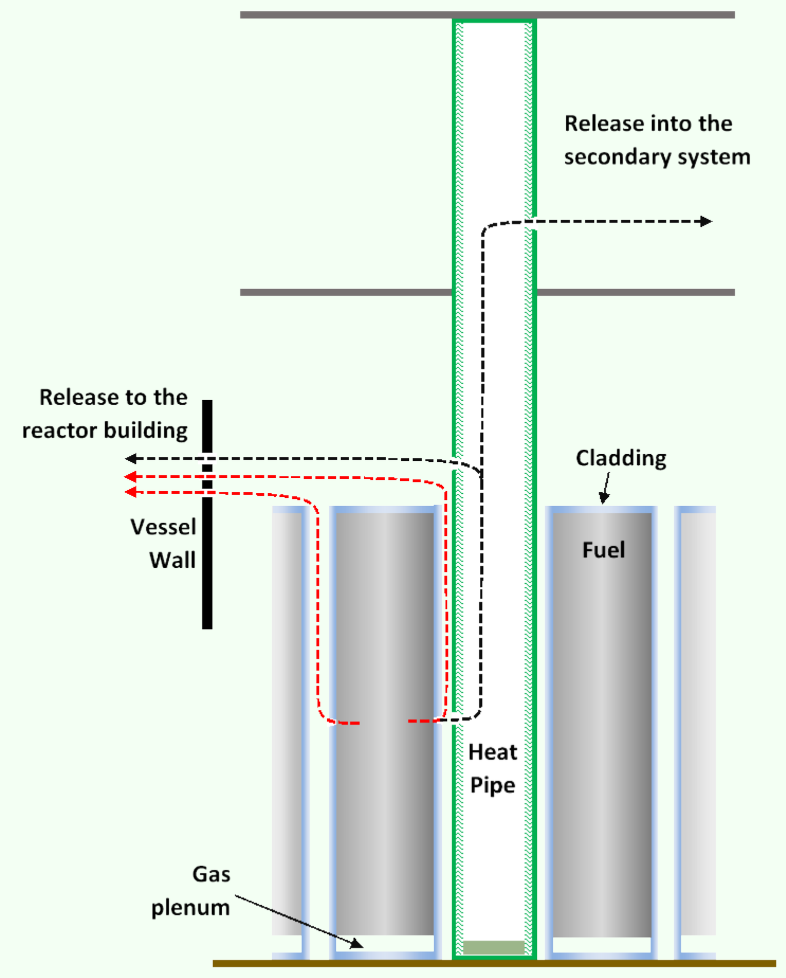


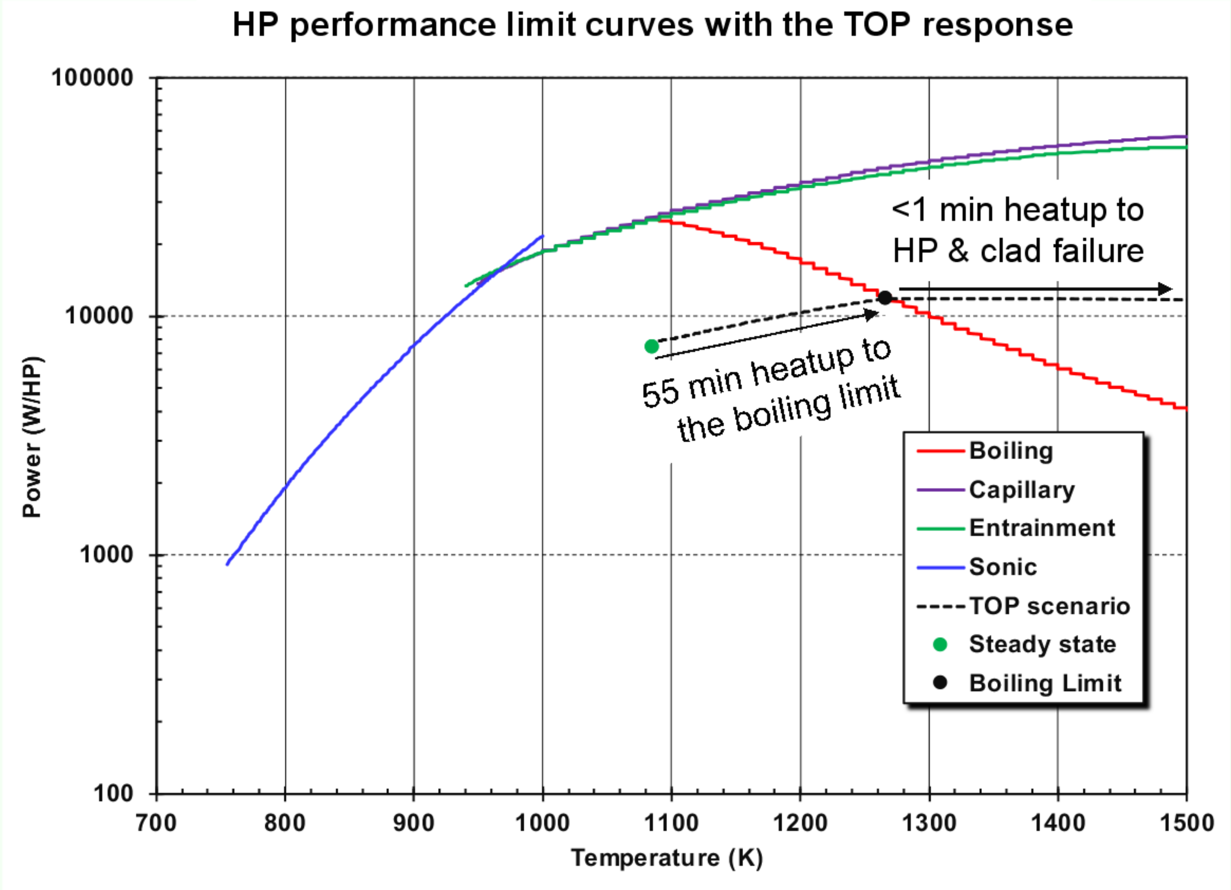
Vessel control volume, flow path, and heat structure nodalization with core package boundaries in blue





Heat Pipe Reactors





Fluoride Salt Cooled High Temperature Reactor (FHR)