MELCOR Emerging Applications

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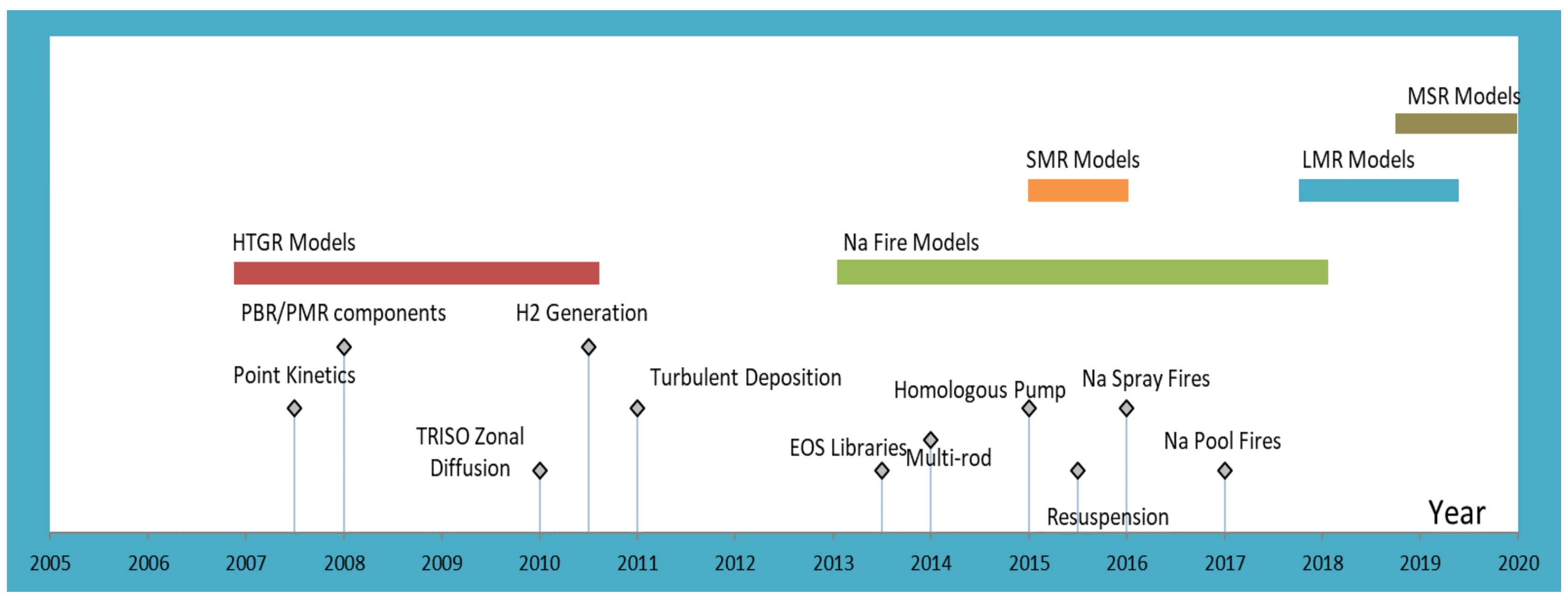
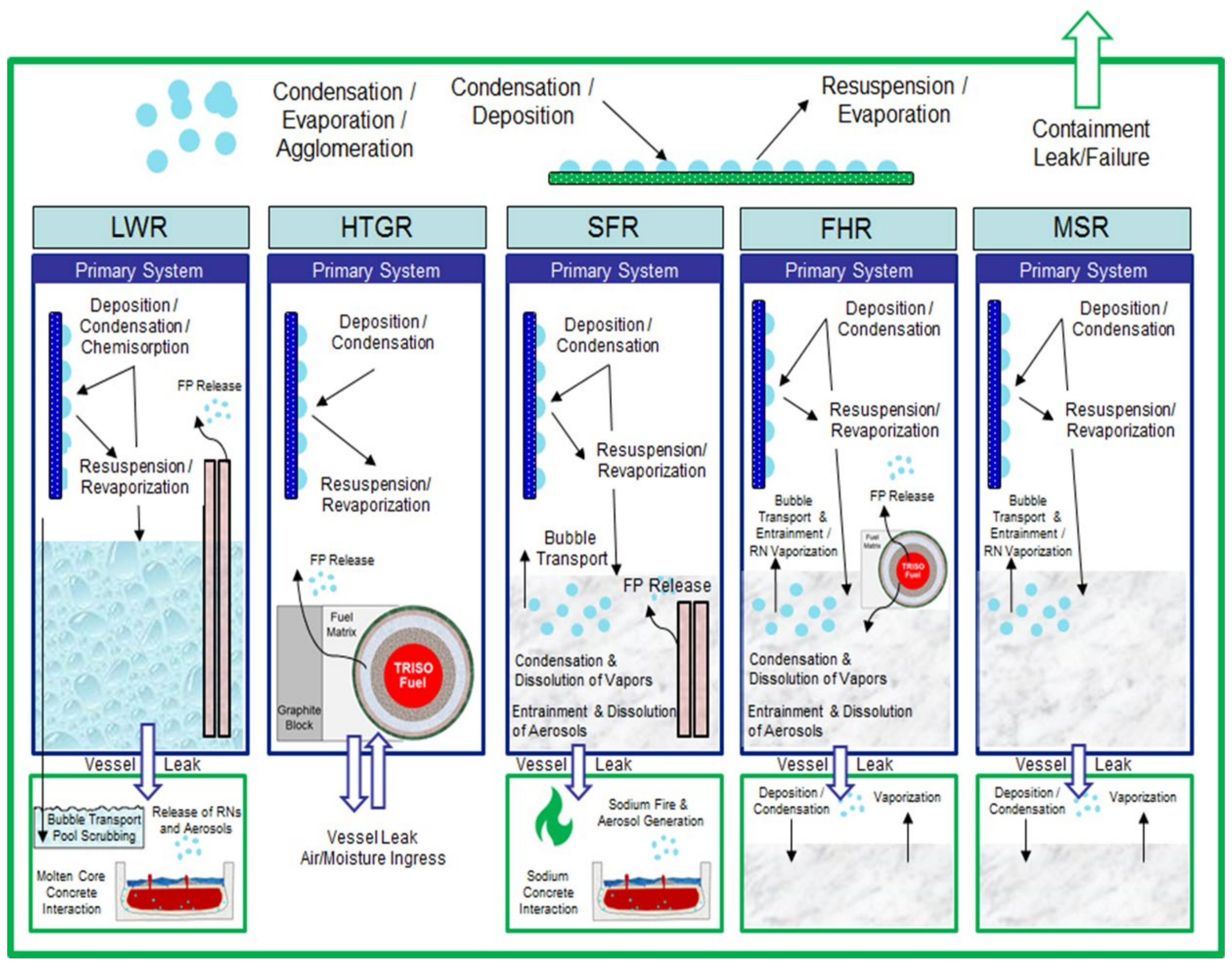
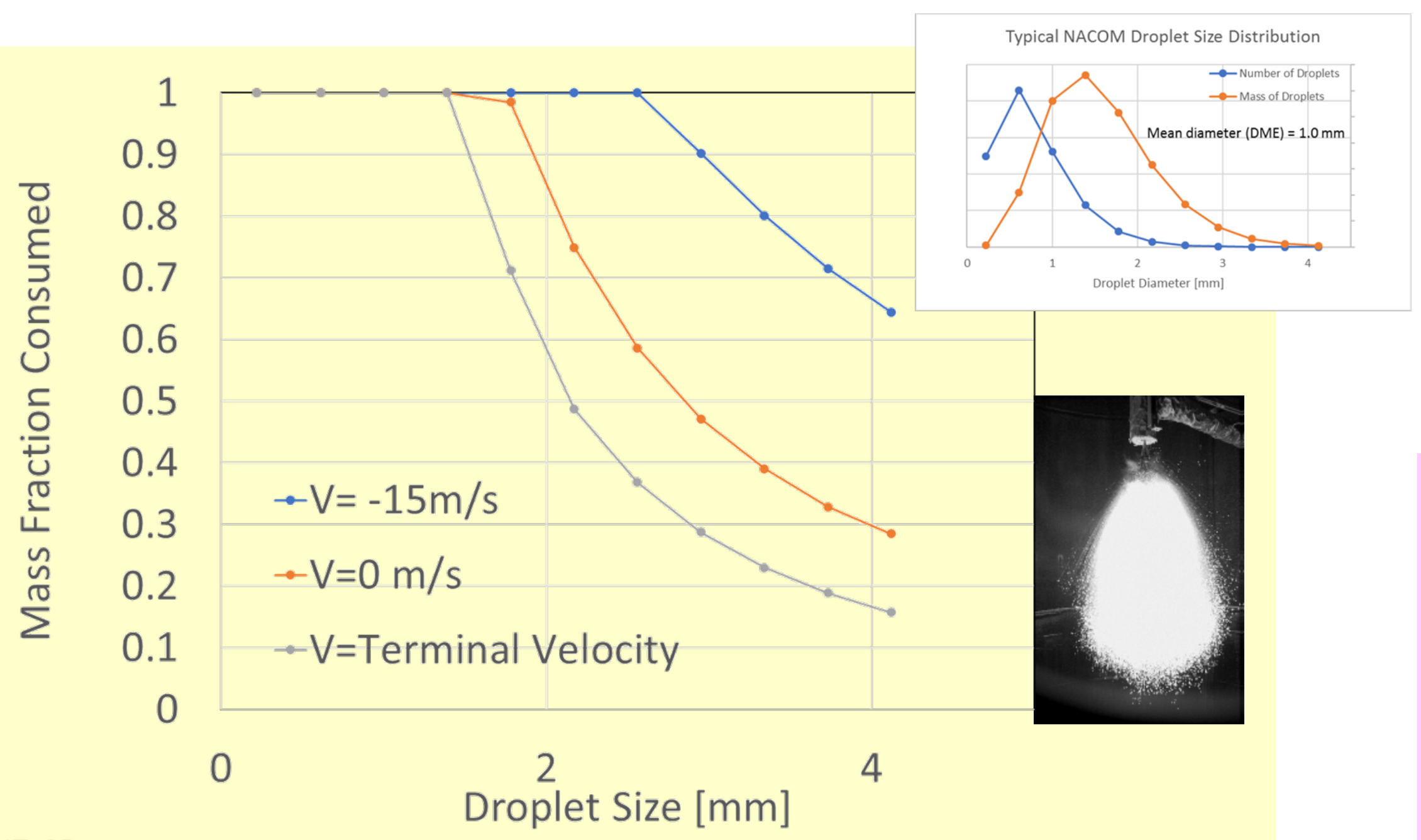
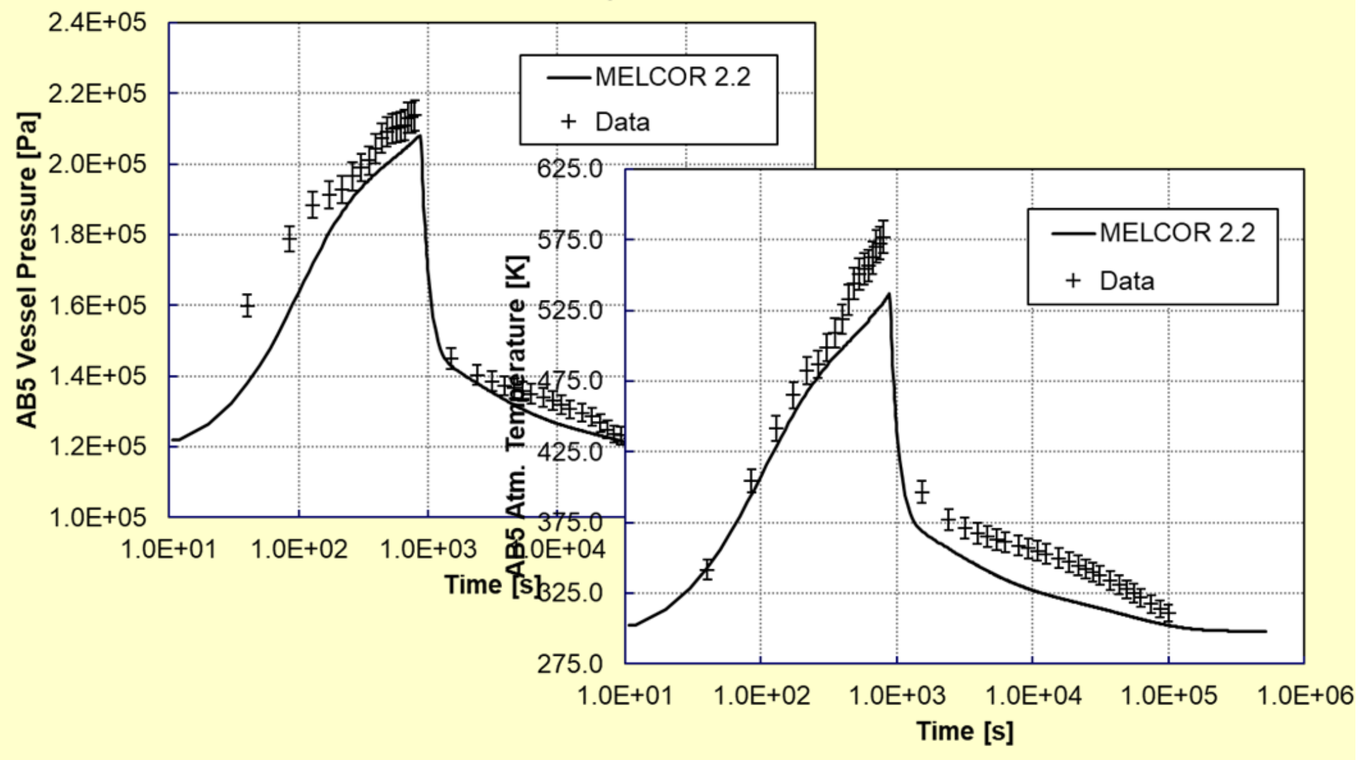


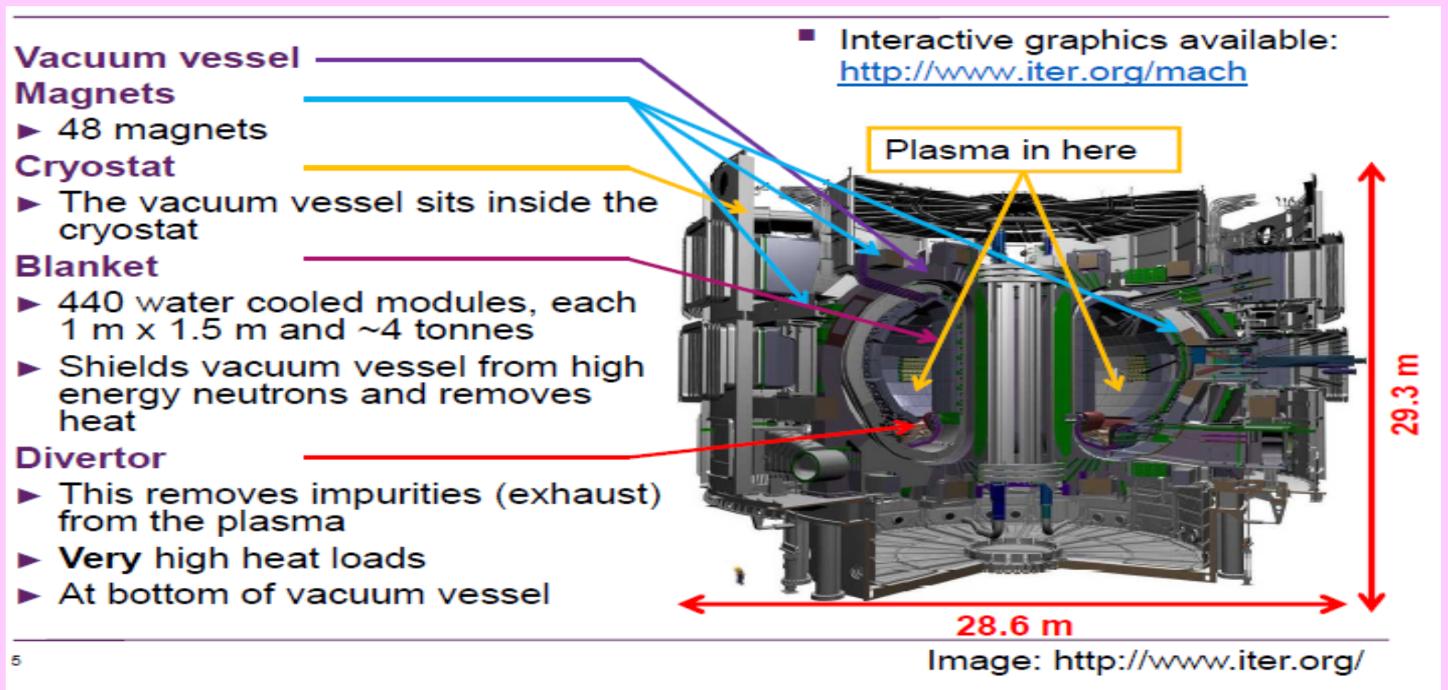


Sodium Reactors

- 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







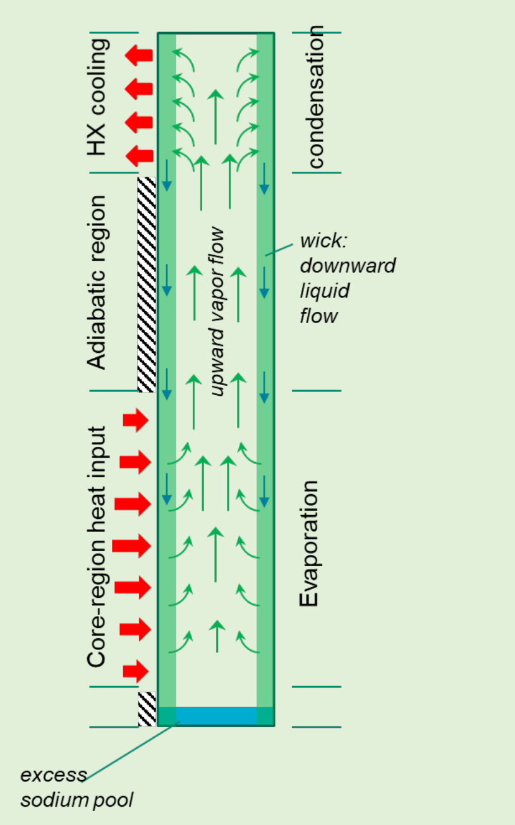
Fusion

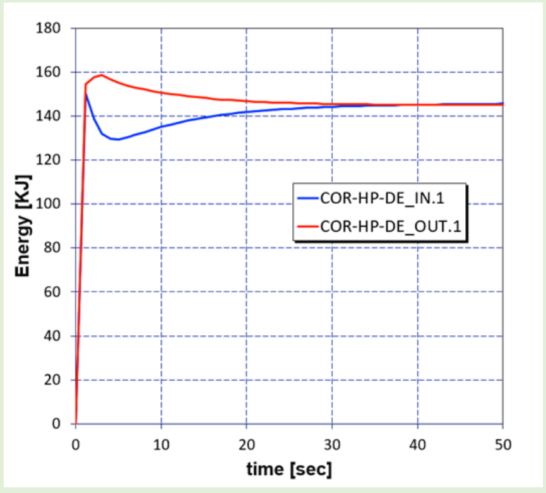
- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

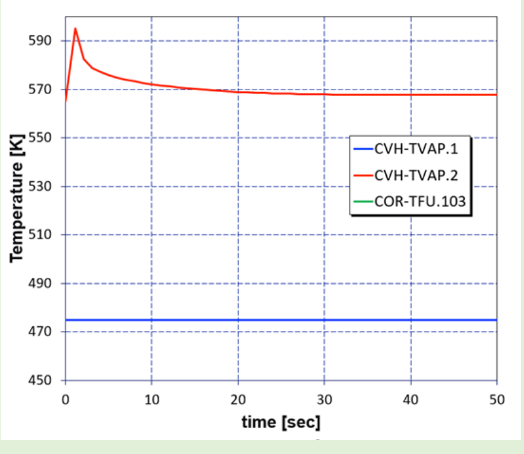
Micro Reactors

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

A Generic Heat Pipe Illustration







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.

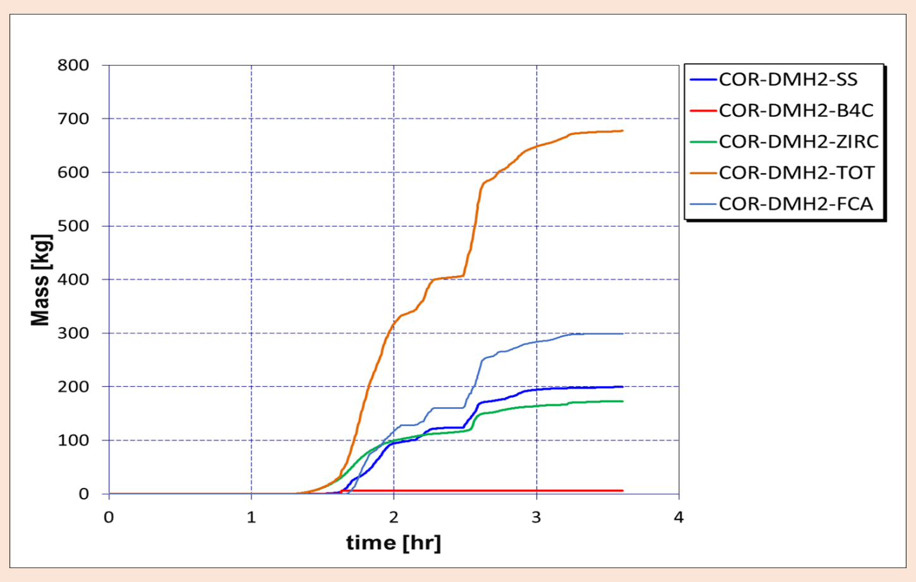
Oxidation Model

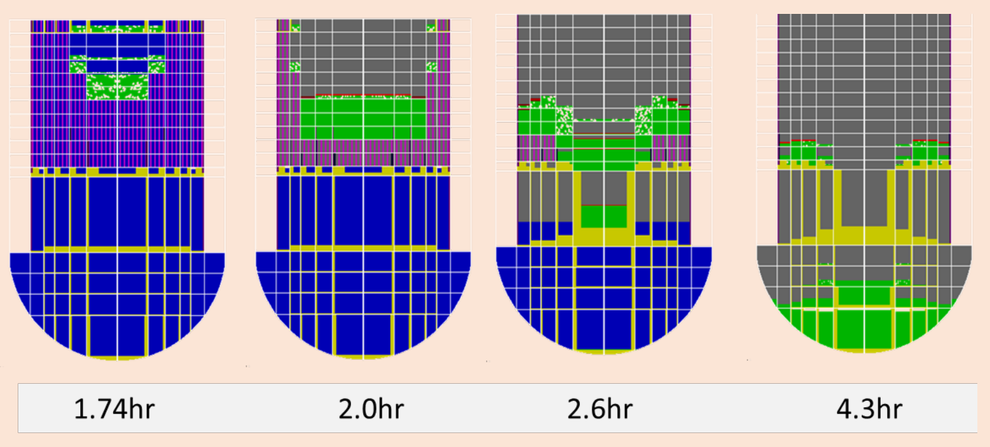
Pre breakaway - Pint, et.al

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:

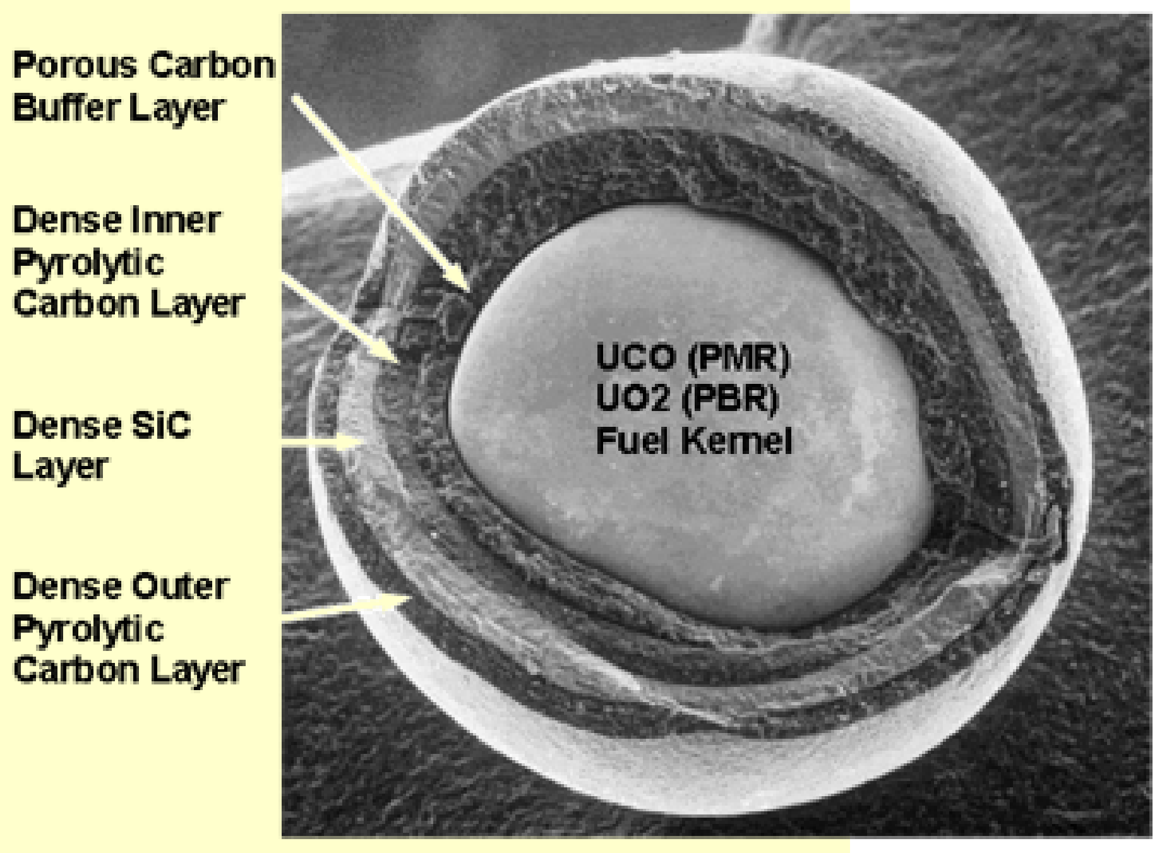
$$\mathrm{Fe} + \frac{4}{3}\mathrm{H_2O} \rightarrow \frac{1}{3}\mathrm{Fe_3O_4} + \frac{4}{3}\mathrm{H_2} + \mathrm{Q_{ox}}$$
$$\mathrm{Cr} + \frac{3}{2}\mathrm{H_2O} \rightarrow \frac{1}{2}\mathrm{Cr_2O_3} + \frac{3}{2}\mathrm{H_2} + \mathrm{Q_{ox}}$$
$$\mathrm{Al} + \frac{3}{2}\mathrm{H_2O} \rightarrow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

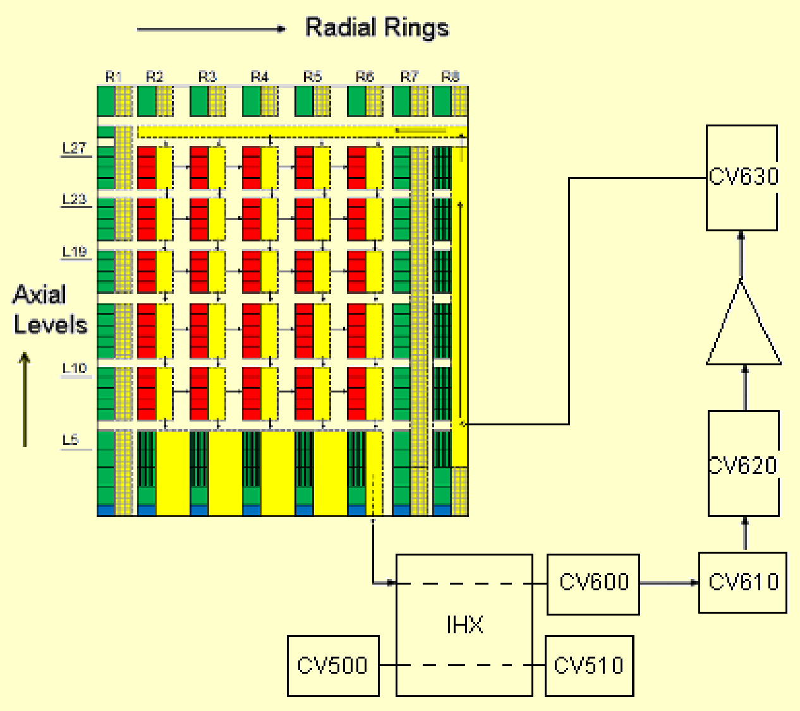


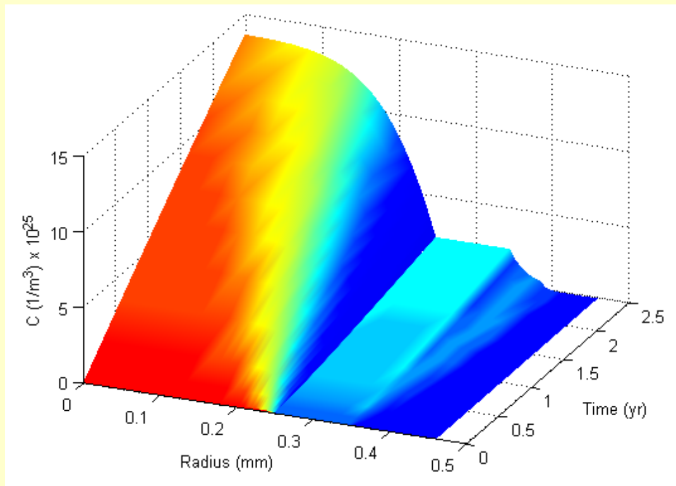


High Temperature Gas Reactors

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 strategy

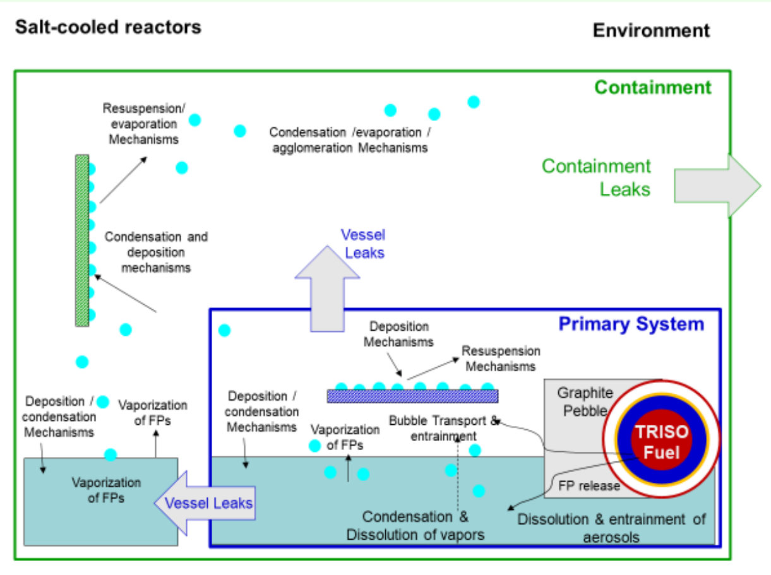


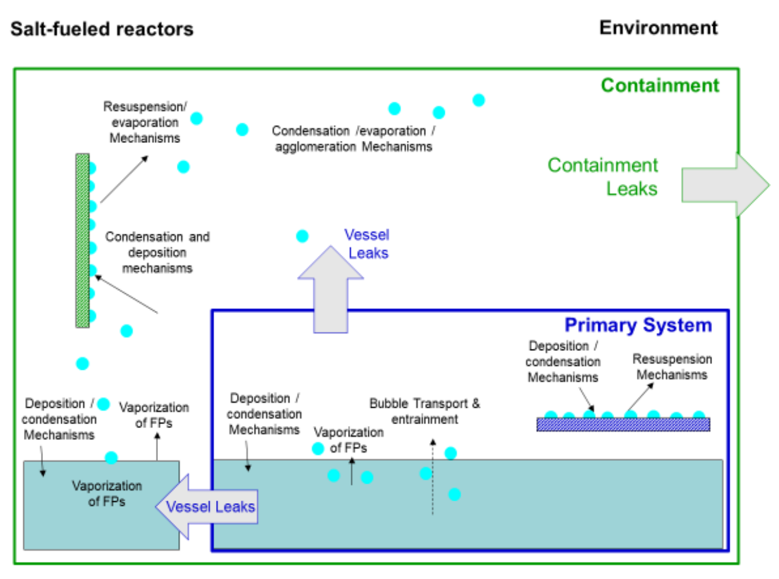


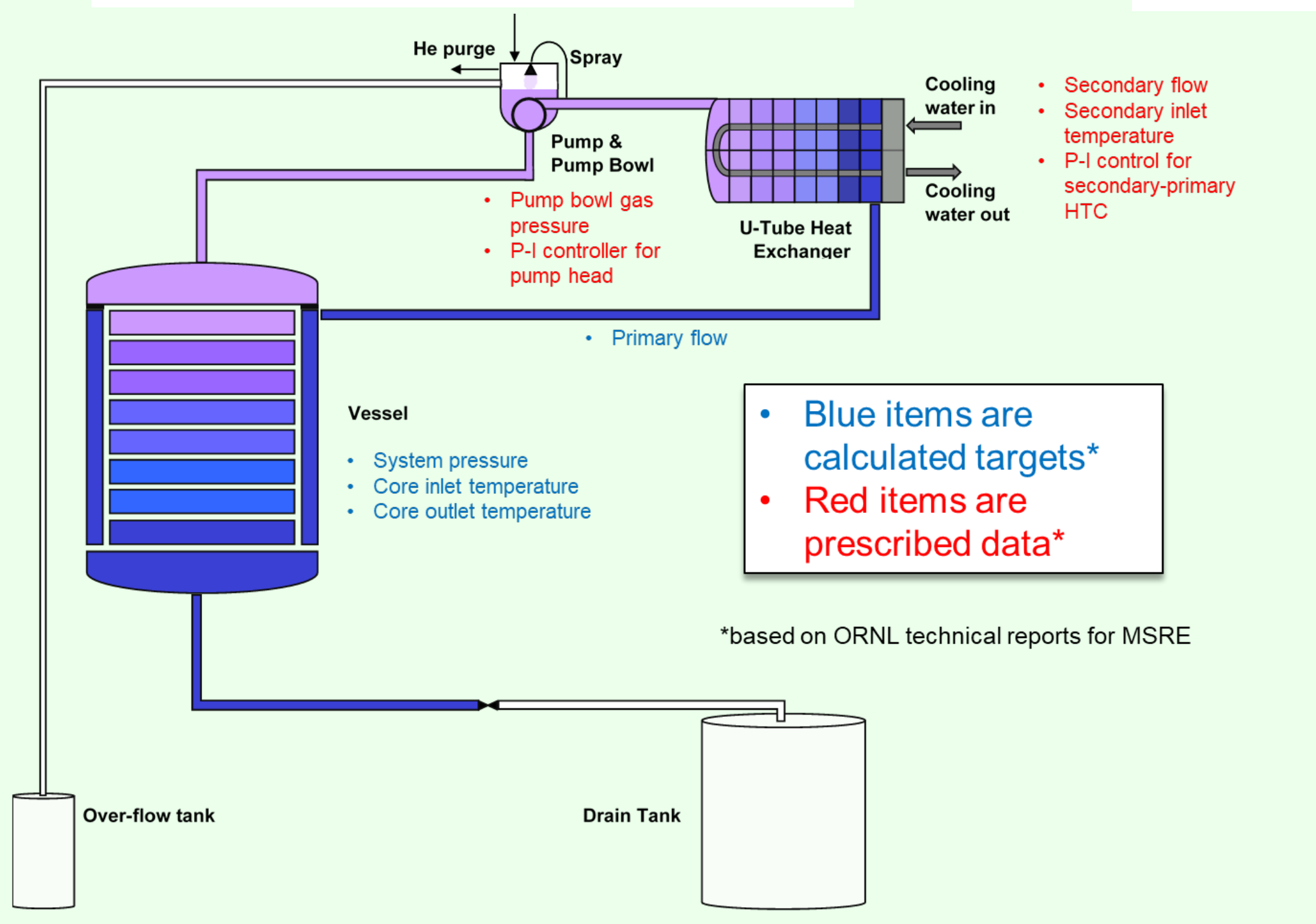


Molten Salt Reactors

- 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

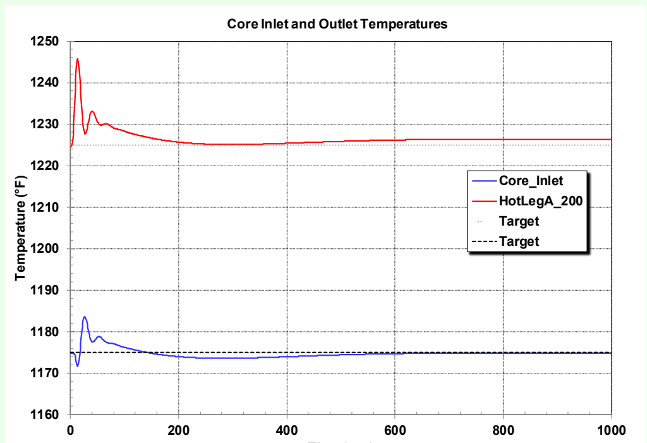




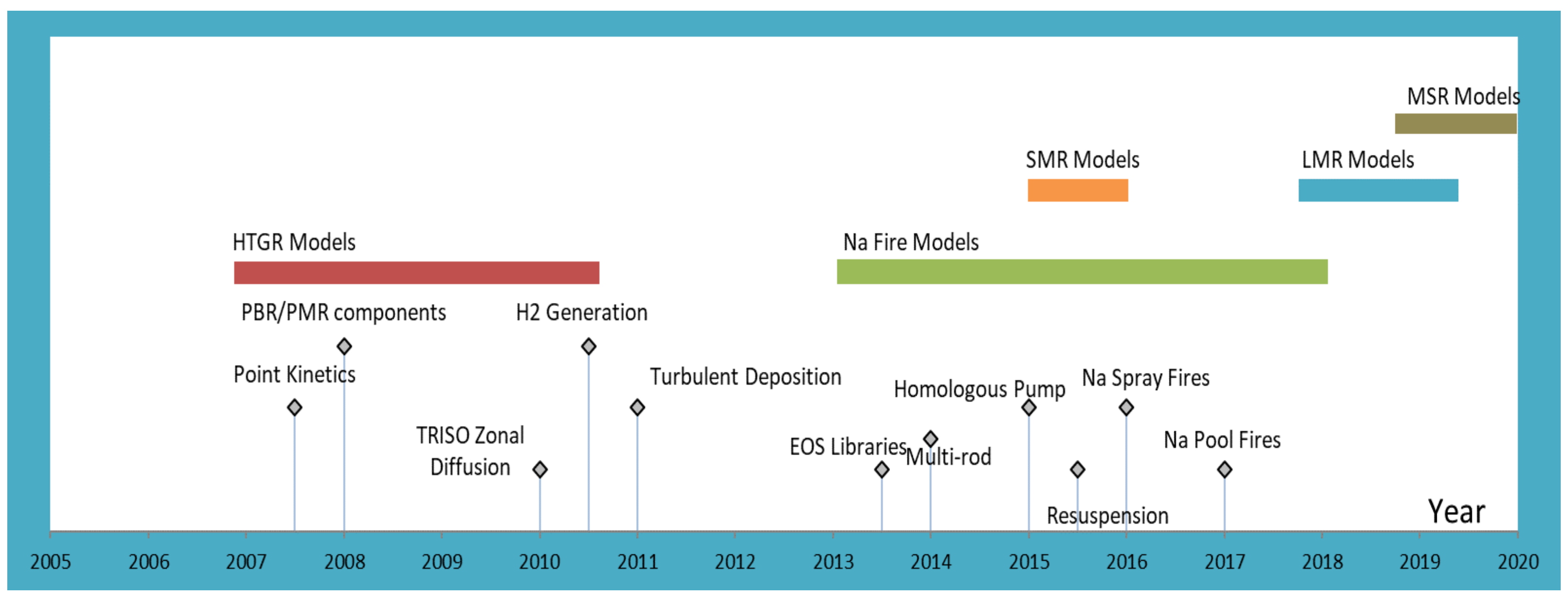


- Blue items are calculated targets*
- Red items are prescribed data*

*based on ORNL technical reports for MSRE



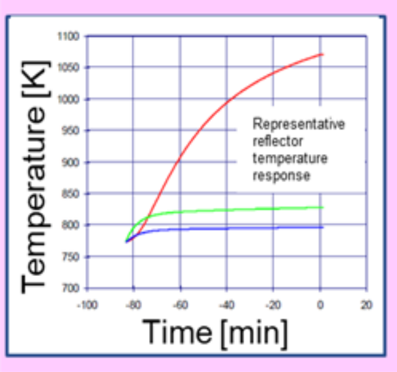
HTGR Reactor Modeling



Transient Accident Methodology

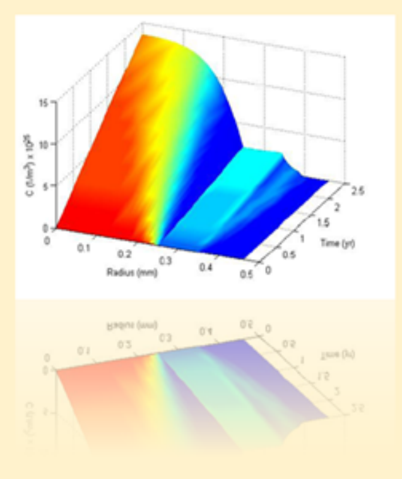
Stage 0:
Normal Operation
Establish thermal state

- *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.*



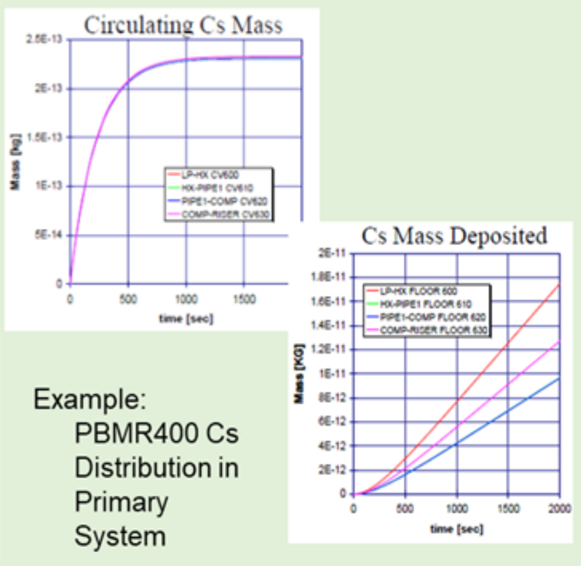
Stage 1:
Normal Operation
Diffusion Calculation

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



Stage 2:
Normal Operation
Transport Calculation

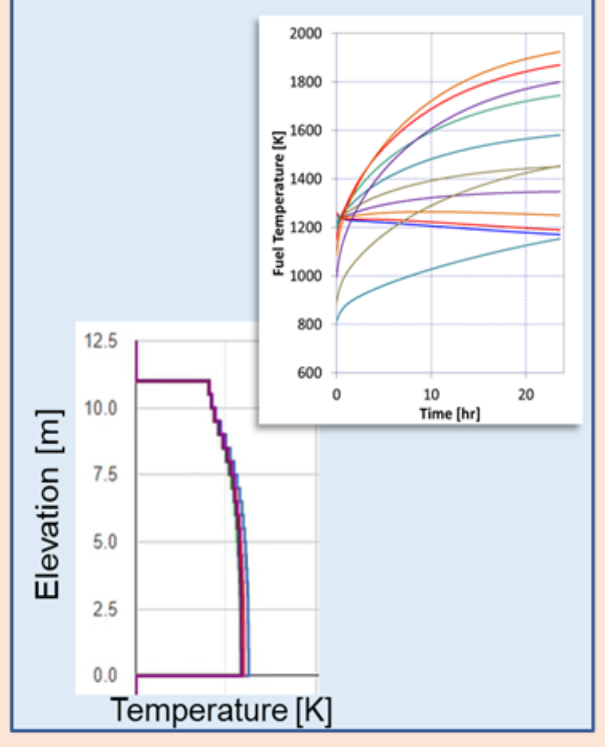
Calculate steady state distribution of radionuclides throughout system during normal operation (deposition on surfaces, convection through flow paths, etc.)



Example:
PBMR400 Cs Distribution in Primary System

Stage 3:
Accident
Diffusion & Transport calculation

Calculate accident progression and radionuclide release

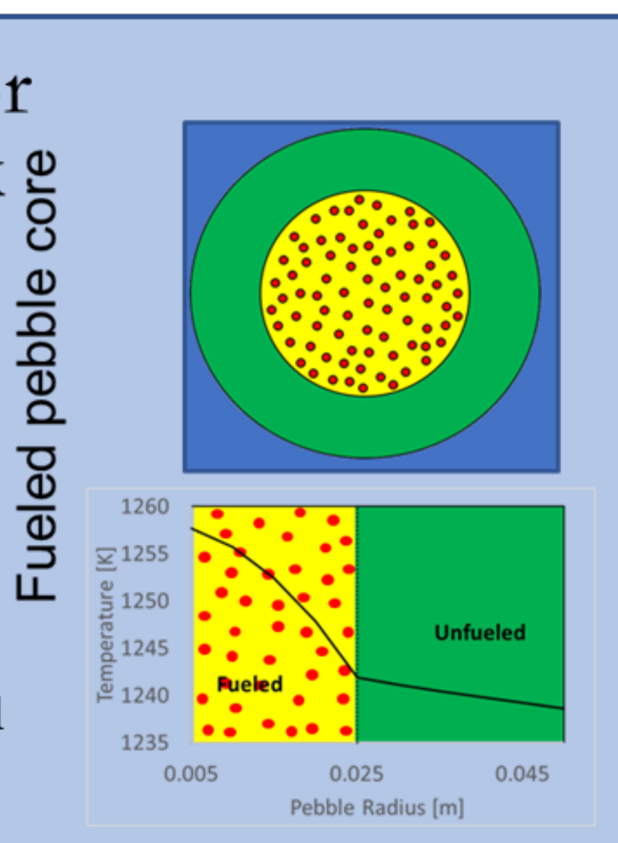


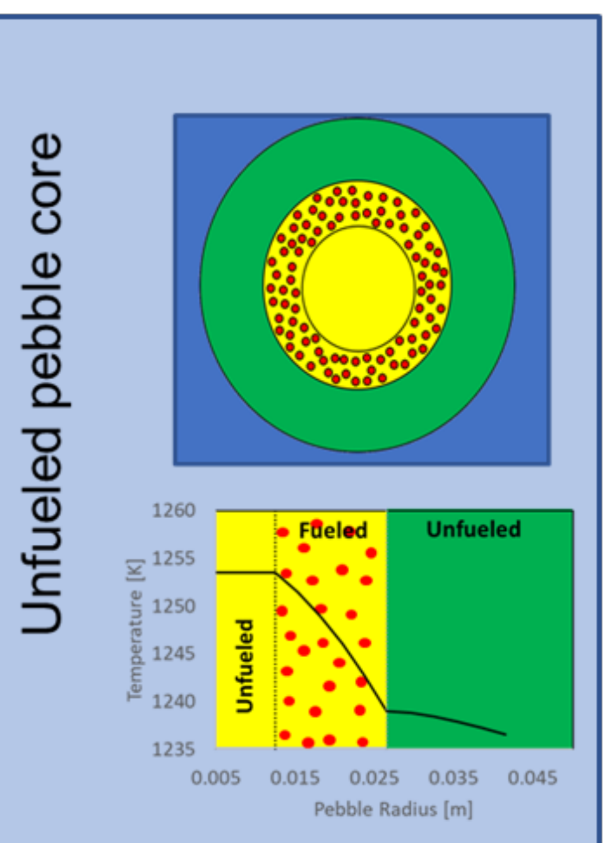
All steps performed in one run with data passed transparently between stages

HTGR Components

Pebble Bed Reactor (PBR) Fuel/Matrix Components

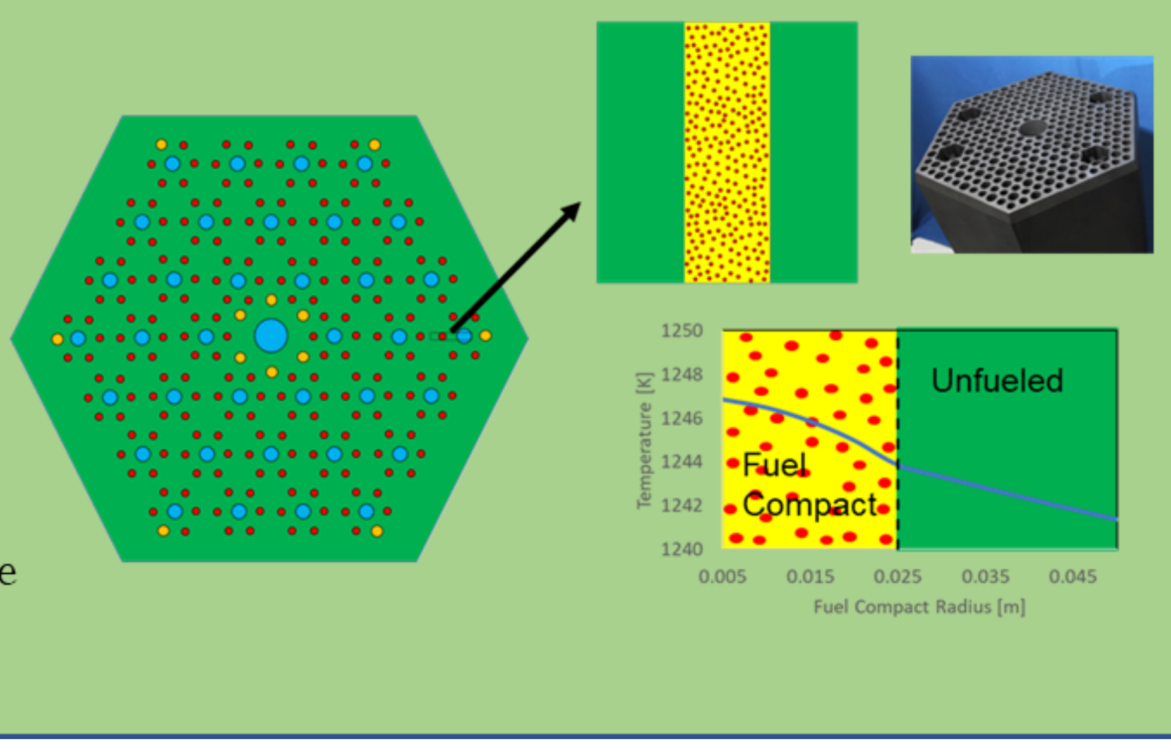
- Fueled part of pebble
- Unfueled shell is modeled as separate component (Matrix)
- Fuel radial temperature profile for sphere
  - Provides peak and surface pebble temperature
  - Modified for unfueled central core

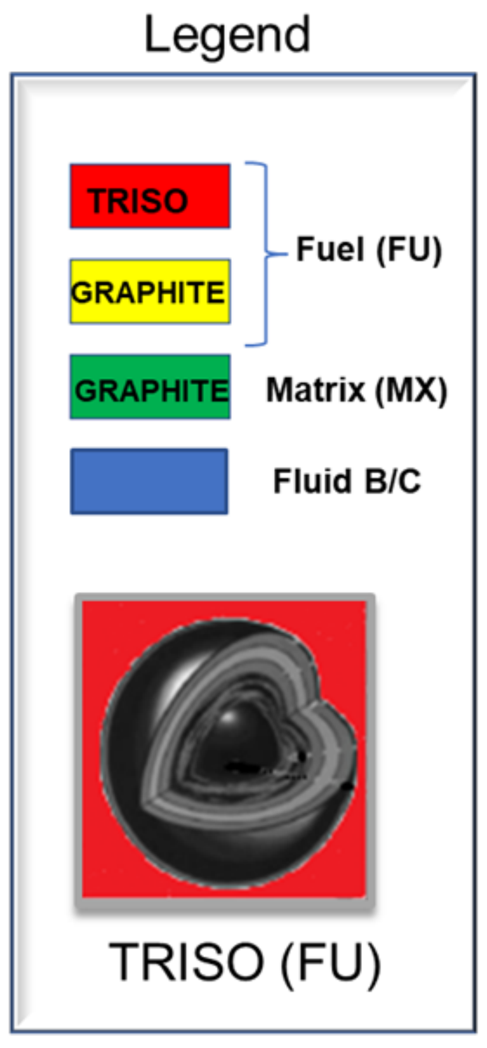




Prismatic Modular Reactor (PMR) Fuel/Matrix Components

- 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

Point Reactor Kinetics

Standard delayed-group treatment

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

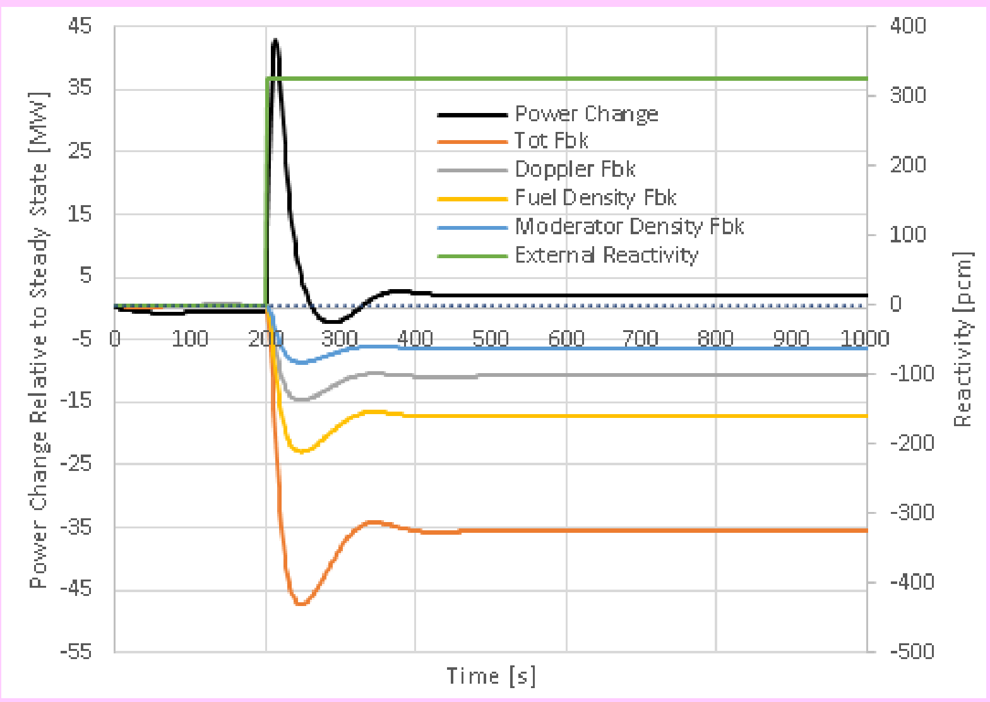
$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right)P - \lambda_i C_i, \qquad for\ i = 1 \ldots 6$$

Kinetics data accessible by sensitivity coefficients

Feedback models

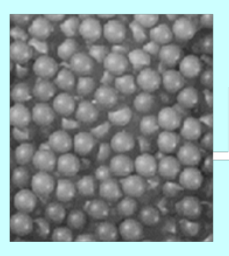
- Control function-specified externalcomponent
- Doppler
- Fuel and moderator density

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



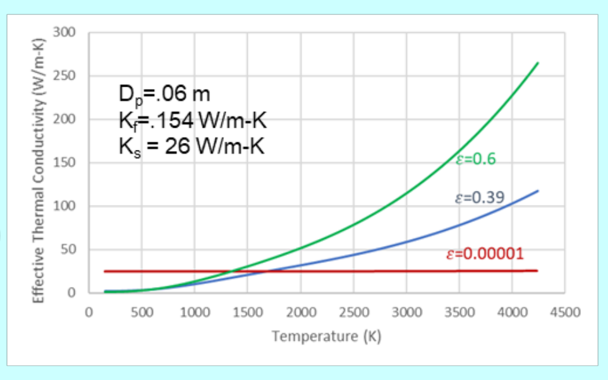
COR Intercell Conduction

Effective conductivity prescription for PBR (bed conductance)

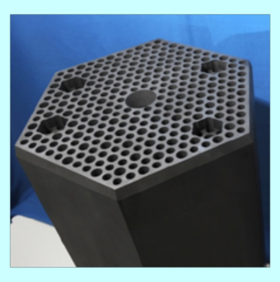


- Zehner-Schlunder-Bauer with Breitbach-Barthels modification to the radiation term

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



Effective conductivity prescription for PMR (continuous solid with pores)



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

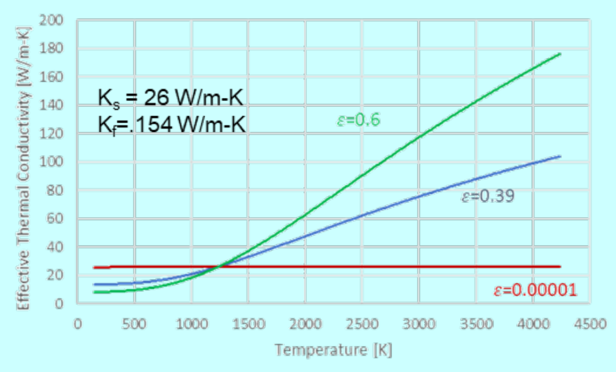
$$k_{eff} = k_s\left[A + (1-A)\frac{\ln\left(1+2B\left(k_{por}/k_s-1\right)\right)}{2B\left(1-k_s/k_{por}\right)}\right]$$

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

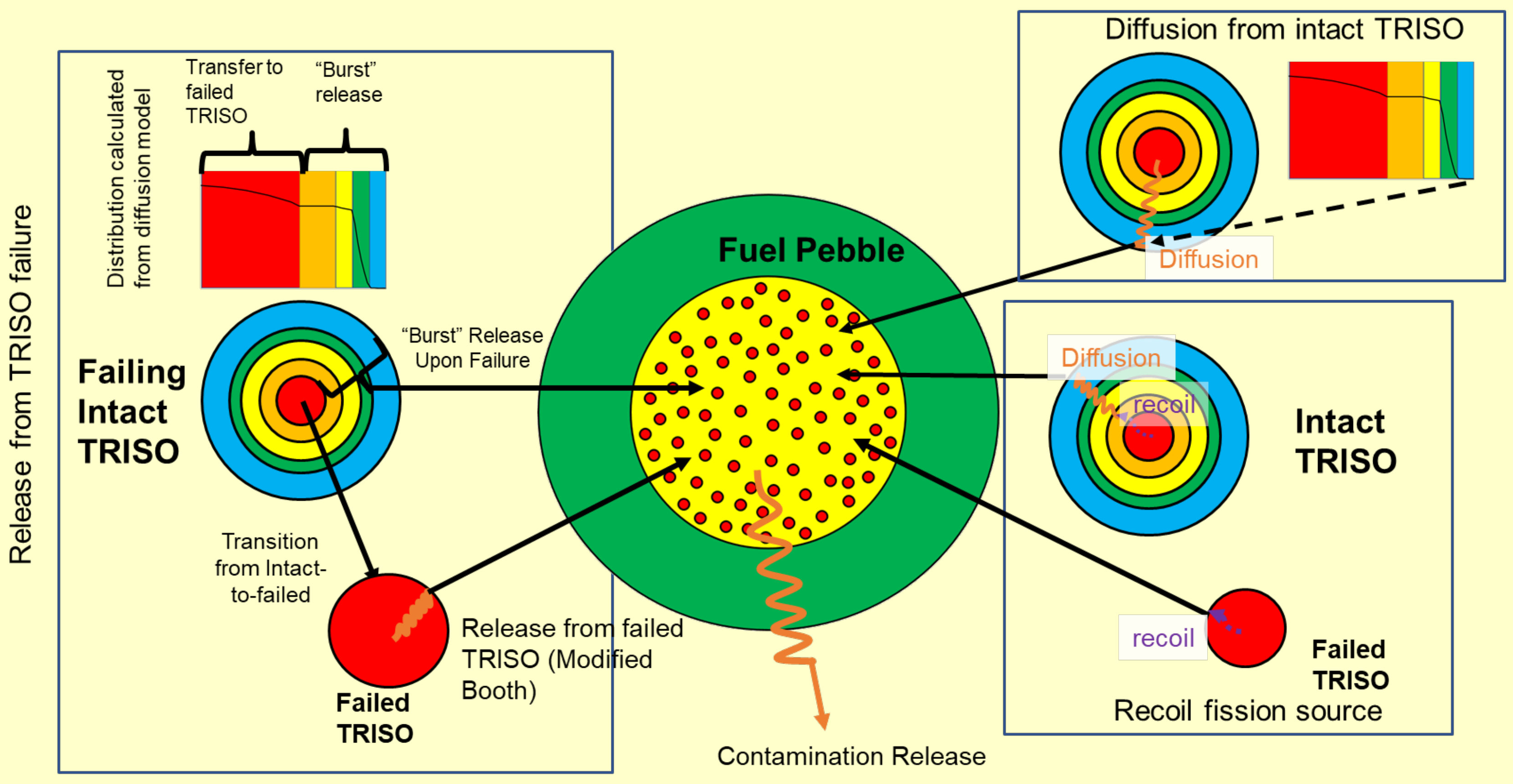
$$k_{rad} = 4\varepsilon_r\sigma T^3 D$$

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

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



Release Models



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

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

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

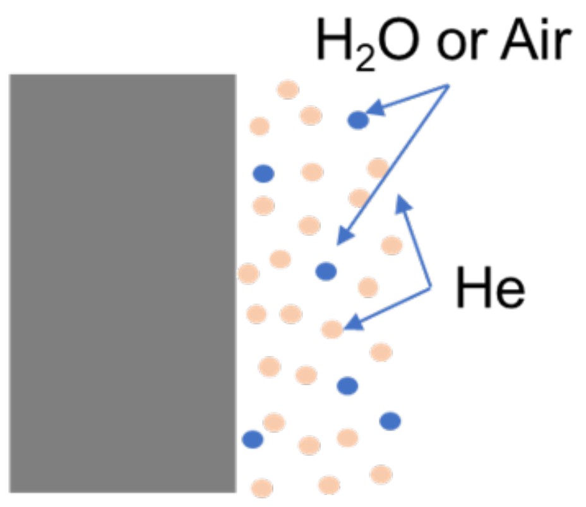
Air oxidation

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

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

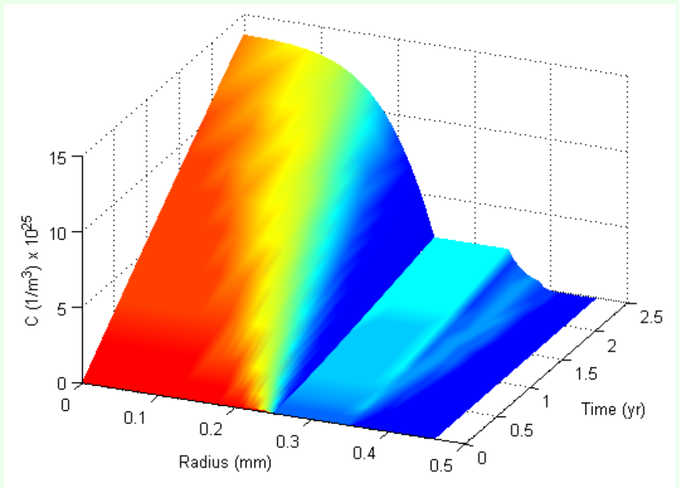


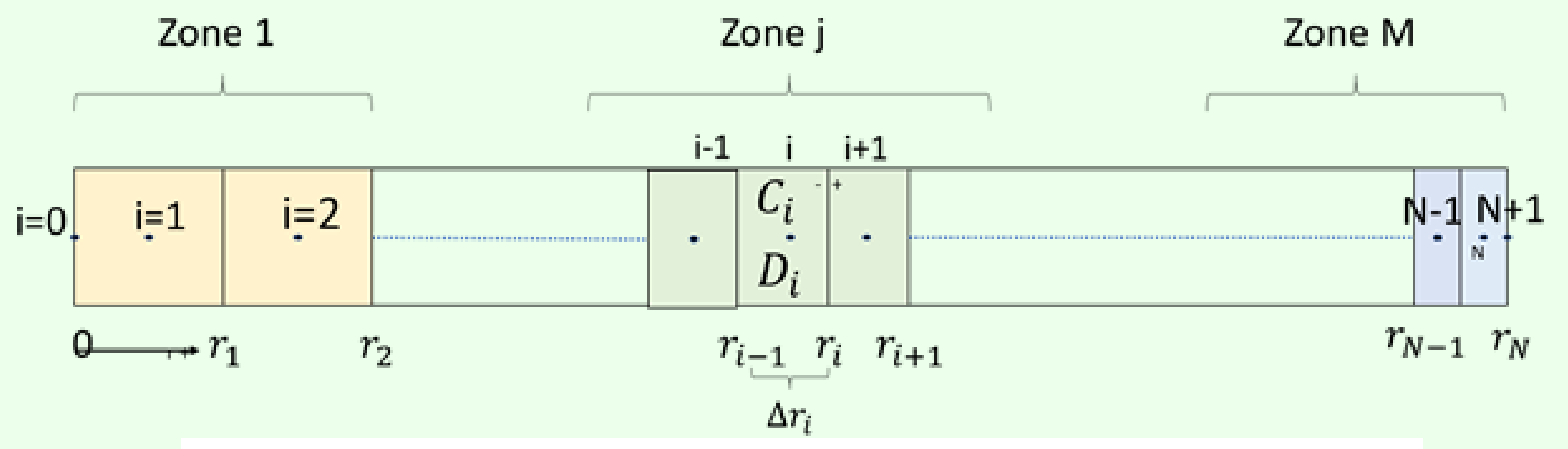
Intact TRISO Particles

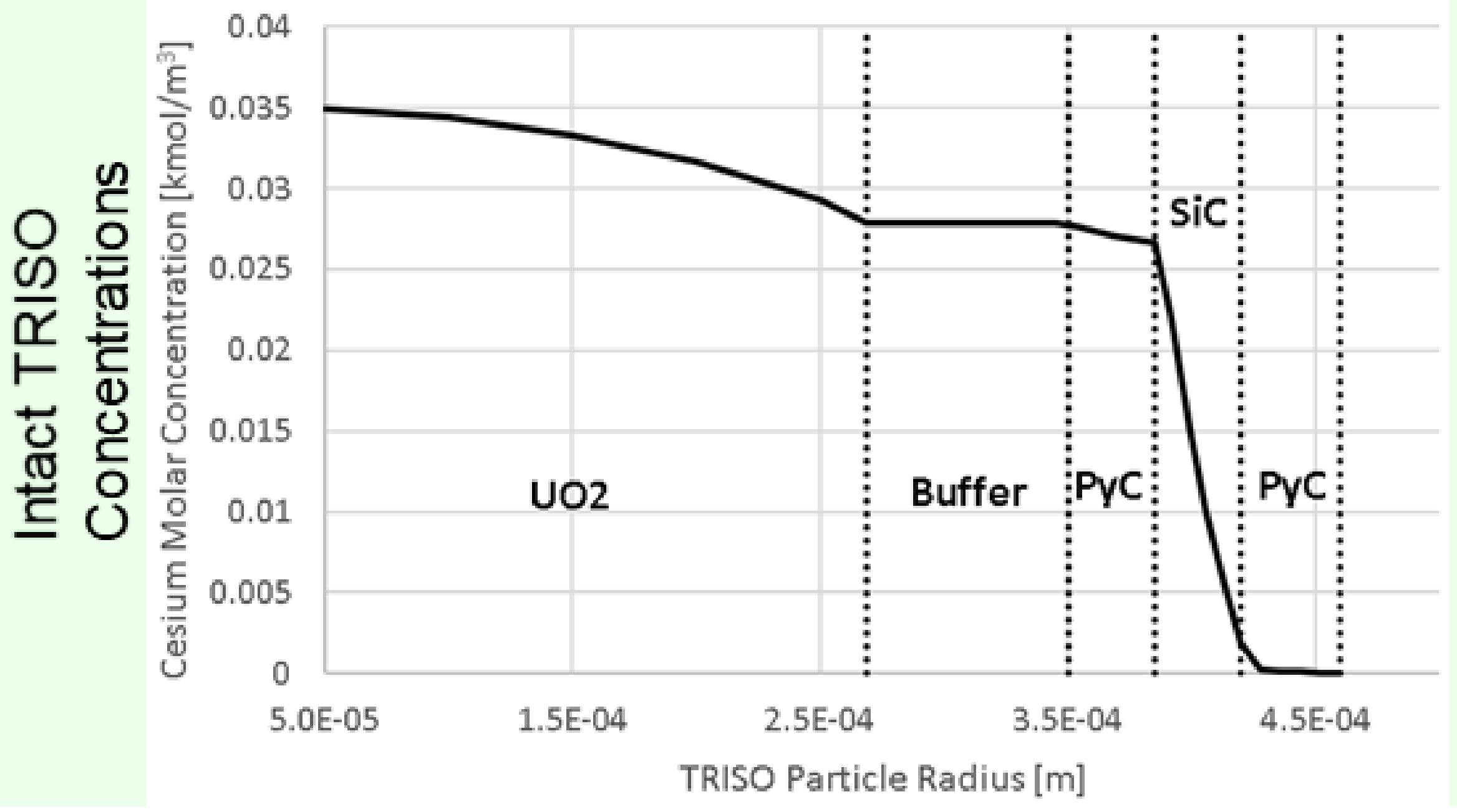
- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

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

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







MELCOR LWR Advancements

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Top-Quenched Debris in Cavity

New Modeling based on CORQUENCH Model

Water-Ingression Model

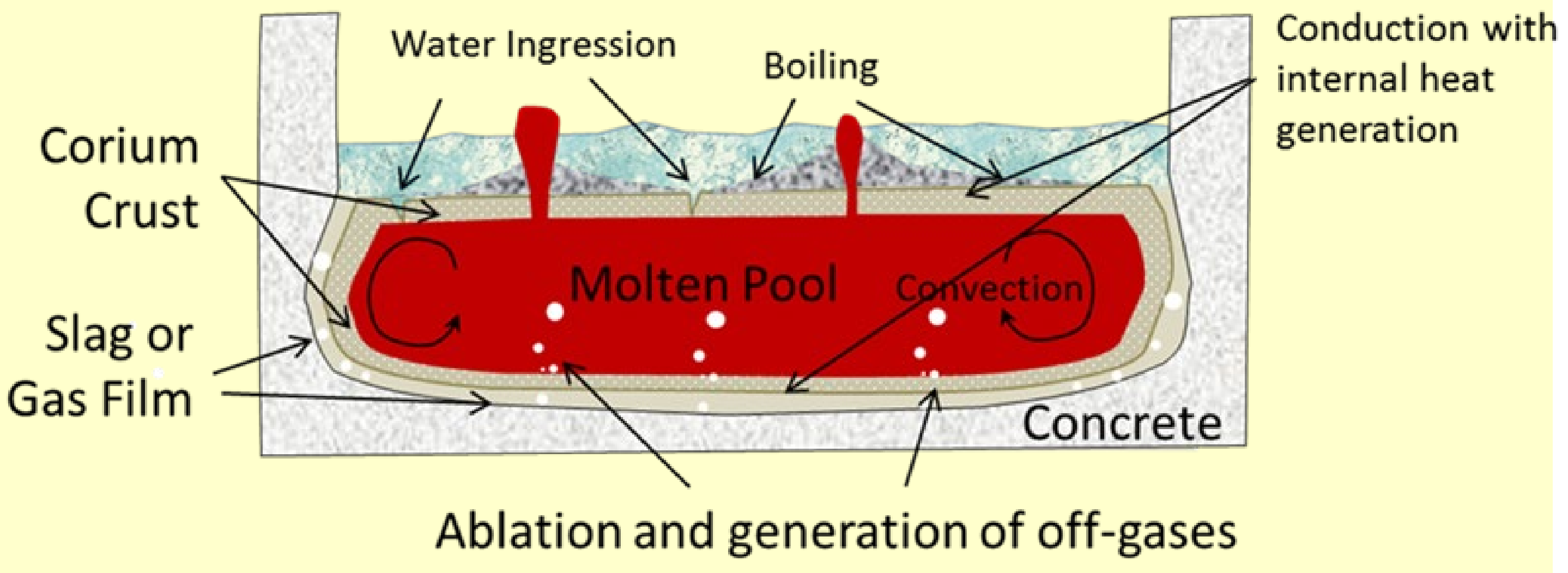
Quenching of the upper crust at the top of the corium debris can lead to a considerable density change (~18%volume) leading to cracking and formation of voids

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.

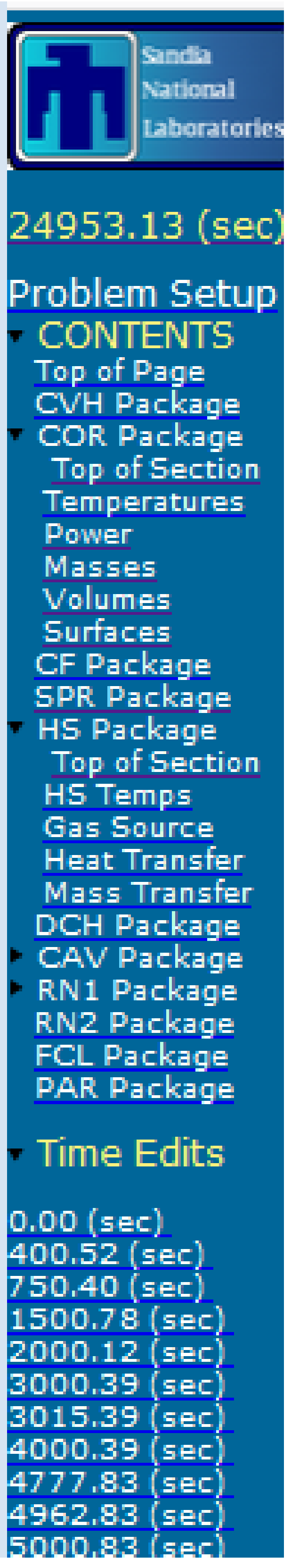
Enhances the coolability of the molten corium by relocating enthalpy from the internal melt through the crust more coolable geometry that is more porous and permeable to water



Fully implemented

Validated

HTML Output



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Problem Setup
- CONTENTS
  - Top of Page
  - CVH Package
  - COR Package
    - Top of Section
    - Temperatures
    - Power
    - Masses
    - Volumes
    - Surfaces
  - CF Package
  - SPR Package
  - HS Package
    - Top of Section
    - HS Temps
    - Gas Source
    - Heat Transfer
    - Mass Transfer
  - DCH Package
  - CAV Package
  - RN1 Package
  - RN2 Package
  - FCL Package
  - PAR Package
- Time Edits

0.00 (sec)
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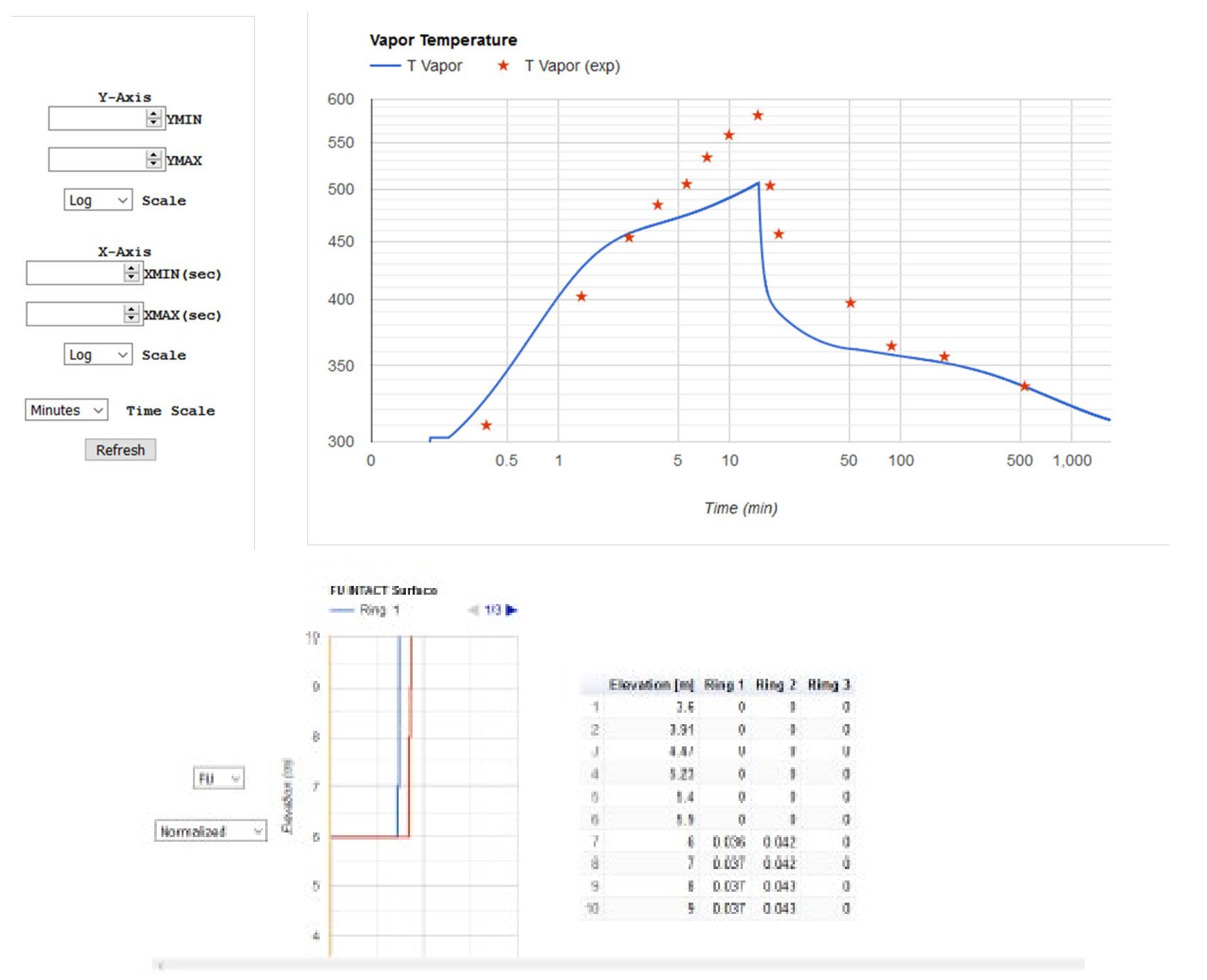
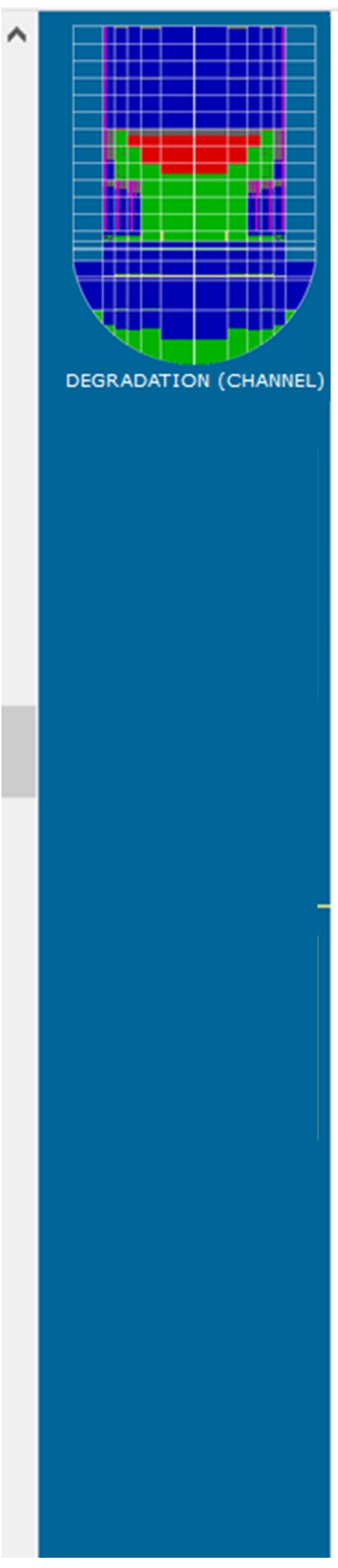
2000.12 (sec)
3000.39 (sec)
3015.39 (sec)
4000.39 (sec)
4777.83 (sec)
4962.83 (sec)
5000.83 (sec)

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

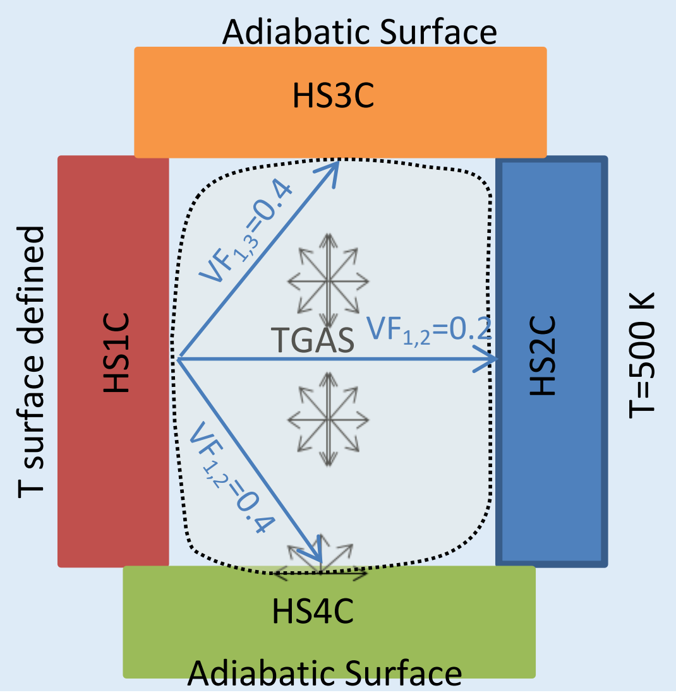
Radiation Enclosure Model

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

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

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

$$q_i = A_i\left(J_i - G_i\right)$$



```
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)

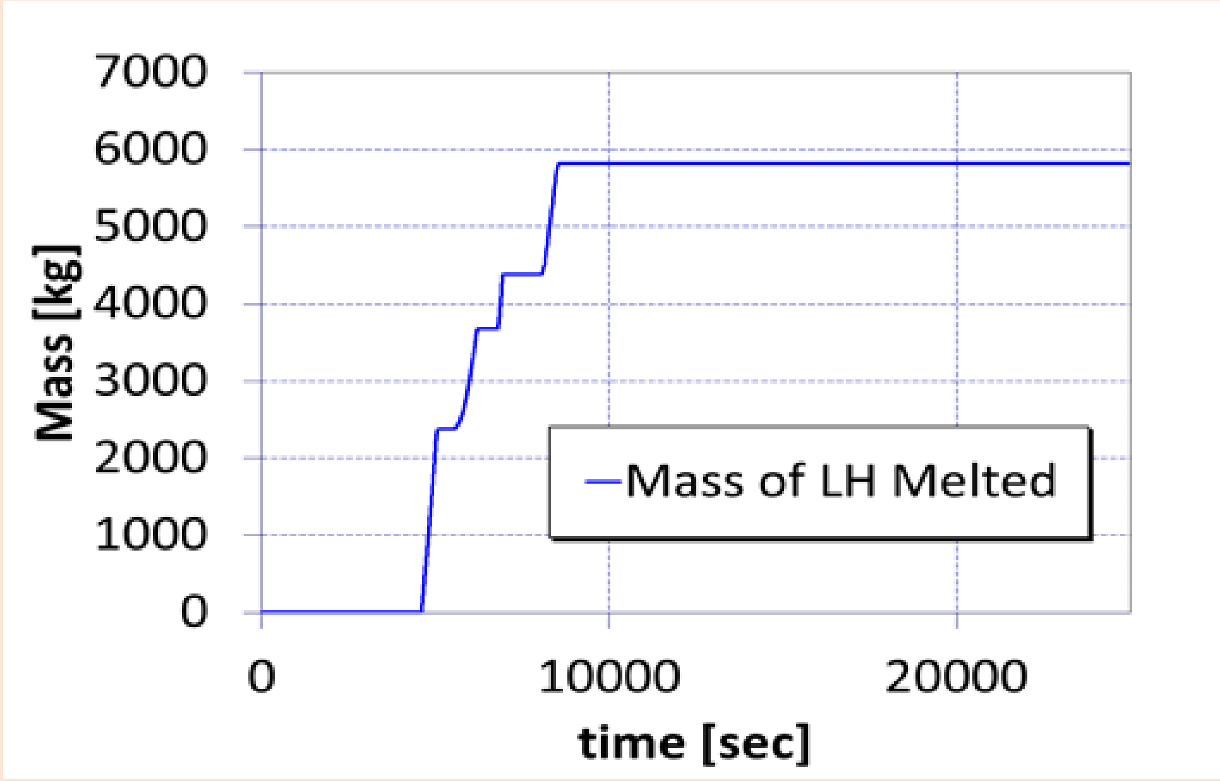
General Oxidation Model makes use of the new UDMs to create a new oxidizable material.

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

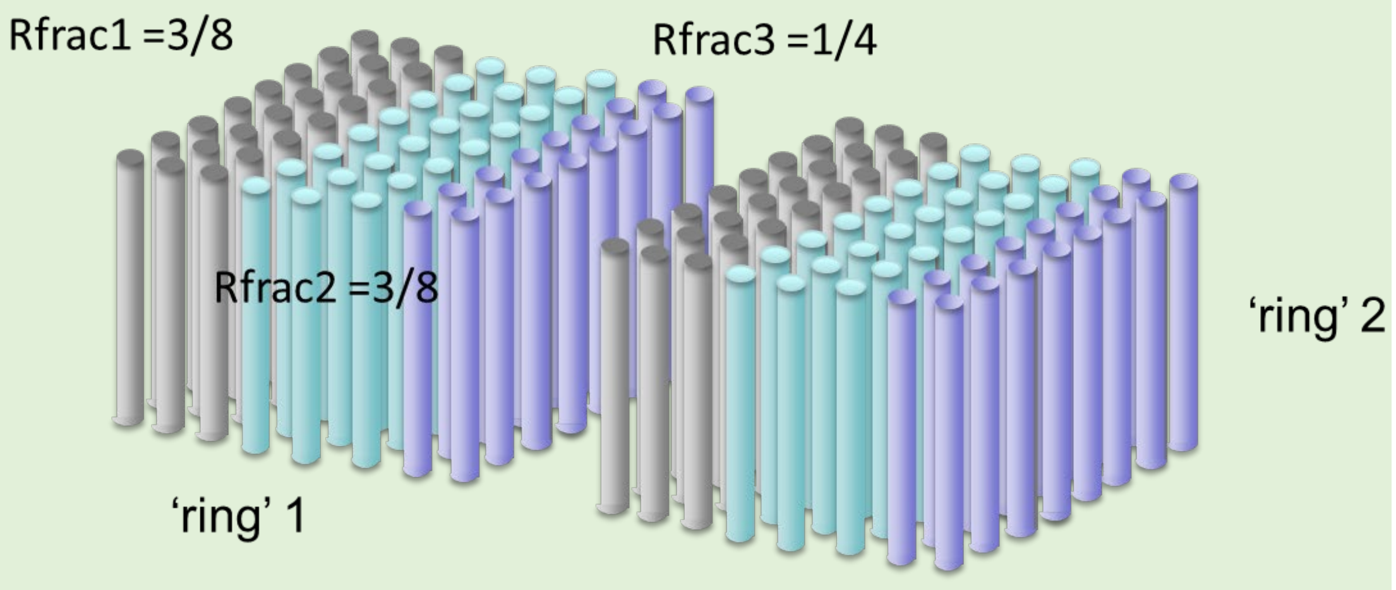


Multi-rod Model

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

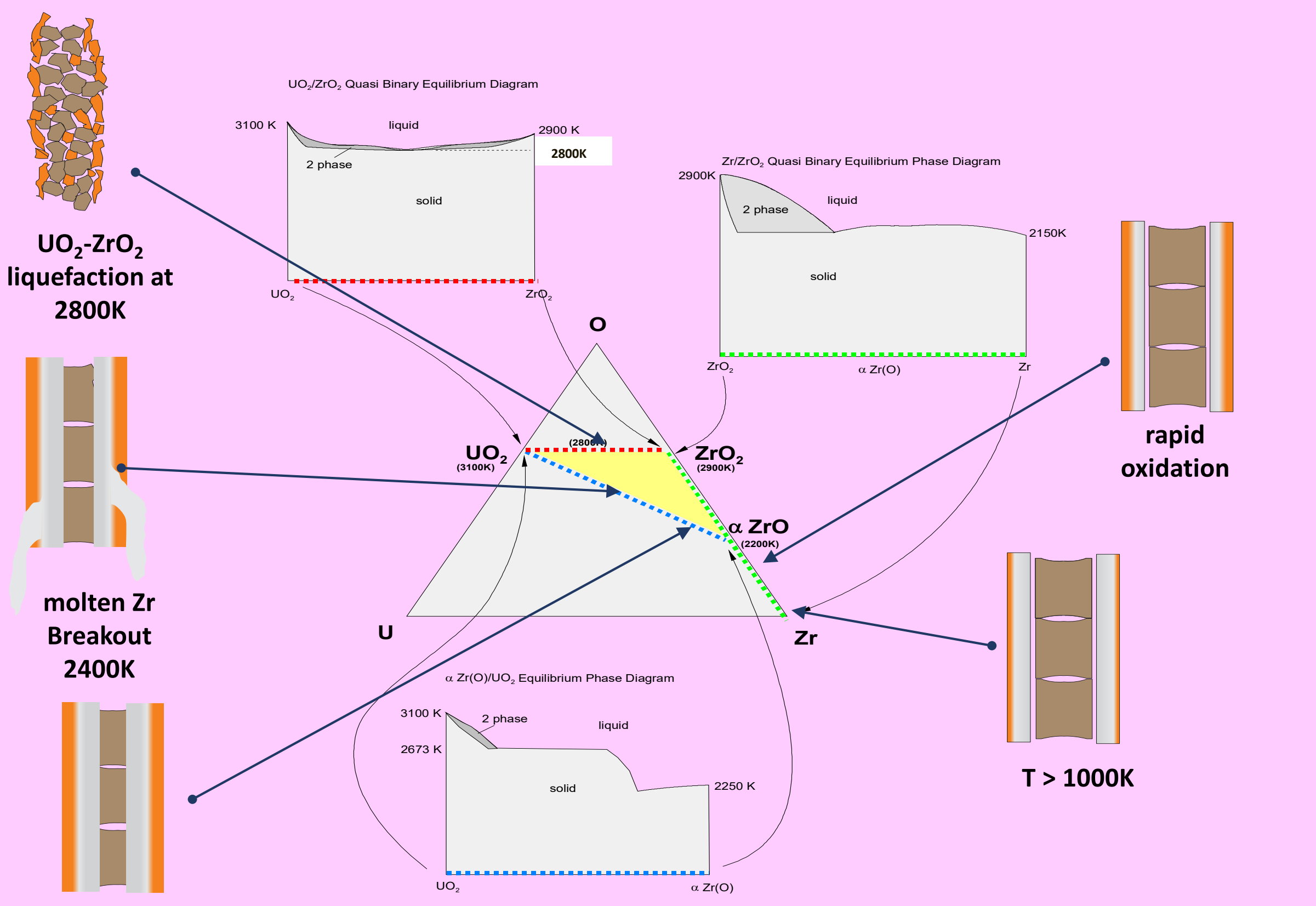


Eutectic Model

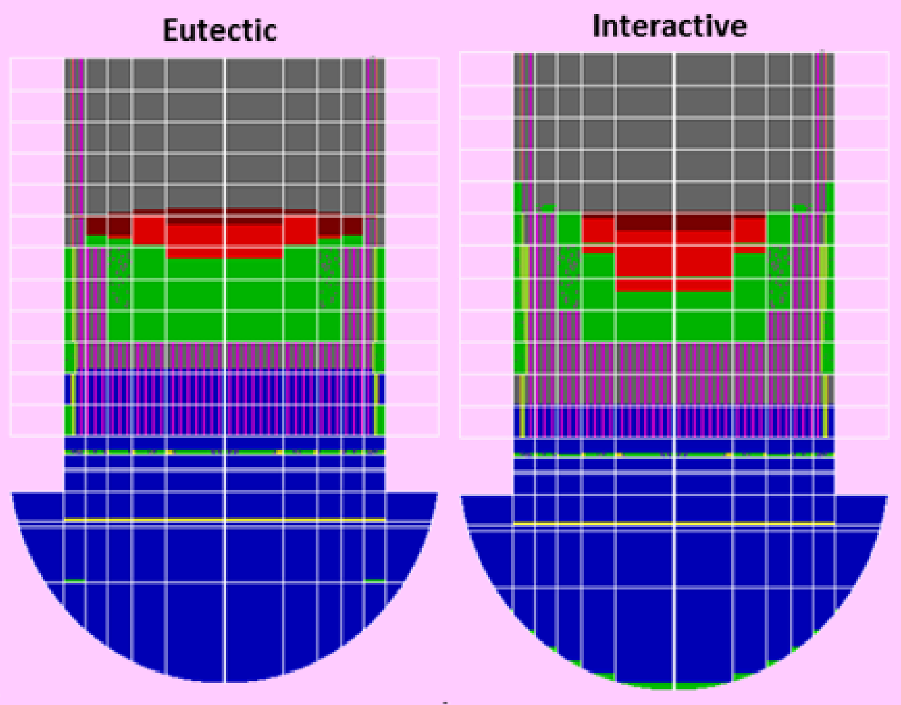
- Composition dependence of melting temperatures
- User specifies eutectic temperature and composition for material pairs
  - Zr/SS, Zr/INC, UO2/ZRO2
- Materials Interactions model
  - Parabolic rate of dissolution reaction accounting for changes to liquidus
  - Liquefaction of ZrO2 in BWR canisters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

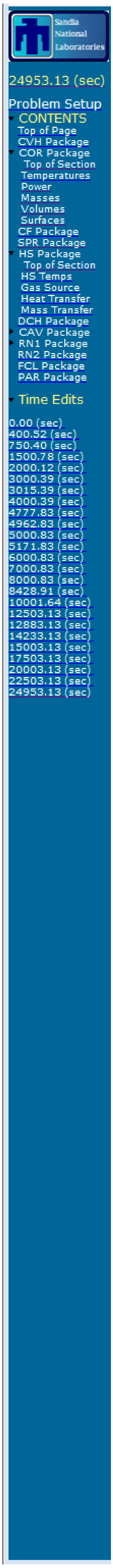


Comparison of Eutectics Model and older interactive materials model



MELCOR HTML Output

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.



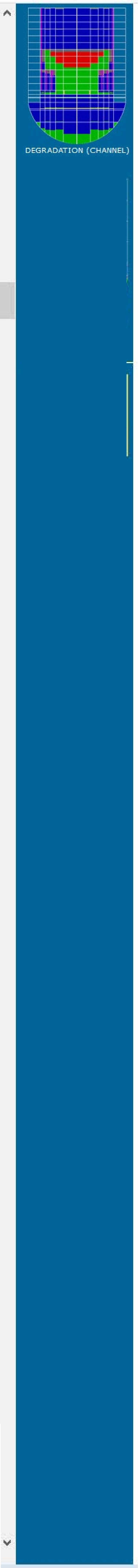
24953.13 (sec)

Problem Setup

- CONTENTS
  - Top of Page
  - CVH Package
  - COR Package
    - Top of Section
    - Temperatures
    - Power
    - Masses
    - Volumes
    - Surfaces
  - CF Package
  - SPR Package
  - HS Package
    - Top of Section
    - HS Temps
    - Gas Source
    - Heat Transfer
    - Mass Transfer
  - DCH Package
  - CAV Package
  - RN1 Package
  - RN2 Package
  - FCL Package
  - PAR Package
- Time Edits

0.00 (sec)
400.52 (sec)
750.40 (sec)
1500.78 (sec)
2000.12 (sec)
3000.39 (sec)
3015.39 (sec)
4000.39 (sec)
4777.83 (sec)
4962.83 (sec)
5000.83 (sec)
5171.83 (sec)
6000.83 (sec)
7000.83 (sec)
8000.83 (sec)
8428.91 (sec)
10001.64 (sec)
12503.13 (sec)
12883.13 (sec)
14233.13 (sec)
15003.13 (sec)
17503.13 (sec)
20003.13 (sec)
22503.13 (sec)
24953.13 (sec)

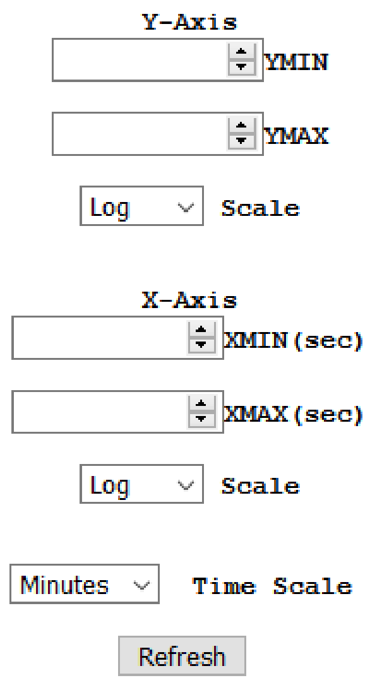
- *Lightning fast hyper-linked navigation to the MELCOR output you're looking for.*
- *Graphical depiction of core degradation*
- *Automatic plot generation for enhanced user efficiency*
  - *Trend plots, profile plots, animated plots*
- *Plots of material property functions, EOS functions, and fluid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

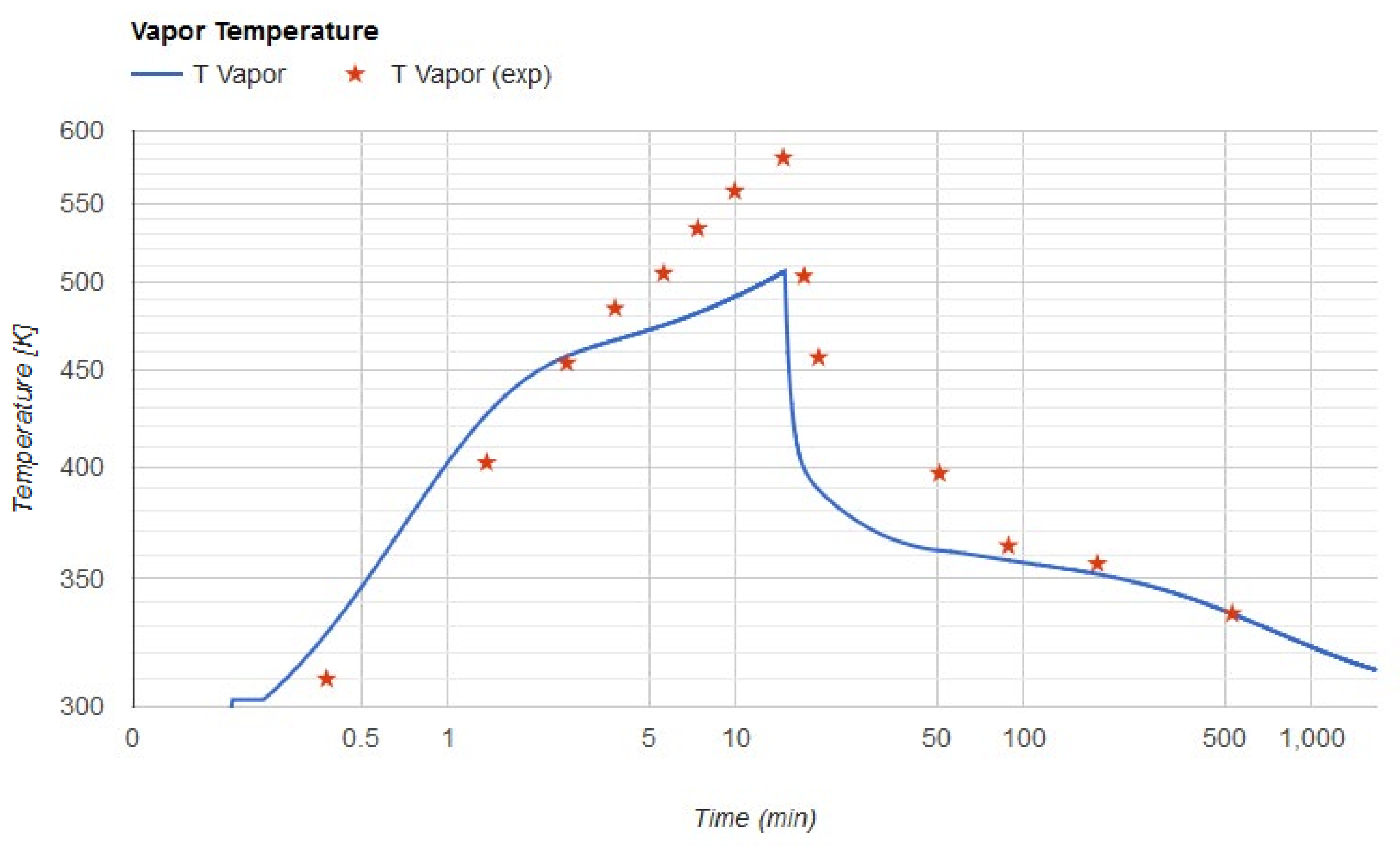


User Customized Plots

- 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'
```

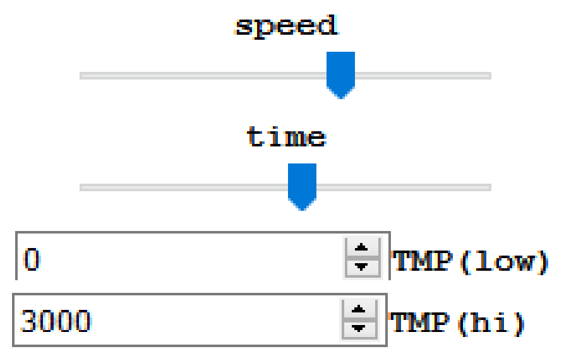




Static and Animated Profiles

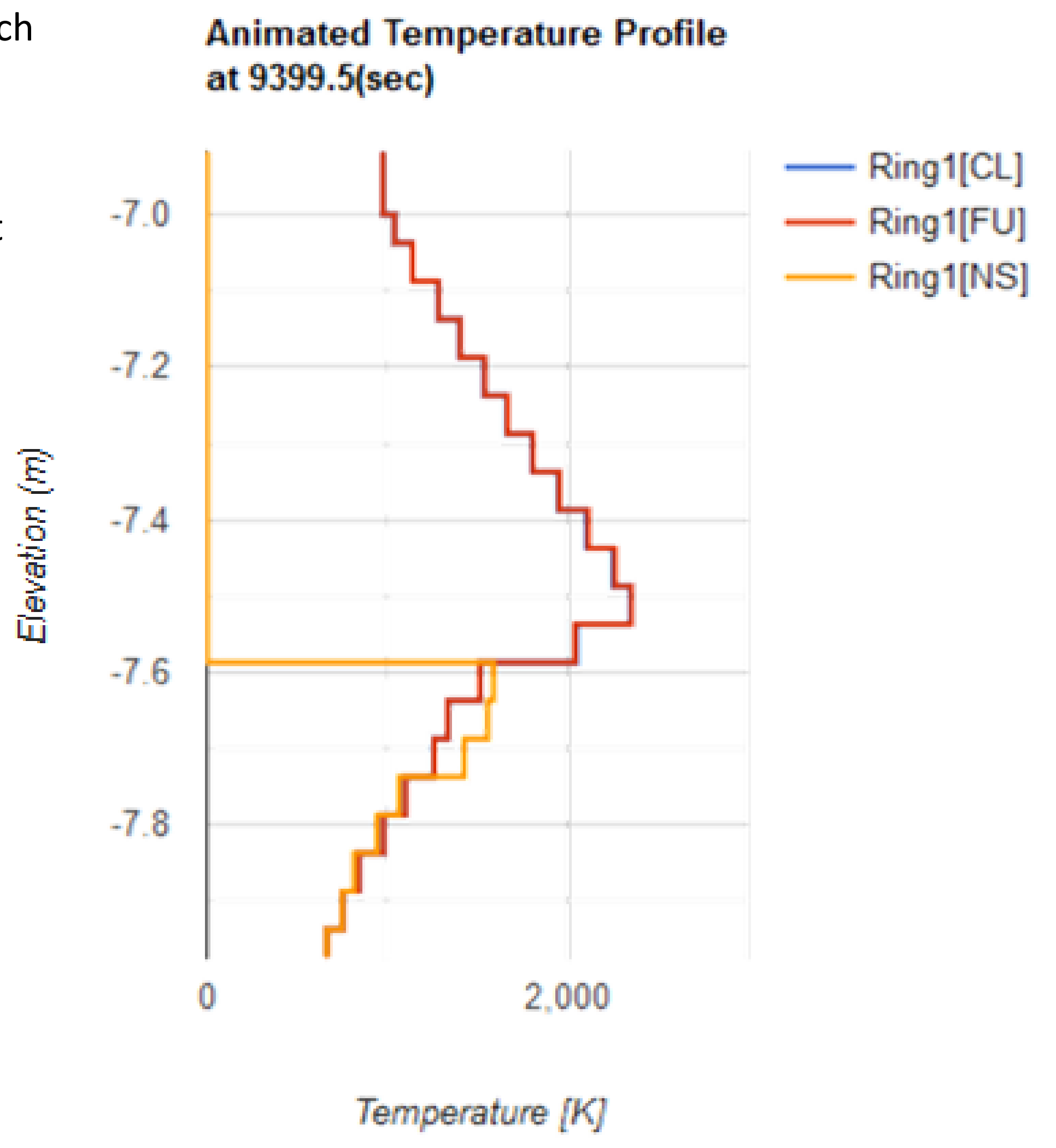
Temperatures, mass, power, surface area, volumes

- 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

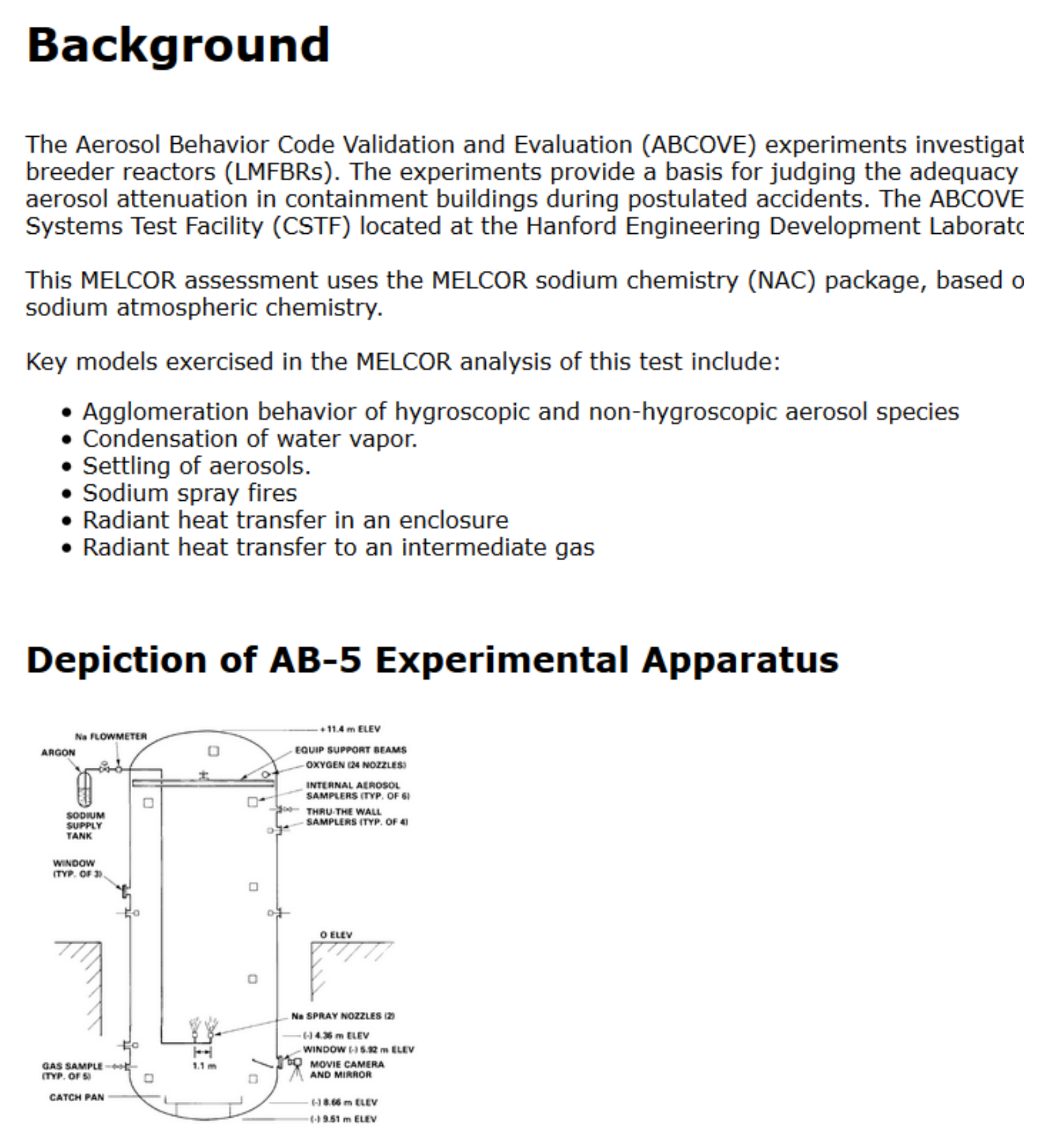


Minimal Input Required

```
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 Laboratc

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

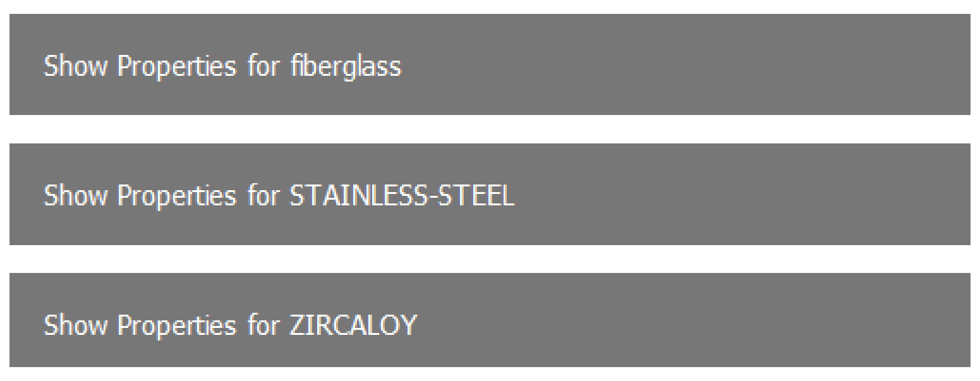
Key models exercised in the MELCOR analysis of this test include:

- 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

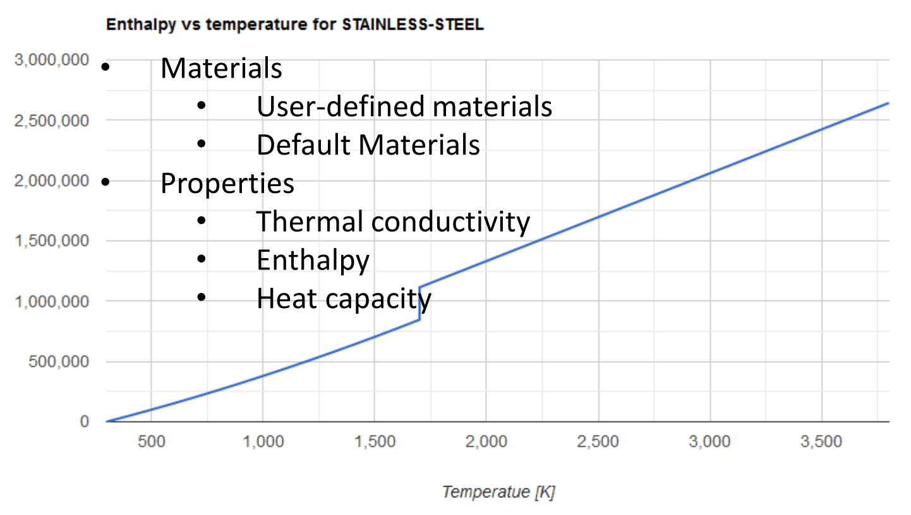
Depiction of AB-5 Experimental Apparatus

Material Property Plots Generated at MELGEN

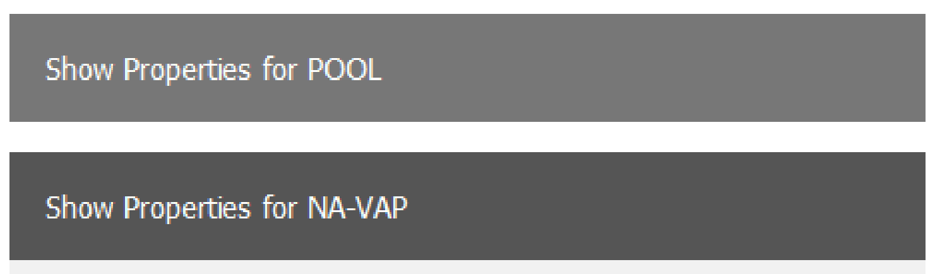
MATERIAL PROPERTIES PACKAGE



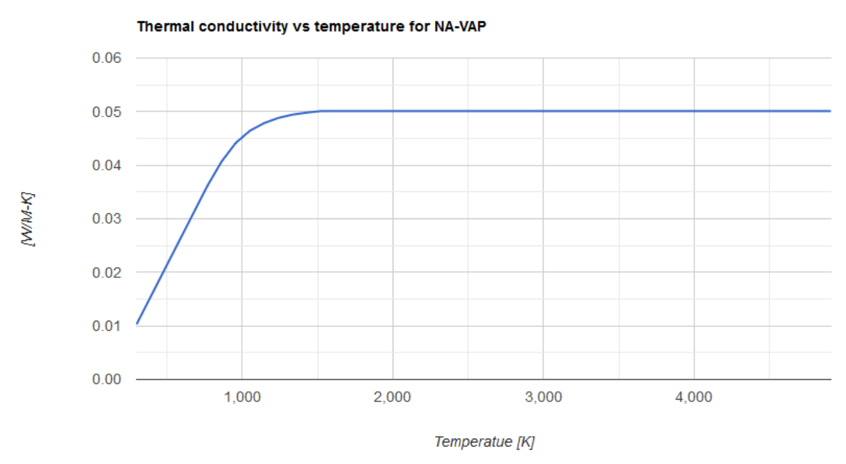
- Materials
  - User-defined materials
  - Default Materials
- Properties
  - Thermal conductivity
  - Enthalpy
  - Heat capacity



NON CONDENSIBLE GAS PACKAGE

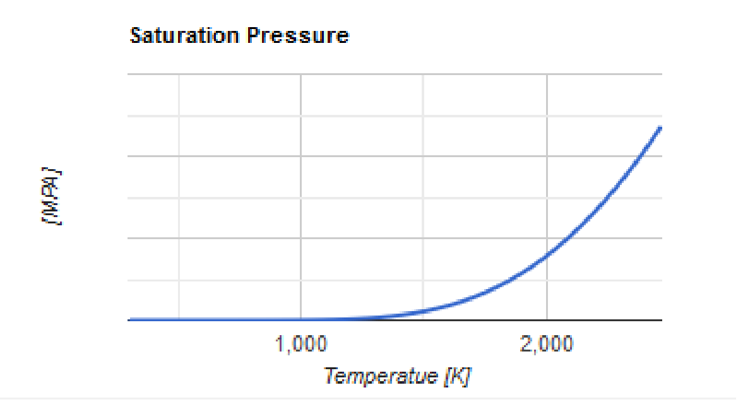


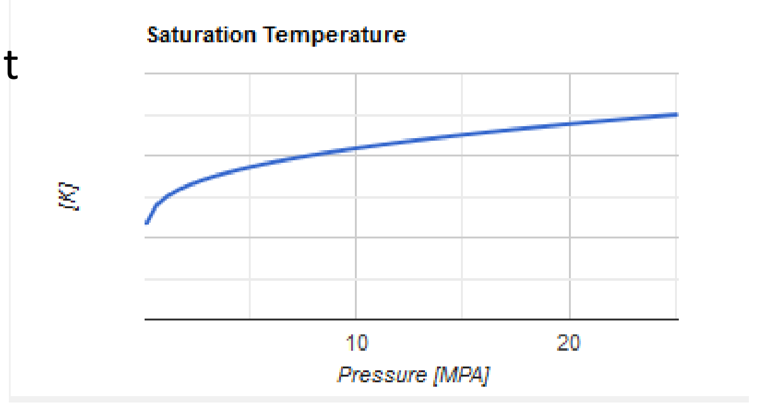
- Viscosity
- Thermal conductivity



EOS PACKAGE

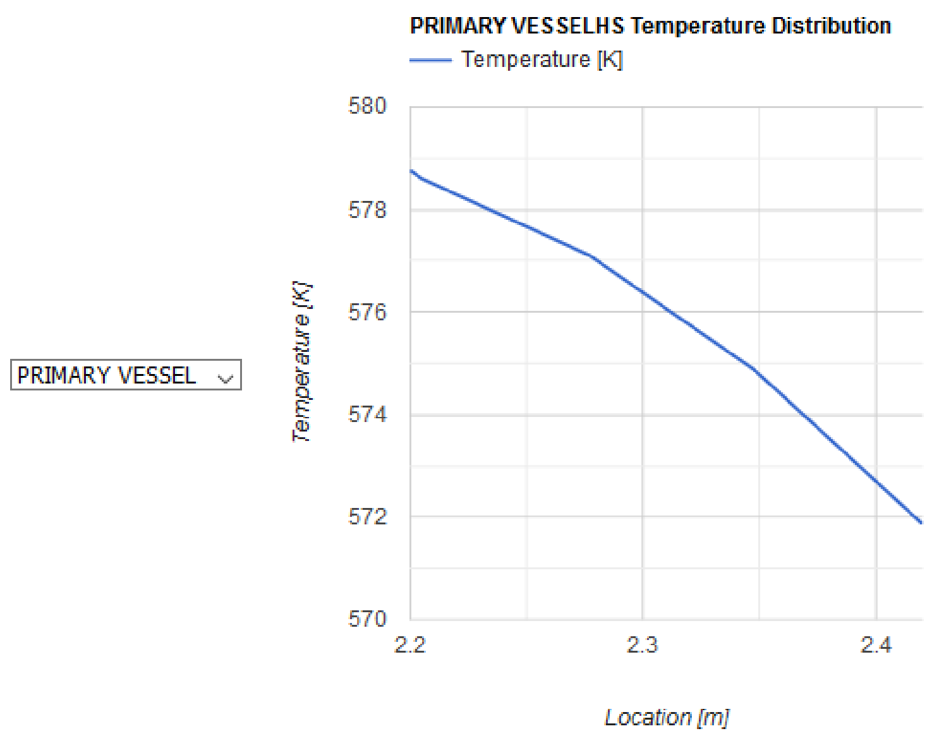
- Saturation Pressure
- Saturation Temperature
- Liquid Density at saturation
- Vapor density at saturation
- Liquid specific enthalpy at saturation pressure
- Vapor specific enthalpy at saturation pressure
- Liquid specific heat
- Vapor specific heat



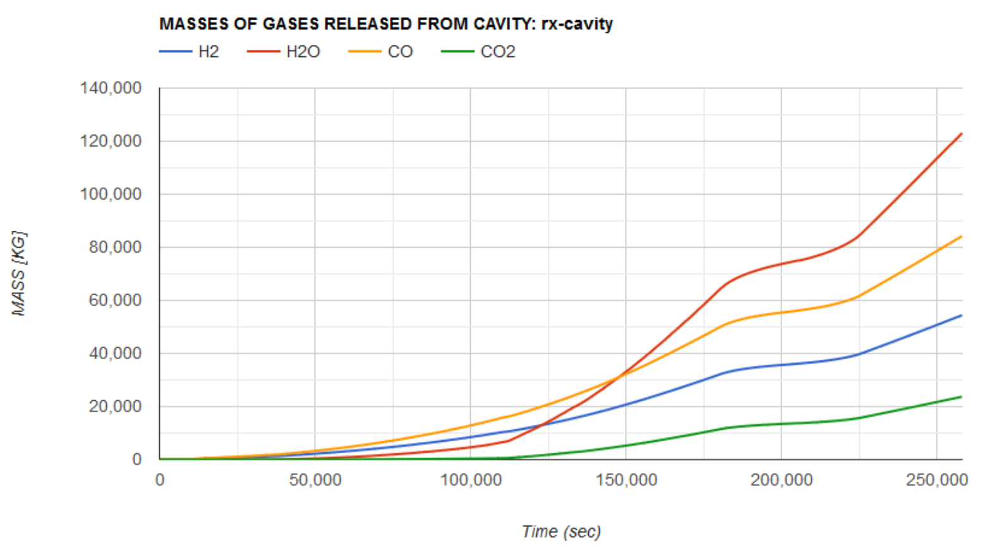


Automatically Generated Model-Dependent Plots

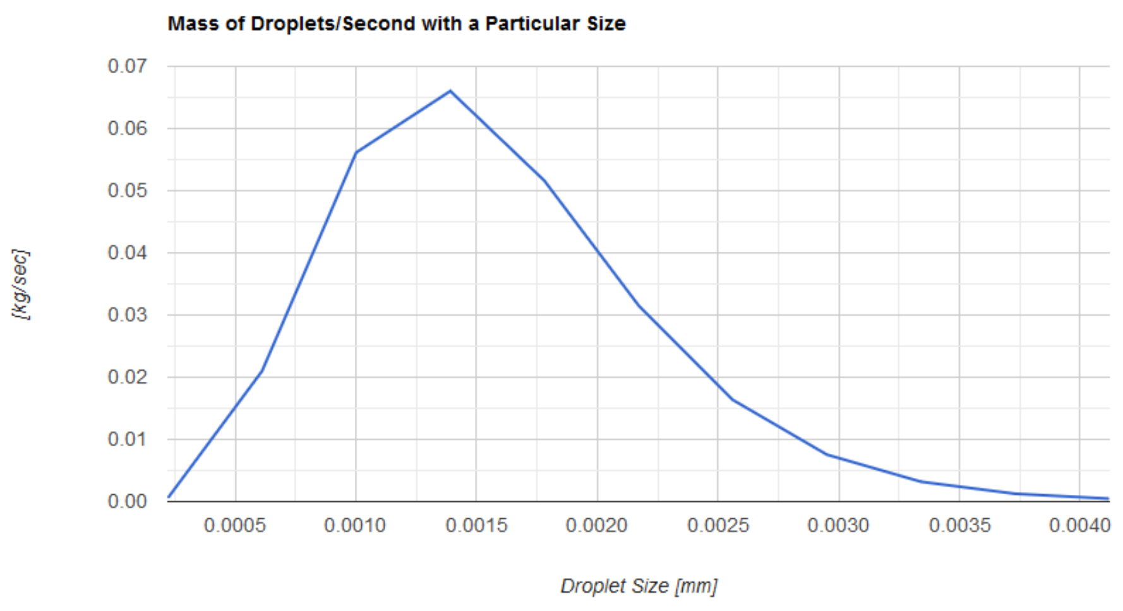
HS PACKAGE



MCCI MODELS



NA SPRAY FIRE MODEL



Now Available in MELCOR 2.2.14770 or Later

Non-LWR Demo Calculations

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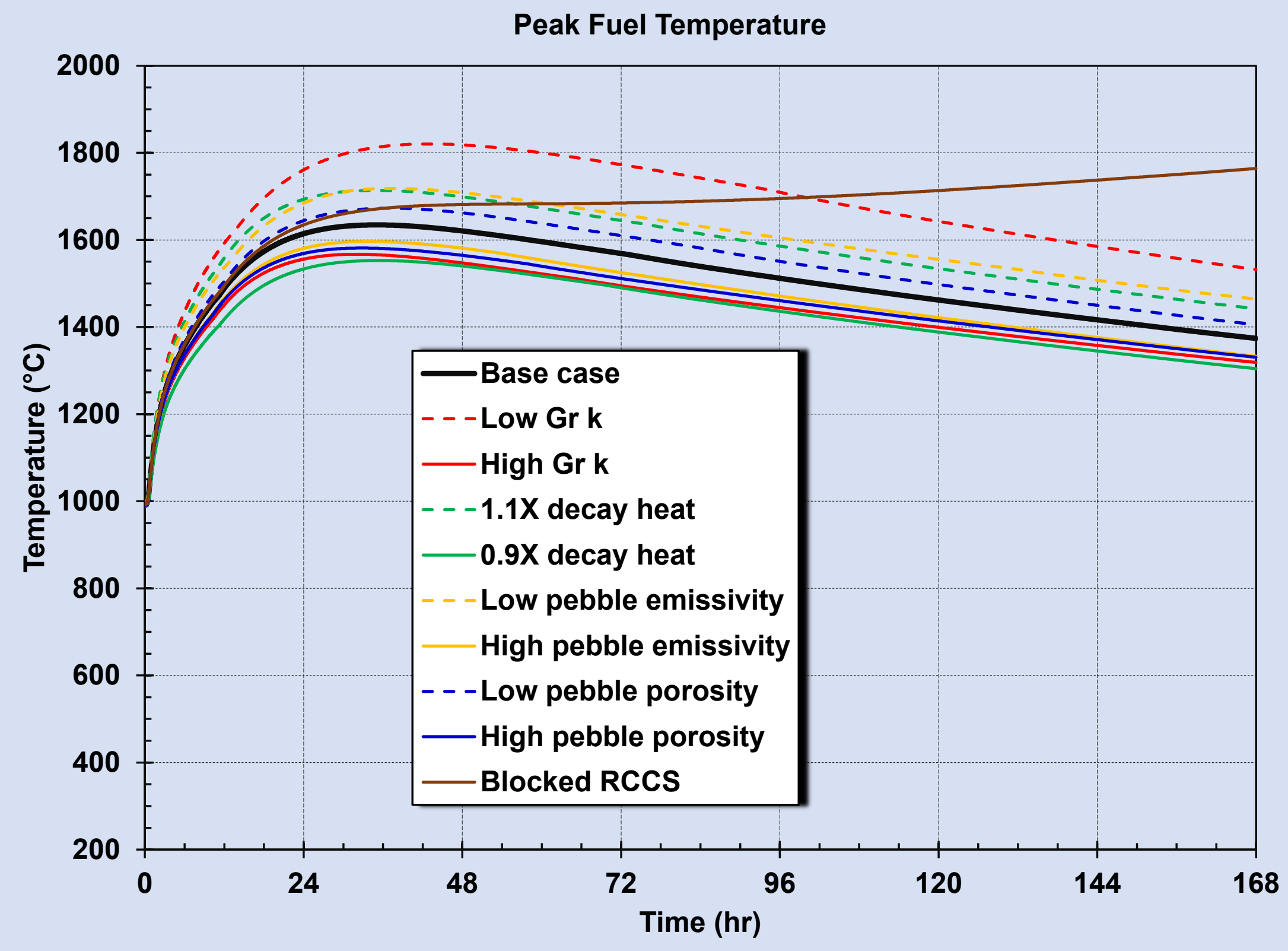
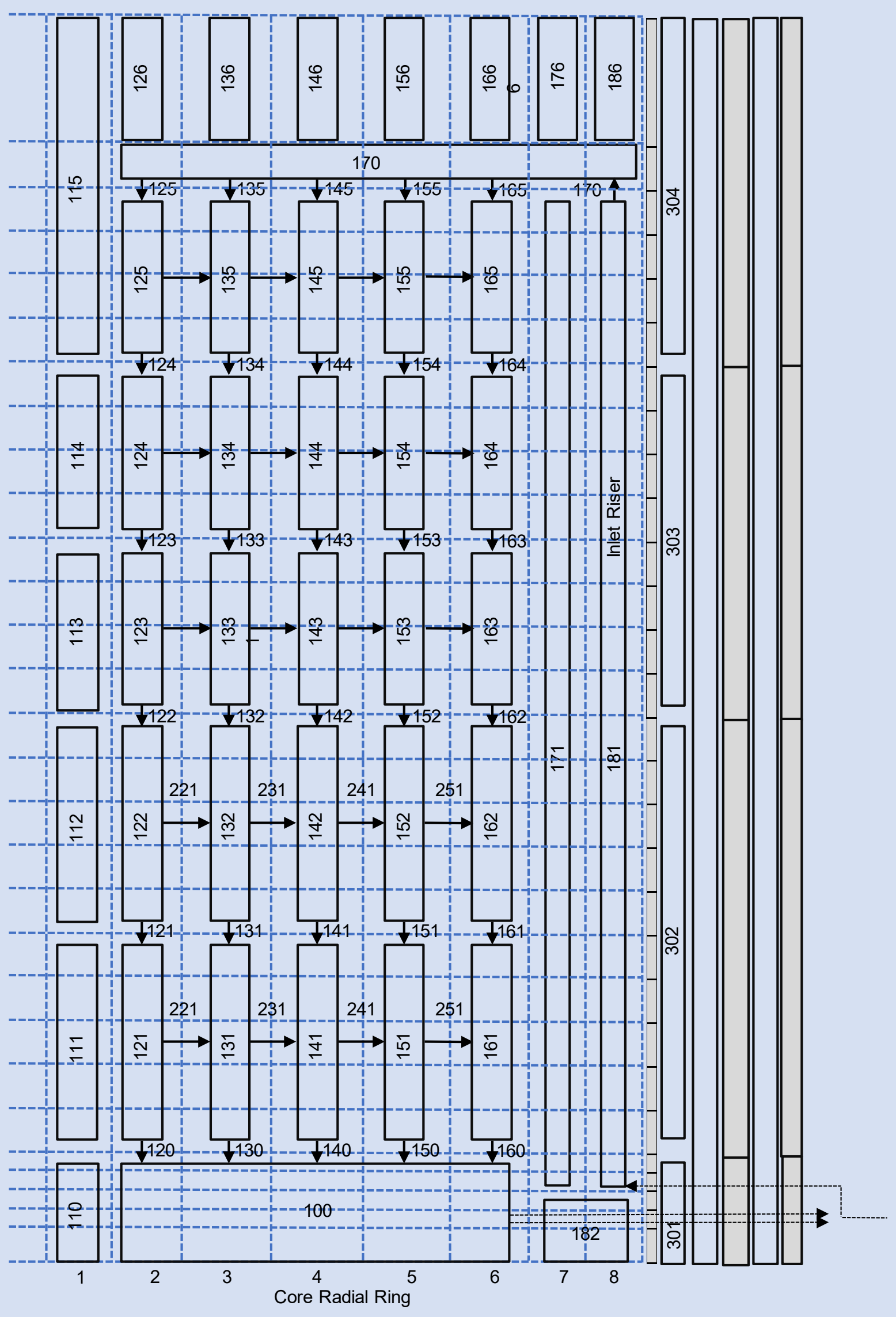
High Temperature Gas Cooled Reactor

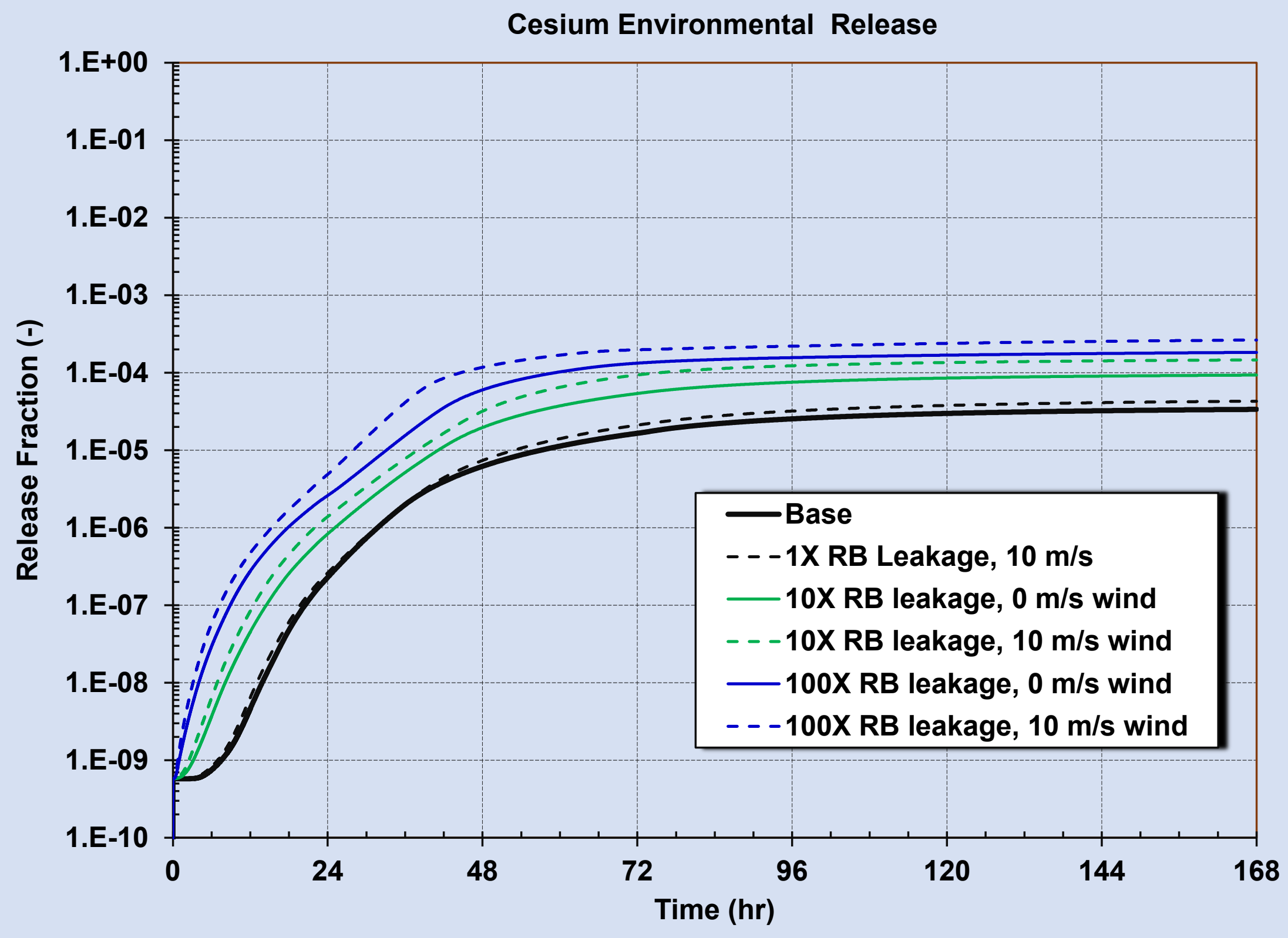
SCALE/MELCOR Non-LWR Source Term Demonstration Project – High-Temperature Gas-Cooled Reactor

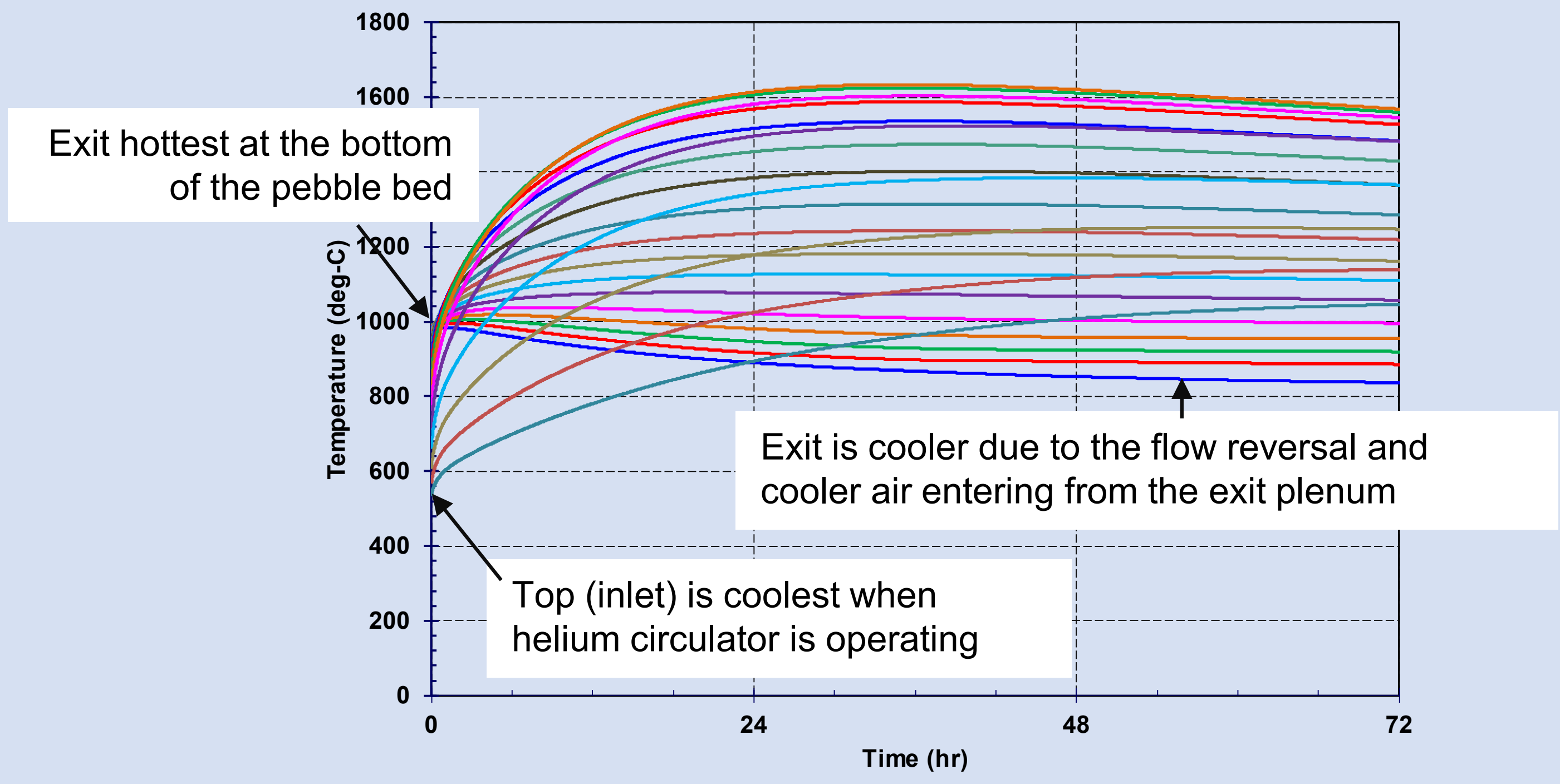
July 2021





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





Exit hottest at the bottom of the pebble bed

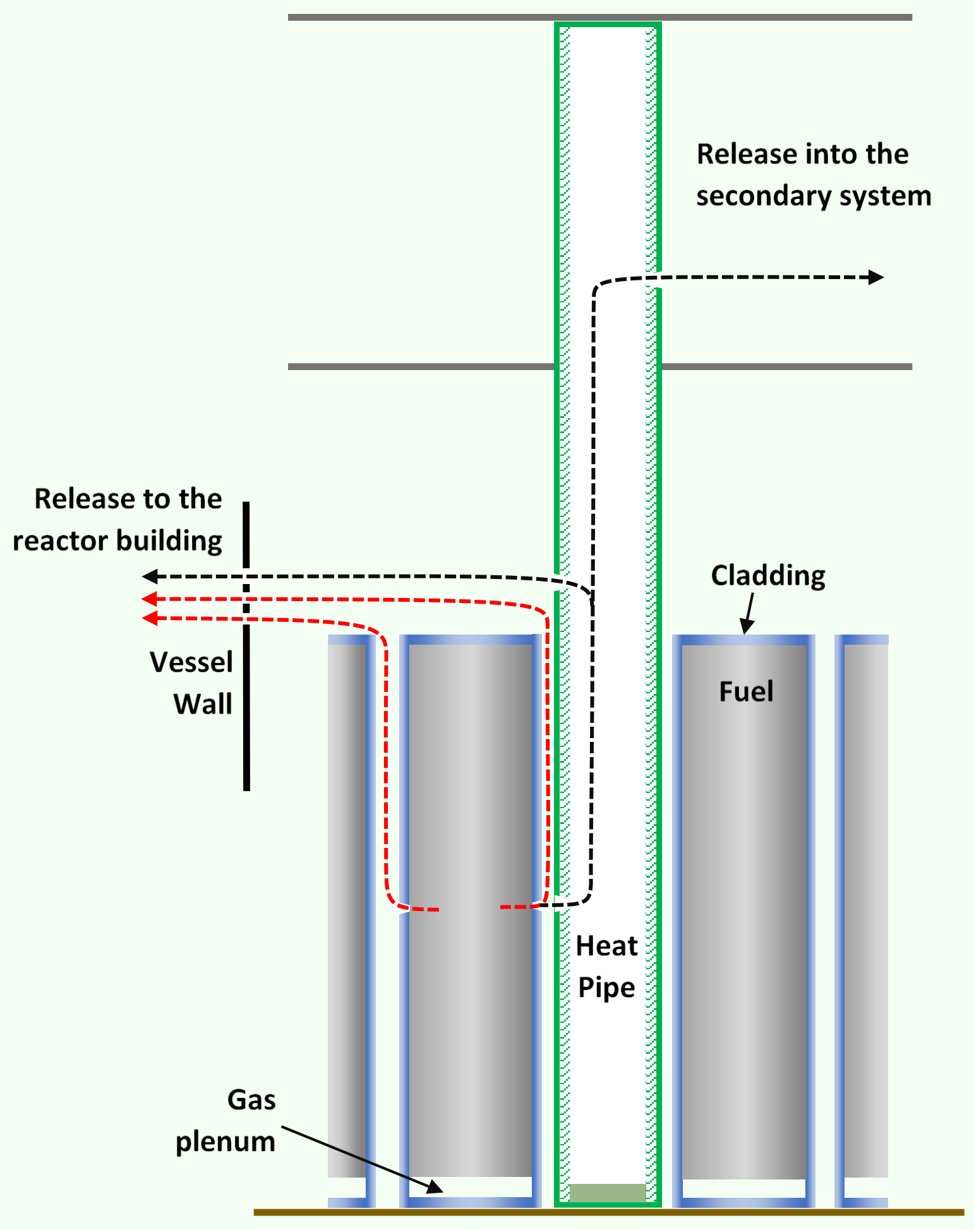
Exit is cooler due to the flow reversal and cooler air entering from the exit plenum

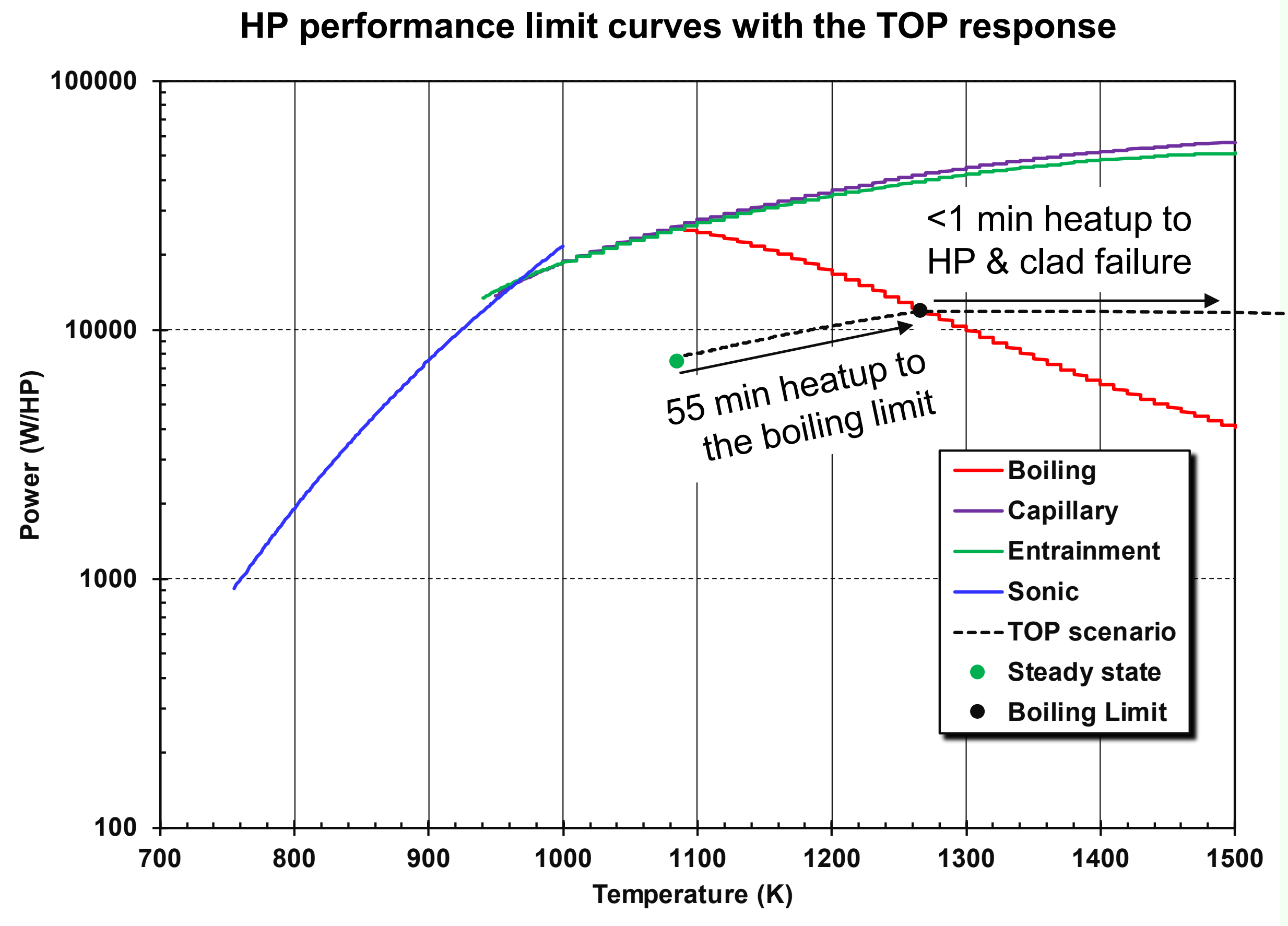
Top (inlet) is coolest when helium circulator is operating

Heat Pipe Reactors

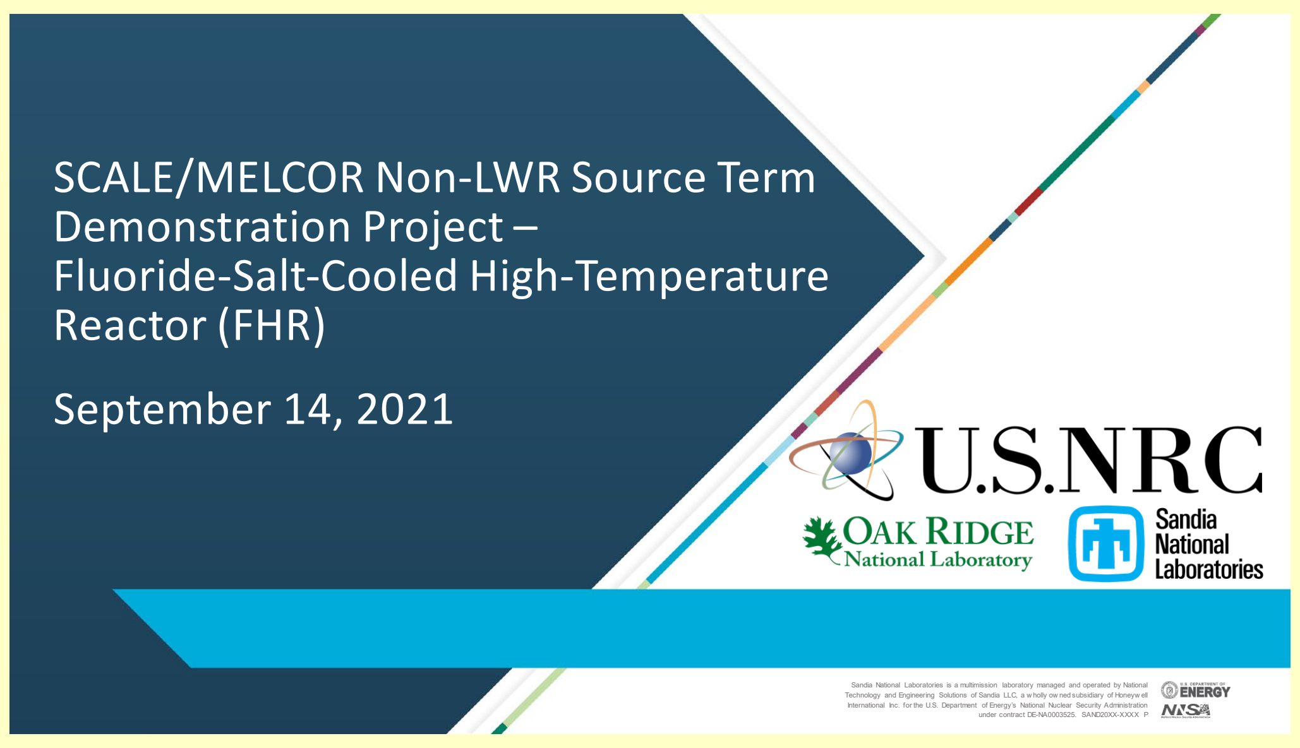
SCALE/MELCOR Non-LWR Source Term Demonstration Project – Heat Pipe Reactor

June 2021



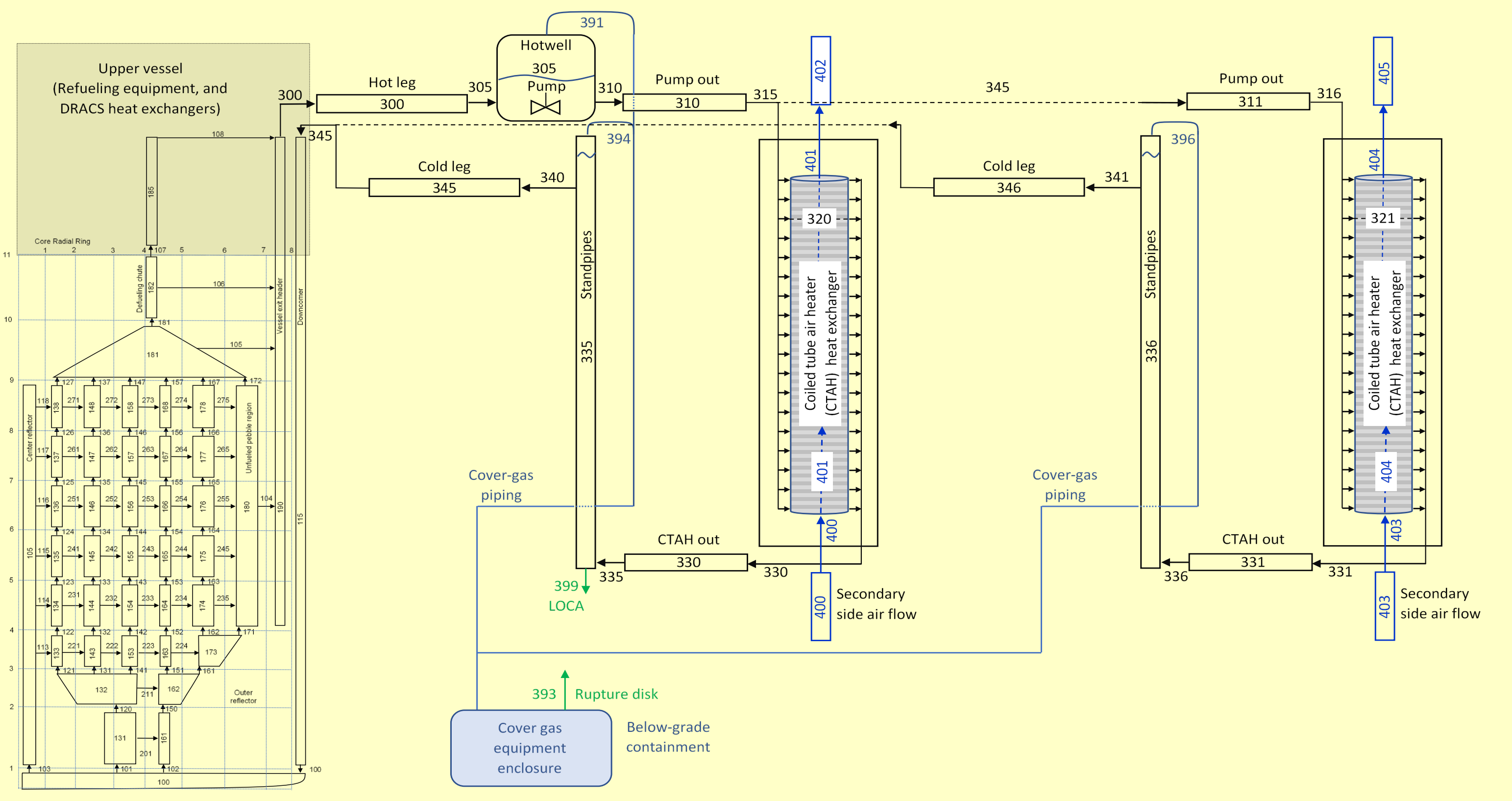


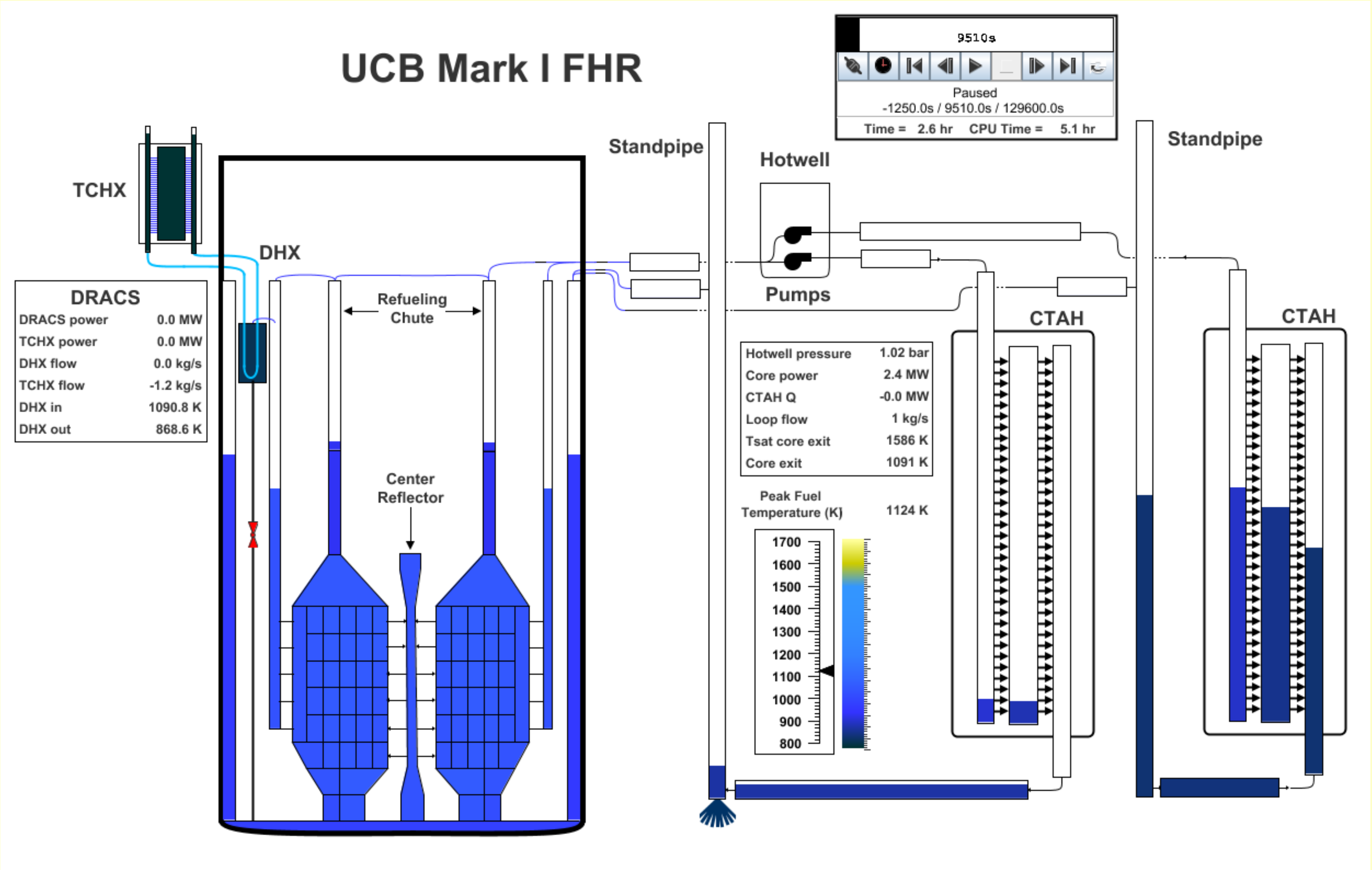
Fluoride Salt Cooled High Temperature Reactor (FHR)



SCALE/MELCOR Non-LWR Source Term Demonstration Project – Fluoride-Salt-Cooled High-Temperature Reactor (FHR)

September 14, 2021

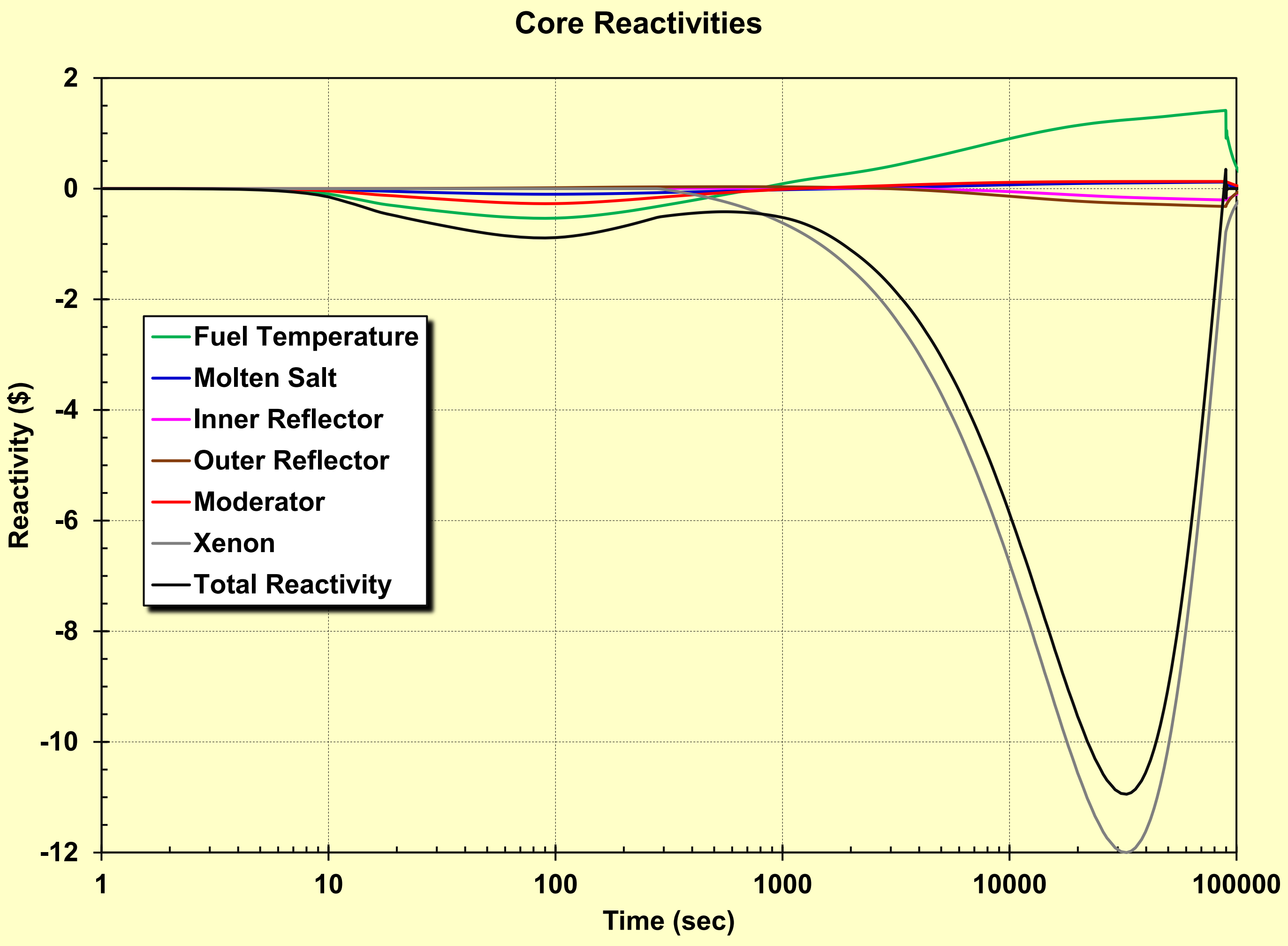




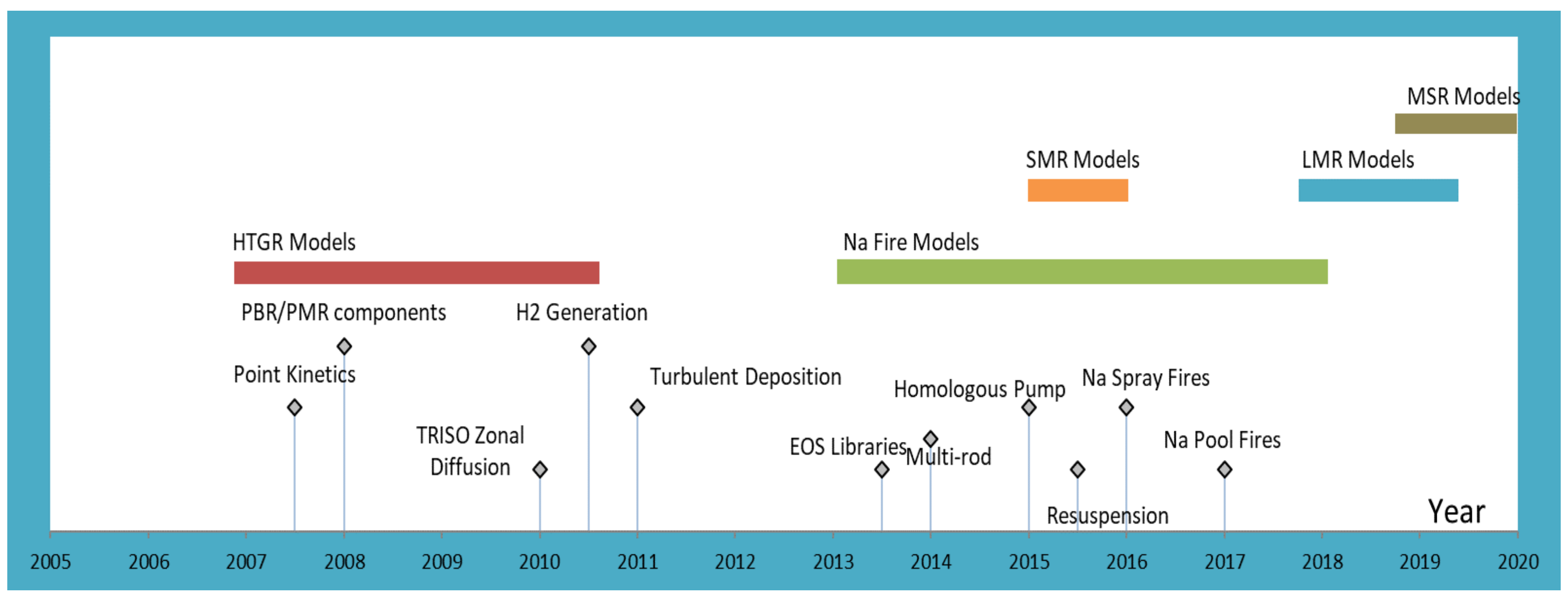
DRACS	
DRACS power	0.0 MW
TCHX power	0.0 MW
DHX flow	0.0 kg/s
TCHX flow	-1.2 kg/s
DHX in	1090.8 K
DHX out	868.6 K

Hotwell pressure	1.02 bar
Core power	2.4 MW
CTAH Q	-0.0 MW
Loop flow	1 kg/s
Tsat core exit	1586 K
Core exit	1091 K

Peak Fuel Temperature (K) 1124 K

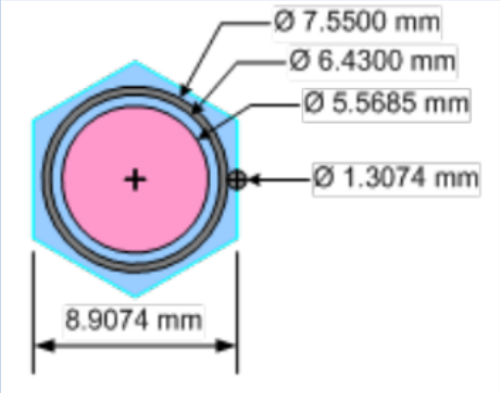


SFR Modeling



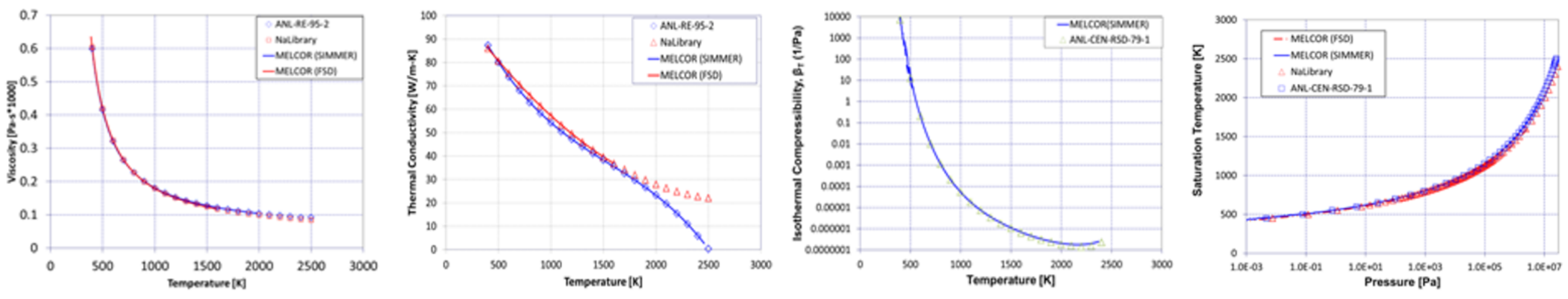
SFR Components (under development)

- SFR to use fuel, clad, cannister, and support/non-support structure
- Bond sodium gap not its own component as of now
  - Existing gap modeling capabilities
  - New models for gap closure, sodium migration to plenum, and attending FP transport
- Pin plenum not its own component as of now
  - Initialization
  - Volume accounting and ideal gas treatment
  - Attending FP transport
  - Pressure calculation
- Expect reflector component could factor into SFR designs
- May revise some intracell and intercell component-wise heat transfer models



Sodium Equation of State (EOS)

- Two alternatives: Fusion Safety Database (FSD) and SIMMER-III
  - FSD uses a soft-sphere EOS model fit to an experimental database
  - SIMMER-III supplemented with experimental data (Fink & Leibowitz)
- Verified EOS on a wide range of thermodynamic conditions
- Enthalpy, heat capacity, heat of fusion, vapor pressure, heat of vaporization, density, thermal conductivity, thermal diffusivity, and thermal expansion
- Demonstration calculations reproduce the experimental database



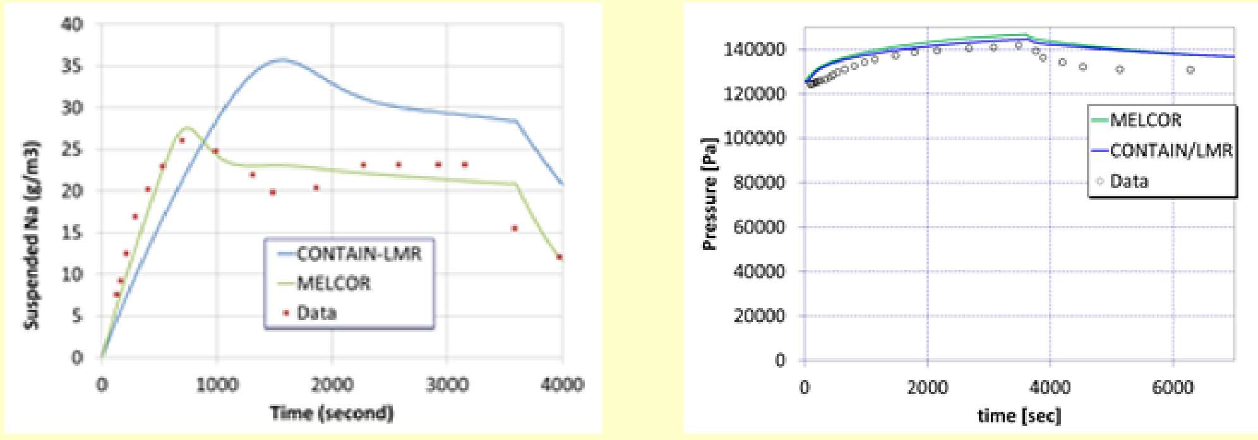
SFR Containment (Ex-Vessel) Models

- Spray and pool fire models from CONTAIN/LMR
- Pool fire
  - Pool fire model from SOFIRE-II based on pool fire tests
  - Predicts rate of oxygen and sodium consumption plus heat evolved from reaction

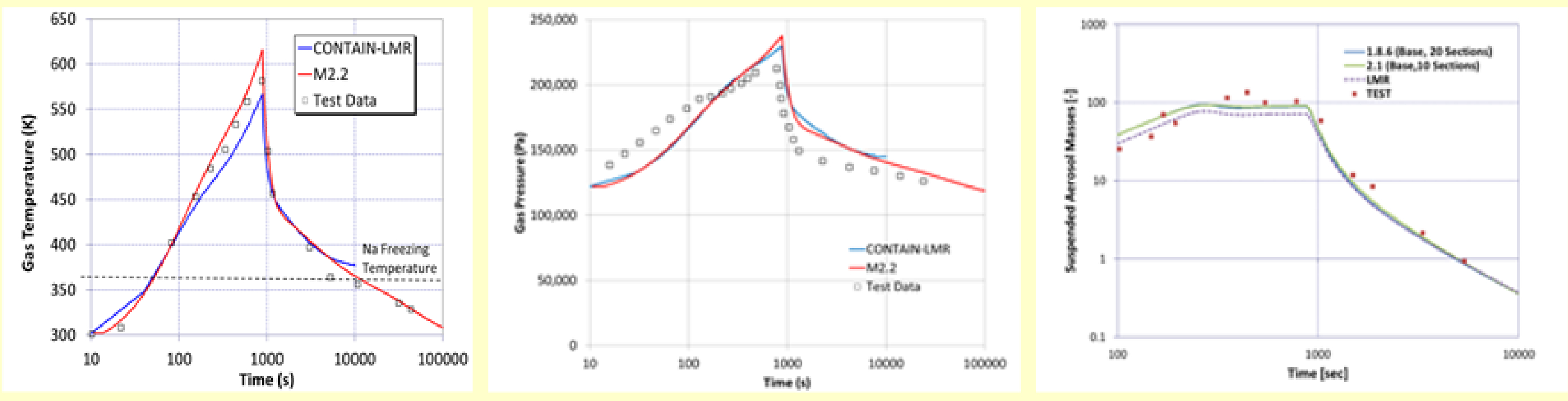
$$(1+f_1)\cdot 2\cdot \mathrm{Na} + \mathrm{O_2} \rightarrow 2\cdot f_1\cdot \mathrm{Na_2O} + (1-f_1)\cdot \mathrm{Na_2O_2} + q(\mathrm{reaction})$$

- Spray fire
  - Spray fire model from NACOM
  - Predict total burned sodium mass as function of droplet size and fall velocity
  - Integrate combustion rate over droplet fall height

- Fire model validation – ABCOVE AB1/AB5
  - AB1 (pool)



  - AB5 (spray)



- Atmospheric chemistry
  - Aerosol/atmosphere
  - Aerosol on surfaces
  - Sodium/water in atmosphere
  - Reactions in hierarchical order
  - Affected through NAC package
  - New RN classes
  - New sensitivity coefficients

$$\mathrm{Na(l)} + \mathrm{H_2O\ (l)} \rightarrow \mathrm{NaOH(a)} + \tfrac{1}{2}\mathrm{H_2}$$

$$2\,\mathrm{Na(g,l)} + \mathrm{H_2O\ (g,l)} \rightarrow \mathrm{Na_2O(a)} + \mathrm{H_2}$$

$$2\,\mathrm{Na(g,l,a)} + \tfrac{1}{2}\mathrm{O_2}\ \text{or}\ \mathrm{O_2} \rightarrow \mathrm{Na_2O(a)}\ \text{or}\ \mathrm{Na_2O_2(a)}$$

$$\mathrm{Na_2O_2(a)} + 2\,\mathrm{Na(g,l)} \rightarrow 2\,\mathrm{Na_2O(a)}$$

$$\mathrm{Na_2O(a)} + \mathrm{H_2O\ (g,l)} \rightarrow 2\mathrm{NaOH(a)}$$

$$\mathrm{Na_2O_2(a)} + \mathrm{H_2O\ (g,l)} \rightarrow 2\mathrm{NaOH(a)} + 0.5\mathrm{O_2}$$

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Transient/Accident Solution Methodology

Stage 1:
Thermal Steady State

Establish COR, CVH, & HS temperatures

Establish steady flow patterns

Initialize any RN form mass outside fuel

Assume thermal hydraulic conditions hold constant over pre-transient stage

Stage 2:
Steady/Pre-Transient Mechanics and Fission Product Transport

Option 1) – User Input
- *Fuel and Clad geometry changes*
- *Pin plena initialization*
- *Fuel swelling/porosity distribution*
- *DCH/RN class mapping to gaseous and solid fission products*
- *End-of-burnup RN class inventory*
  - *Gaseous and solid in fuel*
  - *Solid in bond sodium gap*
  - *Gaseous in pin plena*

Option 2) – Calculated (coming soon)
- *Mechanical response of fuel pins*
  - *Algebraic formulation*
  - *Stress, strain, and displacement*
  - *Bond sodium gap dynamics*
- *Fission gas transport in-pin*
  - *Volume accounting methods*
  - *Ideal gas assumptions*
  - *Empirical models for fuel swelling and porosity dynamics*

Stage 3:
Transient Diffusion & Transport calculation

In-pin dynamics (coming soon)
- *Up to and including pin failure*
- *Fuel molten cavity formation*
- *Fuel and clad dimensional changes*
- *Clad dynamics*
  - *Eutectic thinning*
  - *Mechanical failure*
  - *Candling and conglomerate debris*
  - *Assembly peripheral area (CN,CL)*
- *Clad/pin failure*

RN release from COR to CVH/RN in GRTR

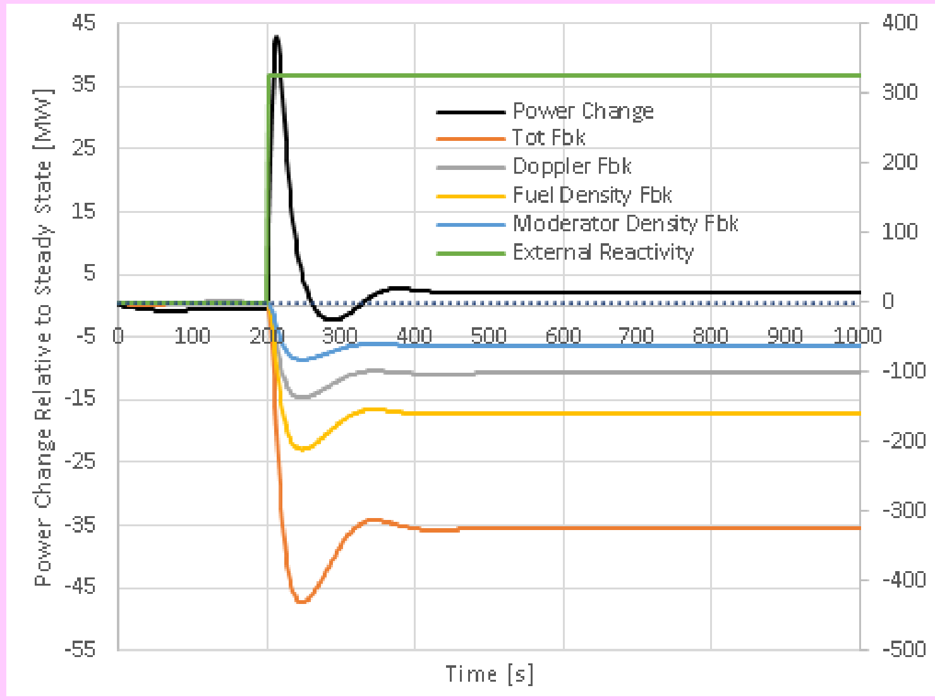
Severe accident phenomena (coming soon)
- *Clad relocation (conventional candling)*
- *Clad relocation (reverse candling)*
- *Fuel relocation in a candling mode*
- *Pin effluents ejection*
  - *Solid (particles, chunks, streamers)*
  - *Molten material and pin gases*

Standard Point Reactor Kinetics Equations

Standard 6 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 external
- Doppler
- Fuel and moderator density
- New for SFRs (under development)
  - Dimension changes and rod bowing
  - Molten fuel/clad
  - Sodium void

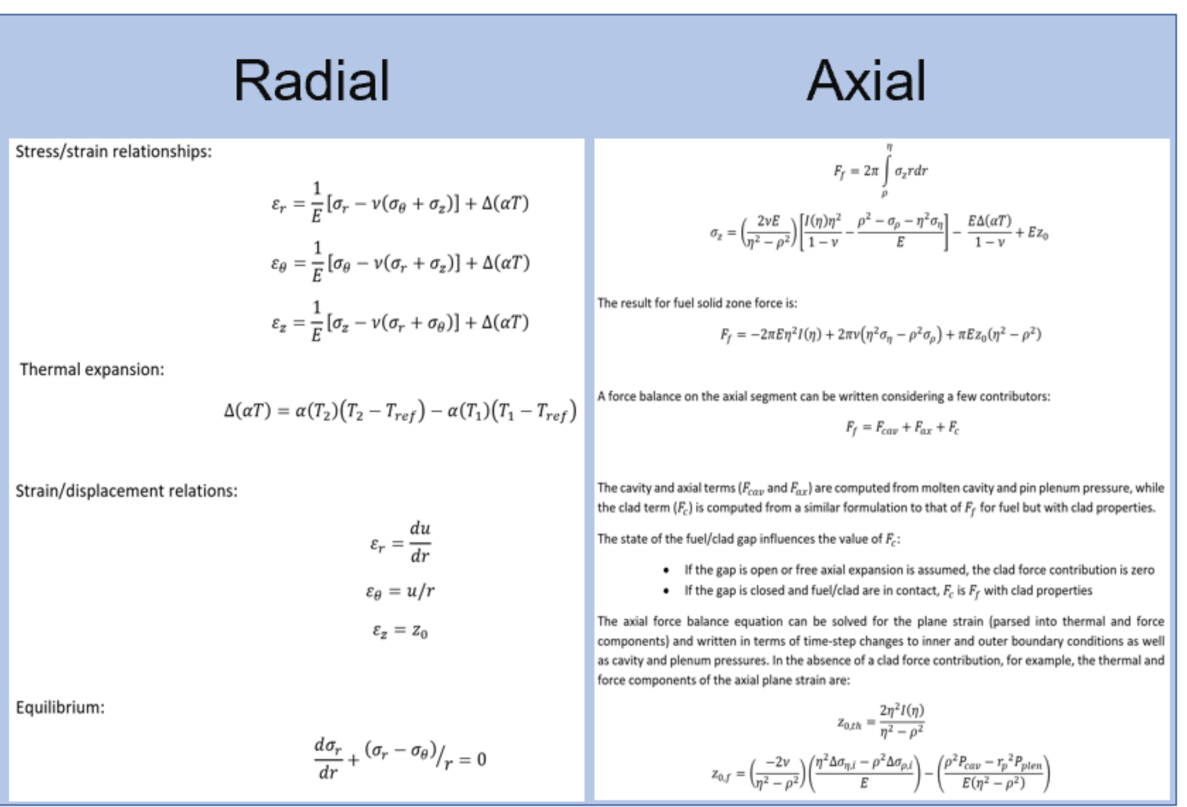
Define core cell ranges over which component average temperatures are taken to inform feedback models

SFR Expanded In-Vessel Modeling

- Pin Mechanics
  - Radial stress/strain/displacement
  - Axial stress/strain
  - Solve iteratively
- Miscellaneous models
  - Fuel swelling
  - Fuel molten cavity formation
  - Pin pressurization
  - Reactivity effects

Radial

Axial



Stress/strain relationships:

$$\varepsilon_r = \frac{1}{E}[\sigma_r - \nu(\sigma_\theta + \sigma_z)] + \Delta(\alpha T)$$

$$\varepsilon_\theta = \frac{1}{E}[\sigma_\theta - \nu(\sigma_r + \sigma_z)] + \Delta(\alpha T)$$

$$\varepsilon_z = \frac{1}{E}[\sigma_z - \nu(\sigma_r + \sigma_\theta)] + \Delta(\alpha T)$$

Thermal expansion:

$$\Delta(\alpha T) = \alpha(T_2)(T_2 - T_{ref}) - \alpha(T_1)(T_1 - T_{ref})$$

Strain/displacement relations:

$$\varepsilon_r = \frac{du}{dr}$$

$$\varepsilon_\theta = u/r$$

$$\varepsilon_z = z_0$$

Equilibrium:

$$\frac{d\sigma_r}{dr} + {(\sigma_r - \sigma_\theta)}/{r} = 0$$

$$F_f = 2\pi\int_\rho^\eta \sigma_z r dr$$

$$\sigma_z = \left(\frac{2\nu E}{\eta^2-\rho^2}\right)\left[\frac{I(\eta)\eta^2}{1-\nu} - \frac{\rho^2-\sigma_\rho-\eta^2\sigma_\eta}{E}\right] - \frac{E\Delta(\alpha T)}{1-\nu} + E z_0$$

The result for fuel solid zone force is:

$$F_f = -2\pi E\eta^2 I(\eta) + 2\pi\nu(\eta^2\sigma_\eta - \rho^2\sigma_\rho) + \pi E z_0(\eta^2 - \rho^2)$$

A force balance on the axial segment can be written considering a few contributors:

$$F_f = F_{cav} + F_{ax} + F_c$$

The cavity and axial terms (F_{cav} and F_{ax}) are computed from molten cavity and pin plenum pressure, while the clad term (F_c) is computed from a similar formulation to that of F_f for fuel but with clad properties.

The state of the fuel/clad gap influences the value of F_c:

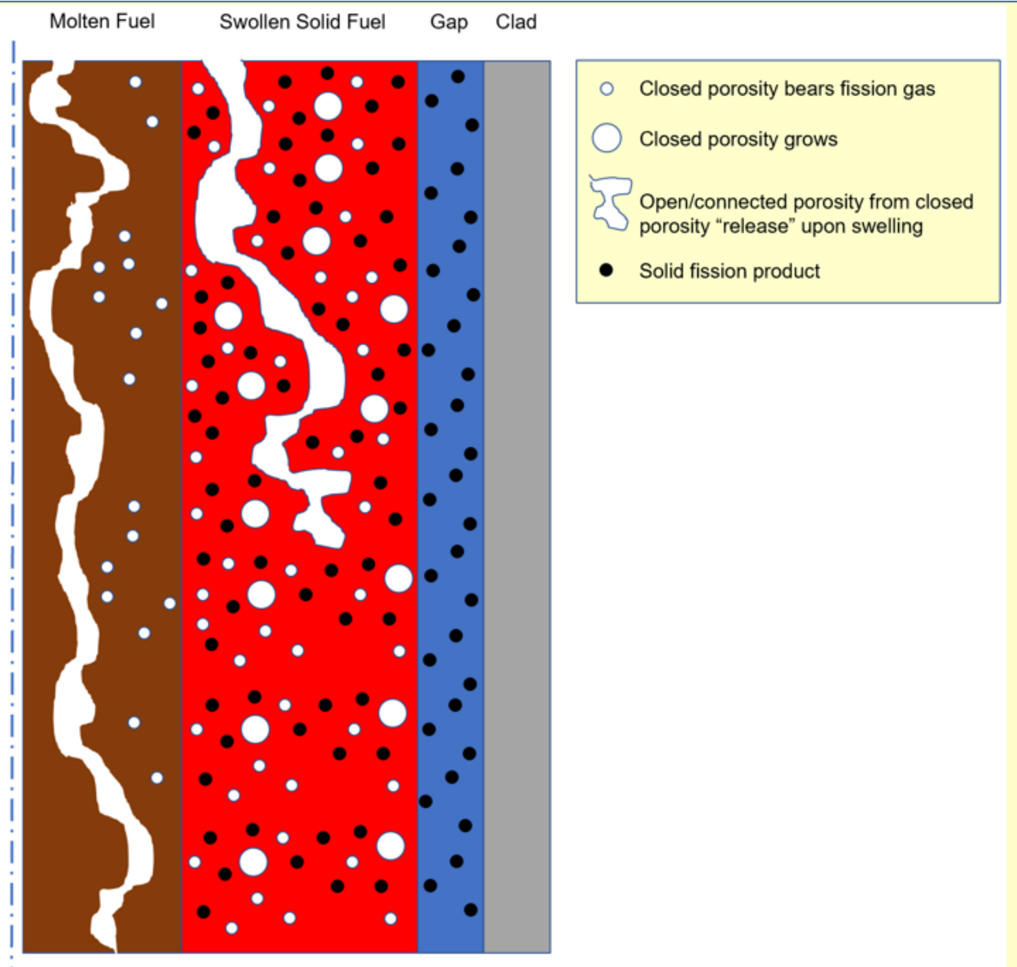
- If the gap is open or free axial expansion is assumed, the clad force contribution is zero
- If the gap is closed and fuel/clad are in contact, F_c is F_f with clad properties

The axial force balance equation can be solved for the plane strain (parsed into thermal and force components) and written in terms of time-step changes to inner and outer boundary conditions as well as cavity and plenum pressures. In the absence of a clad force contribution, for example, the thermal and force components of the axial plane strain are:

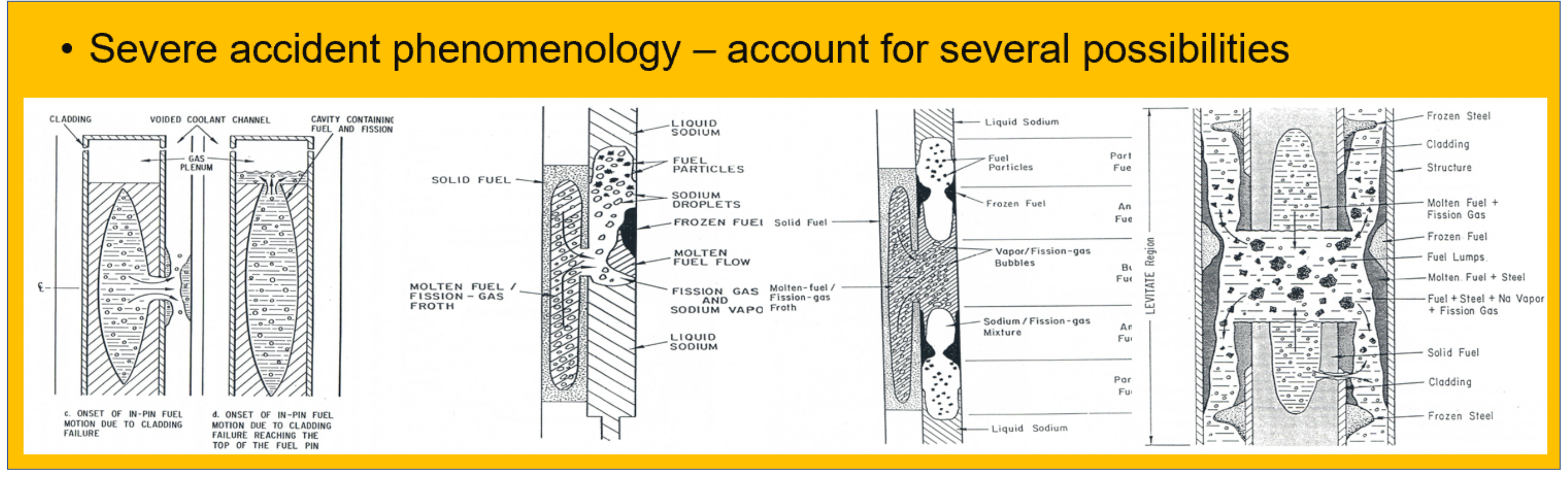
$$z_{0,th} = \frac{2\eta^2 I(\eta)}{\eta^2 - \rho^2}$$

$$z_{0,f} = \left(\frac{-2\nu}{\eta^2-\rho^2}\right)\left(\frac{\eta^2\Delta\sigma_{\eta,i} - \rho^2\Delta\sigma_{\rho,i}}{E}\right) - \left(\frac{\rho^2 P_{cav} - r_p{}^2 P_{plen}}{E(\eta^2-\rho^2)}\right)$$

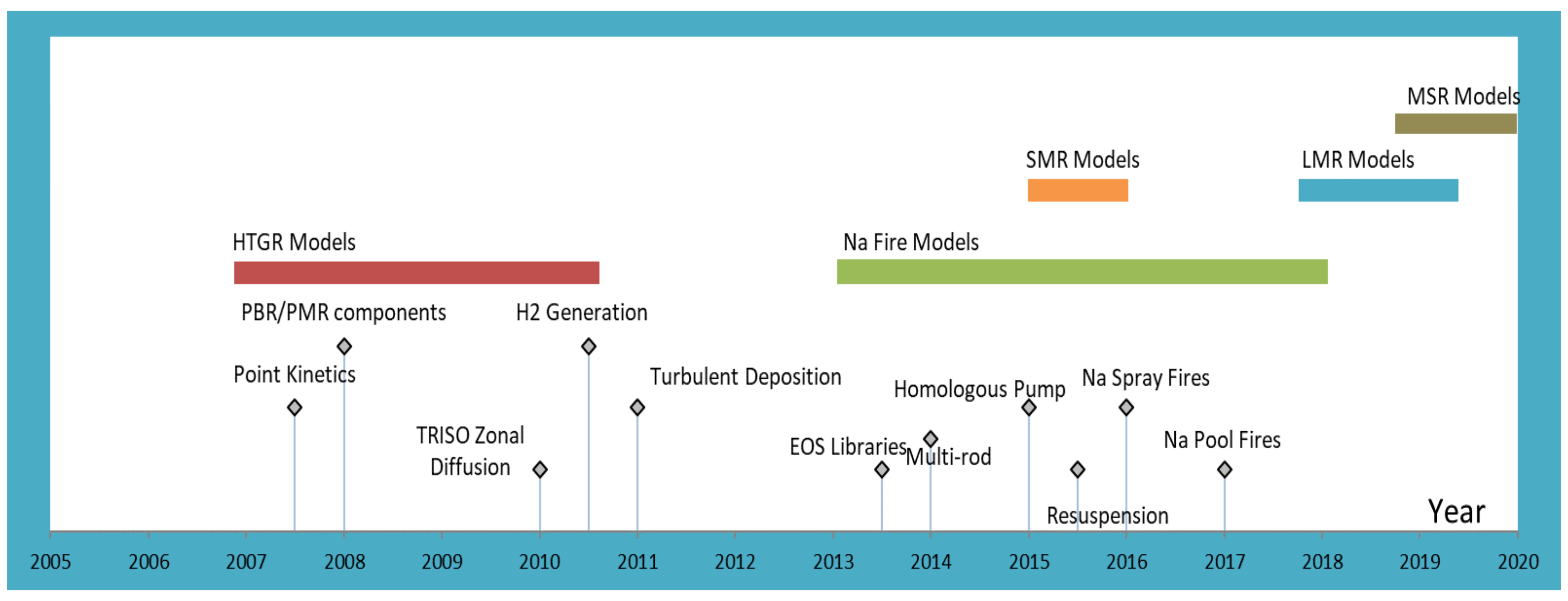
- Fission gas dynamics in-pin
  - Forms closed porosity in solid fuel
  - Closed porosity grows
  - Closed porosity "releases" – swelling
  - Open/connected porosity
    - Forms from closed porosity release
    - A "free volume" in pin
    - Communicates with pin plenum
    - At pin plenum pressure
  - Molten fuel
    - Forms as solid melts
    - Subsumes open/closed porosity
  - RN class inventory migrates as volume



- Severe accident phenomenology – account for several possibilities



MSR Modeling



Transient/Accident Solution Methodology

Stage 1:
Thermal Hydraulic
Steady State

Establish COR, CVH, & HS temperatures

Establish steady flow patterns

Initialize or source in RN form-wise mass

Stage 2:
Pre-Transient

Fluid fuel point kinetics

GRTR framework governs form-wise transfer to some steady distribution of RN class mass across user-defined RN forms

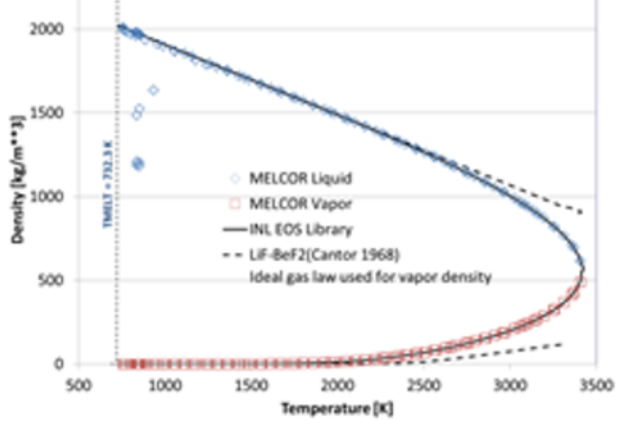
Stage 3:
Transient

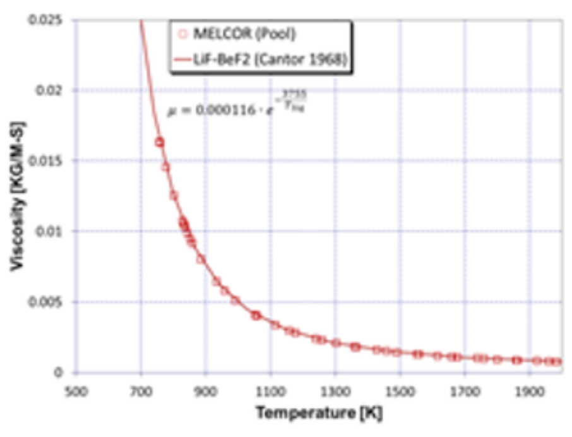
Fluid fuel point kinetics governs power according to flow reactivity excursions

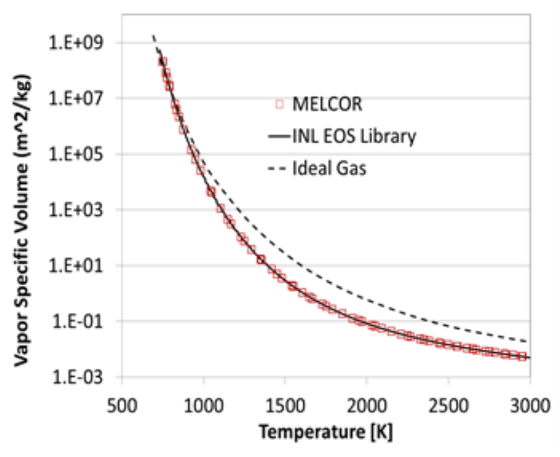
GRTR moves RN class mass between forms
- *Thermodynamic conditions evolve*
- *Vapors, aerosols, and RN package physics are still in play within GRTR*
- *User-directed transfers between user-defined forms or internal models*

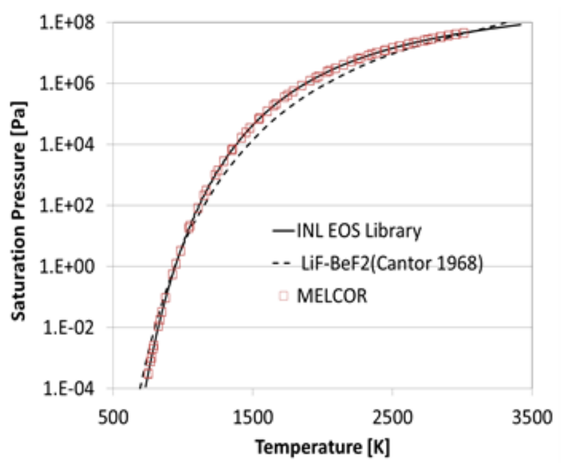
FLiBe Equation of State (EOS)

- Property database based on ORNL publication
- Verified EOS on a wide range of thermodynamic conditions
- Demonstration calculations reproduce the experimental database
- Provisions exist for salt freezing (solid phase) from liquid phase



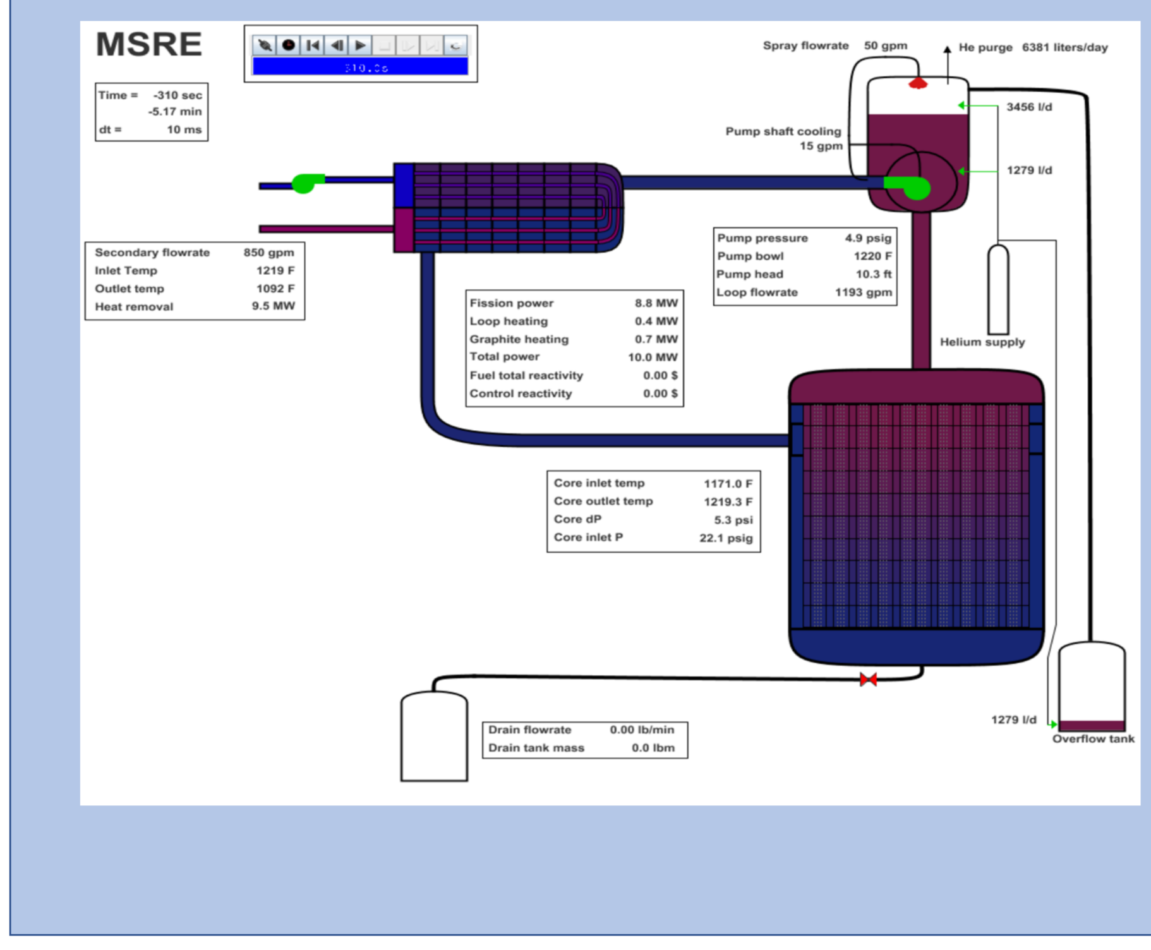




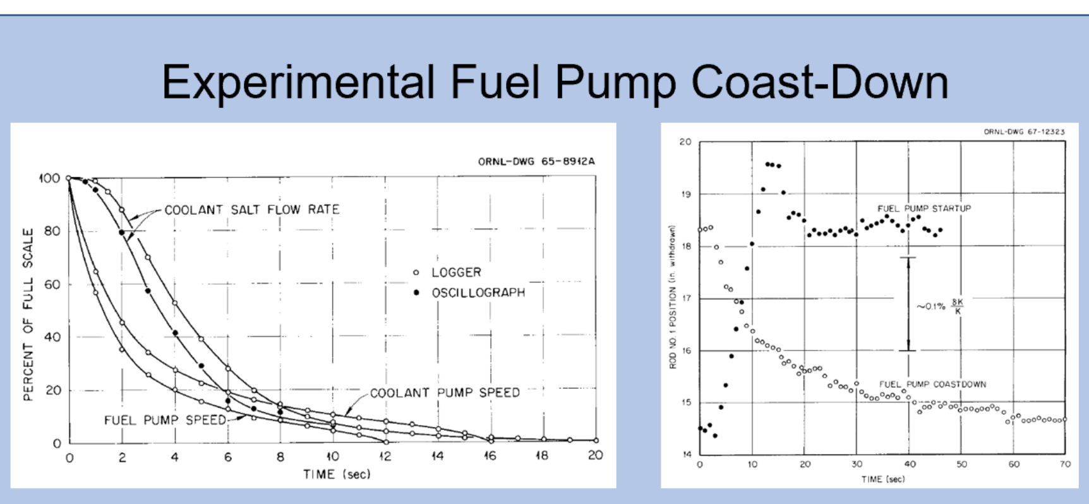


ORNL MSRE Zero-Power Flow Coast-Down Benchmark

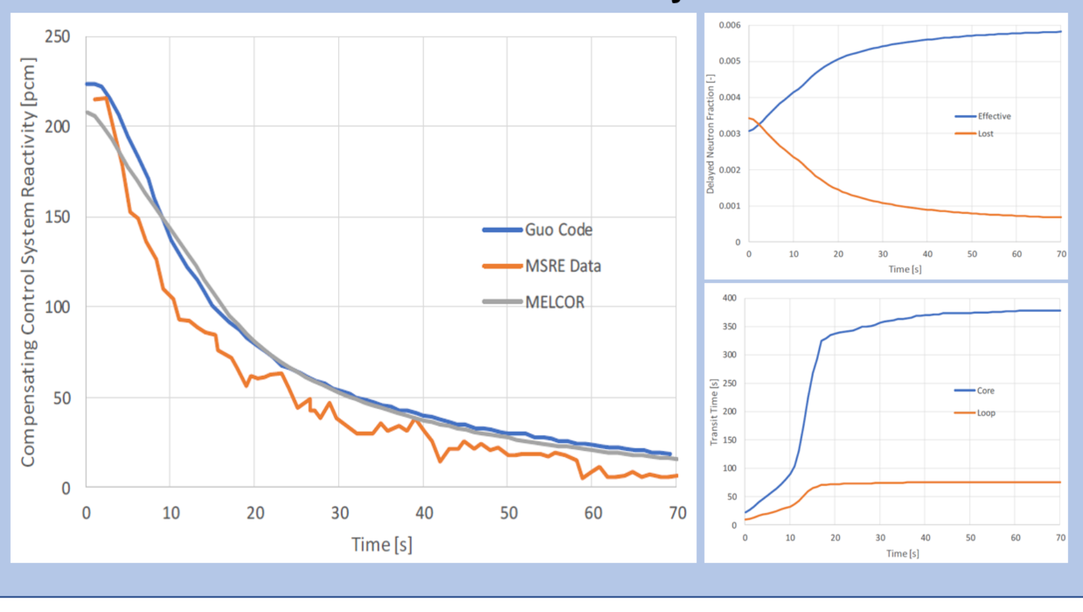
Simplified ORNL MSRE Input Model



Experimental Fuel Pump Coast-Down

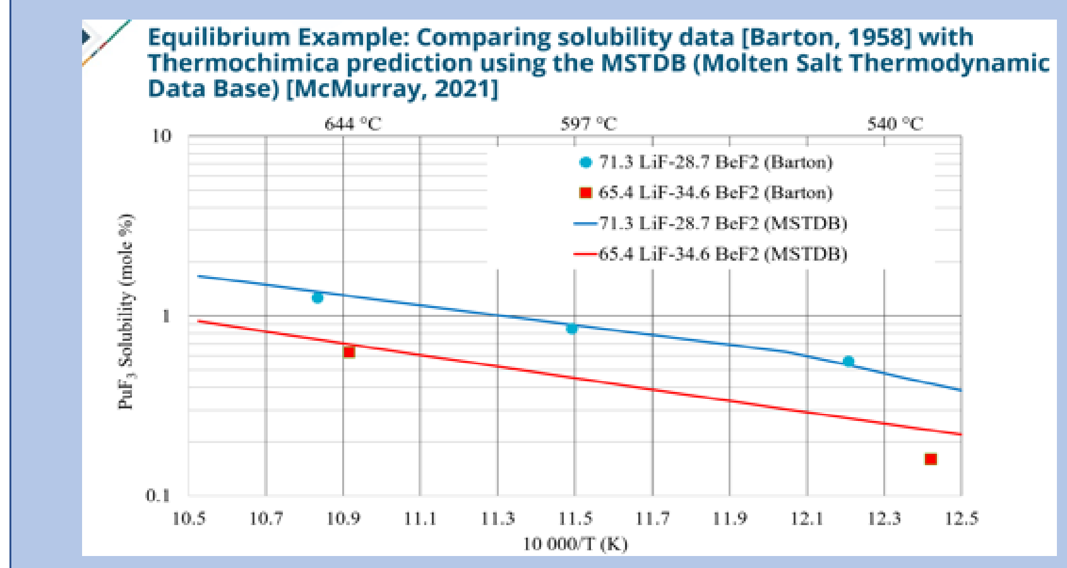


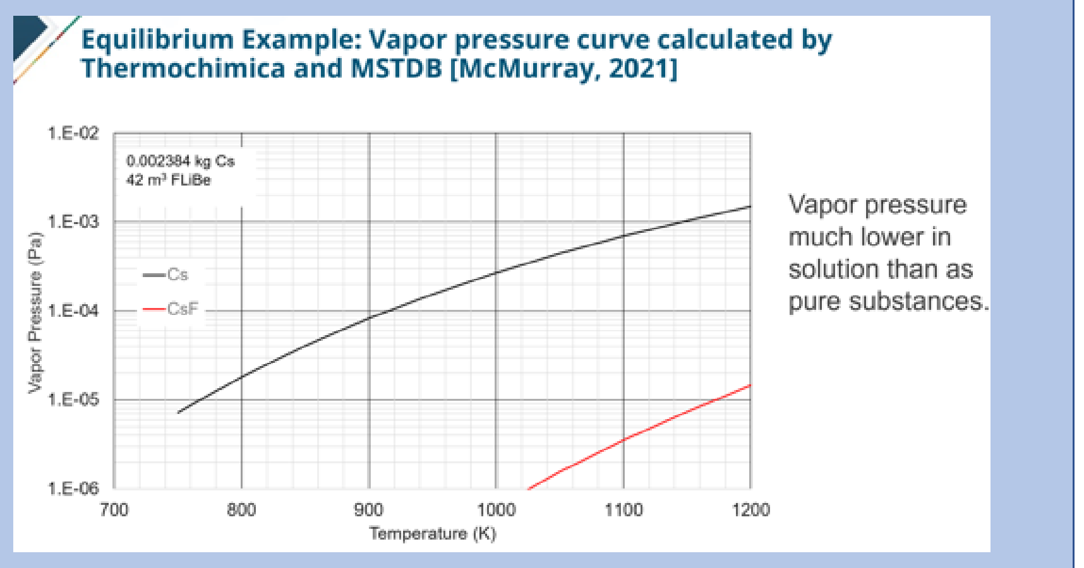
MELCOR Flow Reactivity Benchmark



Thermochemistry and Data Needs

- MELCOR capabilities are in place to use data as available
- MELCOR can utilize Gibbs Energy Minimization type tools (e.g. Thermochimica)

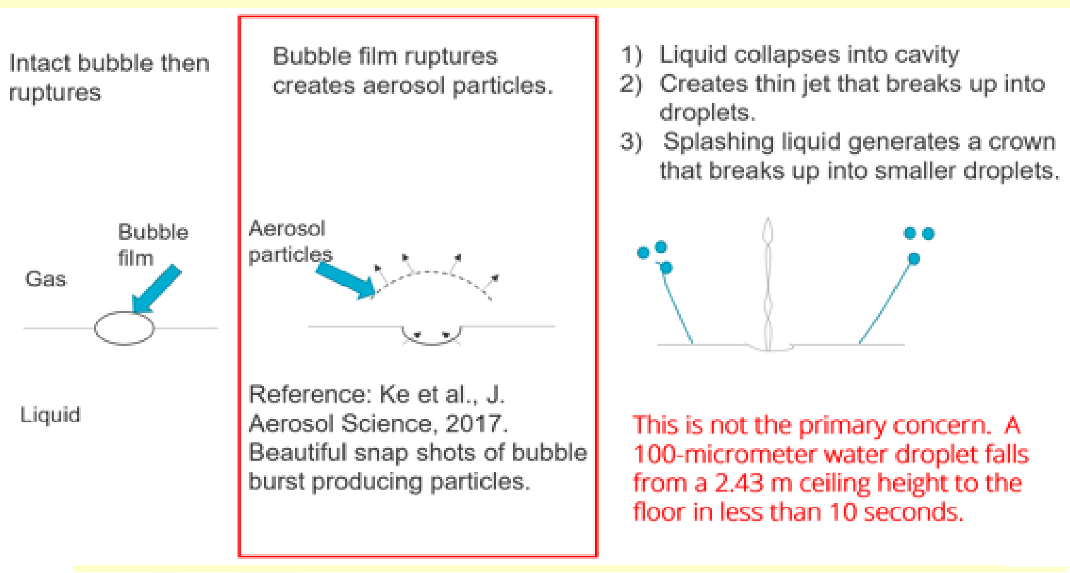

Equilibrium Example: Comparing solubility data [Barton, 1958] with Thermochimica prediction using the MSTDB (Molten Salt Thermodynamic Data Base) [McMurray, 2021]


Equilibrium Example: Vapor pressure curve calculated by Thermochimica and MSTDB [McMurray, 2021]

Vapor pressure much lower in solution than as pure substances.

- Thermo databases available in FactSage format:
  - MSTDB w/ 2 systems:
    - Fluoride: Pu-U-Th-Nd-Ce-La-Cs-Rb-Ni- Ca-K- Na-F-Be-Li
    - Chloride: Pu-U- Ce- Cs-Rb-Ni-Fe-Cr-Ca-K-Cl-Al-Mg-Na- Li
  - JRC database: Pu-U-Th-Ce-La-Cs-I-Zr-Rb-Ca-K-Cl-Mg-Na-F-Be-Li
- Databases under active development, needs for severe accidents include:
  - High temperatures (beyond normal operating range)
  - Fission product elements in row 5 of periodic table (Sr, I, Ag, etc.)
  - Species introduced during possible severe accidents (air, water vapor)

- Gas bubbling/agitation and burst in molten salt is a case-in-point that well-designed experiments targeting certain data needs are valuable

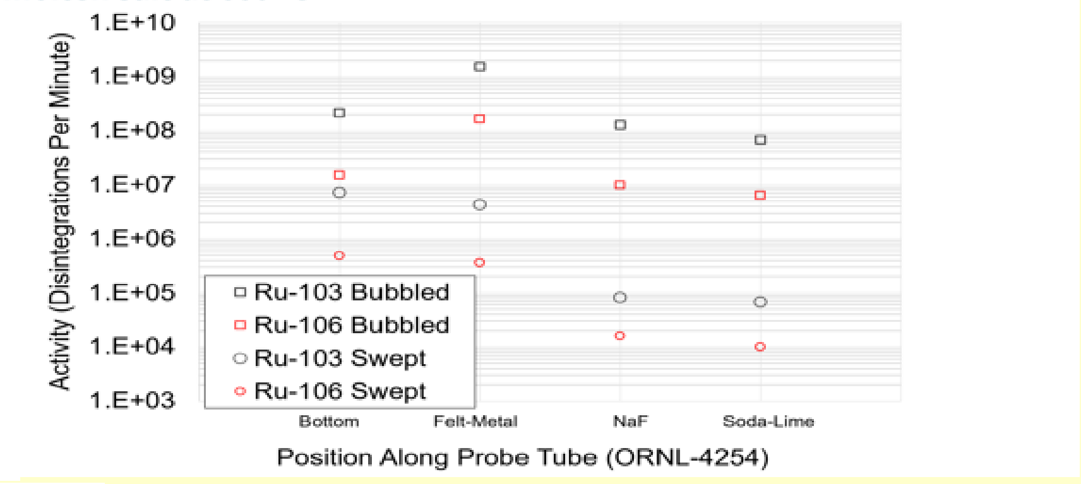


Reference: Ke et al., J. Aerosol Science, 2017. Beautiful snap shots of bubble burst producing particles.

1) Liquid collapses into cavity
2) Creates thin jet that breaks up into droplets.
3) Splashing liquid generates a crown that breaks up into smaller droplets.

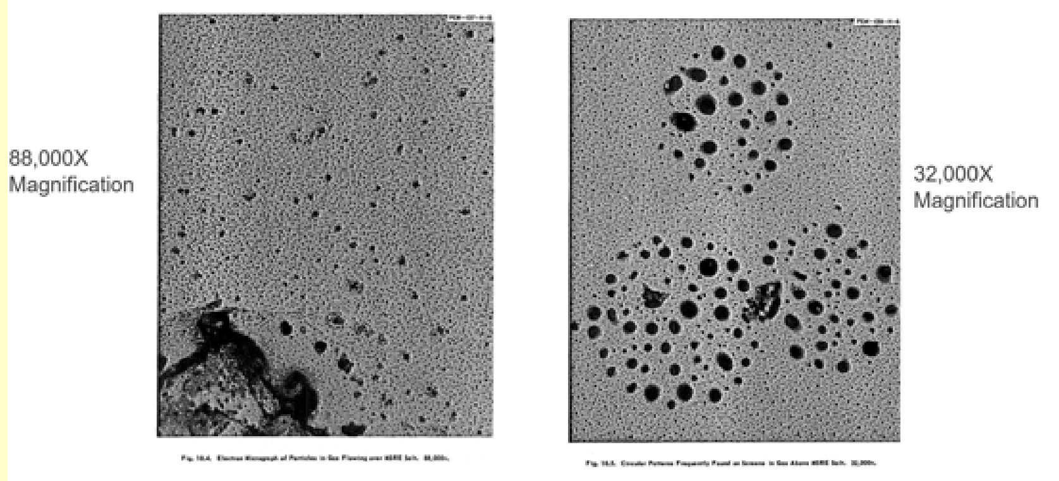
This is not the primary concern. A 100-micrometer water droplet falls from a 2.43 m ceiling height to the floor in less than 10 seconds.

Radioactive particle release for some experiments but not all, increased dramatically with gas bubbled up 3 inches (7.6 cm) through 50-g MSRE molten salt at 600 °C



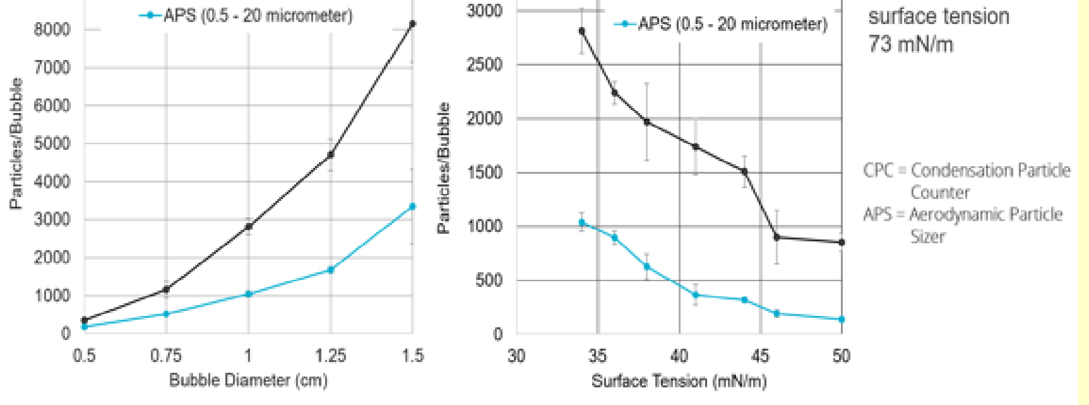
Electron microscope images of particles collected from sweeping above a 50-gram molten salt sample [ORNL-4254].

Three Sizes: Mostly 3.5 – 18 nm, 100-200 nm, and larger sizes



Respirable (< 10 micron aerodynamic diameter) particles released from molten salt during benign operations. This is important!

Aerosol particles generated by a single bursting bubble of an aqueous solution [Ke et al., 2017].



Water at 25 °C, surface tension 73 mN/m

CPC = Condensation Particle Counter
APS = Aerodynamic Particle Sizer

- Larger bubbles rupture with thousands more respirable aerosol particles per bubble.
- Higher surface tension results in thousands fewer respirable aerosol particles.

Fluid Fuel Point Reactor Kinetics Equations

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

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

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

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

Where:

$P(t)$= Thermal power due to fission 0

C_i^C= delayed neutron precursor group i inventory/concentration in-core

C_i^L= delayed neutron precursor group i inventory/concentration ex-core (in loop)

S_0= Thermal power generation rate due to neutron source

$\rho(t) = \frac{k-1}{k}$= Reactivity for k the effective multiplication factor

$\bar{\beta}$= Effective delayed neutron fraction

β= Delayed neutron fraction (static, in absence of drift effects)

$\Lambda = {}^{1}/_{\nu V \Sigma_f}$= Neutron generation time

$\tau_{C/L} = {}^{M_{C/L}}/_{\dot{m}}$ = Residence time of precursors (core, loop, respectively)

$V_{C/L}$= Fluid volume (core, loop, respectively)

λ_i= Decay constant of delayed neutron precursor group i

A – In-Vessel DNP gain by fission
B – In-Vessel DNP loss by decay, flow
C – In-Vessel DNP gain by Ex-Vessel DNP flow
D – Ex-Vessel DNP gain by In-Vessel DNP flow
E – Ex-Vessel DNP loss by decay, flow

Under these assumptions, the steady form of the FFPRK equations is:

$$\frac{dP(0)}{dt} = 0 = \left(\frac{\Delta\rho_0 - \bar{\beta}(0)}{\Lambda}\right)P_0 + \sum_{i=1}^{6}\lambda_i C_{i,0}^C = \left(\frac{\Delta\rho_0 - \beta + \beta_{lost}(0)}{\Lambda}\right)P_0 + \sum_{i=1}^{6}\lambda_i C_{i,0}^C$$

$$\frac{dC_i^C(0)}{dt} = 0 = \left(\frac{\beta_i}{\Lambda}\right)P_0 - \left(\lambda_i + {}^{2}/_{\tau_C}\right)C_{i,0}^C + \left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^{2}/_{\tau_L}\right)C_{i,0}^L, \qquad i = 1 \ldots 6$$

$$\frac{dC_i^L(0)}{dt} = 0 = \left(\frac{V_C}{\tau_C V_L}\right)C_{i,0}^C - \left(\lambda_i + {}^{1}/_{\tau_L}\right)C_{i,0}^L, \qquad i = 1 \ldots 6$$

Solving for DNP cohorts:

$$C_{i,0}^C = \alpha_i P_0, \qquad i = 1 \ldots 6$$

$$C_{i,0}^L = \gamma_i \alpha_i P_0 = \gamma_i C_{i,0}^C, \qquad i = 1 \ldots 6$$

$$\gamma_i = {\left(\frac{V_C}{\tau_C V_L}\right)}\Big/{\left(\lambda_i + {}^{1}/_{\tau_L}\right)}, \qquad i = 1 \ldots 6$$

$$\alpha_i = {\left(\frac{\beta_i}{\Lambda}\right)}\Big/{\left[\left(\lambda_i + {}^{2}/_{\tau_C}\right) - \gamma_i\left(\left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^{2}/_{\tau_L}\right)\right)\right]}, \qquad i = 1 \ldots 6$$

Solving for the bias reactivity and the time-zero effective delayed neutron fraction:

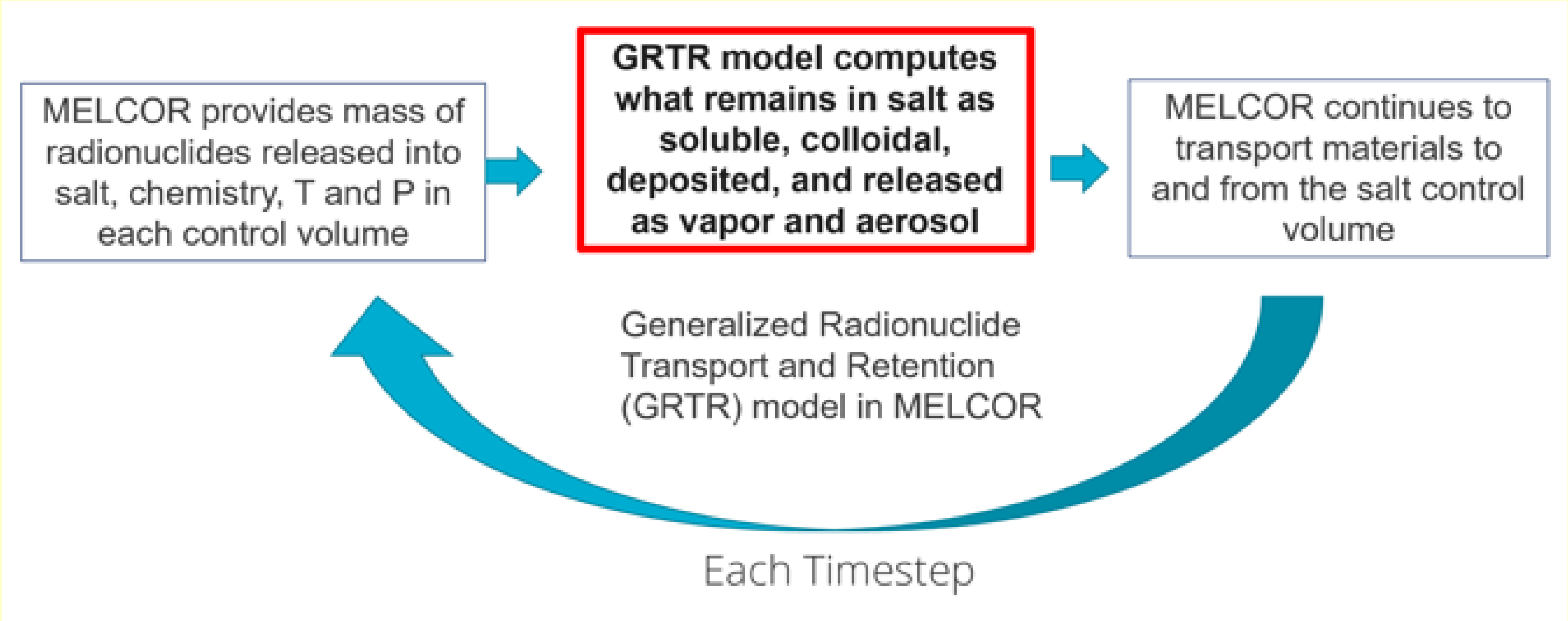
$$\Delta\rho_0 = \beta - \Lambda\sum_{i=1}^{6}\lambda_i\alpha_i(1+\gamma_i)$$

$$\bar{\beta}(0) = \beta - \beta_{lost}(0) = \beta - \Lambda\sum_{i=1}^{6}\lambda_i\gamma_i\alpha_i$$

GRTR Modeling Framework

- GRTR affected through CVH and RN1
  - CVH input declares:
    - User-defined forms and their characteristics (sectionwise, nonsectionwise, HS deposition)
    - Transfers between user-defined forms and from user-defined forms to built-in forms
    - Control functions can direct transfers
    - Limited built-in form-wise transfer physics models
    - Limited ability to employ Gibbs Energy Minimization tools like Thermochimica
  - RN1 input declares:
    - Initial user-defined form-wise mass by class and control volume
    - Sources for user-defined form-wise mass by class and control volume
  - If COR package is active, require a mapping for user-defined form-wise release

- GRTR applied to MSRs



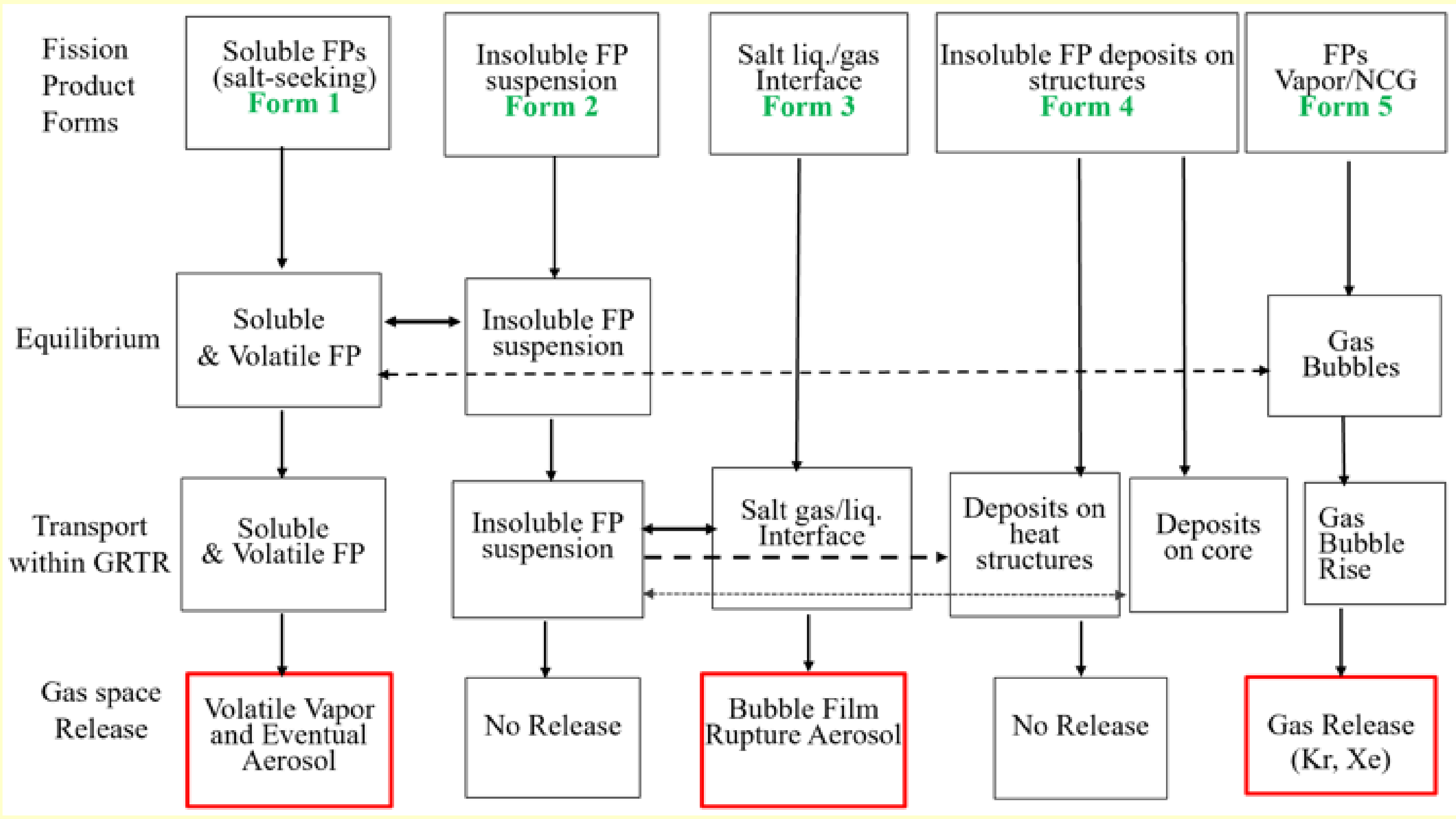
MELCOR provides mass of radionuclides released into salt, chemistry, T and P in each control volume

GRTR model computes what remains in salt as soluble, colloidal, deposited, and released as vapor and aerosol

MELCOR continues to transport materials to and from the salt control volume

Generalized Radionuclide Transport and Retention (GRTR) model in MELCOR

Each Timestep



- In MSR context, GRTR can account for:
  - Dissolved mass and its coming out of solution
  - Colloidal (insoluble) mass and its transport
  - Generation of aerosol at a free surface as bubbles burst
  - Vaporization
  - Aerosol dynamics according to conventional MELCOR physics models
  - HS deposition of any of the above forms
  - Advection of any of the above with CVH/FL flows
  - Use of control functions or built-in models or Thermochimica for form-wise transfers