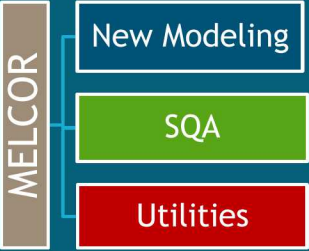
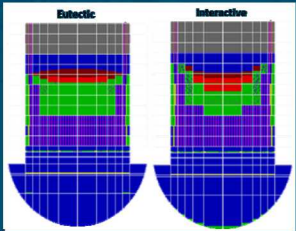
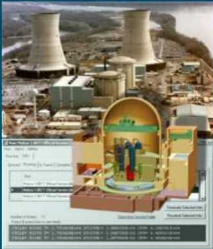




SAND2019-6157PE



# MELCOR Code Development Status MCAP 2019



Larry Humphries, Sandia National Laboratories

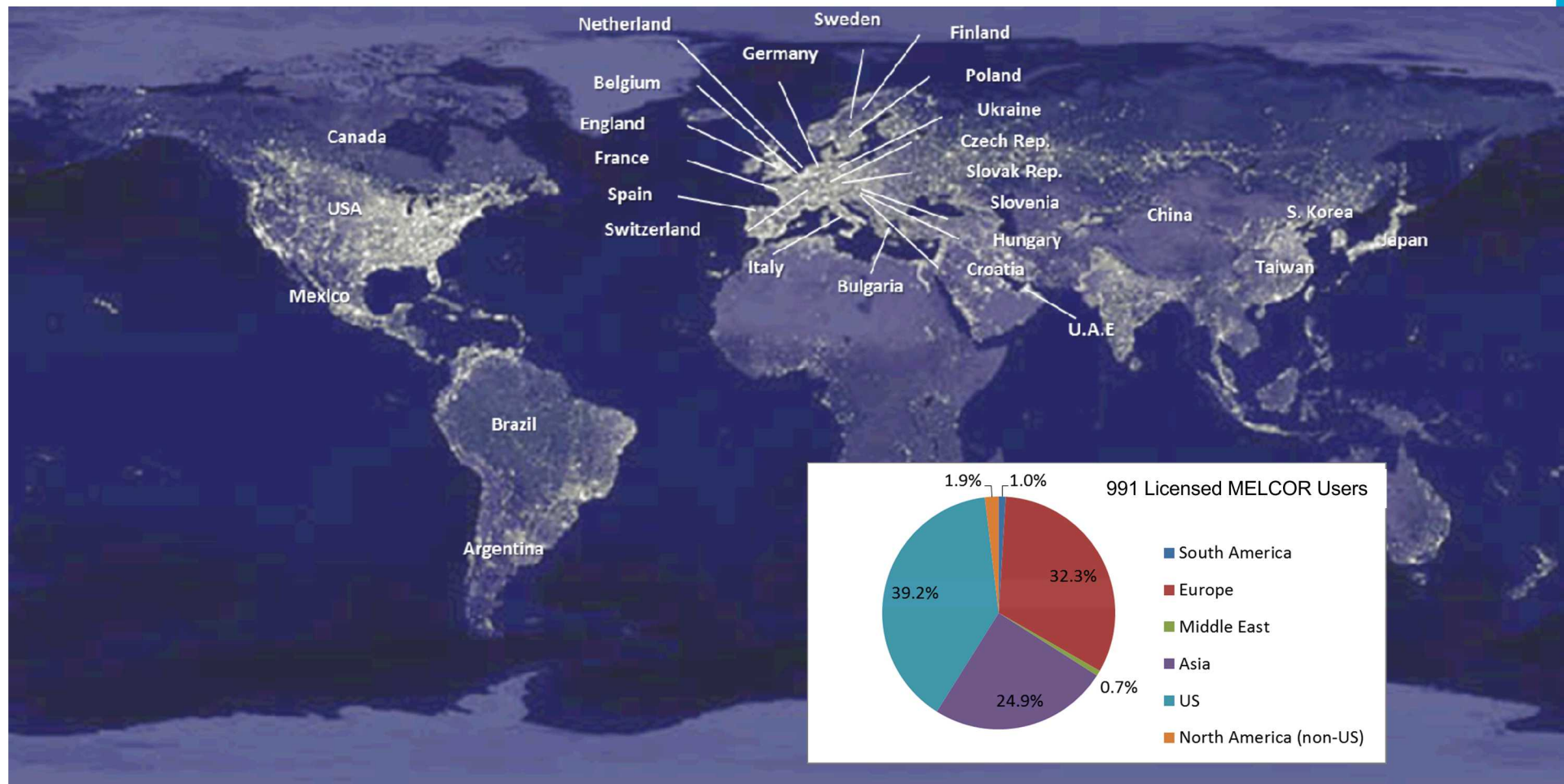
PRESENTED BY

Larry Humphries, Sandia National Laboratories



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# International Use of MELCOR



# MELCOR Workshops & Meetings

## 2018 Asian MELCOR User Group (AMUG)

- Hosted by CRIEPI (Japan)
- August 2018
- MELCOR/MACCS Topics

## 2019 European MELCOR User Group (EMUG)

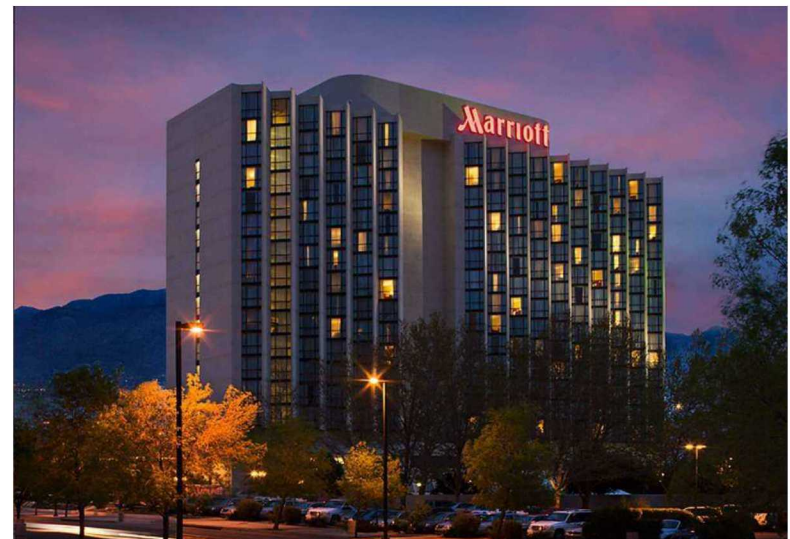
- Hosted by Paul-Scherrer Institute (PSI)
- Workshop on COR Package (April 3)
- April 4-5, 2019

## 2019 CSARP/MCAP/MELCOR Workshop

- CSARP (June 3-5), MCAP (June 5-6), Workshop (June 6 afternoon)
- Albuquerque, NM
- 1/2 day workshop with focused topics on ex-vessel corium modeling

## 2019 Asian MELCOR User Group

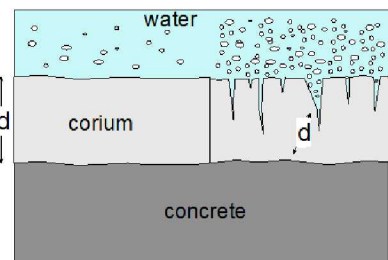
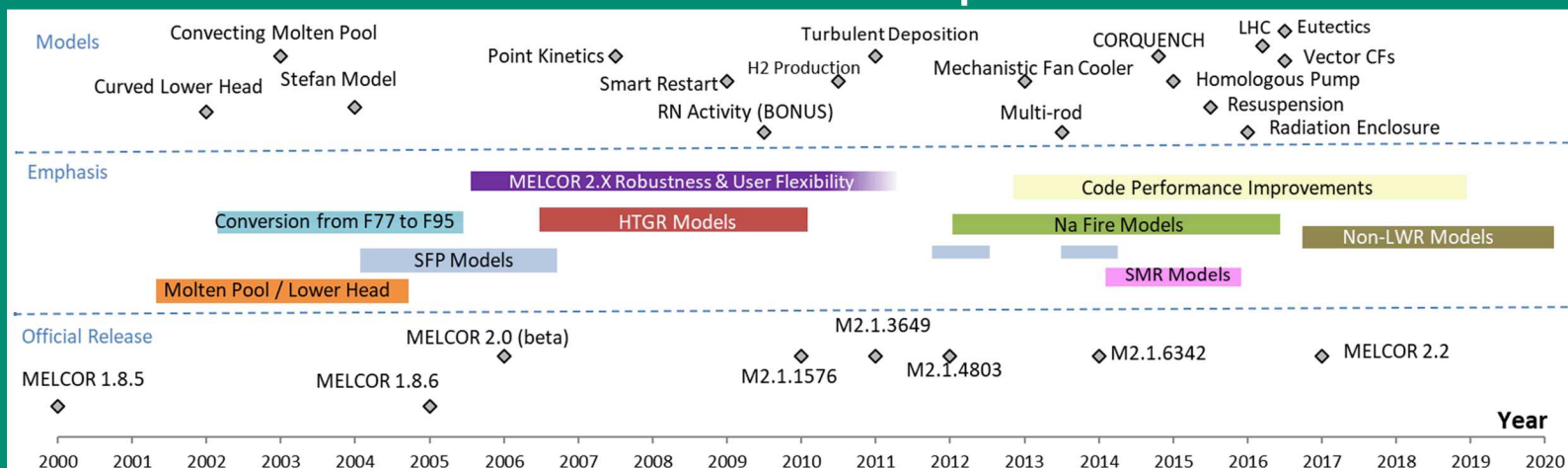
- Hosted by KAERI
- November 2019?





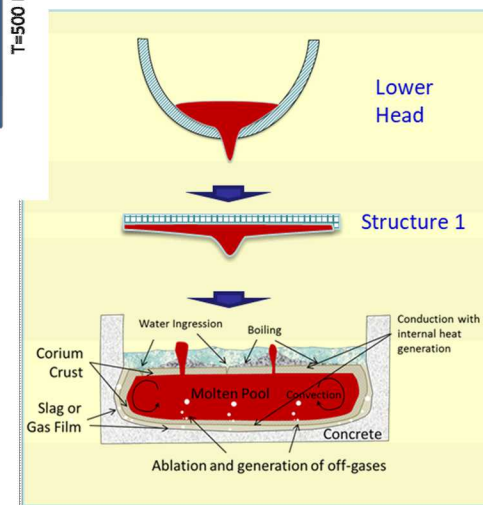
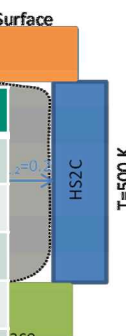
# MELCOR Model Development

## MELCOR Code Development



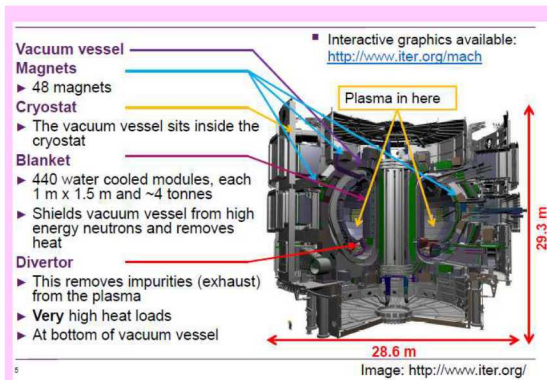
### M2x Official Code Releases

Version	Date
2.2.13519?	June 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





# Application Driven Development Non-Reactor Applications



## Fusion

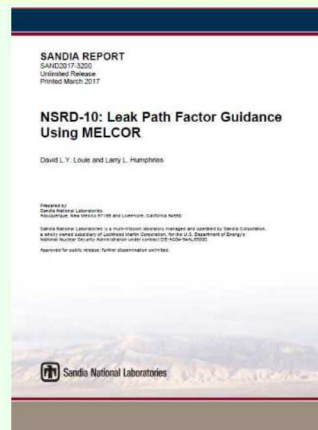
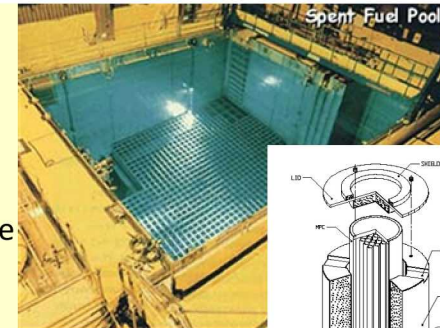
- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

## Spent Fuel

Spent fuel pool risk studies

Multi-unit accidents (large area destruction)

Dry Storage



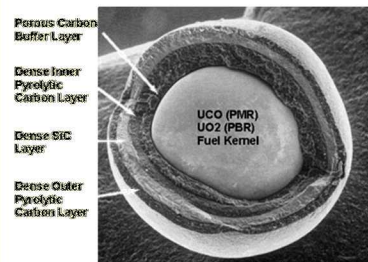
## Non-Nuclear Facilities

- Leak Path Factor Calculations (LPF)
  - Release of hazardous materials from facilities, buildings, confined spaces
- DOE Safety Toolbox code
- DOE nuclear facility users
  - Pantex
  - Hanford
  - Los Alamos
  - Savannah River Site

# Application Driven Development MELCOR 2.2 Emerging Applications

## HTGR Reactors

- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- Modified Fuel components (PMR/PBR)
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure



## Sodium Reactors

### Sodium Properties

- Sodium Equation of State
- Sodium Thermo-mechanical properties



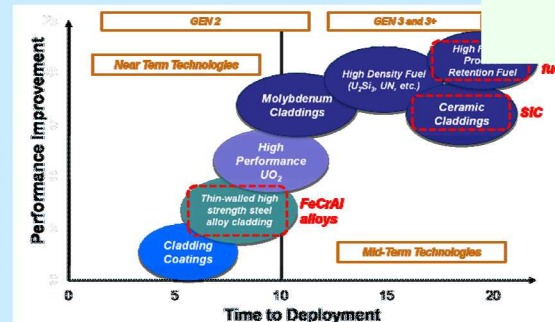
### Containment Modeling

- Sodium pool fire model
- Sodium spray fire model
- Atmospheric chemistry model
- Sodium-concrete interaction

## Molten Salt Reactors

- Properties for LiF-BeF<sub>2</sub> have been added
  - Equation of State
  - Thermal-mechanical properties

## Accident Tolerant Fuels



# LWR/Non-LWR/ATF Fuels Development

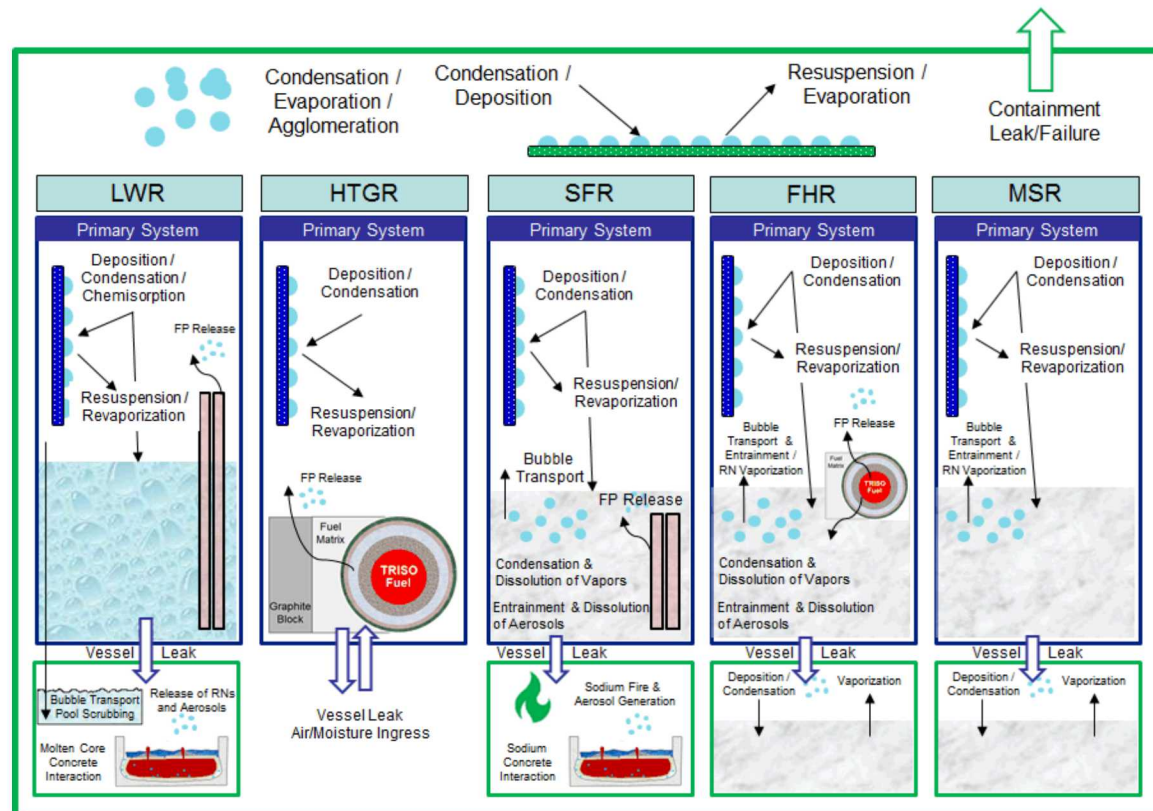
LWR and General MELCOR development

Advanced Technology Fuels (ATF)

Non-LWR Reactors

- HTGR
- Sodium
- Molten Salts

Spent Fuel Pools



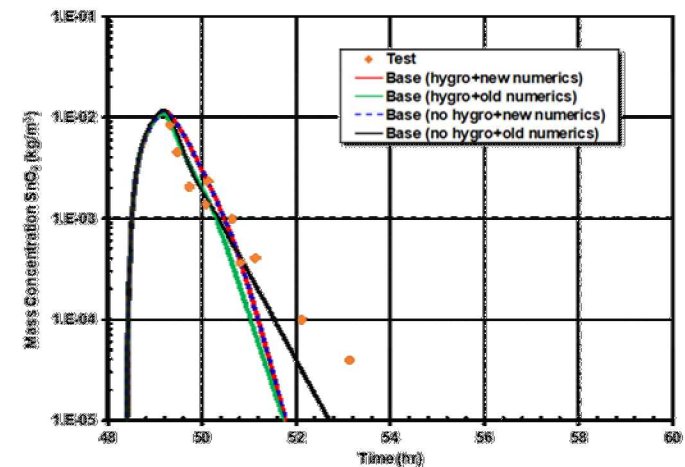
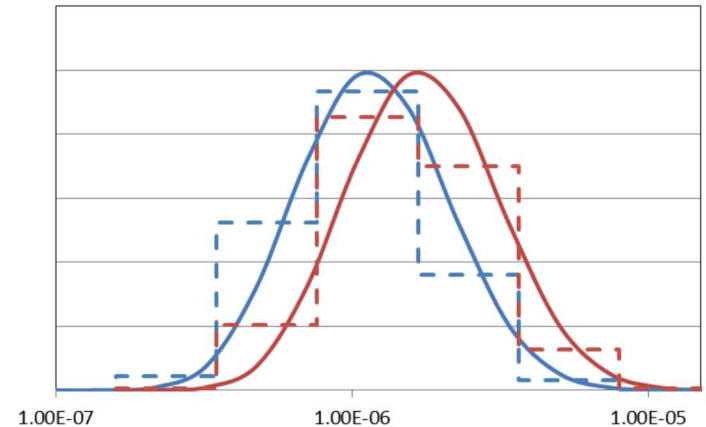


# Vapor Condensation/Hygroscopic Model (new default)

New condensation/evaporation algorithm significantly reduces numerical diffusion of aerosol growth

- Better resolution of aerosol mass within a section (particle size bin).
- Number mean particle mass tracked in addition to total mass
- Previously aerosol particles growing into a section were automatically uniformly spread across size bin, but now higher order resolution within a bin to be used.

Validation tests show much less sensitivity to whether the hygroscopic model is active or not.



# Sub-cooled Heat Transfer

## New Default



- ◆ New COR default enables lower head segment-to-pool heat transfer when segment surface temperature is sub-cooled with respect to the pool
  - ◆ Becomes default in 2019 release
- ◆ Previously, outer surfaces of LH segments submerged in a CAV/LHC pool do not transfer heat unless surfaces are superheated with respect to the pool
- ◆ No new physics, apply existing convection correlations (HS subroutine)
- ◆ 5th field **ILHHT** on **COR\_MS** - “1”/“ACTIVE” to deactivate

!	IEUMOD	IHSDT	IDTDZ	ICORCV	ILHT	
COR_MS	0	0	0	0	1	! Activate sub-cooled LH HT to pool

# Heat Transfer Coefficients for Lower Head New Default

10

Parameters for modeling heat transfer to the lower head are provided on the COR\_LHF record.

User specifies heat transfer for the following:

- Debris to penetrations
- Debris to lower head
- Heat transfer from oxidic molten pool to lower head
- Heat transfer for 'stray' metallic molten pool to lower head

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

Using Thermal Conductivity of Material at 1700 K

User can optionally specify a control function for each HTC

Previous default: All heat transfer coefficients were assumed to be 1000.0 W/m<sup>2</sup>-k

- Completely arbitrary and not always representative
- Does not reflect thermal conductivities of materials and composition
- Does not reflect conduction path which is dependent on nodalization

MELCOR 2019 release default: an internal model for calculating heat transfer.

- Available for PD to LH and MP1 to LH and MP2 to LH
- Model uses locally calculated thermal conductivity and a conduction path using half the current calculated component height
- These internal models will become default in next code release

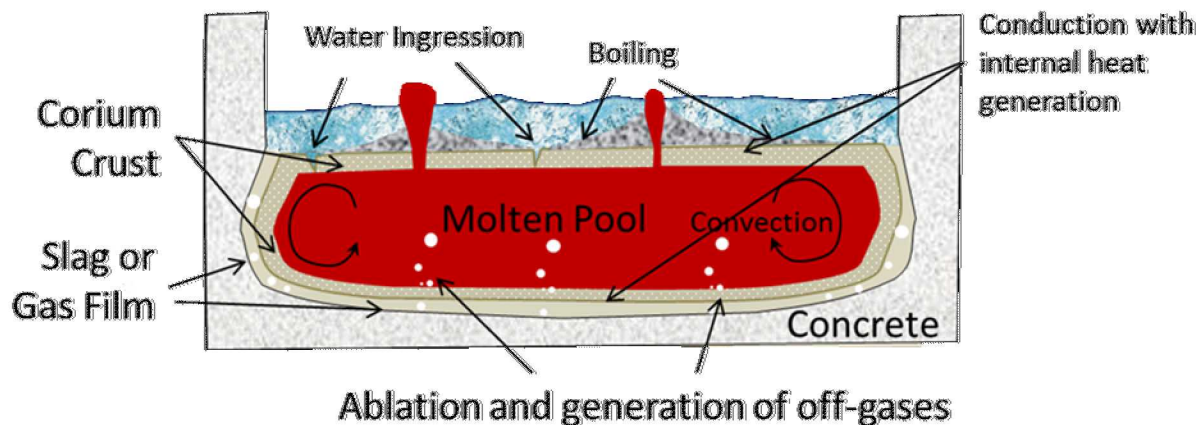
## Example

```
!          HDBPH/CF HDBLH/CF HMPOLH/CF HMPMLH/CF TPFAIL      CDISPEN
COR_LHF 1.00E-02 1.00E+02 MODEL      MODEL      1525.0      1.0
```



# New Modeling for Top-Quenched Debris in Cavity

11



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

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

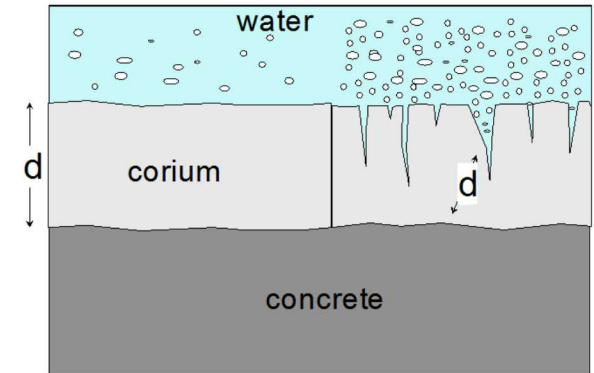
Molten corium extruded through crust by entrainment from decomposition gases as they escape through fissures and defects in the crust.

- Enhance 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

# Pre 2015 MELCOR Best Practice

- Water ingress will increase the contact surface area between water and the corium
- Decrease the conduction path length through the corium, both of which will enhance the heat transfer through the crust

$$Q = -A \cdot k \frac{dT}{dz} \sim -\frac{A}{d} k \Delta T \sim -\frac{A}{d} k \Delta T$$



- MELCOR best practice attempted to account for this effect by applying a thermal conductivity multiplier
  - Based on benchmarking against MACE tests
- MELCOR model development is focusing on improvements in the CAV package to capture water ingress and melt eruptions
  - New porous layer for debris relocating above crust
  - New porous crust layer
  - Dense crust layer

# CORCON/CORQUENCH Model



## Enhanced Conductivity (2010)

CAV\_U 9  
...  
5 BOILING value 10.0  
6 COND.OX mult 5.0  
7 COND.MET mult 5.0  
8 HTRINT multip 1.0  
9 HTRSIDE multip 1.0

## Modified Enhanced Conductivity (2012)

CAV\_U 10  
...  
5 BOILING value 10.0  
6 COND.OX mult 1.0  
7 COND.MET mult 1.0  
8 HTRINT multip 5.0  
9 HTRSIDE STAND  
10 COND.CRUST 3.0

## Water Ingression (2015)

CAV\_U 10  
...  
5 BOILING VALUE 10.0  
6 COND.OX MULT 1.0  
7 COND.MET MULT 1.0  
8 COND.CRUST 1.0  
9 WATINGR ON  
10 ERUPT ON

**2018:**  
**Still current best practice**

**2019 Release: Default**



# Extensions to the CF Package (September 2016)



## 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

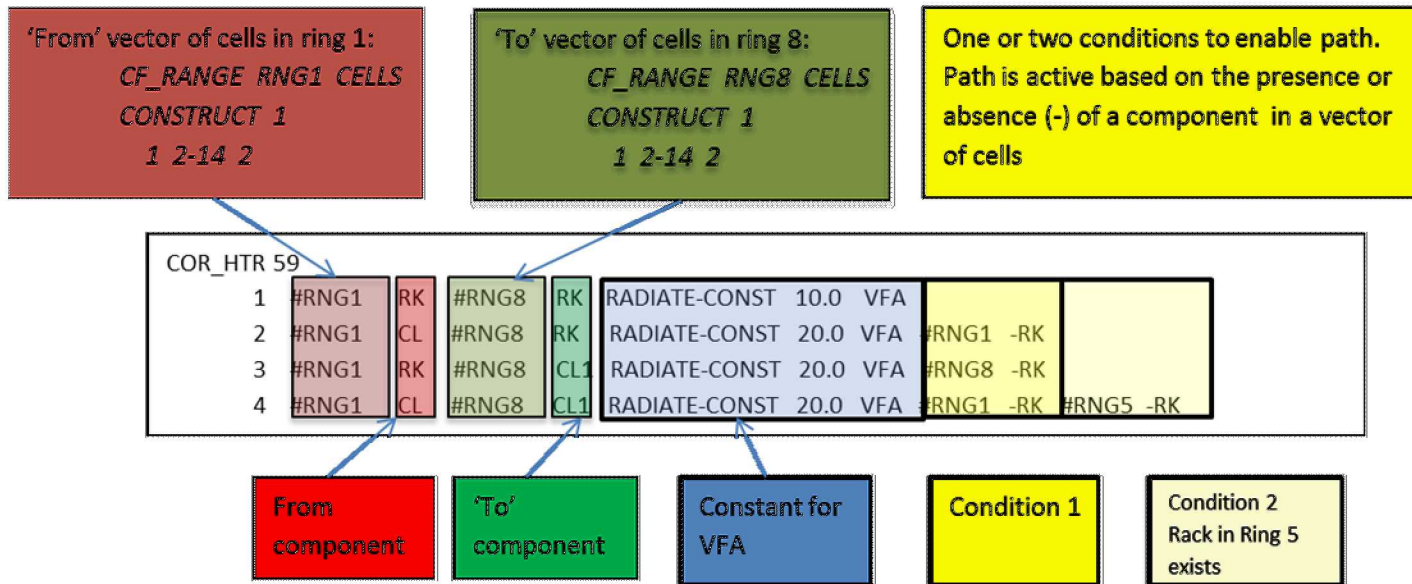
## Analytic Control Functions

- 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

# Vectorized COR\_HTR Input



Reduces number of input records significantly.

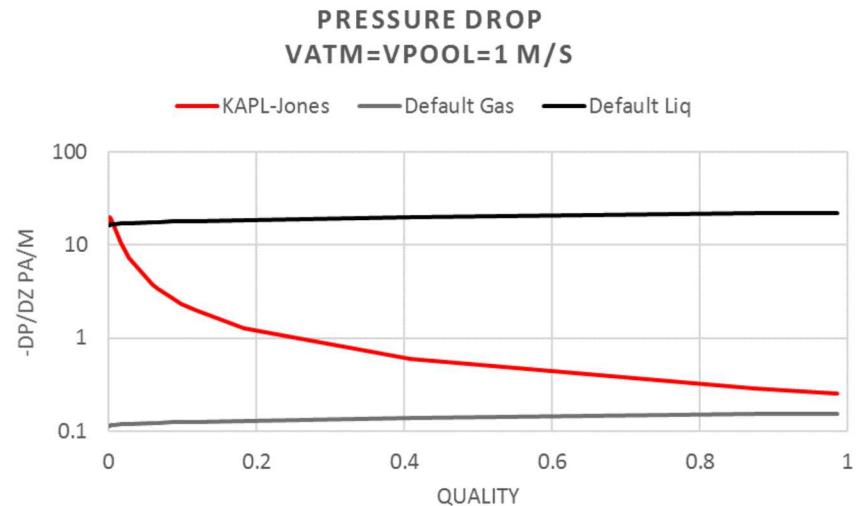
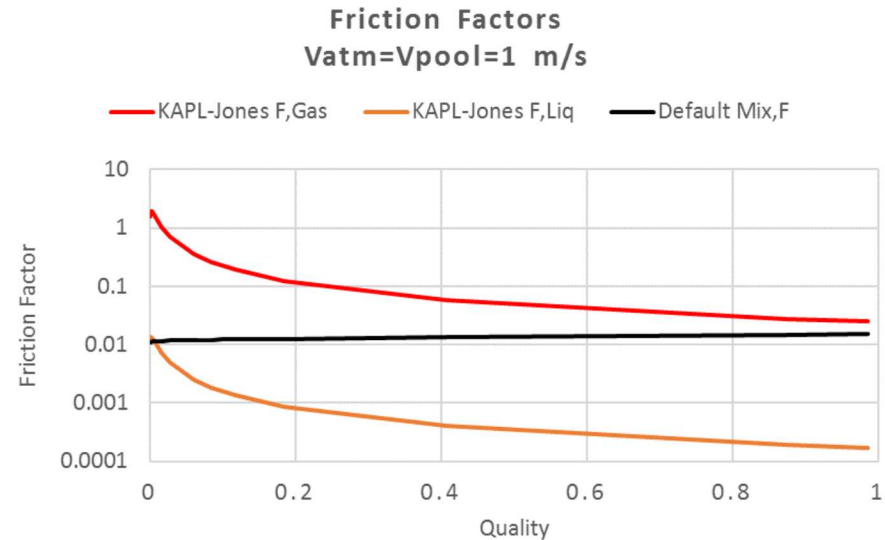
- Otherwise input is required cell by cell.
- Unnecessary CF logic required to determine existence of components.
- Difficult to read (QA)
  - Input for a cell is scattered among COR\_HTR records and multiple CF records
- One example reduced number of records from over 7000 records to under 100

# Two-Phase Friction Factor 2019 MELCOR Code Release

16

A user-defined friction factor is available with three available options:

- a single friction factor applied to both fields,
- two-separate friction factors specified for each field independently,
- or a homogenous treatment where either a gas- or liquid-only correlation is used.





# MELCOR Debris Spreading Model

## Released in 2013



By default, corium relocated to the cavity will spread instantaneously

Users are able to specify a spreading radius through a CF or TF

Current model development adds an internally calculated spreading radius.

- Balance between gravitational and viscous forces

### **CAV\_SP** – Definition of Parametric Debris Spreading Optional

This record may be used to model the spreading of debris in the cavity. Users can define a maximum debris radius as a function of time through a tabular function, control function, channel of an external data file, or an internal model.

#### (1) SOURCE

Source of data for maximum debris radius as a function of time

1 or 'TF'

Use data from tabular function.

-1 or 'CF'

Use data from control function.

2 or 'CHANNELEDF',

Use data from channel of external data file NameCF\_TF\_EDF.

0 or 'MODEL',

This option allows the code to internally calculate the debris radius as a function of time. However, this option requires the initial debris radius (RADTINI).

If SOURCE = 0, the following record is required:

(2) RADTINI - Initial time-dependent debris radius for the internal model

# Homologous Pump Model

## July 2015

Transient Pump operation characterized by

- Rotational speed
- Volumetric flow rate
- Dynamic head
- Hydraulic torque

Pump characteristic curves or four quadrant curves

- Any one of the above quantities can be expressed as a function of any other two
  - Dynamic head and hydraulic torque are expressed as functions of volumetric flow and rotational speed ratios
    - Eight curves for the dynamic head
    - Eight curves for hydraulic torque
- Empirically characterized by manufacturer
- Similarities to RELAP and TRACE models

Curve Definitions

- Built-in pump curves
  - Semi-scale
  - Loft
- User defined curves
  - Uses tabular function (32 TFs for full coverage)
  - If user does not define all modes, error occurs when pump enters undefined domain
- Universal correlation
  - Systematic approach for predicting pump performance where data does not exist
  - Fits to several data sets (including LOFT & Semiscale)
  - Only valid in normal operating mode
  - Lahssun, Jedral. Universal Correlations for Predicting Complete Pump Performance Characteristics. 2004.

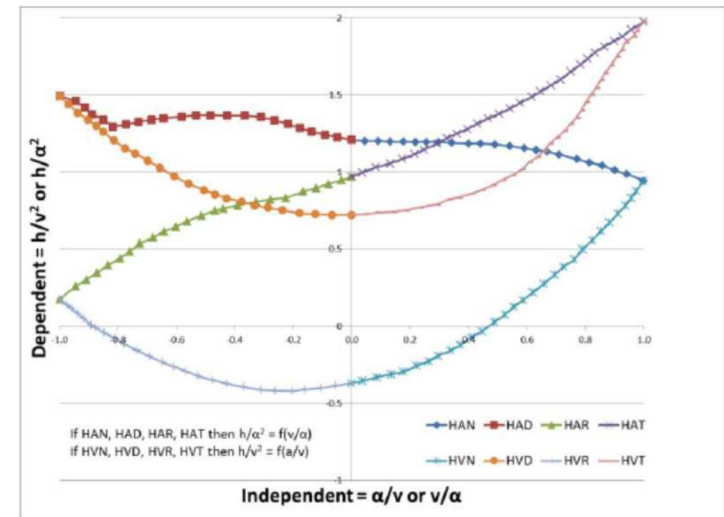


Figure 1. Semiscale single-phase head curve

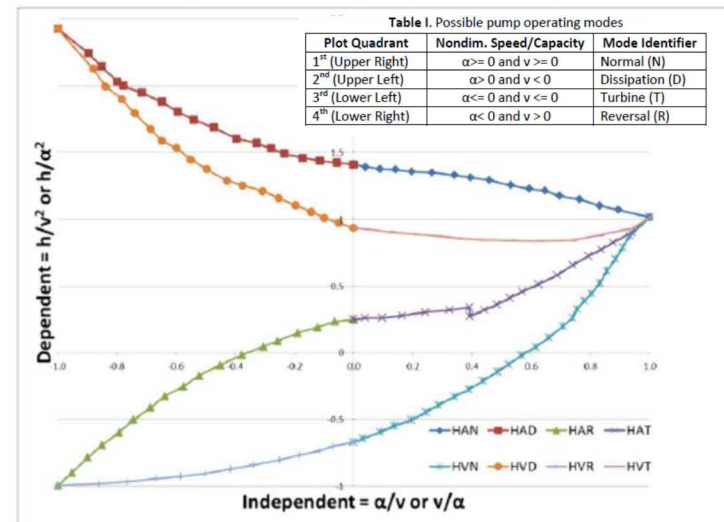


Figure 4. LOFT single-phase head curve

$$\alpha = \frac{\omega}{\omega_R} \text{ and } v = \frac{Q}{Q_R}, \text{ for rated speed and capacity } \omega_R, Q_R$$

# MELCOR Terry Turbine Model(s) Overview

## September 2017

Terry turbine pressure-stage model (rapid steam expansion across nozzles)

- Isentropic steam expansion or analytical Wilson point approach to capture phase non-equilibrium effects
- Back-pressure effects for either under-expanded or over-expanded flow

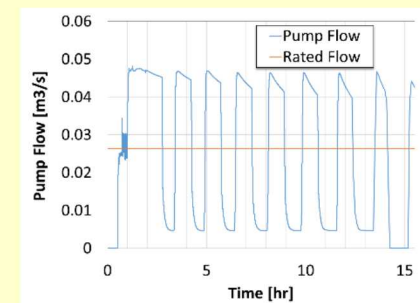
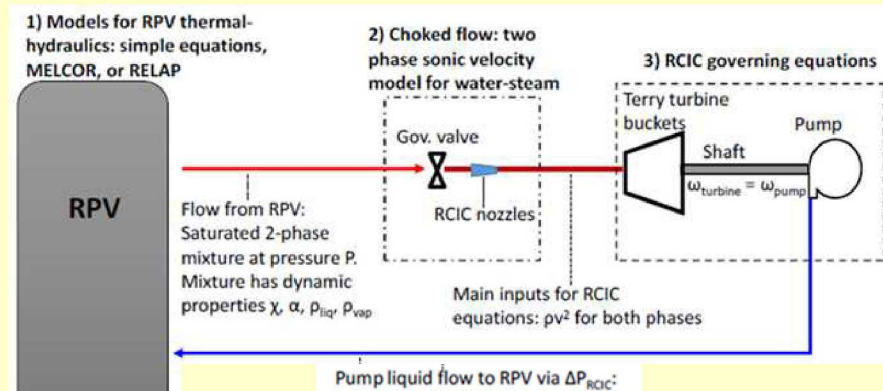
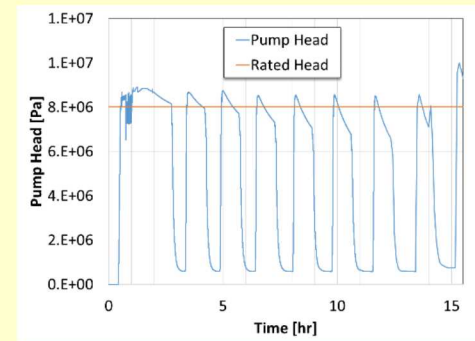
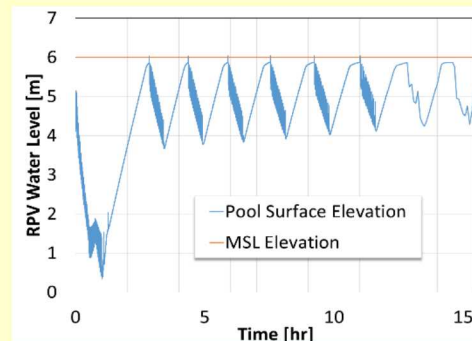
Terry turbine compound velocity-stage model (impulse of steam on turbine rotor)

- Interfaces to pressure-stage model
- Predicts rotor torque from initial impingement of steam plus subsequent stages (reversing chambers)

Turbo-shaft model

- Rigid coupling of the turbine to the homologous pump model
- Solves a torque-inertia equation to govern turbo-shaft speed

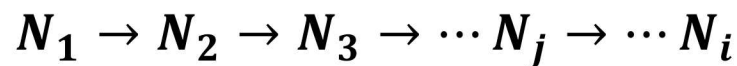
*New models exercised on a pseudo-Fukushima RCIC.*



# MELCOR Activity Calculations (BONUS)

## Bateman Equations (December 2009)

General Radioactive Decay  
Chain



Sources and losses

$$\frac{dN_i}{dt} = \sum_{j=1}^{i-1} \lambda_j N_j - \lambda_i N_i$$

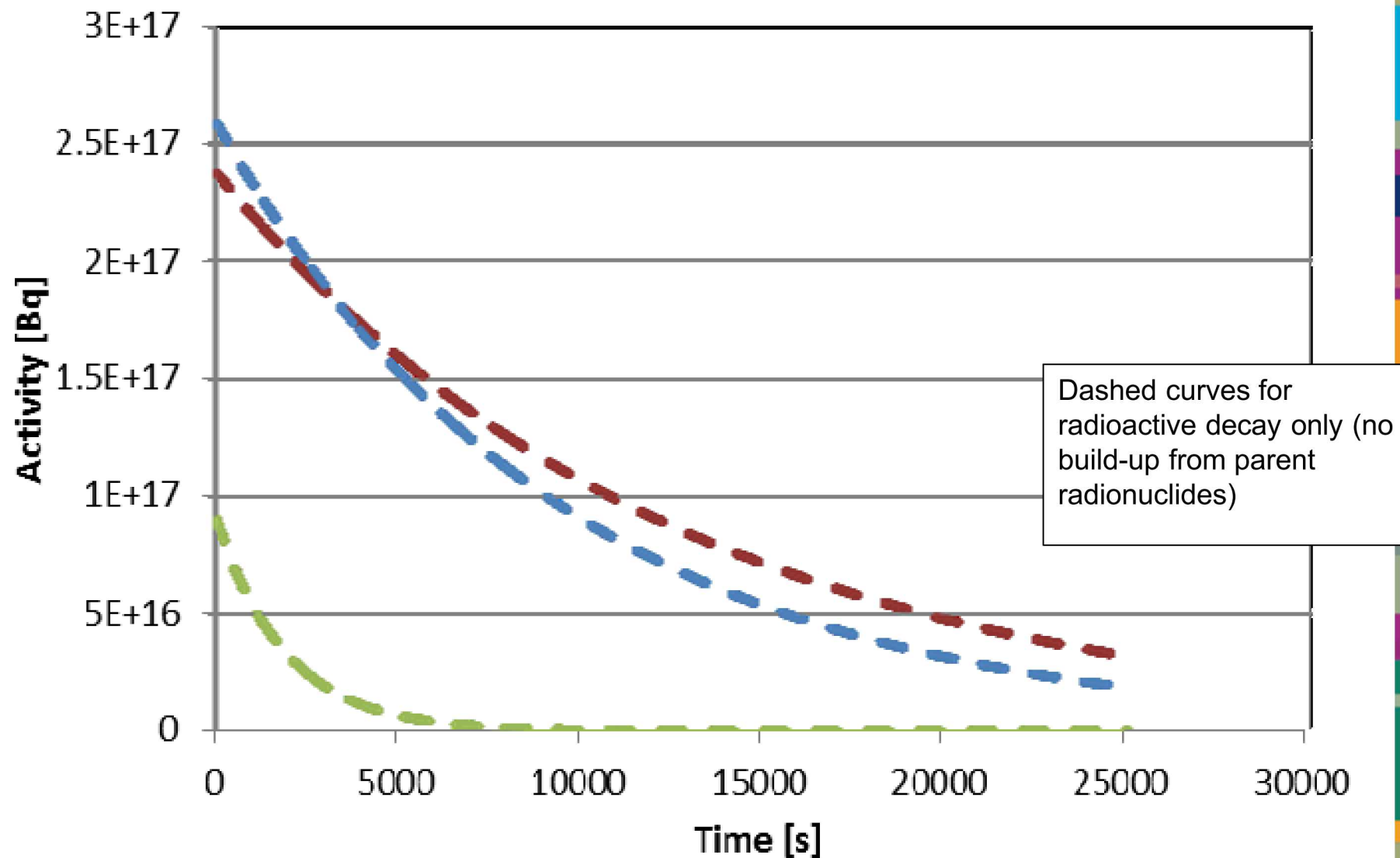
Solution

$$N_i(t) = \lambda_1 \lambda_2 \cdots \lambda_{i-1} N_1(0) \sum_{j=1}^i \frac{e^{-\lambda_i t}}{\prod_{k \neq j} (\lambda_k - \lambda_j)}$$

- Isobaric  $\beta$  and  $\gamma$  decays of fission products are considered
- Thermal neutron capture also taken into account
- Daughter products defined in file Fpchains.in
- Significant interest in activity models expressed at EMUG
- Decay chain modeling listed in NRC SOW



# Decay and Build-up (A=83)



# Dose Plot Variable

Plot variables for dose estimate recently added (April 2018)

- Doses calculated for each surface or volumes in DCH\_SUR table
- BONUS-DOSE.isur (Rad/hr)
  - isur corresponds to table entry in DCH\_SUR table
  - Optional characteristic length, CHARL, provided by user (in red)
    - Real value for word 4 indicates characteristic length.
    - Otherwise, 4<sup>th</sup> word should be KEY.
    - For CVOLUME – CHARL = radius of volume used by flux calculation
      - Default is calculated from atmospheric volume assuming spherical volume
    - For HS surface – CHARL = orthogonal distance from surface to dose ‘detector’
      - Default is 1 m from surface

Example				
DCH_SUR	4	! N TYPE	NAME	CHARL IKEY
1	CVH	CORE-INLET		ALL
2	LHS	INLET-FLOOR	1.25	ISOTOPE 'Cs-137' 'I-131'
3	CVH	'CONTAINMENT'	0.9	ALL
4	LHS	'CORWALL6'		ISOTOPE 'Cs-137' 'I-131'

- Gamma energy from user files

- 1<sup>st</sup> uses gamma energy from FissProd.in file
- Overwrites with any gamma energy on 3<sup>rd</sup> field in inventory file.

## Gamma dose rate in air

$$\dot{D}_i^\gamma = (5.77 \times 10^{-5}) \phi_i E_i \left( \frac{\mu_{a,i}}{\rho} \right)_{air}$$

### Where

- $\dot{D}_i^\gamma$  - gamma dose rate of the  $i^{\text{th}}$  isotope [Rad/hr]
- $\phi_i$  - gamma flux of the  $i^{\text{th}}$  isotope [ $1/(\text{cm}^2 \text{ s})$ ]
- $E_i$  - gamma energy of the  $i^{\text{th}}$  isotope [MeV]
- $\left( \frac{\mu_a}{\rho} \right)_{air}$  - mass absorption coefficient for air at  $E_i$  [ $\text{cm}^2/\text{g}$ ]

### Assume mono-energetic gammas for each isotope

- In reality, gammas interactive with matter before reaching detector, creating an energy spectrum

**For each isotope of interest, this approach amounts to estimating the gamma flux at a detector**

# Two Fluxes Available May 2018



**Uniform and spherical source with a detector located at the center of the sphere**

$$\phi_i = (3.7 \times 10^{10}) \frac{A_i}{V \rho_{air} \left( \frac{\mu_s}{\rho} \right)_{air}} \left( 1 - e^{-\rho_{air} R \left( \frac{\mu_s}{\rho} \right)_{air}} \right)$$

■ Where

$A_i$  = activity for the  $i^{\text{th}}$  isotope (Ci),

$R$  = equivalent spherical radius of volume  $V$  ( $\text{cm}^3$ ),

$\rho_{air}$  = density of air ( $\text{g}/\text{cm}^3$ ),

$\left( \frac{\mu_s}{\rho_{air}} \right)$  = total attenuation coefficient of air at  $E_i$  ( $\text{cm}^2/\text{g}$ ),

and  $V$  = volume of MELCOR control volume(s) of interest ( $\text{cm}^3$ ).

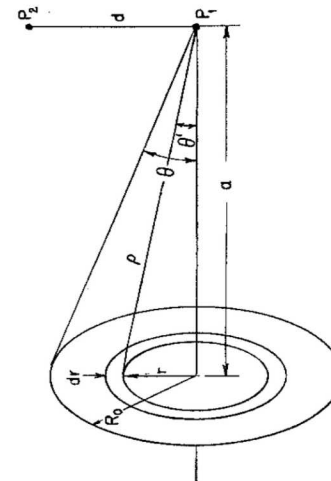
■ **Assumptions:**

- Mono-energetic flux
- Mono-energetic gamma particles from each isotope reach the detector
- attenuation coefficient: consider energy dependence or treat as a constant

**Uniform and planar, circular source with a detector located a distance 'a' from center.**

$$\phi_i = \frac{A_i}{2 \cdot \pi \cdot R_o^2} [E_1(b_1) - E_1(b_1 \sec \theta)]$$

$$E_n(b) = b^{n-1} \int_{b_n}^{\infty} \frac{e^t}{t^n} dt \quad (\text{Exponential integral})$$





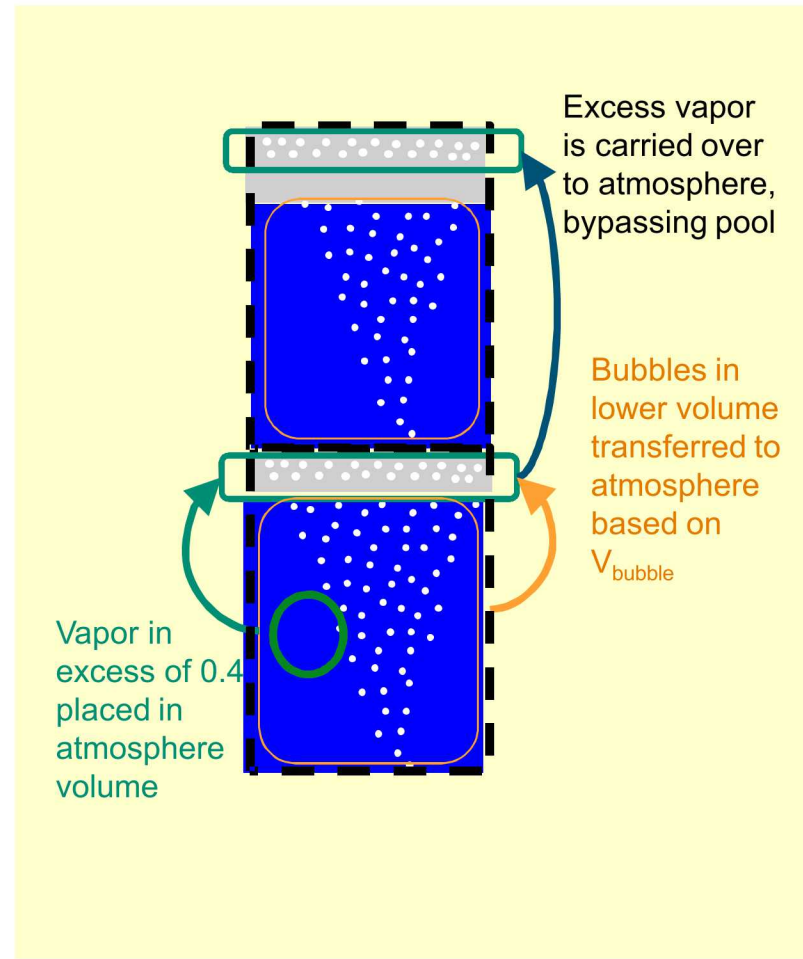
# Bubble Rise Model

Boiling may cause vapor bubbles to appear in a pool

- Either as a result of flashing or heat deposition in the pool
- Only occurs with non-equilibrium model since NCG not present in pool.

Bubble rise model

- Volume flow of bubbles varies linearly from zero at bottom of CV to a value of  $J_{\max}$  at the top
- Constant rise velocity,  $v_o = 0.3$  (SC4407)
- Maximum void fraction in pool is 0.4 (SC4407)
- Formulated for a single CV volume
- Bubble density assumed to be zero at bottom of all CVs
- Excess bubbles placed in atmosphere carry over to atmosphere in receiving volumes, bypassing pool



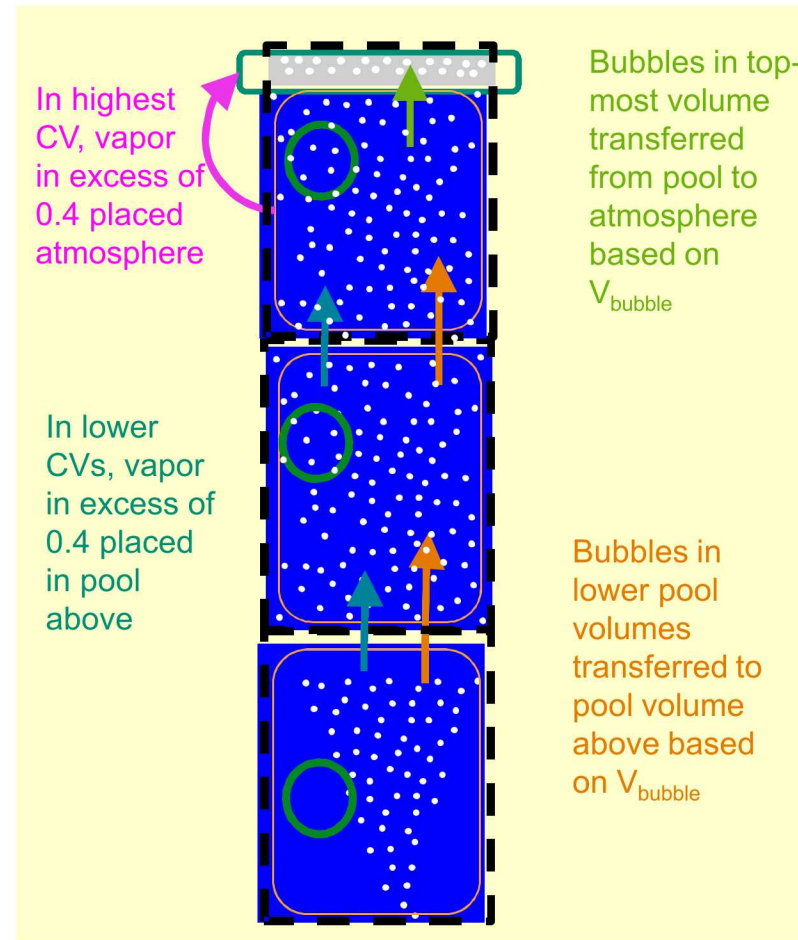
# Modified Bubble Rise Model

## March 2019

User defines a collection of stacked CVs for which the bubble model interacts

```
CV_ID 'CV108' 108
CV_TYP 'CVTYPE01' 1
```

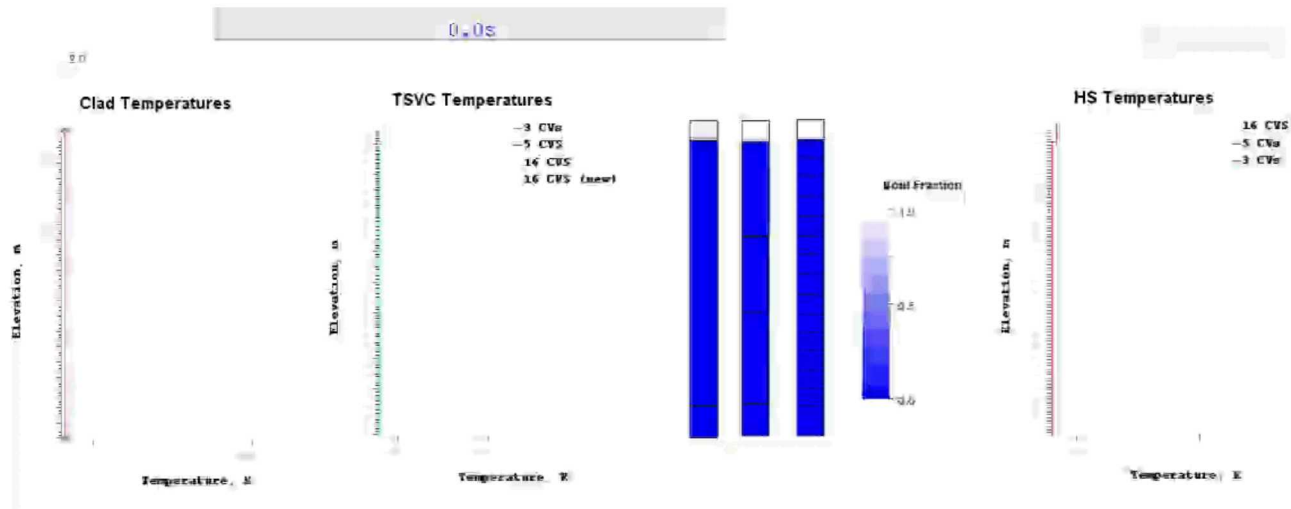
- Bubble rise leads to transfer of mass across the pool/atmosphere interface only in uppermost volume (with a nonzero pool mass).
- Bubble model transfers mass from pool in lower CV to pool in CV directly above.
- Vapor in excess of 0.4 is placed in cell atmosphere volume only in the uppermost CV, otherwise placed in pool above.



User-defined CV stack

Additional changes required for SPARC model

# NEPTUN Experiment



CV16 (new) represents new formulation of the bubble rise model

- Somewhat improved temperature response
- For stratified suppression pool, bubbles could be condensed in pool.

# Melt Ejection From Failed Vessel

Two models for determining debris mass available for ejection

- Default Slurry/Oatmeal Model

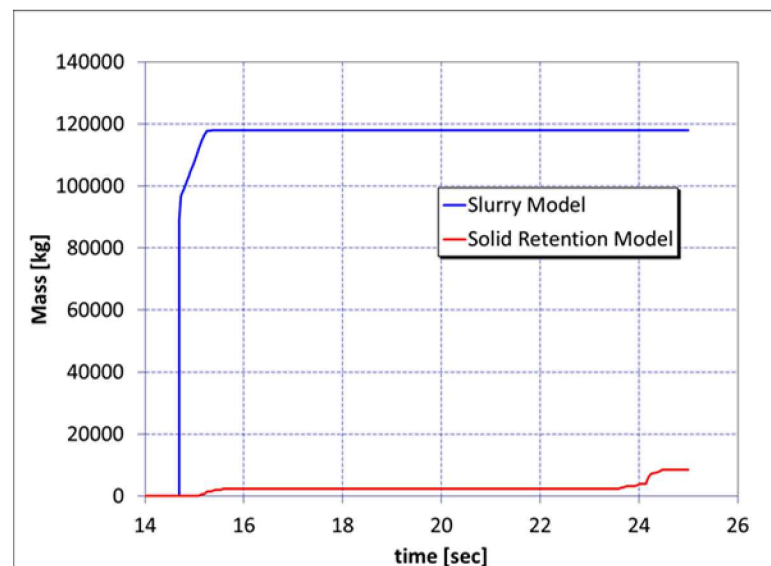
- The total debris mass and molten pool material masses
  - Regardless of whether they are molten or not
- May lead to ejection of more solid debris than is realistic

- Alternate Model - Solid retention

- SS, Zr,  $\text{UO}_2$  liquid masses available for ejection
- SSOX, CRP mass multiplied by SS melt fraction (assumed proportional mixing)
- $\text{ZrO}_2$  mass multiplied by Zr melt fraction (assumed proportional mixing)
- $\text{UO}_2$  solid mass (fraction assumed in candling model)
- Currently enabled on COR\_TST record

- Possible Future Modeling

- Initially use solid retention model
  - Small localized failure
  - Fused debris mass in lower head
- Switch to slurry model
  - Vessel further degrades with possible melting
- Control function can be used to switch between models



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

## (9) IDEJ

Disable switch for solid debris ejection model.

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



# MELCOR Eutectic Temperature

## Initial repair May 2017

### UO<sub>2</sub>-INT/ZRO<sub>2</sub>-INT

Melt temperature for UO<sub>2</sub> & ZrO<sub>2</sub> is the same for intact materials as it is for conglomerate.

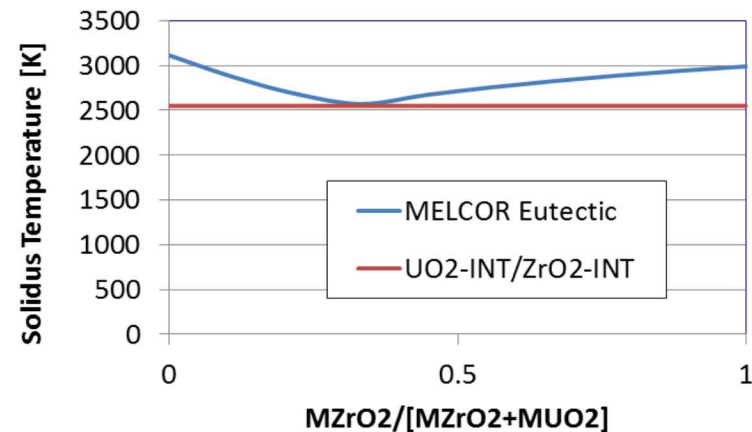
Does not depend on composition

### Eutectic Model

Melt temperature of intact material uses elemental melting points while conglomerate uses eutectic temperature

- Liquefaction of solids in contact from calculated rates

Melt temperature dependent on composition



***The existing MELCOR eutectics model provides a framework from which a new MELCOR model may be constructed***

# Dissolution of solids by molten mixture

Dissolution will proceed until the addition of solid lowers the updated gross mixture enthalpy to the liquidus enthalpy associated with the updated mixture composition

Or until the parabolic rate limitation associated with the dissolution reaction has been exceeded for the given timestep.

The solution is iterative

Component	Solids Dissolved by Mixture
Cladding	UO <sub>2</sub> from intact fuel ZrO <sub>2</sub> from intact cladding
Canister	ZrO <sub>2</sub> from intact canister ZrO <sub>2</sub> from intact cladding (A) UO <sub>2</sub> from intact fuel
Other structure SS or NS (steel only)	steel oxide from the same other structure
Other structure NS (BWR control rod)	steel oxide from the same other structure ZrO <sub>2</sub> from intact canister (A) Zr from intact canister (A)
Other structure NS (PWR control rod)	steel oxide from the same other structure (B) Zr from the same other structure ZrO <sub>2</sub> from intact cladding (A) UO <sub>2</sub> from intact fuel (A)
Particulate debris	UO <sub>2</sub> from particulate debris ZrO <sub>2</sub> from particulate debris ZrO <sub>2</sub> from intact cladding UO <sub>2</sub> from intact fuel
(A)	indicates solid is attacked only if there is no holdup of the mixture in the component.
(B)	indicates solid is attacked only if the mixture is being held up by the component

$$(x_j^f)^2 = (x_j^i)^2 + K_j \Delta t$$

$$K_j = A_j \exp(B_j / T)$$

where

$x_j^f$  = final mass fraction of material j,

$x_j^i$  = initial mass fraction of material j,

$\Delta t$  = timestep (s), and

$$A_{ZrO_2} = 1.47 \times 10^{14}$$

$$A_{UO_2} = 1.02 \times 10^{15}$$

$$B_{ZrO_2} = 8.01 \times 10^4$$

$$B_{UO_2} = 8.14 \times 10^4$$

# Multi-Rod Model

## October 2015

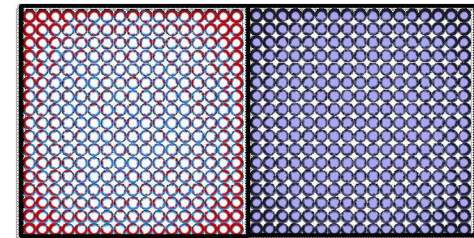
31

### Motivation

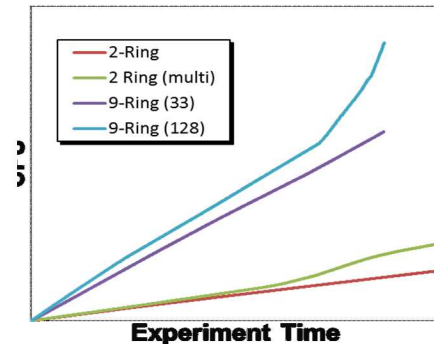
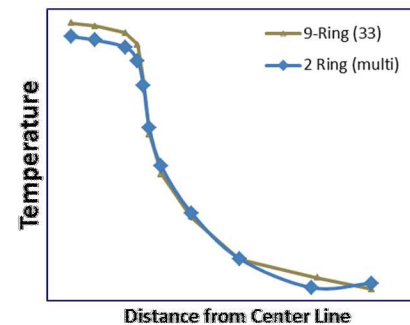
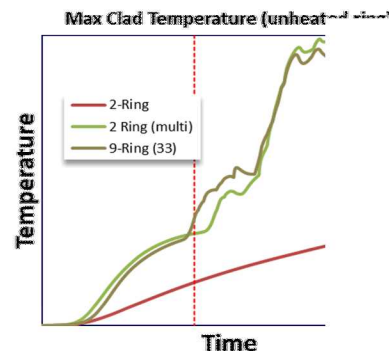
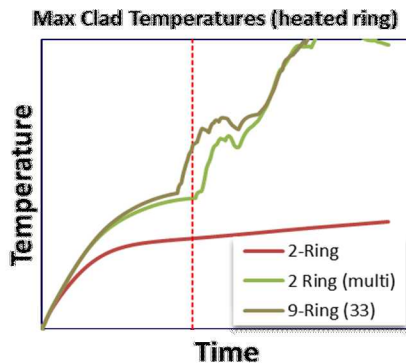
- It is desirable to model an entire assembly within a single MELCOR ring

### Challenge

- When hot assembly reaches ignition, heat transfer to cold assembly is problematic



Hot Assembly Cold Assembly



### Validation

- Validation was performed against the Sandia PWR Spent Fuel Pool Experiments
- Comparisons between 2-ring (2 rods) model; 2-ring, (9 rods) model; and 9-ring model.
- CPU time is greatly reduced for multi-rod model
- Simplified input requirements
- Fuel rod degradation modeling is nearly complete
- Recently extended to PWR reactor type in addition to PWR-SFP



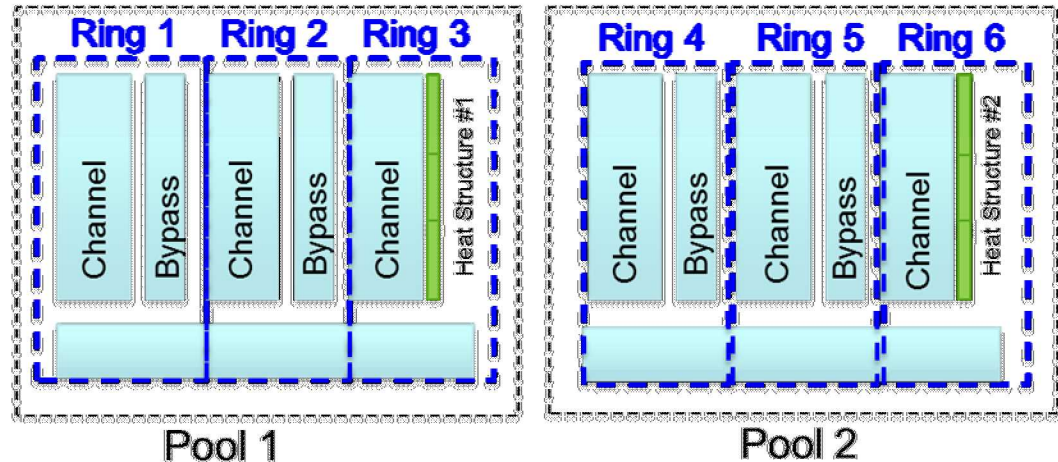
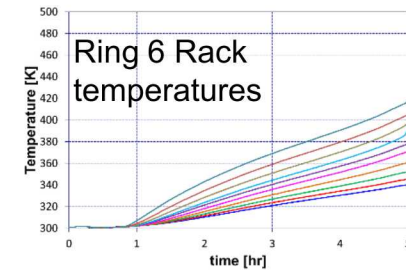
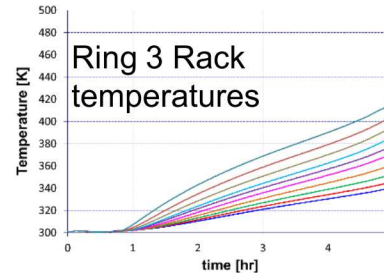
# COR\_HTR extended to HS (Application)

Two connected spent fuel pools

Rods near boundary radiate to concrete wall.

Modification enables heat transfer to heat structures other than boundary heat structures

Pool 1 & 2 Rack (and HS) temperatures are equivalent.



## Caveats

- Emissivity of boundary HS can be specified by user for SFP reactor types
  - HS\_LBR record
  - A value of 0.9999 is assumed for boundary heat structures for all other reactor types
- Input is required to connect the HS surface to the COR cell
  - HS\_LBF record
  - Otherwise DTDZ model will not use the structure for calculating local TSVC



# Miscellaneous New Models: MACCS Multi-ring release

## Motivation

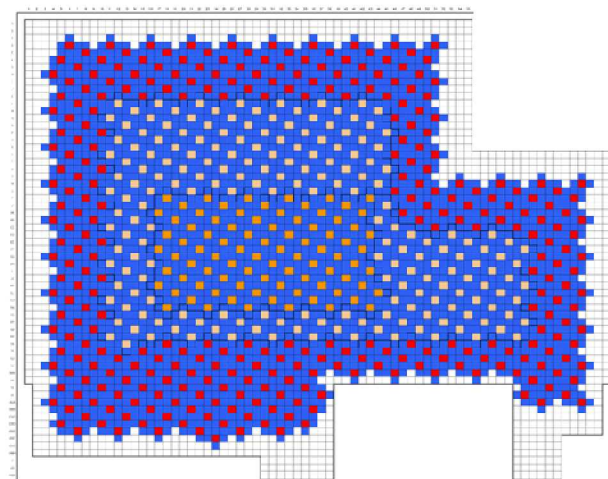
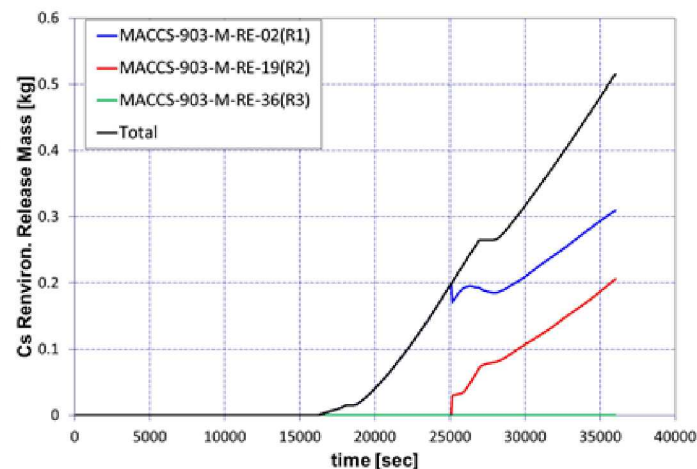
- Burnup and therefore activity for distinct rings may be vastly different. Recently, MACCS has been modified to allow it to distinguish masses provided by MELCOR by batch (ring). MACCS then will associate different activities for a class, dependent on the ring of origination
- The problem is that once RN mass is released, it can no longer be distinguished by originating ring.

New variable for approximating mass release by offload batch (ring)

- Not really a new model
- Creation of a plot variable in the binary plot file
- **This is an approximation in obtaining a plot variable**

Previously implemented by KC Wagner through use of control functions.

- Control function description can be quite lengthy even for a two-ring model



# ATF Design Concepts

- Near Term
  - Coated Cladding
    - Multiple vendors
    - Standard zirconium alloy material with thin coating applied to outside
    - Intent is to reduce corrosion and metal-water reaction
  - Doped fuel pellets
    - Reduce PCI by increasing pellet creep
  - Steel cladding (FeCrAl)
- Long Term
  - SiC (ceramic composite) Cladding
    - Pursued by multiple vendors
  - $U_3Si_2$  fuel pellets
    - Higher fuel density
    - Limited information on fuel performance
  - Lightbridge
    - Helical cruciform fuel rods
    - Metallic fuel co-extruded with clad

# Helical SG HTC in MELCOR 2.2

## August 2017

Helical Steam Generator (HSG) Heat Transfer Coefficients were implemented in MELCOR 2.2

Subroutines added for calculations of HSG heat transfer coefficients

Subroutine HSGhtcSubcool for subcooled boiling

Subroutine HSGhtcbl for two-phase flow

Subroutine HSGhtcat for super-heated steam [ Eq. (9) ]

### 2.4 Correlation for secondary superheated steam flow (inside tubes)

The heat transfer coefficient for secondary superheated steam in a forced-convection condition is calculated in Eq. (9). Steam properties are used.

$$h = \frac{1}{26.2} \left( \frac{k}{d_i} \right) \frac{Pr}{(Pr^{2/3} - 0.074)} Re^{4/5} \left( \frac{d_i}{D_c} \right)^{1/10} \left[ 1 + \frac{0.098}{\{Re(d_i/D_c)^2\}^{0.2}} \right] \quad \dots \text{Eq. (9)}$$

Sensitivity Coefficients added for the user to adjust code calculation

# Zukauskas Heat Transfer Coefficient

## October 2015

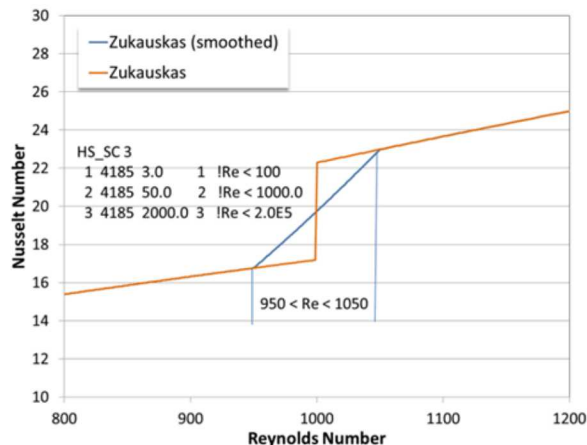
Heat transfer for external cross-flow across a tube bundle

- Aligned or staggered

Implemented as option for HS boundary condition (HS\_LB & HS\_RB IBCL=2 or ZUKAUSKAS).

Correction factor  $C_2(N_L)$  can be specified or determined from number of rows

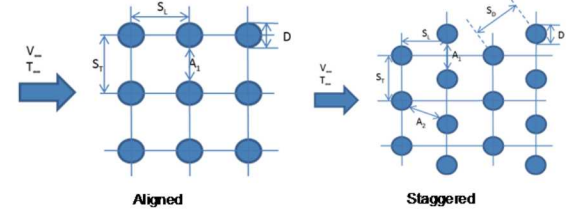
Option to smooth at discontinuities



$$Nu_D = C_2(N_L) C Re_{D,max}^m Pr^n \left( \frac{Pr}{Pr_s} \right)^{0.25}$$

Aligned:

$$V_{max} = \frac{S_T}{S_T - D} V$$



Staggered:

$$\text{if } S_D = \left[ S_L^2 + \left( \frac{S_T}{2} \right)^2 \right]^{1/2} < \frac{S_T + D}{2}$$

else

$$V_{max} = \frac{S_T}{2(S_D - D)} V$$

$$V_{max} = \frac{S_T}{S_T - D} V$$

	$Re_{D,max}$	Condition	C	m	n
Aligned	$10 < Re_{D,max} < 100$		0.8	0.4	0.36
	$100 < Re_{D,max} < 1000$	$Pr < 10$	0.51	0.5	0.37
		$Pr > 10$	0.51	0.5	0.36
	$1000 < Re_{D,max} \leq 2 \times 10^5$		0.27	0.63	0.36
	$2 \times 10^5 < Re_{D,max} \leq 2 \times 10^6$		0.021	0.84	0.36
Staggered	$10 < Re_{D,max} < 100$		0.9	0.4	0.36
	$100 < Re_{D,max} < 1000$	$Pr < 10$	0.51	0.5	0.37
		$Pr > 10$	0.51	0.5	0.36
	$1000 < Re_{D,max} \leq 2 \times 10^5$	$S_T/S_L < 2$	$0.35(S_T/S_L)^{1/5}$	0.6	0.36
		$S_T/S_L > 2$	0.4	0.6	0.36
	$2 \times 10^5 < Re_{D,max} \leq 2 \times 10^6$		0.022	0.84	0.36



# Core Catcher / Ex-Vessel Structure Model

## July 2016

New model for simulating core catcher assembly (assemblies) outside the lower head.

- Can also be used to simulate multiple lower heads or secondary pressure vessels
  - Debris relocated from lower head to core catcher via transfer process
  - Allow for multiple core catcher objects (pressure vessels) connected via transfer processes

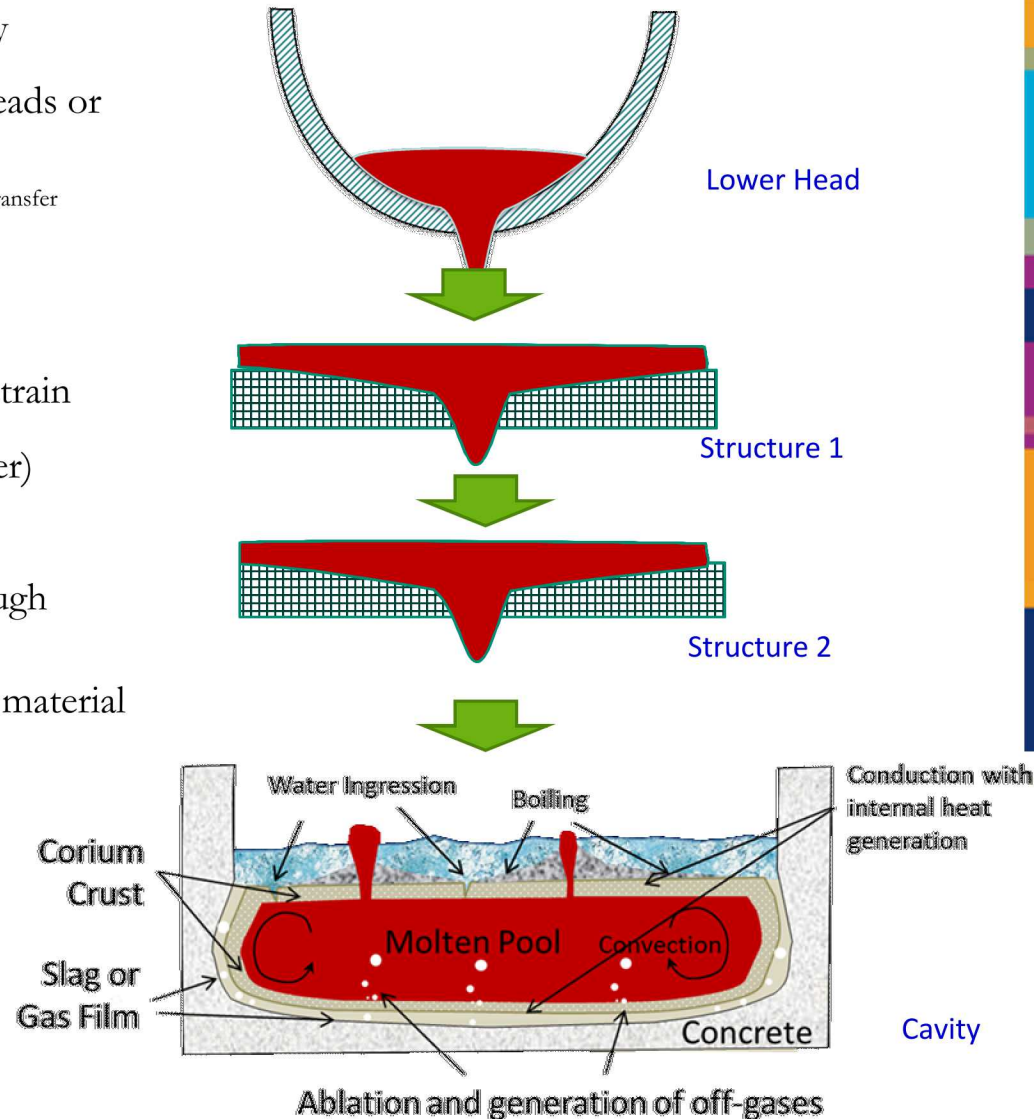
2-D core catcher nodalized through the wall

- Through-wall and transverse heat conduction
- CV volumes serve as boundary conditions
- Available volume between structures can constrain melt relocation
- Heat transfer between debris and 'upper' (inner) structure
  - Radiation
  - Possible contact
- Material composition of structure varies through mesh
  - Allows insulation or other non-structural material
- Allow for vessel structure to melt and molten material become part of molten debris.
  - Simple eutectics
- Homogeneous molten debris
- Crust between molten debris and structure
- Special features (like penetrations) modeled

Multiple failure criteria

- Failure by melt-through
- Failure by control function
- Secondary Pressure Vessel
  - Larson-Miller Creep
  - Yield Stress

Work completed in September 2015



# Multi HS Radiation Enclosure Model

## September 2016

### Previous HS radiation model

- Radiation defined only for surface pairs
- Radiation to gas performed independently for each surface
- Does not account for transmissivity of gas

### New enclosure model

- Multiple enclosure networks, each with multiple heat structures defined by the user.
- Memory dynamically allocated
- User defines all surfaces exchanging radiant heat
- Matrix of view factors connecting surfaces
- Participating gas
- Transmissivity accounts for reduction in radiation between surfaces
- Only 1 CV associated with all surfaces
- User supplies beam length (similar to COR package)

### Recent (Aug 2017) model improvements

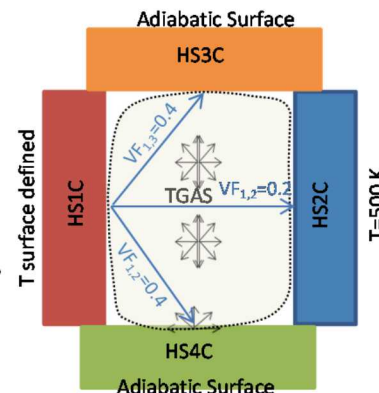
- Continuation of view factor records onto new line
- View factors can now be specified by control functions.
- Sum of view factors for a surface cannot exceed 1.0
- Radiation to pool surface
- When pool covers a participating surface on a HS, the pool surface replaces that HS surface in the enclosure network.

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

$$J_i = (1 - \epsilon_i) \cdot \sum_j^N [F_{ji} \cdot \tau_{ji} \cdot J_j] + \epsilon_i \cdot \sigma \cdot T_i^4 + \rho_i \epsilon_i E_{\text{em}}$$

$$G_i = \sum_j^N [A_j \cdot F_{ji} \cdot \tau_{ji} \cdot J_j] / A_i + \epsilon_i E_{\text{em}}$$

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



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	IT	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				

# Re-suspension Model

## September 2015

Deposited material can be re-suspended

- All sections for which the lower section boundary particle diameter is greater than a critical diameter
- Critical diameter is calculated from gas flow conditions

$$D_{\text{crit}} = \frac{4 \times 10^{-5}}{\pi \tau_{\text{wall}}} \text{ (m)},$$

$$\tau_{\text{wall}} = \frac{f \rho v^2}{2} \text{ (N/m}^2\text{)}$$

Wall shear stress

$$f = \frac{0.0791}{\text{Re}^{0.25}}$$

- Uses CV velocity
- Critical diameter can be specified by user
  - Control function
  - Constant value

By default, surfaces do not re-suspend

Wet surfaces cannot re-suspend.

- Pools and surfaces with condensed water

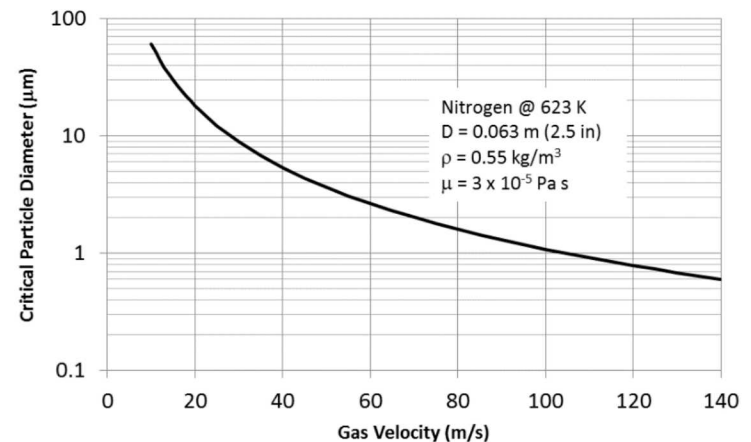
Relaxation time for resuspension

Reference

- “Liftoff Model for MELCOR,” Mike Young
- SAND2015-6119

Validation against Tests

- STORM tests (SR11 and SR12)
- Validation against LACE tests



### Examples

To fully activate resuspension, specify a value of **FractResuspend** as 1.0, and let **MELCOR** determine the critical diameter:

HS\_LBAR 1. ! Left surface

HS\_RBAR 1. ! Right surface

# High Temperature Gas Reactor February 2012+

## Reactor Components

- PBR Reactor components
- PMR Reactor Components

## Materials

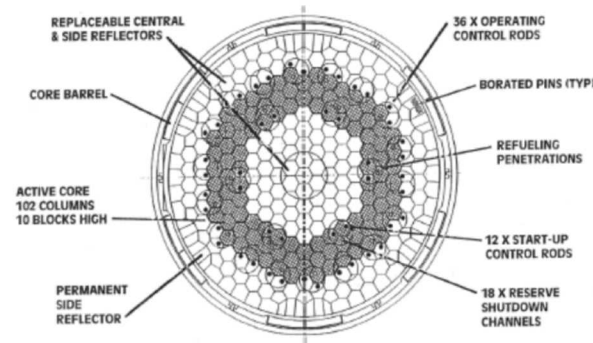
- TRISO Fuel Modeling
  - Fission product release modeling
- Helium Treatment
- Graphite modeling
  - Oxidation Models

## Graphite Dust Modeling

- Aerosol physics models
  - Turbulent Deposition
  - Resuspension

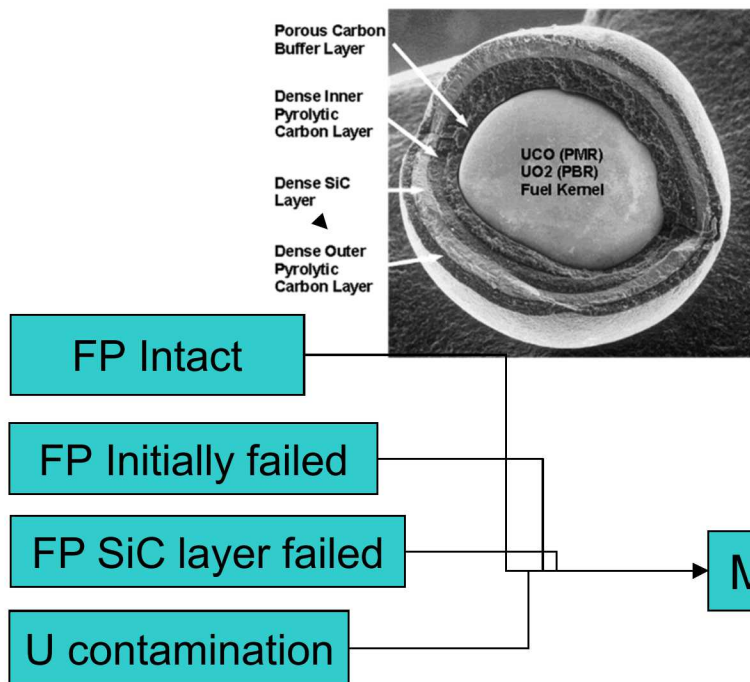
## Point Kinetics Model

Steady state initialization and  
transient solution strategy





# MELCOR FP Release Model



- TRISO particle failure
  - Intact particles: SiC layer acting as a pressure vessel and retaining fission products
  - Failed particles: Initially defective, already-failed or ineffective SiC layer
- Uranium contamination of matrix (generation of fission products outside TRISO particles)
- Diffusional release from intact and failed TRISO particles

## Particle Release

- Particles fail at different times during accident
  - Convolution integral of failure rate and release fraction

$$F_{tot}(t) = \int_0^t \frac{dF_w(\tau)}{d\tau} F_R(t - \tau) d\tau$$

$F_{tot}$  = Total release fraction  
 $F_w$  = Failure fraction  
 $F_R$  = Release fraction of particle

## Diffusional Release

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

$$D(T) = D_o e^{-Q/RT}$$

$m=2$  (spherical)

$C$  = Concentration (kmol/m<sup>3</sup>)

$\lambda$  = Decay constant (1/s)

$S$  = Source term (kmol/m<sup>3</sup>-s)

$D$  = Effective Diffusion coefficient (m<sup>2</sup>/s)

# Coolant Modeling Considerations

## Helium

- An ideal gas approach was chosen as an acceptable approximation
  - expected  $< 1\%$  error for anticipated temperature and pressure range of HTGRs

## DTDZ Model

- User specifies the flow direction to be down for HTGR application

## PBR

- Coolant friction factor is for pebble bed (default Ergun equation) when PBR model is invoked
  - Achenbach or KTA correlation should be used for HTGR
- Coolant heat transfer uses pebble bed heat transfer coefficients (user input modified KTA)

## Air Ingress scenarios

- The counter-current stratified flow model enables the user to couple two such flow paths and compute momentum exchange of the single-phase, two-component, counter-current flow as consistent with correlations of Epstein and Kenton.

# Graphite Modeling

- Oxidation of graphite by steam and air
  - The air oxidation rate is implemented as (Richards, 1987)

$$R_{OX} = 122.19 \exp\left(-\frac{20129}{T}\right) P^{0.5}$$

- The steam oxidation model is implemented as (Richards, 1988)

$$R_{OX,steam} = \frac{k_4 P_{H_2O}}{1 + k_5 P_{H_2}^{0.5} + k_6 P_{H_2O}} \quad k_i = K_i \exp\left(-\frac{E_i}{RT}\right)$$

- Maximum rates limited by gaseous diffusion to surface
- Reaction Products
  - The air reaction produces CO/CO<sub>2</sub>
  - Steam reaction produces CO and H<sub>2</sub>
  - The CO/CO<sub>2</sub> mole ratio is given as (Kim and NO, 2006)

$$f_{CO/CO_2} = 7396 e^{-69604/RT}$$

# New Aerosol Physics Models

## Turbulent deposition and deposition in bends

### Particle Diffusion Regime

- Davies equation

$$V_d^* = \frac{3\sqrt{3}}{29\pi\tau_*^{1/3}} Sc^{-2/3} \tau_*^{1/3} + K\tau_*^2$$

### Eddy Diffusion –Impaction Regime

$$V_d^* = \frac{3\sqrt{3}}{29\pi\tau_*^{1/3}} Sc^{-2/3} \tau_*^{1/3} + K\tau_*^2$$

K is determined empirically or from a Fick's law equation (Wood)

### Inertia Moderated Regime

- Deposition velocity is either constant

$$V_d^* = \sqrt{\frac{f}{2}} \quad 10 \leq \tau_* \leq 270$$

- Or may decrease with increasing dimensionless relaxation time

$$V_d^* = \frac{2.6}{\sqrt{\tau_*}} \left(1 - \frac{50}{\tau_*}\right) \quad \tau_* \geq 270$$

### PUI Model for deposition in bends

- Pui bend model
- Merrill's bend model
- McFarland's bend model

## Resuspension model

- All sections for which the lower section boundary particle diameter is greater than a critical diameter
- Critical diameter is calculated from gas flow conditions

$$D_{\text{crit}} = \frac{4 \times 10^{-5}}{\pi \tau_{\text{wall}}} \text{ (m)}, \quad \tau_{\text{wall}} = \frac{f \rho v^2}{2} \text{ (N/m}^2\text{)} \quad f = \frac{0.0791}{\text{Re}^{0.25}}$$

- Uses CV velocity
- Critical diameter can be specified by user
  - Control function
  - Constant value
- Relaxation time for resuspension
- Reference
  - "Liftoff Model for MELCOR," Mike Young
  - SAND2015-6119

### Example

To fully activate resuspension, specify a value of **FractResuspend** as 1.0, and let MELCOR determine the critical diameter:

HS\_LBAR 1. ! Left surface

HS\_RBAR 1. ! Right surface



# Point Kinetics Model

Point kinetics for operating reactor

$$\frac{dn}{dt} = \frac{\rho - \beta}{\Lambda} n + \sum_{i=1}^6 \lambda_i C_i + S_0$$

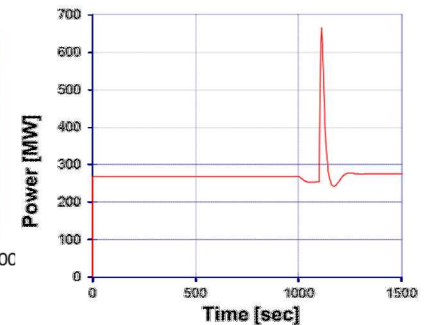
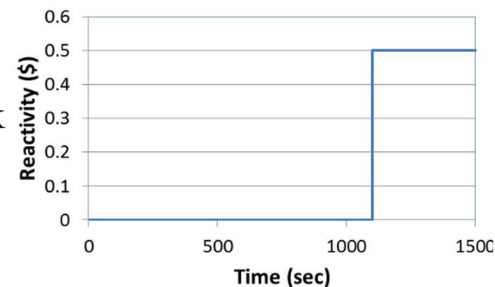
$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n - \lambda_i C_i$$

- Unconditionally stable over wide range of timesteps
  - Exponential matrix approximated with a 7<sup>th</sup> order Pade(3,3) function
- Temperature-dependent reactivity feedback from COR components
  - Fuel/Moderator/Reflector generalized weighting for spatially averaged feedback
- External reactivity insertion via control functions
  - Generalized and flexible
  - 2018 EMUG Presentation (Helman)

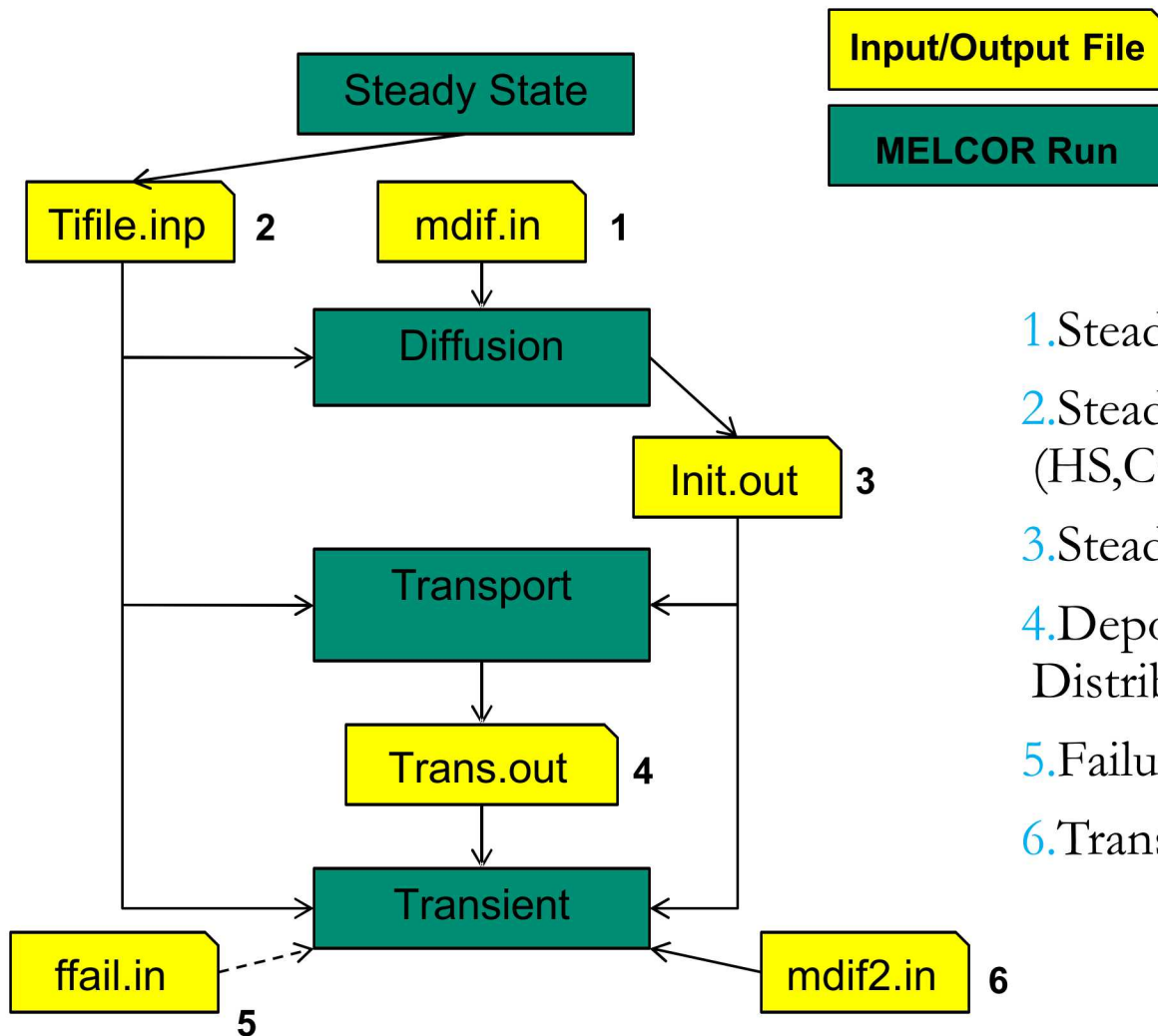
## Simple Sample Problem

- Initial power level is 268 MW
- Control Function used to insert \$0.50 reactivity step at 1100s
- Doppler feedback from fuel and moderator
- PK Model turned on at 1000 s
- Example Input:
 

```
- !          NTPCOR  RNTPCOR  ICFGAP  ICFFIS  CFNAME
- COR_TP    NO      NO      NO      NO
- ! trigger PK on at 1000s
- !          TINIT   QINIT    FUEL    MODERATOR
- COR_PKM01 1000.0  2.68e8  UO2     GRAPH
- !          EXTREACCF          NEUSRCECF
- COR_PKM02 'Reactivity'
```



# HTGR – Analysis Strategy



1. Steady State Diffusion Input
2. Steady State Temperatures (HS,COR)
3. Steady State FP Distributions
4. Deposited FP Primary Distributions
5. Failure Fraction Input
6. Transient Diffusion Input

# HTGR Input Simplified

## New in 2019 Code Release

Previously, input acquired and runs performed with a sequence of rigidly-formatted input/output files

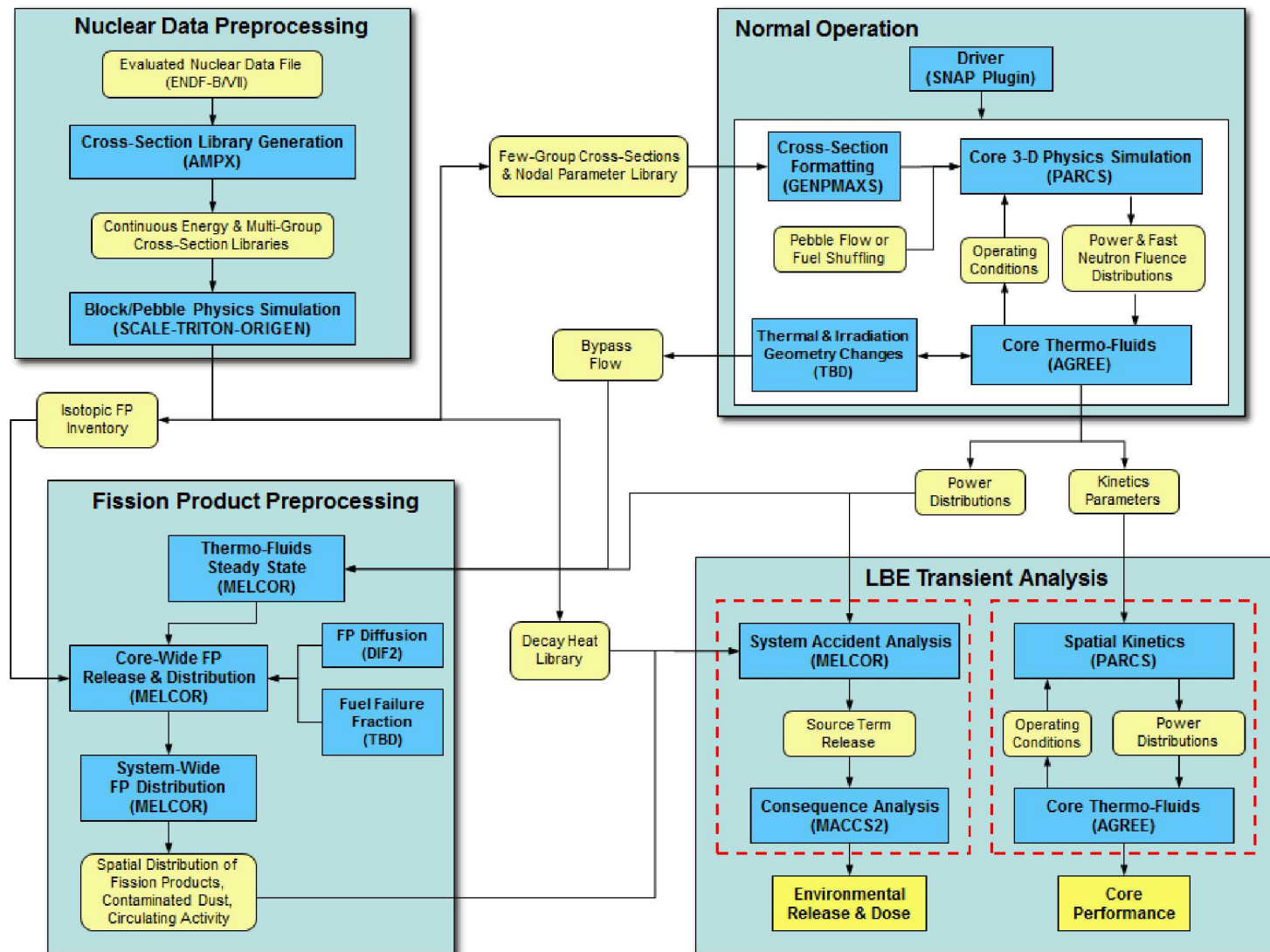
Now have “block” COR input structures to acquire “global” and “model-wise”

- COR\_DIFFGX records for global input for diffusional transport/release model
  - Burnup time, number of “models” to employ, total number of fission product species to track
  - TRISO fuel parameters (density, mass per fuel unit, particles per fuel unit, initial failed fraction, etc.)
  - Tracked fission product species molecular weights and decay constants
  - Model identifier numbers
- COR\_DIFFMX records for model-wise input for diffusional transport/release model
  - Configuration parameters for each model (intact TRISO, failed TRISO, missing SiC, matrix, etc.)
  - Computational grids
  - Diffusion coefficients by fission product species
  - Partition coefficient and/or sorption isotherm data

In a single run while marching forward in problem time, can now sequentially execute...

- Steady-state diffusion (computed in a single time-step since steady-state)
- Steady-state transport (using release as determined from steady-state diffusion)
- Transient diffusion/release
  - ...without restarts and without extra input/output files

# HTGR – Evaluation Model



\* ACRS Future Plant Designs Subcommittee, April 5, 2011



# High Temp Gas-Cooled Reactors

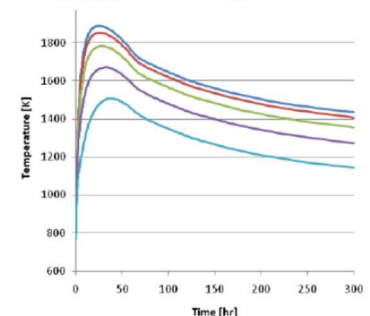
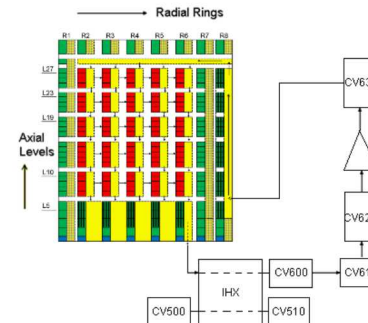
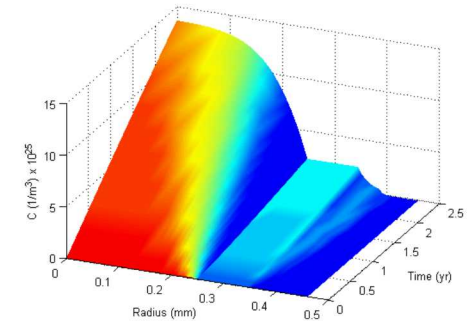
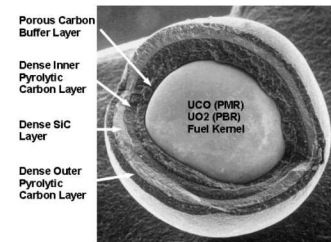
## Existing Modeling Capabilities

- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- Modified clad (CL) component (PMR/PBR)
- Core conduction
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure
- Graphite dust transport
  - Turbulent deposition, Resuspension
- Basic balance-of-plant models (Turbomachinery, Heat exchangers)
- Momentum exchange between adjacent flow paths (lock-exchange air ingress)
- Graphite oxidation
 
$$\frac{\partial C}{\partial t} = \frac{1}{r^m} \frac{\partial}{\partial r} \left( r^m D \frac{\partial C}{\partial r} \right) - \lambda C + S$$

$m=1$  (cylindrical)  
 $m=2$  (spherical)

## Existing Modeling Gaps

- New designs use  $UC_x$  fuels rather than  $UO_2$



# MELCOR/CONTAIN-LMR Implementation



Phase 1 – Implement sodium as replacement to the working fluid for a MELCOR calculation

- Implement properties & Equations Of State (EOS) from the fusion safety database
- Implement properties & EOS based on SIMMER-III

Phase 2 – Review of CONTAIN-LMR and preparation of design documents

- Detailed examination of LMR models with regards to implementation into MELCOR architecture
- Updating CONTAIN-LMR and CONTAIN2 to MELCOR development standard

Phase 3 – Implementation and Validation of:

- Implementation of CONTAIN/LMR models into CONTAIN2
- Sodium spray fires (ongoing)
- Atmospheric chemistry (ongoing)
- Sodium pool chemistry (ongoing)

Phase 4 – Implementation and Validation of:

- Condensation of sodium
- Sodium-concrete interactions (SLAM model)

# Sodium Coolant in MELCOR 2.2

## February 2016

Sodium Working fluid

- Implement Sodium Equations of State (EOS)
- Implement Sodium thermal-mechanical properties

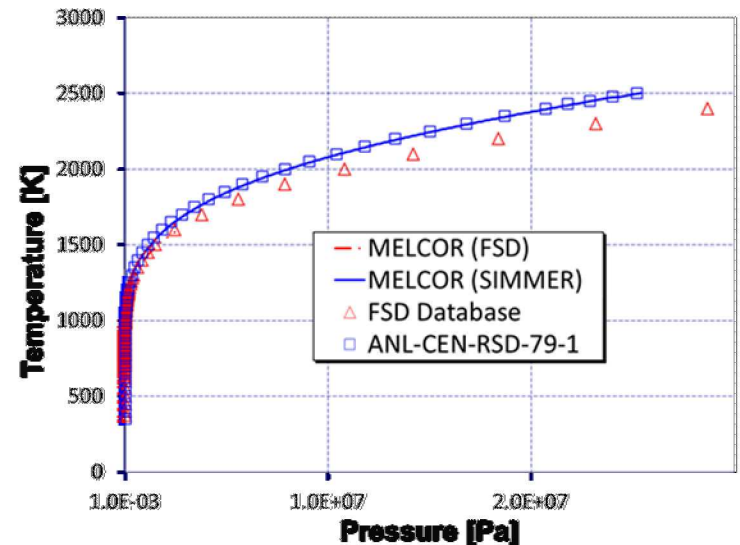
Two models implemented

- Fusion safety database (FSD) based on soft sphere EOS
  - Na (tpfna), FLiBe (tpffi), Pb-Li (tpflipb), He (tpfhe), N2(tpfn2)
- SIMMER database

Sodium properties for FSD are mainly read from an input file, so it is easy to adapt for other liquid metal fluids

Test problems have been created demonstrating model capability

Some improvement for FSD database were made last FY



# Spray Fire Chemistry

## November 2018

Based on NACOM spray model from BNL

- Input requirement: fall height, mean diameter and source
- Internal droplet size distribution (11 bins) from Nukiyama-Tanasama correlation
- Reactions considered:
  - (S1)  $2\text{Na} + \frac{1}{2}\text{O}_2 \rightarrow \text{Na}_2\text{O}$ ,
  - (S2)  $2\text{Na} + \text{O}_2 \rightarrow \text{Na}_2\text{O}_2$
- Fixed ratio of peroxide and monoxide

$$\frac{1.3478 \cdot F_{\text{Na}_2\text{O}_2}}{1.6957 - 0.3479 \cdot F_{\text{Na}_2\text{O}_2}}$$

- Predicted quantities include:
  - Mass of Na (spray, burned, pool),  $\text{O}_2$ (consumed),  $\text{Na}_2\text{O}_2 + \text{Na}_2\text{O}$ (produced)
  - Energy of reactions

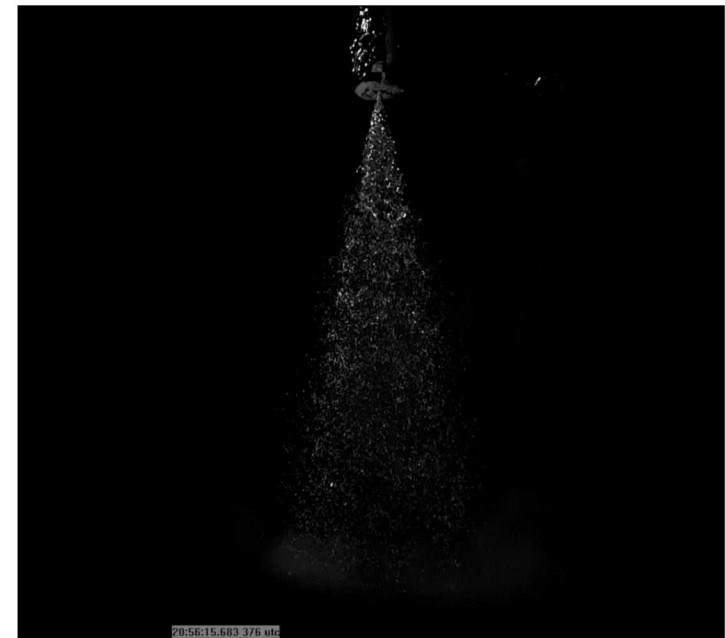
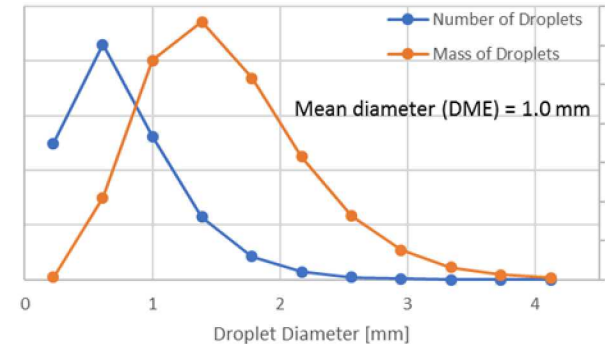
Enhancements

- Droplet acceleration model
- Pre-ignition burn rate
- Adjustment to heat of combustion to include heat of vaporization
  - $\text{Na}_2\text{O}$  from 9.18 to 13.71 MJ/kg of sodium
  - $\text{Na}_2\text{O}_2$  from 10.46 to 15.88 MJ/kg of sodium

Missing from model

- Maximum droplet size
- Radiant heat loss from droplets
- Swarm effects

Typical NACOM Droplet Size Distribution





# Pool Fire Model

## November 2018

Based on SOFIRE II code from ANL

- Reactions considered:

- $2 \text{ Na} + \text{O}_2 \rightarrow \text{Na}_2\text{O}_2$ , 10.97 MJ/kg
- $4 \text{ Na} + \text{O}_2 \rightarrow 2 \text{ Na}_2\text{O}$ , 9.05 MJ/kg
- Half of the heat produced by these reactions is assigned to the sodium pool, while the other half is assigned to atmospheric gases above the pool.

- Reactions depend on the oxygen diffusion as:

$$D = \frac{6.4315 \times 10^{-5}}{P} T^{1.823}$$

- Input requirement:

- F1 – fraction of  $\text{O}_2$  consumed for monoxide, F2 – fraction of reaction heat to pool, F3 – fraction of peroxide mass to pool, & F4 – fraction of monoxide mass to pool

Predicted quantities:

- Mass of Na(pool, burned),  $\text{O}_2$ (consumed),  $\text{Na}_2\text{O}_2 + \text{Na}_2\text{O}$ (produced)
- Energy of reactions

Model Extensions

- Radiation Heat Transfer Between Heat Structures and Pool Surface
- Heat Transfer Between Pool and Atmosphere
- CONTAIN/LMR uses film temperature for evaluating many thermodynamic properties.
- User controllable pool surface area
  - User-specified surface area (control function)



# Atmospheric Chemistry

## New in 2019 Code Release



A number of reactions have been considered:

- $\text{Na(l)} + \text{H}_2\text{O (l)} \rightarrow \text{NaOH(a)} + \frac{1}{2} \text{H}_2$
- $2 \text{Na(g, l)} + \text{H}_2\text{O (g, l)} \rightarrow \text{Na}_2\text{O(a)} + \text{H}_2$
- $2 \text{Na(g, l, a)} + \frac{1}{2} \text{O}_2 \text{ or } \text{O}_2 \rightarrow \text{Na}_2\text{O(a)} \text{ or } \text{Na}_2\text{O}_2(\text{a})$
- $\text{Na}_2\text{O}_2(\text{a}) + 2 \text{Na(g, l)} \rightarrow 2 \text{Na}_2\text{O(a)}$
- $\text{Na}_2\text{O(a)} + \text{H}_2\text{O (g, l)} \rightarrow 2 \text{NaOH(a)}$
- $\text{Na}_2\text{O}_2(\text{a}) + \text{H}_2\text{O (g, l)} \rightarrow 2 \text{NaOH(a)} + 0.5 \text{O}_2$

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)

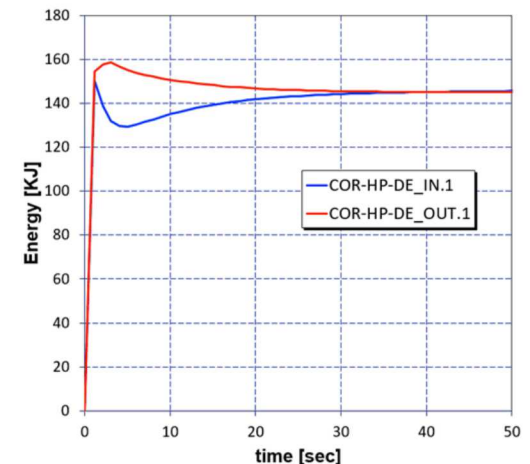
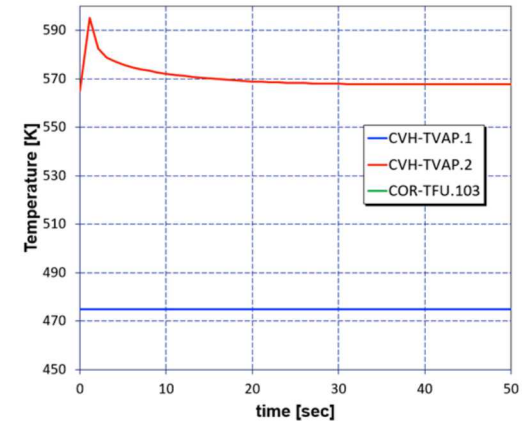
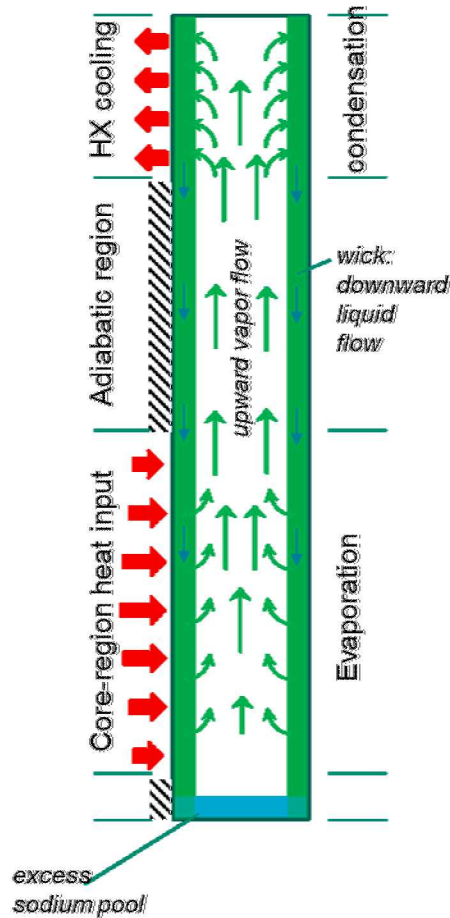
Outputs

- Reaction number, reaction energy, byproducts (Na classes,  $\text{H}_2$ ), gas and liquid consumed (Na,  $\text{H}_2\text{O}$ ,  $\text{O}_2$ )

# Heat Pipe Model New in 2019 Code Release

- MELCOR 2 model for simulation of Heat Pipes (HP) to transfer heat from the fuel to the secondary coolant flow.
- As implemented, the HP model is grouped with the COR package with interfaces to RN and CVH package.
  - COR provides a heat flux boundary condition to the evaporator region.
  - The HP model provides an energy source (from the condensor region) to CVH
  - Models of different fidelity and applicability (steady state, transient, 0D to 3D, . . .) can be written and be available for use. They would all used the same interfaces to COR and CVH.

**A Generic Heat Pipe Illustration**



# Aerosol Radiation Model

## New in 2019 Code Release

Aerosol cloud emissivity derived per Pilat and Ensor

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

Where  $C_{\lambda m}$  is the user defined parameter kmx,

- Input as part of the radiation enclosure model.
- $f_m$  is the total aerosol mass concentration ( $\text{kg}/\text{m}^3$ ) calculated by the code.

$C_{\lambda m}$  in this equation is provided to allow the user to account for the effects of wavelength, index of refraction, particle size distribution, and aerosol particle material density.

$C_{\lambda m} = 1$ , corresponds to soot-like particles with a density of  $2000 \text{ kg}/\text{m}^3$ .

M. J. Pilat and D. S. Ensor, "Plume Opacity and Particulate Mass Concentration," *Atmospheric Environment*, Vol. 4, pp. 163-173, 1970.



# Radionuclide Transfer between Pool & Atmosphere

## New in 2019 Code Release

Radionuclides condensed in a pool stay there until the pool evaporates, at which time

- Aerosols are distributed between the floor heat structures and flow-through areas

New model allows the user to specify a control function to release radionuclides in pool back into the atmosphere.

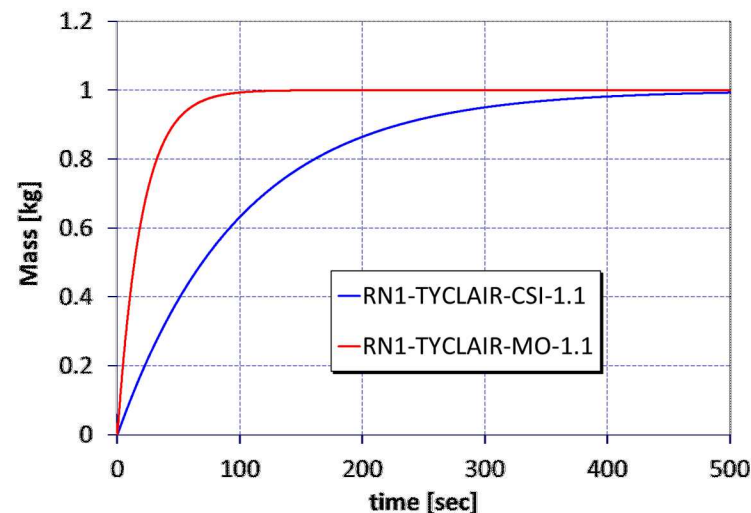
- User specifies table (for each CV) of radionuclides and CFs for calculating RN transfer

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

- $C_{RN}$  is the concentration of radionuclide, RN in volume, ICV
- CF defines the fractional transfer rate
- Aerosols placed in smallest section
  - Alternatively, user can specify section to receive aerosol

Example Input:

```
CV_RNP 2
1 CSI DECAY2
2 MO DECAY
```



Example case:

- 1 kg of CSI specified in pool at  $t=0$  sec
- 1 kg of MO specified in pool at  $t=0$  sec
- Input specifies a constant CF of  $0.01 \text{ sec}^{-1}$  for CSI
- Input specifies a constant CF of  $0.05 \text{ sec}^{-1}$  for MO
- Plot shows release to atmosphere over time.

# Sodium Fast Reactors

## Existing Modeling Capabilities

### 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 model (in development)

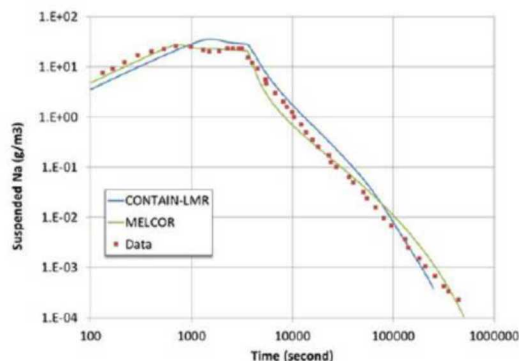


Figure 33. Suspended Na Aerosol Mass - ABI

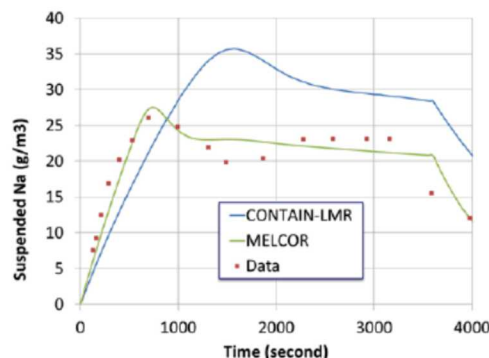


Figure 34. Suspended Na Aerosol Mass-ABI

## Existing Modeling Gaps

- SFR Core modeling
  - Fuel thermal-mechanical properties
  - Fuel fission product release
  - Fission product transport modeling
    - FP speciation & chemistry
    - Bubble transport through a sodium pool
  - Core degradation models
    - SASS4A surrogate model
- Containment Modeling
  - Capability for having more than one working fluid
  - Vaporization rates of RNs from sodium pool surface
  - Radionuclide entrainment near pool surface during fires
    - Transport of FP in sodium drops
  - Hot gas layer formation during sodium fires.
  - Oxygen entrainment into a pool fire
  - Sodium water reactions
  - Sodium aerosol aging

# Molten Salt Reactors

Properties for LiF-BeF<sub>2</sub> have been added

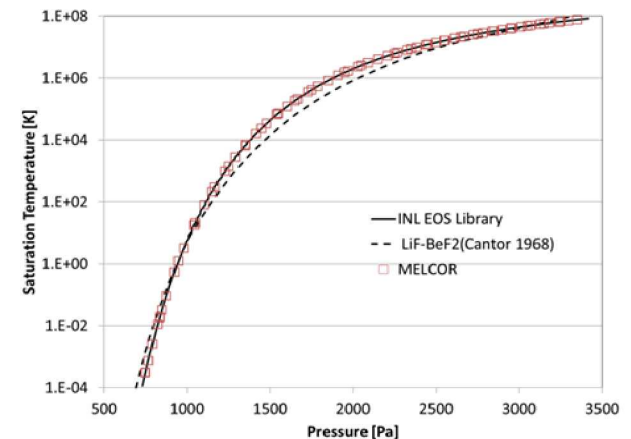
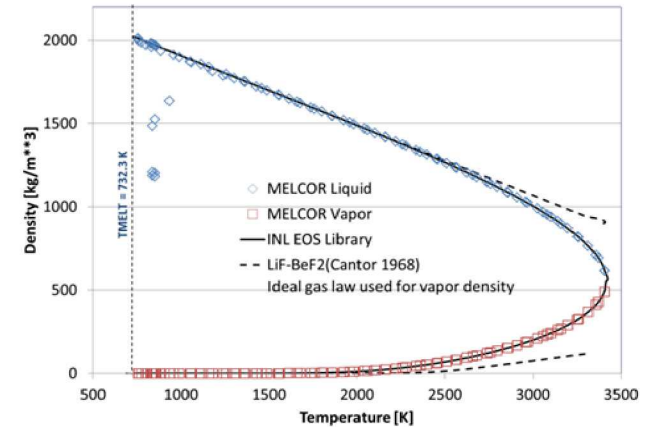
- Equation of State
  - Current capability
- Thermal-mechanical properties
  - Current capability
- EOS for other molten salt fluids would need to be developed
  - Minor modeling gap

Fission product modeling

- Fission product interaction with coolant, speciation, vaporization, and chemistry
  - Moderate modeling gap

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
  - COR package representation no longer applicable but structures can be represented by HS package
  - Calculation of neutronics kinetics for flowing fuel
    - Significant modeling gap.

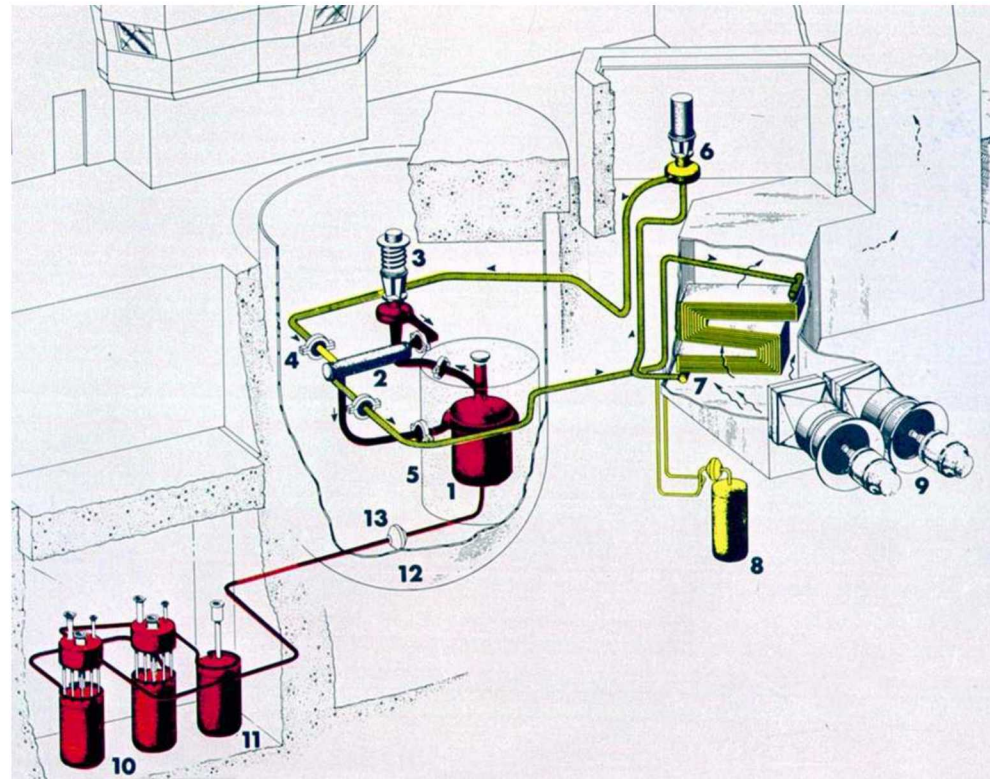




# MSRE MELCOR V2.2 Model New Benchmark 2019

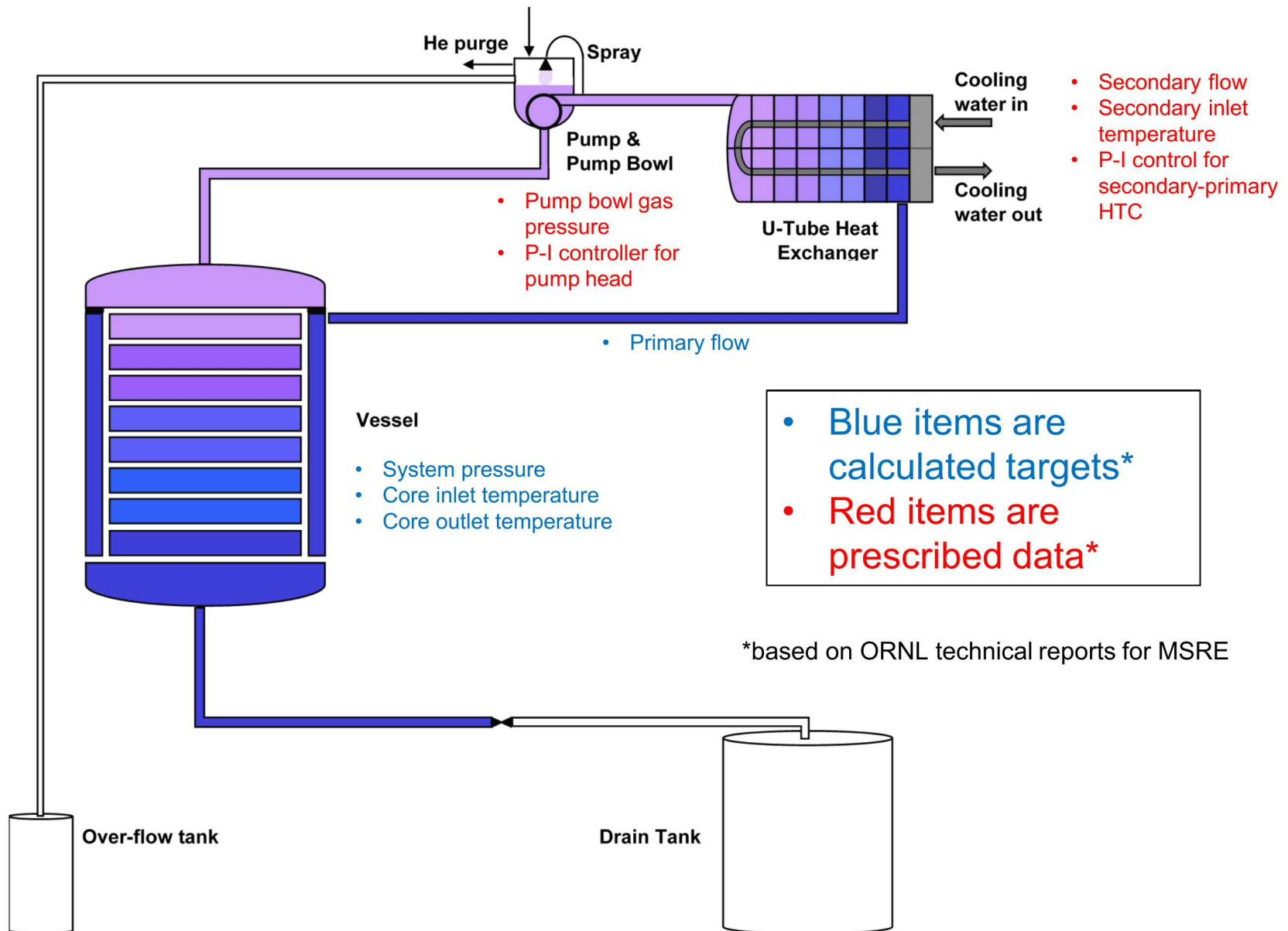
The MELCOR MSRE model includes the following features

- **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

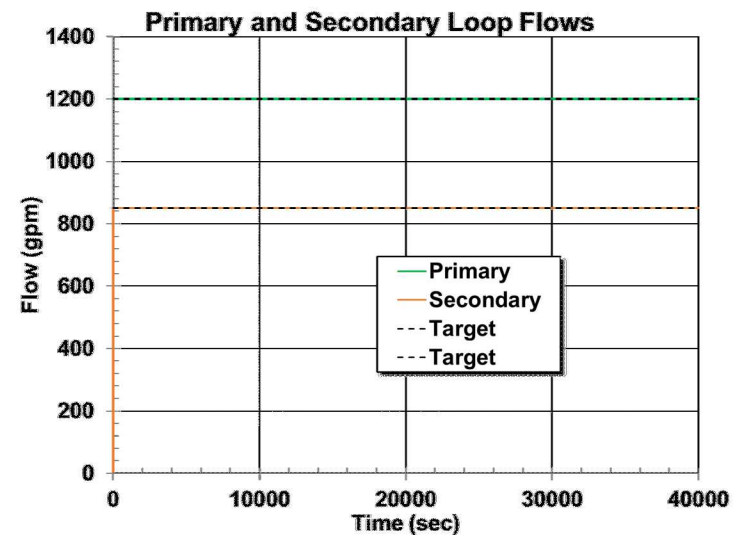
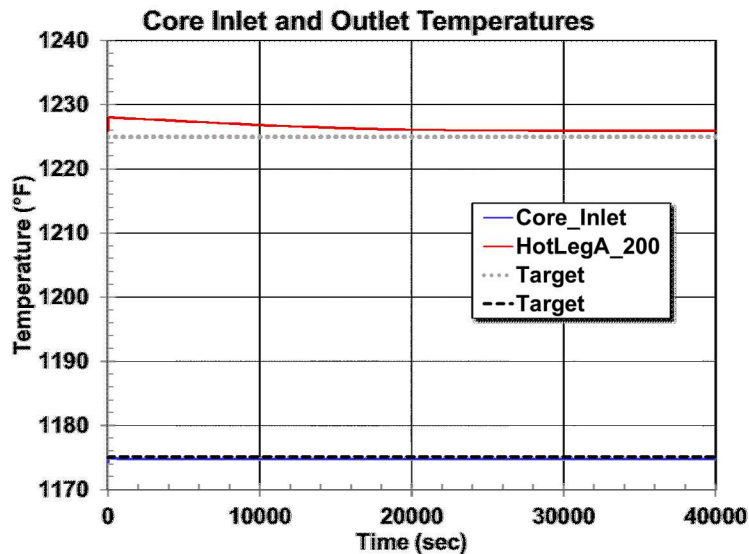
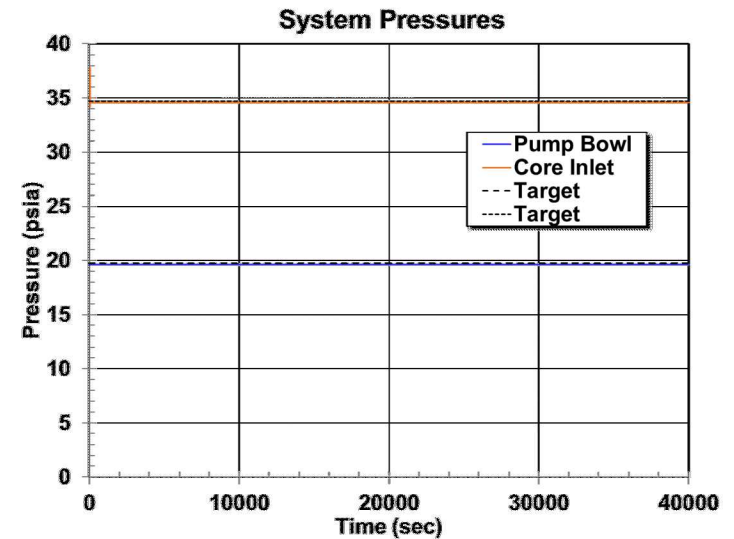
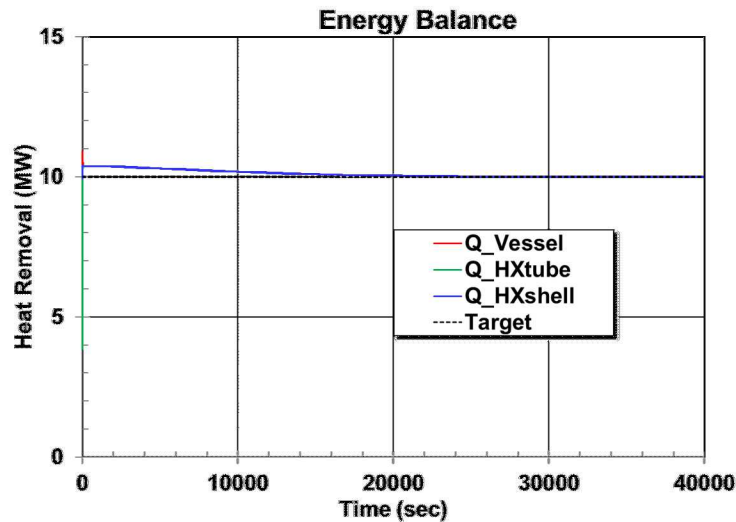




# MELCOR V2.2 MSRE Model – Operating Conditions



# MELCOR MSRE Results



# Molten Salt Road Map

## Molten Salt Properties

- Develop EOS for various salts
- Validation of properties and EOS

## Fission Product Modeling

- Interactions with coolant, speciation, vaporization, and chemistry

## Core Modeling

- Use existing capabilities in MELCOR to model advection of fission products and decay heat.
- Add models for neutronics kinetics
- Models for plate-out of salts on surfaces



# Coupling to MELCOR through control functions

## New for M2.x in 2019 Code Release



### Why would anyone need to couple to MELCOR?

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

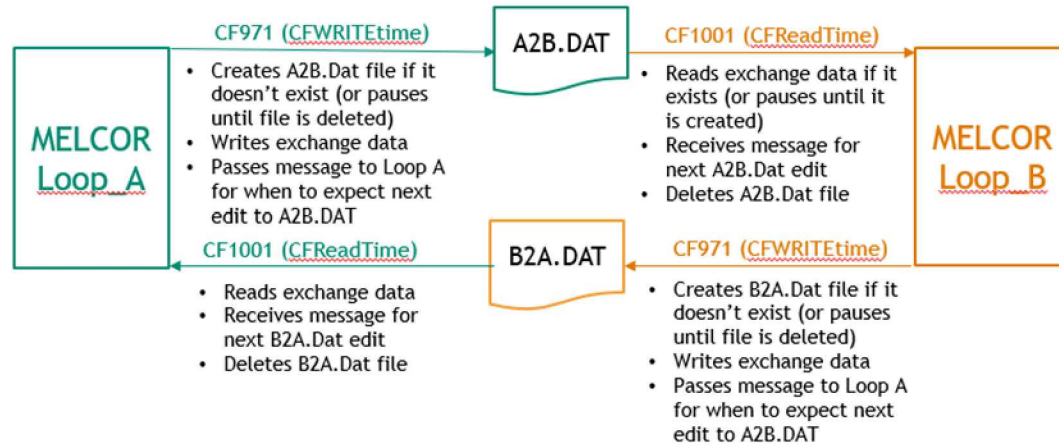
- Integrated accident analysis is necessary to capture the complex coupling between a myriad of interactive phenomenon involving movement of fission products, core materials, and safety systems.
- A calculation performed with a single, integrated code as opposed to a distributed system of codes reduces 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

However, the rare need for coupling to MELCOR may still exist

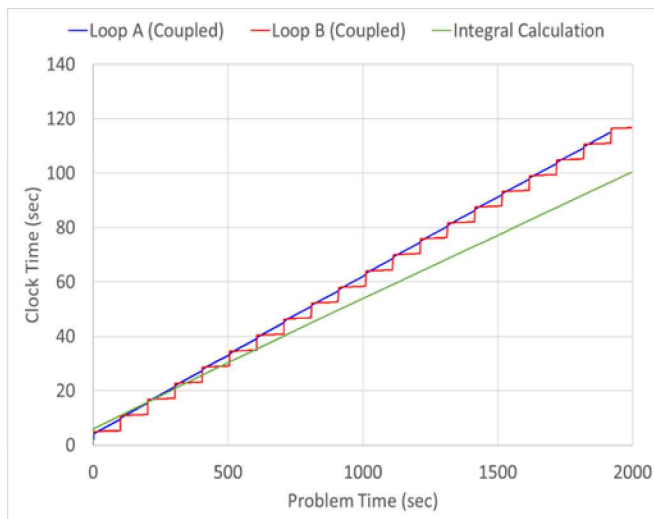
- Development of new models for possible future integration into the code
- Internal requirement for using a specific code to model a particular aspect of the source term calculation.



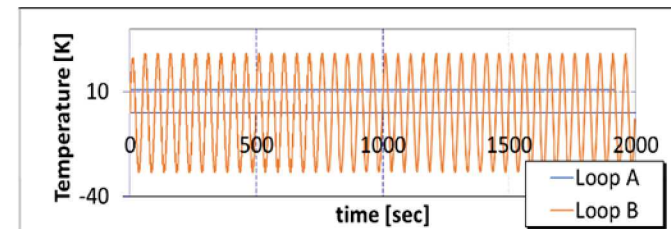
# Coupling MELCOR through Read/Write CFs



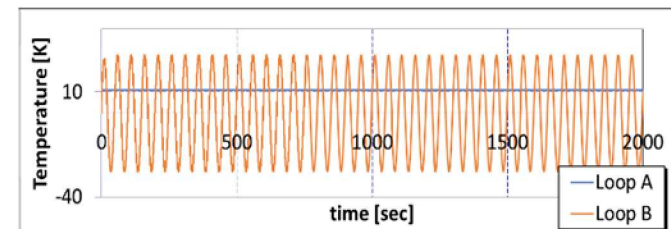
## Comparison of a coupled calculation to the analogous integral calculation



Coupled Calculation



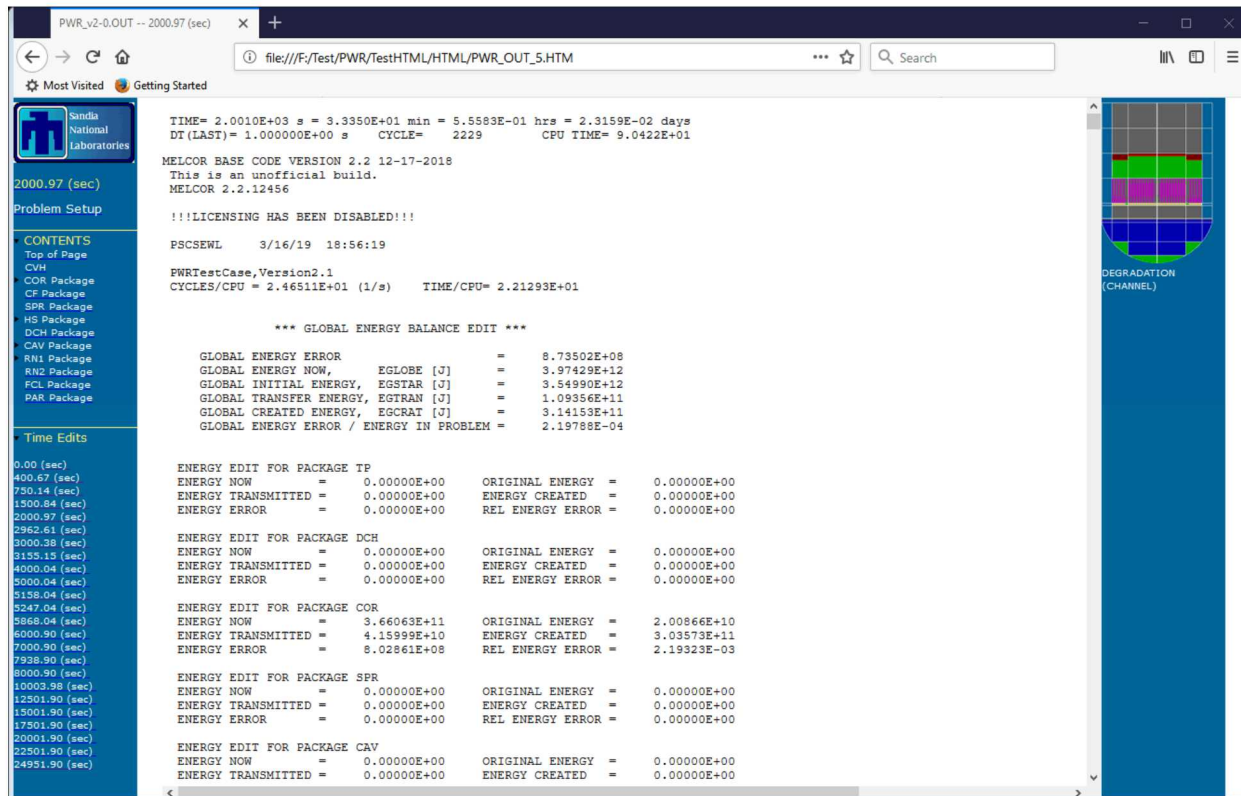
Integral Calculation



# MELCOR HTML Output Extended in MELCOR 2019 Release

HTML Output for MELCOR has been available for several years

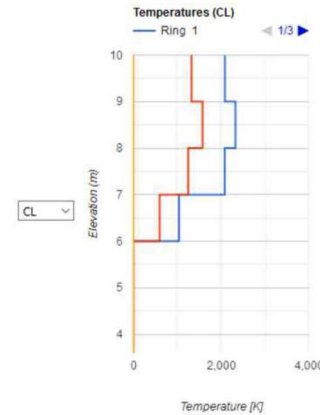
- Text output distributed among multiple files
  - File generated for each output time
  - Hyperlinks between files
  - Convenience in navigation.
- Graphical depiction of core degradation taken from PTFREAD coding several years back.
- Not often used by the general user community



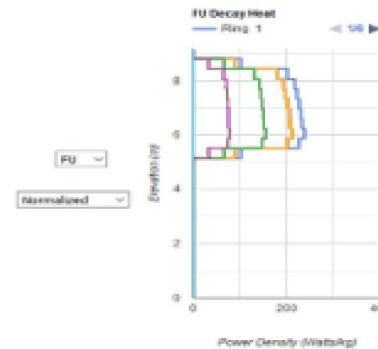
# MELCOR HTML Output

## Recent updates to HTML output

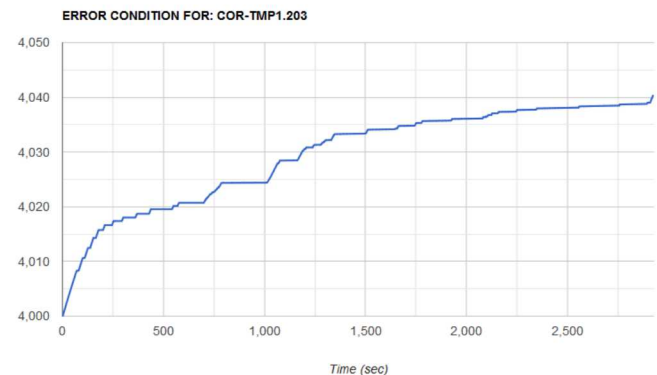
- Uses an 'included' file for time history
  - Speeds up MELCOR generation of HTML files
- Graphical depiction of output data recently added (hopefully next official code release)
  - Several data types for COR package added
    - Temperature profiles
    - Power profiles (decay, oxidation, convection, conduction, radiation)
    - Masses of materials in channel and bypass
    - Component volumes
    - Subgrid frozen volumes
  - Generation of time history plots at end of calculation (TEND or Failed State)
    - Standard plotfiles (CPU, Waterlevels, Core Damage, H2 Generation)
    - User specified plotfiles
    - Error-dependent plots
  - Some data types can be normalized by COR cell mass or volume.
  - Currently using Google Charts
    - Requires that data be exported externally for rendering
    - Investigating other options for internally rendering data (data privacy)



Elevation [m]	Ring 1	Ring 2	Ring 3
1	3.6	0	0
2	3.91	0	0
3	4.47	0	0
4	5.23	0	0
5	5.4	0	0
6	5.9	0	0
7	6	1,039.71	598.06
8	7	2,086.78	1,249.8
9	8	2,330.18	1,577.54
10	9	2,090.75	1,328.79



Elevation [m]	Ring 1	Ring 2	Ring 3	Ring 4	Ring 5	Ring 6
1	0	0	0	0	0	0
2	0.93	0	0	0	0	0
3	1.42	0	0	0	0	0
4	1.91	0	0	0	0	0
5	2.4	0	0	0	0	0
6	4.59	0	0	0	0	0
7	5.13	101.8	90.92	90.1	66.41	33.41
8	5.5	226.8	202.5	200.6	147.7	74.04
9	5.96	238.1	212.6	218.7	155.1	77.73
10	6.23	232.3	207.4	205.5	151.3	75.82
11	6.6	230.5	206.8	203.9	150.2	75.24
12	6.96	227.1	202.8	201	148	74.16
13	7.33	222.5	198.7	196.9	145	72.65
14	7.69	217.7	194.4	192.6	141.8	71.08
15	8.06	201.1	179.5	177.9	131	65.68
16	8.42	101.5	90.64	89.82	66.21	33.31
17	8.79	0	0	0	0	0



# MELCOR Dashboard Beta Release

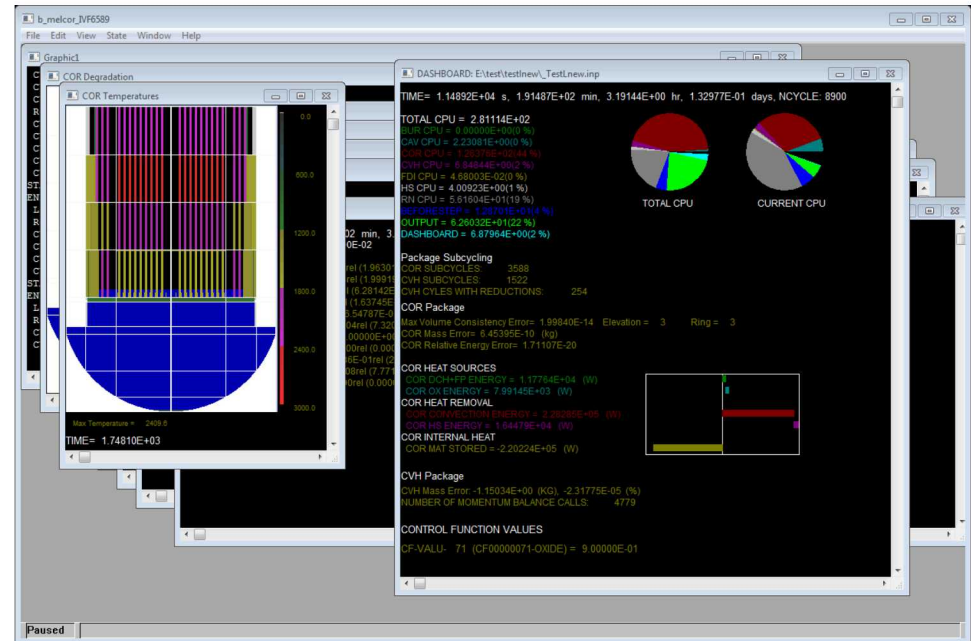
## Part of MELCOR 2019 Release



```

E:\test\testnew\b_melcor_IVF6587.exe
Records of Restart File: DEMON v2-0.RST
NCYCLE= 0 TIME= 0.0000E+00
RESTART REQUESTED FROM LAST AVAILABLE CYCLE
Restart requested from NCYCLE= -1 Read from NCYCLE= 0
RESTART REQUESTED FROM LAST AVAILABLE CYCLE
START: CREATING HTML OUTPUT FILE....
END: CREATING HTML OUTPUT FILE 1.14 (SEC)
Listing written TIME= 0.0000E+00 CYCLE= 0
/SMESAGE/ TIME= 0.0000E+00 CYCLE= 0
CA000001 - MESSAGE FROM CAVITY PACKAGE
CAVITY CAVITY GOING TO SLEEP
CYCLE= 0 T= 0.000000E+00 DT(INC)= 1.000000E+00 CPU= 0.000000E+00
CYCLE= 100 T= 9.960397E+01 DT(MAX)= 1.000000E+00 CPU= 2.839218E+00
CYCLE= 200 T= 1.996040E+02 DT(MAX)= 1.000000E+00 CPU= 4.446028E+00
Restart written TIME= 2.006040E+02 CYCLE= 201
CYCLE= 300 T= 2.996040E+02 DT(MAX)= 1.000000E+00 CPU= 6.084039E+00
CYCLE= 400 T= 3.996040E+02 DT(MAX)= 1.000000E+00 CPU= 7.612849E+00
START: CREATING HTML OUTPUT FILE....
END: CREATING HTML OUTPUT FILE 0.90 (SEC)
Listing written TIME= 4.006040E+02 CYCLE= 401
Restart written TIME= 4.006040E+02 CYCLE= 401
keyboard input sensed - enter RETURN and then complete message with second RETURN
  
```

Console Application

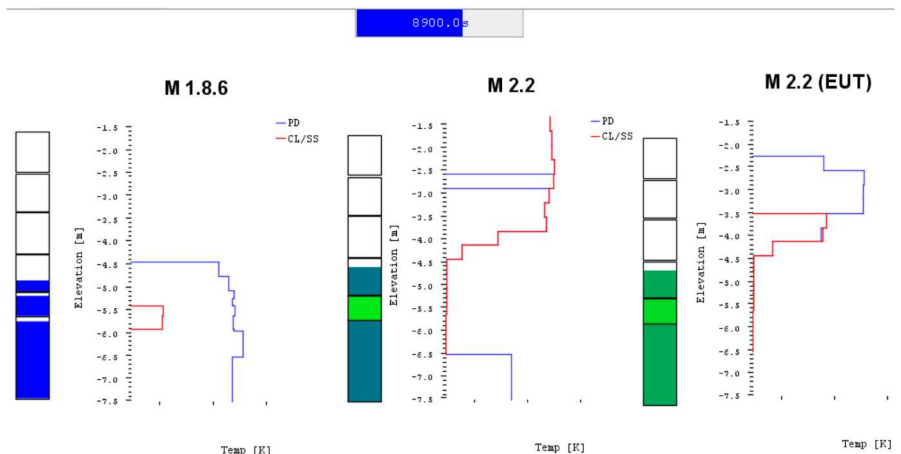
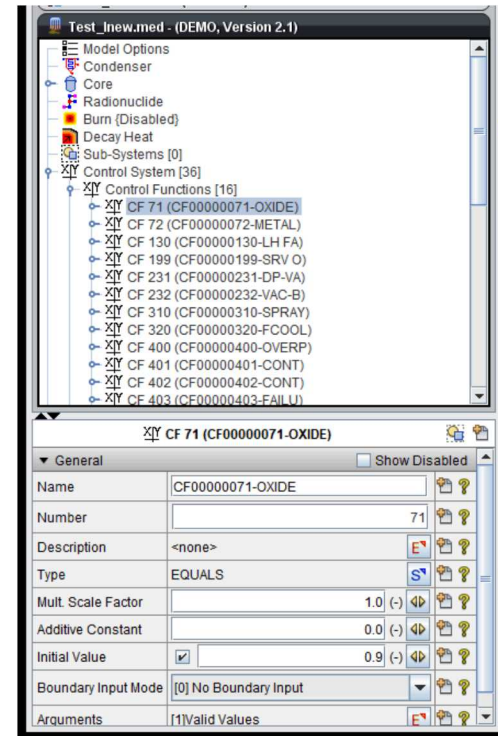


QuickWin Application

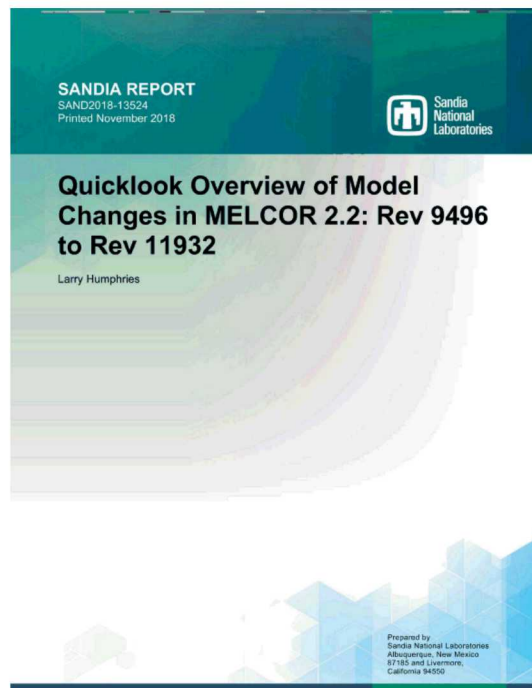


# SNAP Upgrade (Coming)

- 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?

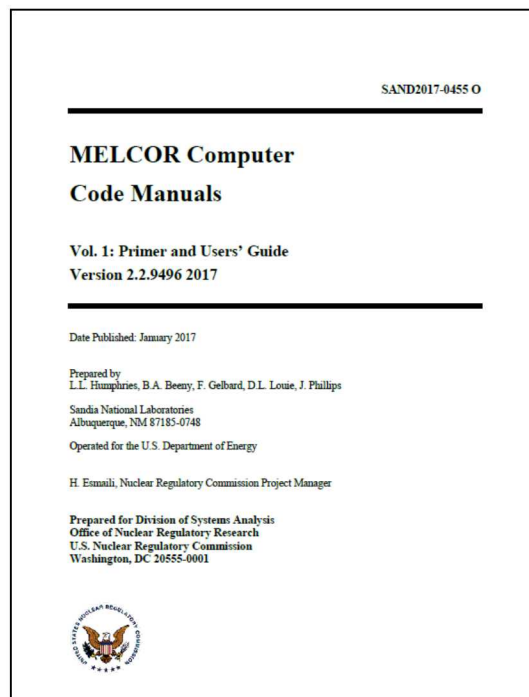


# MELCOR 2.2.11932 Code Release (November 30, 2018)



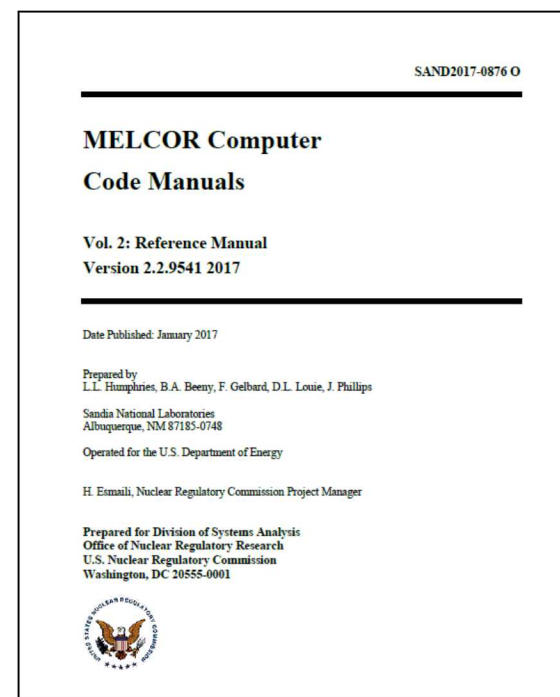
## MELCOR 2.2 Quicklook Overview of Model Changes in MELCOR 2.2

SAND2018-13524



## Volume I: User Guide

SAND2018-13559 O



## Volume II: Reference Manual

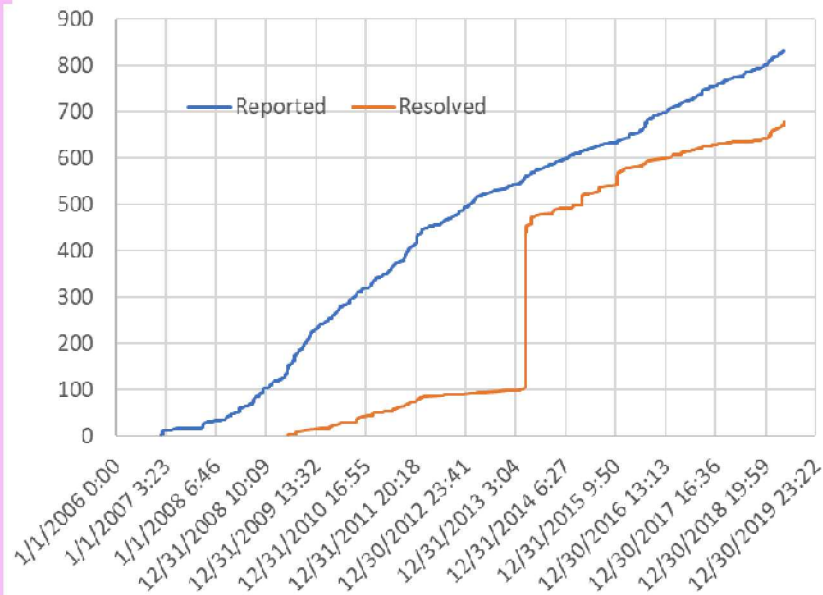
SAND2018-13560 O

New release by end of June

# MELCOR Runtime and Robustness

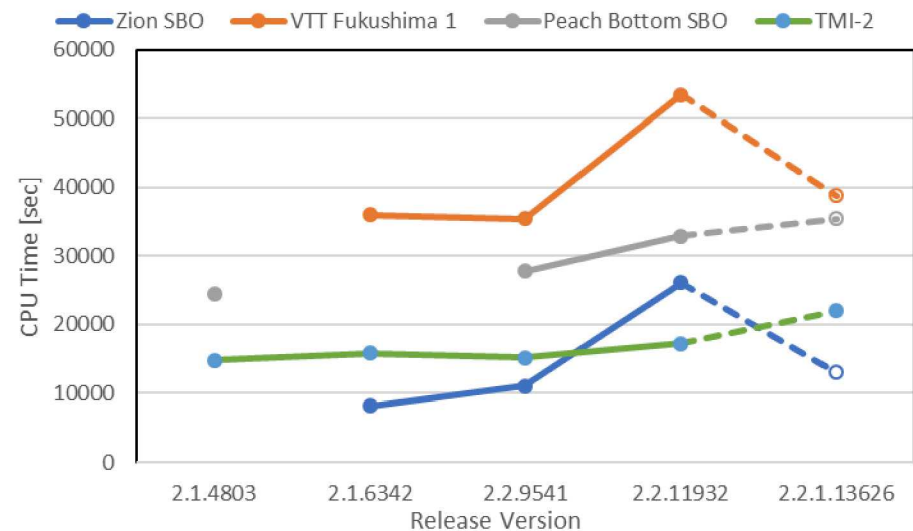
## Code Corrections & Modeling Improvements

- Corrections to reported bugs
- Model reviews
- Targeted efforts to improve code performance
  - Examination of calculations showing time step reduction scenarios.



## Code Performance Improvements

- Enabled extension of Fukushima simulation time
  - 100 hours => 500 hours



## Robustness Improvements

- 2013 (Surry UA)
  - 75% success rate
- 2015 (Peach Bottom UA)
  - 84% success rate
- 2017 (Sequoyah UA)
  - 95% success rate
- 2019 (Peach Bottom UA)
  - M2.2.13369
  - 95% success rate

# Cases in MELCOR Assessment Report - SAND2015-6693 R

## MELCOR ANALYTIC ASSESSMENT

- Saturated Liquid Depressurization
- Adiabatic Expansion of Hydrogen
- Transient Heat Flow in a Semi-Infinite Heat Slab
- Cooling of Heat Structures in a Fluid
- Radial Heat Conduction in Annular Structures
- Establishment of Flow

## MELCOR ASSESSMENTS AGAINST EXPERIMENTS

- Analysis of ABCOVE AB5 and AB6 Aerosol Experiments
- Analysis of ACE Pool Scrubbing Experiments
- Analysis of AHMED 1993 NaOH Experiments
- Analysis of the Bethsy 6.9c Experiment (ISP-38)
- Analysis of Containment System Experiment for Spray-A9 Test
- Analysis of the Cora 13 (ISP

## 31) Experiment

- Analysis of Aerosol Behavior from the Demona-B3 Experiment
- Analysis of Level Swell from the General Electric Large Vessel Blowdown and Level Swell Experiment – 5801-13
- Containment Analysis from the JAERI Spray Experiments
- Analysis of LACE LA-4 Experiment
- Analysis of LOFT LP-FP-2 Experiment
- Analysis of Critical Flow from the Marviken CFT-21 and JIT-1 Experiments
- Analysis of Marviken-V Aerosol Transport Test (ATT-4)
- Analysis of NTS Hydrogen Burn Combustion Tests
- Analysis of the Nuclear Power Engineering Corporation (NUPEC) Mixing Tests
- Analysis of the PHEBUS FPT-1 Experiment

- Analysis of the PHEBUS FPT-3 Experiment
- Analysis of the POSEIDON Integral Experiments under Hot Pool Conditions
- Analysis of STORM Aerosol Mechanical Deposition Tests
- Melt Coolability and Concrete Interaction Experiments
  - CCI-1, CCI-2, and CCI-3

## NEW ASSESSMENTS IN NEXT REVISION

- LACE LA3 (Turbulent Deposition)
- HDR-V44
- ISP-45 (QUENCH-6)
- TMI-2 Accident
- STORM (resuspension phase)
- ABCOVE AB1 and AB5 (Sodium)
- NEPTUN 5006 and 5007



# Cross-walk and Model Uncertainty

Where validation data exists,  
codes give reasonable agreement

During core degradation, codes  
diverge

- Distinct core degradation models

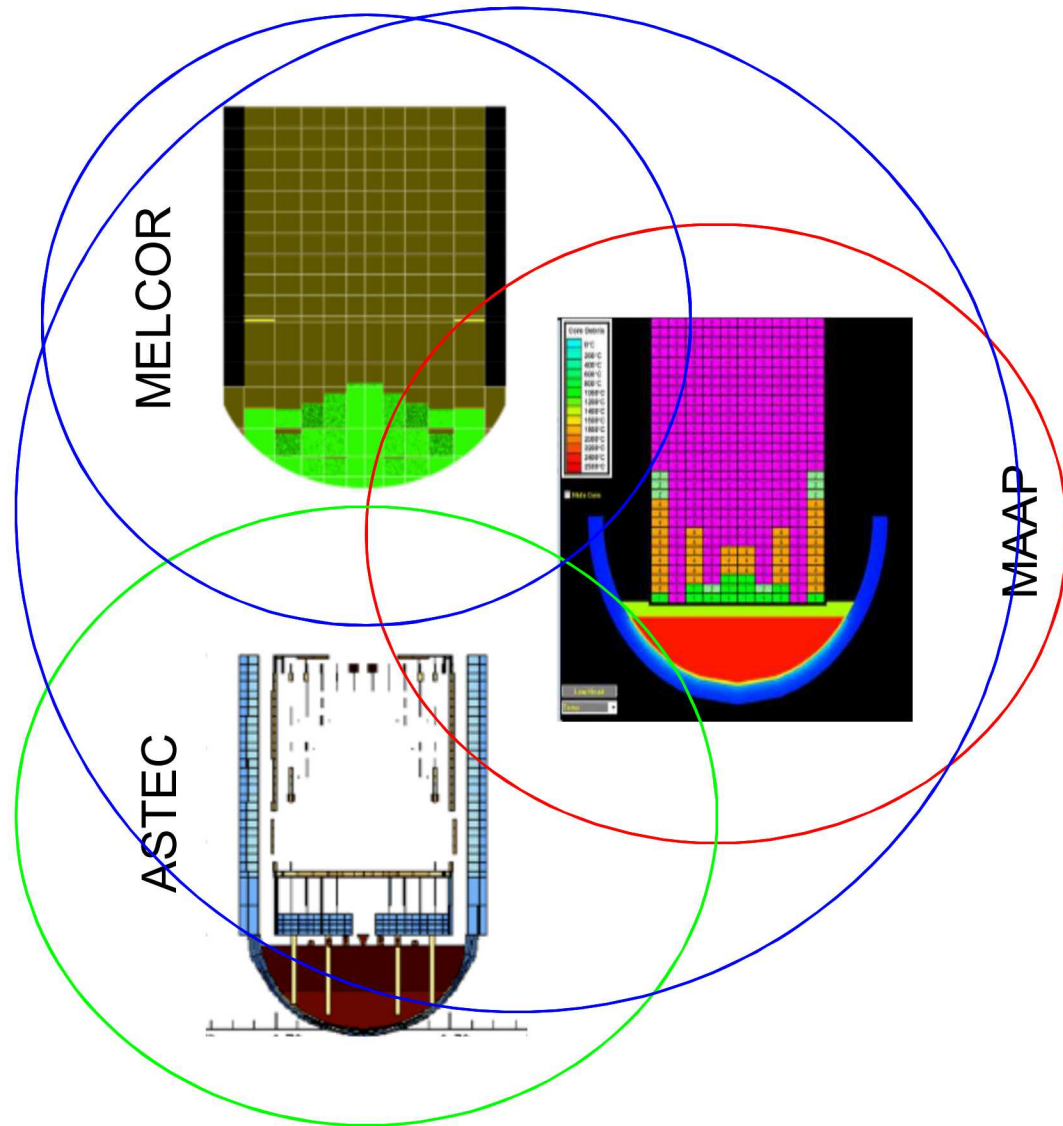
- ASTEC – Melting only
- MELCOR – minimum porosity
- MAAP – molten-pool crust

What can code development  
gain from this activity?

- Potential reduction in MELCOR uncertainty
- Uncertainty analyses capture the uncertainty of a particular code model but do not capture the uncertainty from the possible core degradation paradigms

- Extend the domain of MELCOR to capture other code model paradigms

- Extend the domain of MELCOR to capture other code model paradigms

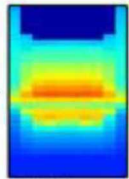
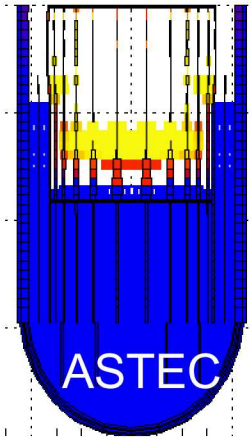


# XWALK- MELCOR (Original)



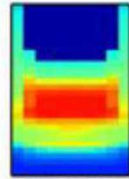
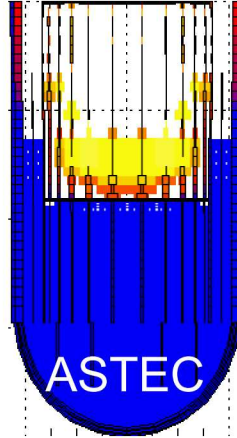
ASTEC/MAAP

4.5 hr



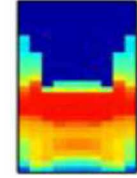
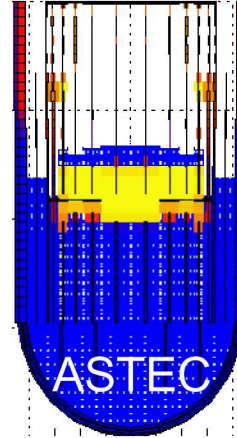
MAAP

5.5 hr



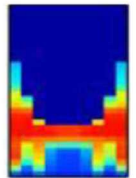
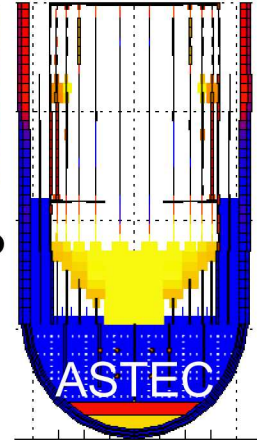
MAAP

7.0 hr



MAAP

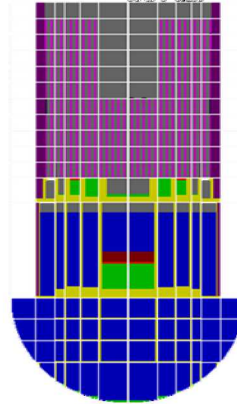
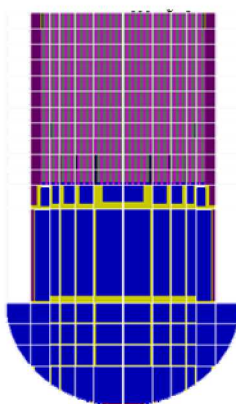
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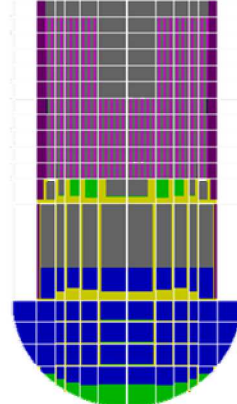
MAAP

MELCOR

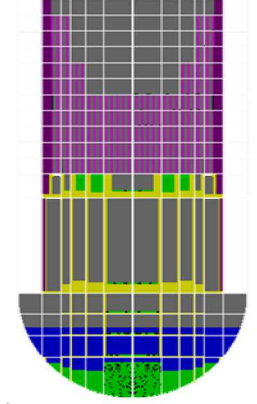
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7.0 hr



9.0 hr

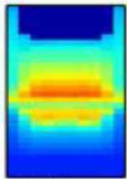
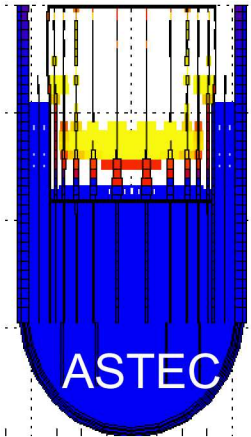


# XWALK- MELCOR (Modified)



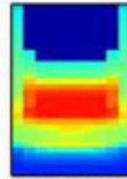
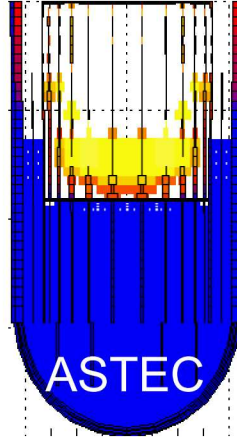
ASTEC/MAAP

4.5 hr



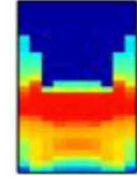
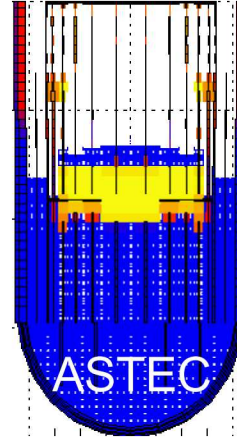
MAAP

5.5 hr



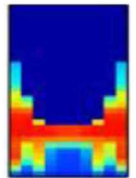
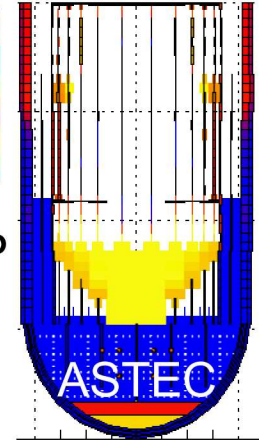
MAAP

7.0 hr



MAAP

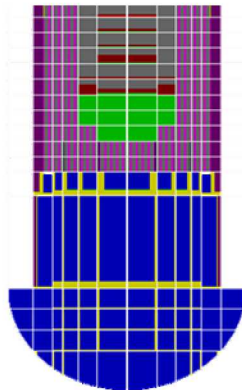
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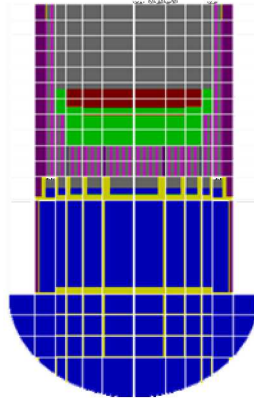
MAAP

MELCOR

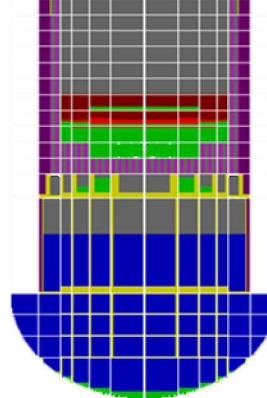
4.65 hr



5.5 hr



7.0 hr



9.3 hr

