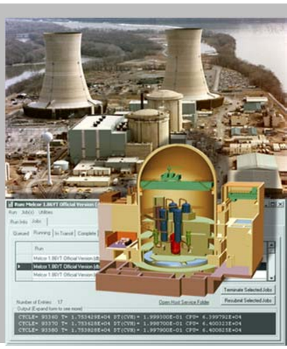
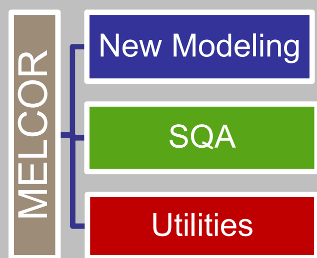
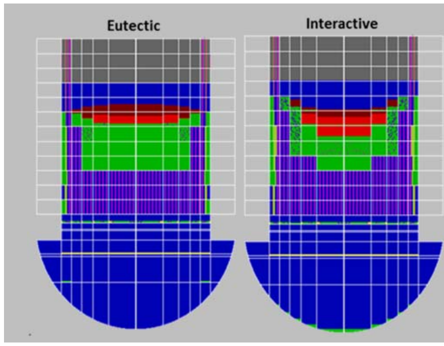






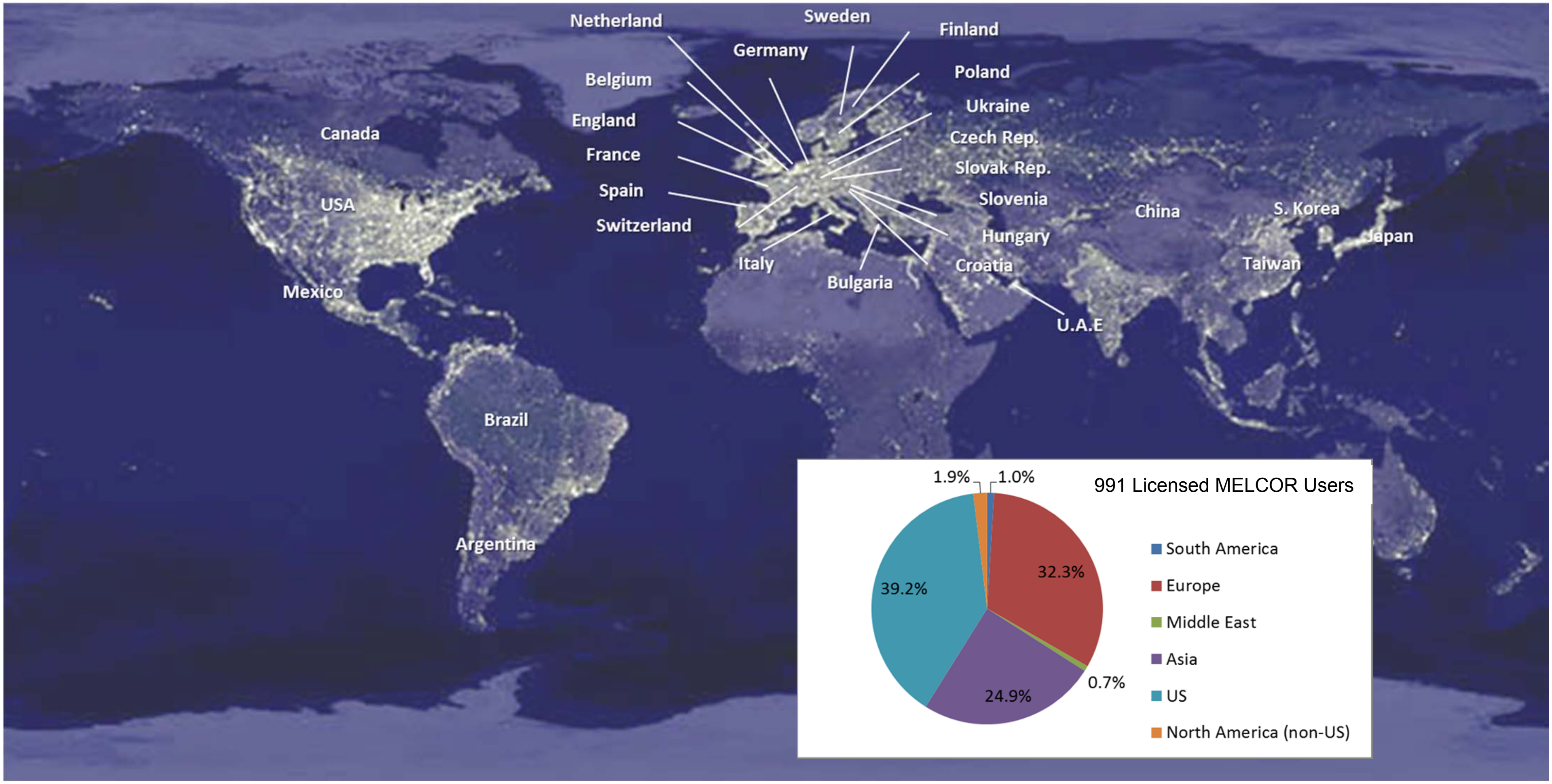
MELCOR Code Development Status
EMUG 2018

Presented by Larry Humphries

llhumph@sandia.gov

SAND2018-4219 C

International Use of MELCOR



MELCOR Workshops & Meetings

Sandia National Laboratories

- 2017 Asian MELCOR User Group (AMUG)
  - Hosted by KAERI (S Korea)
  - November 6– 8, 2017 (tentative)
  - MELCOR/MACCS Topics
- 2018 European MELCOR User Group (EMUG)
  - Hosted by University of Zagreb
  - Workshop on RN Package (April 25)
  - April 26-27, 2017
- 2018 CSARP/MCAP/MELCOR Workshop
  - CSARP (June 5-7), MCAP (June 7-8), Workshop (June 11-15)
  - Rockville, MD
  - General MELCOR workshop with some focused topics
- 2018 Asian MELCOR User Group (AMUG)
  - Hosted by CRIEPI (Japan)
  - August 2018
  - MELCOR/MACCS Topics

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
  - Improvement of runtime (for 100 hours) Rev. 5864 ➔ Now
    - 1F1 – 4 day calc. = 4 day CPU ➔ 500 hours calc. = 50 hours CPU
    - 1F3 - 4 day calc. = 8 days CPU ➔ 500 hours calc. = ~150 hours CPU
  - Enabled extension of Fukushima simulation time
    - 100 hours => 500 hours
- Robustness Improvements
  - 2013 – 75% success rate
  - 2015 - 84% success rate
  - 2017 (Recent Sequoyah UA) – 95% success rate

MELCOR
New Modeling
SQA
Utilities

2018 Workshop Agenda (CSARP)

- Monday (MELCOR overview, Primer, SNAP, MELCOR I/O)
- Tuesday (CVH/FL, Data & Control, Containment, Heat Structures)
- Wednesday (HS, Vapor & Aerosols, COR, CAV/RN)
- Thursday (Validation, SFP, HTGR)
- Friday
  - Sodium Models
  - Lower Head modeling
  - Eutectics models
  - Modeling filters and using MACCS flow paths
  - Activity models
  - RN ESF Models

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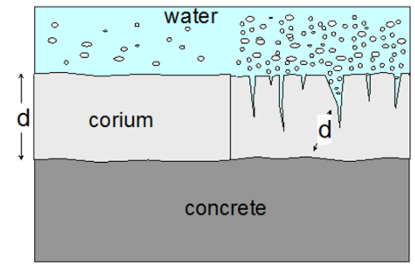
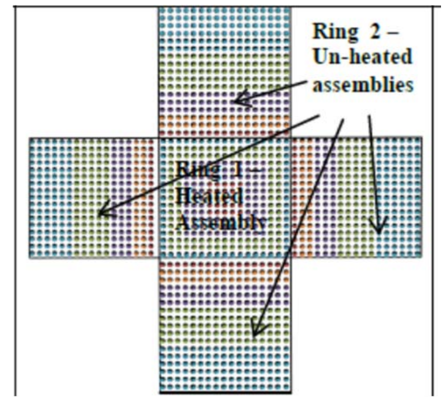
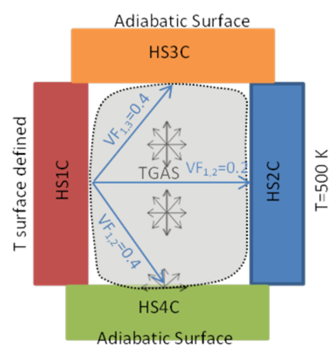
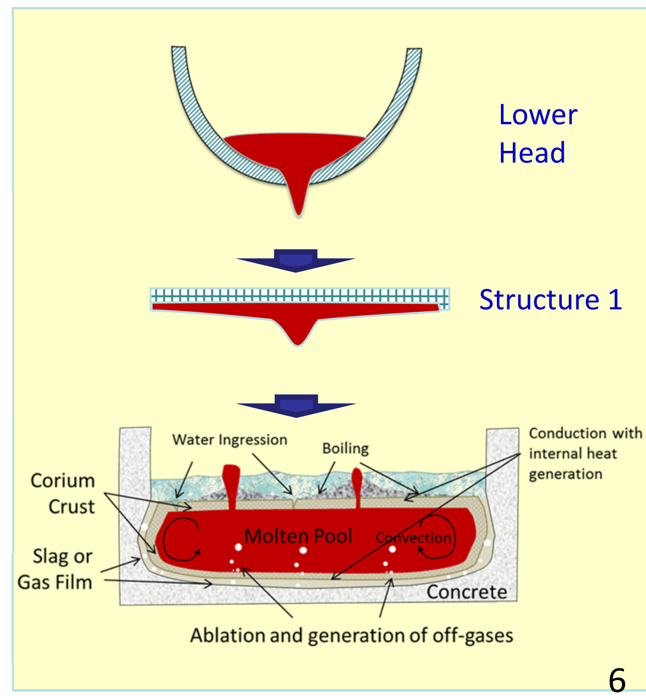
New Model Development Tasks (2014-2017)

- Completed
  - Fuel Rod Collapse Model (NRC)
  - Homologous pump model (NRC)
  - Multi-HS radiation enclosure model
  - Aerosol re-suspension model
  - Zukauskas heat transfer coefficient (external cross-flow across a tube bundle)
  - Core Catcher (multiple containment vessels)
  - Multiple fuel rod types in a COR cell (NRC)
  - Generalized Fission Product Release Model
  - New debris cooling models added to CAV package (NRC)
    - Water-ingression
    - Melt eruption through crust
  - Spreading model implemented into CAV package (NRC)
  - Eutectics Model (NRC)
  - RCIC Terry Turbine model (NRC)
  - Miscellaneous models and code improvements (NRC)
    - LAG CF
    - MACCS Multi-Ring Release
    - Valve Flow Coefficient
    - Non-dimensional parameters
- In Progress or future
  - Vectorized Control Functions (NRC)
  - CONTAIN/LMR models for liquid metal reactors
  - CVH/FL Numerics (NRC)

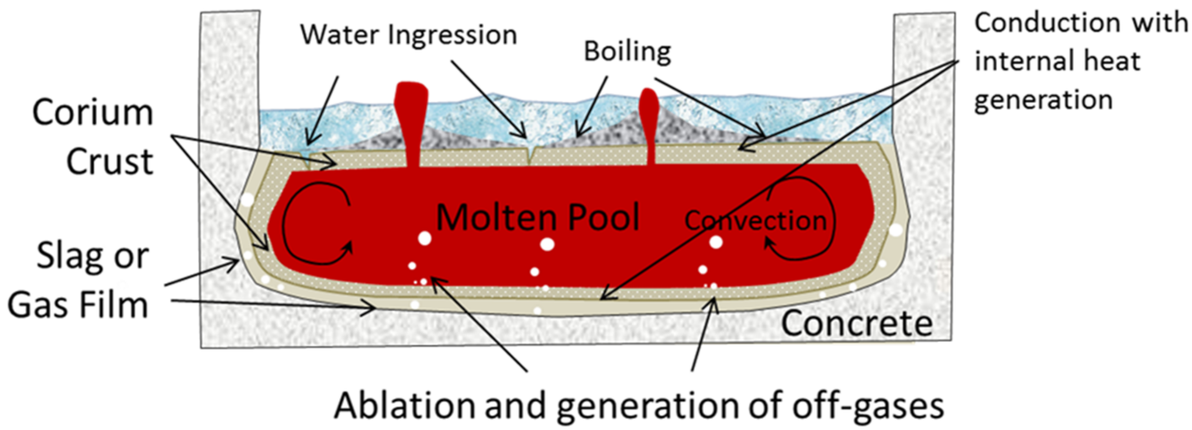








New Modeling for Top-Quenched Debris in Cavity



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

MELCOR | New Modeling | SQA | Utilities

Pre 2015 MELCOR Best Practice

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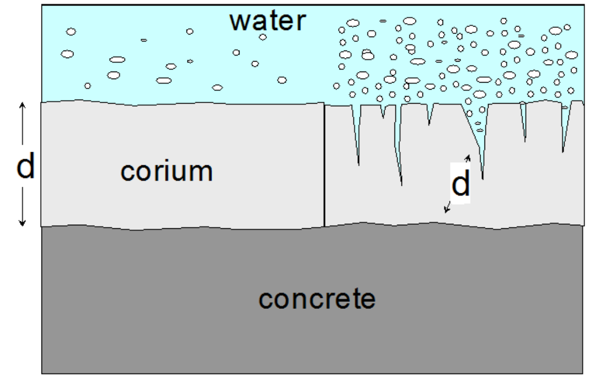
- Water ingression will increase the contact surface area between water and the corium
- Decrease the conduction path length through the corium, both of which will enhance the heat transfer through the crust



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

- 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 ingression and melt eruptions
  - New porous layer for debris relocating above crust
  - New porous crust layer
  - Dense crust layer

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CORCON/CORQUENCH Model

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Still current best practice

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

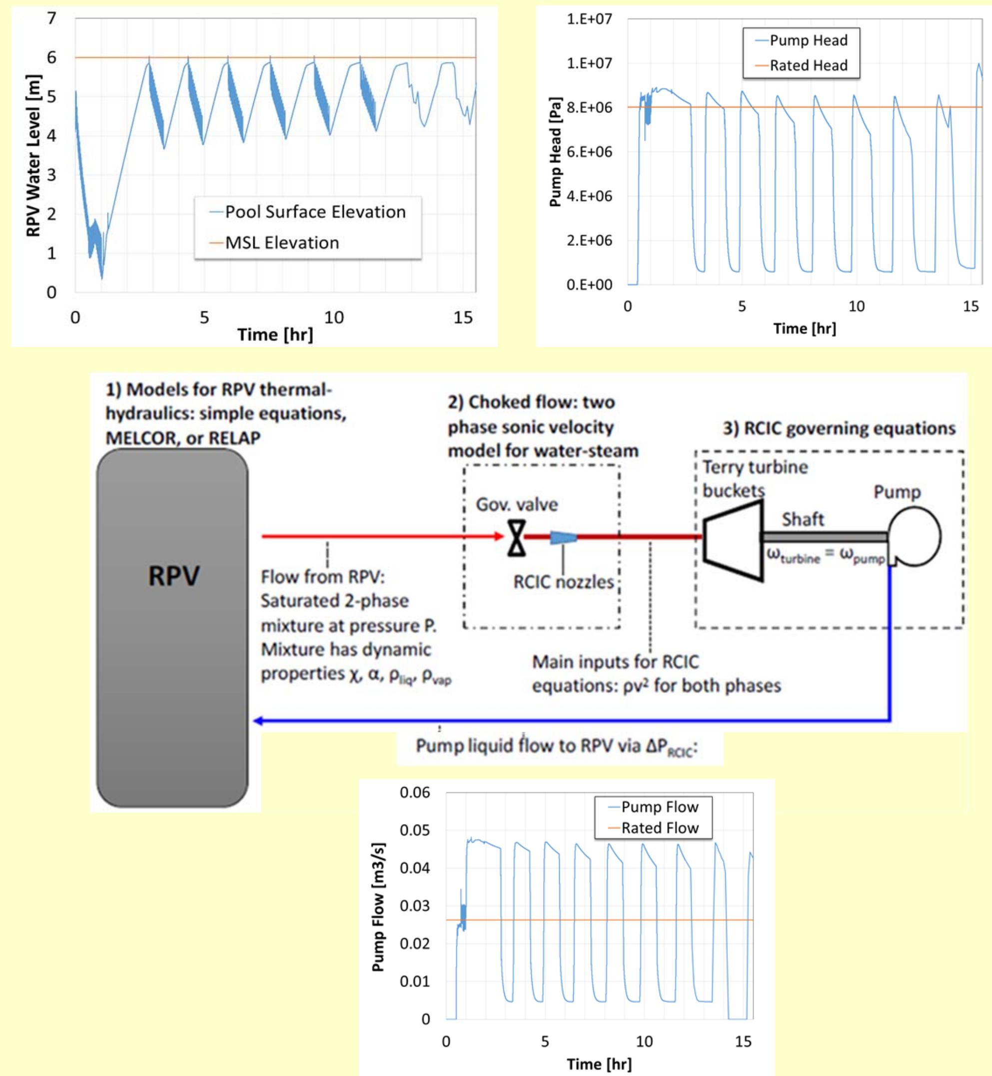
9 WATINGR ON

10 ERUPT ON

MELCOR Terry Turbine Model(s) Overview

- 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.



Helical SG HTC in MELCOR 2.2

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.

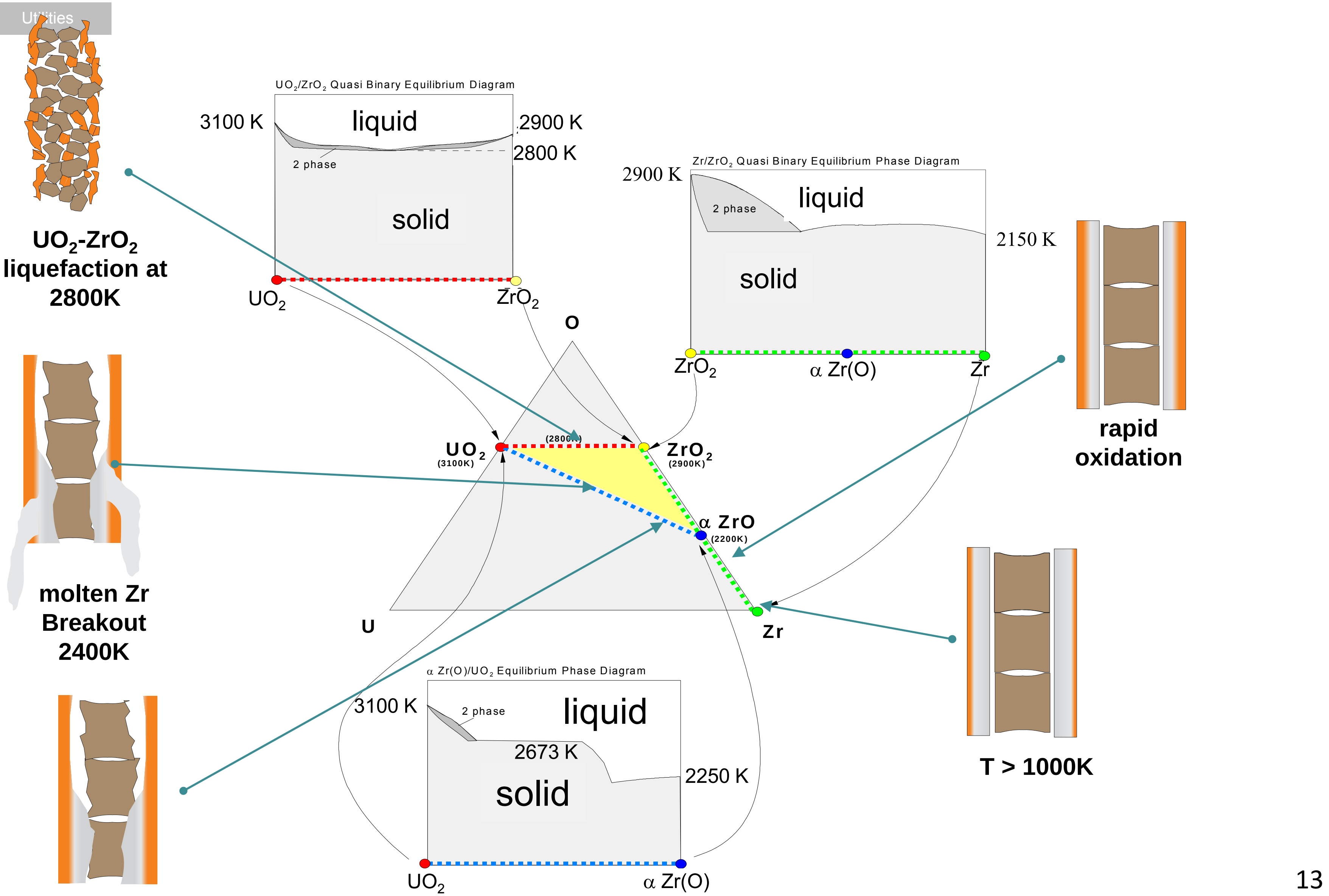
$$h = \frac{1}{26.2}\left(\frac{k}{d_i}\right)\frac{Pr}{(Pr^{2/3}-0.074)}Re^{4/5}\left(\frac{d_i}{D_c}\right)^{1/10}\left[1+\frac{0.098}{\{Re(^{d_i}/_{D_c})^2\}^{0.2}}\right] \quad \cdots \text{ Eq. (9)}$$

Sensitivity Coefficients added for the user to adjust code calculation

MELCOR Eutectic Model Overview

- Eutectics model has been in the code since M1.8.2
  - Eutectic model was not functioning since at least M1.8.5
    - UO2-INT and ZRO2-INT have been used to reduce melt temperature and modify enthalpy curves as an alternate approach
      - Applied globally to intact and conglomerate fields
    - Effective melt temperature was user specified with no default.
- Recent work was done to revive eutectic model.
  - Only applies to conglomerate
    - Liquefaction of solids in contact using calculated rates
  - Two candling routines were used depending on whether eutectics active
    - Routines were recently unified
  - Numerous calls to mixture enthalpy routines were reviewed and corrected.
  - Eutectics model undergoing beta testing
    - Passes all mass energy conservation tests
    - Validation testing with TMI & X-walk

U/Zr/O Ternary Phase Diagrams



MELCOR Eutectic Temperature

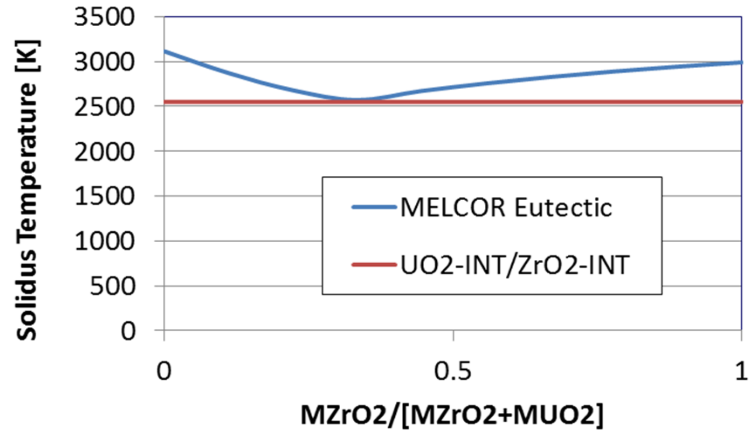
UO2-INT/ZRO2-INT

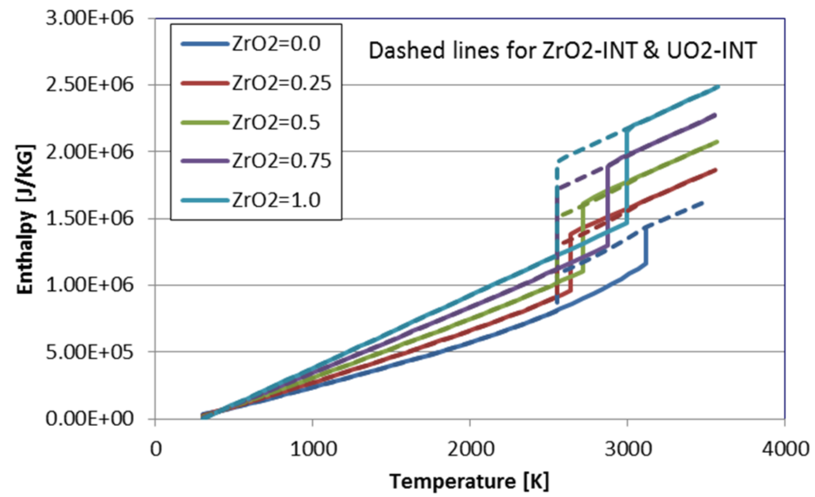
- Melt temperature for UO2 & ZrO2 is the same for intact materials as it is for conglomerate.
- Does not depend on composition

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





Eutectic Model Input

- New Input for the Eutectic model

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

COR_EUT 0 enables the model w/o additional records & uses defaults

PairMelt can be one of the following:

ZR/SS (or 1), ZR/INC (or 2), UO2/ZRO2 (or 3)

TM is the Solidus temperature for the eutectic pair

F1 is the molar ratio of the first member in the pair at the eutectic temperature

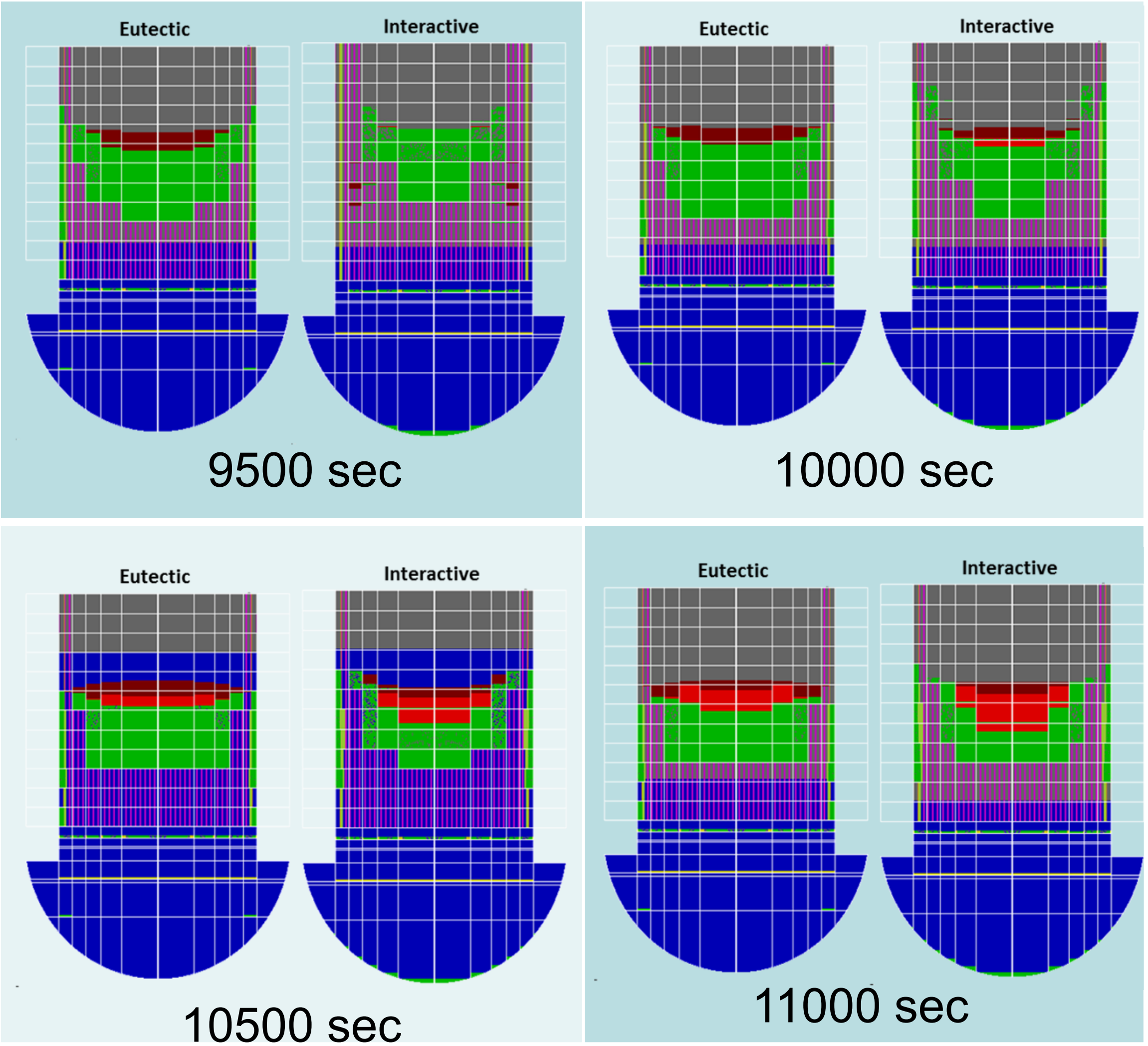
- Obsolete input for activating eutectic model
  - COR_MS IEUMOD
    - Message will indicate new input method.
      - ERROR: The Eutectics model is enabled on COR_EUT
- Interactive materials should not be used along with the eutectic model

```
MP_INPUT
      MP_ID 'ZRO2-INT'
            MP_PRC 5600.0 2502.0 707000.0 ! density, melt temp, latent heat
      MP_ID 'UO2-INT'
            MP_PRC 10960.0 2502.0 274000.0! density, melt temp, latent heat
COR_INPUT
      COR_MAT 2  !      CORMAT      MATNAM
            1      UO2      'UO2-INT'
            2      ZRO2     'ZRO2-INT'
```

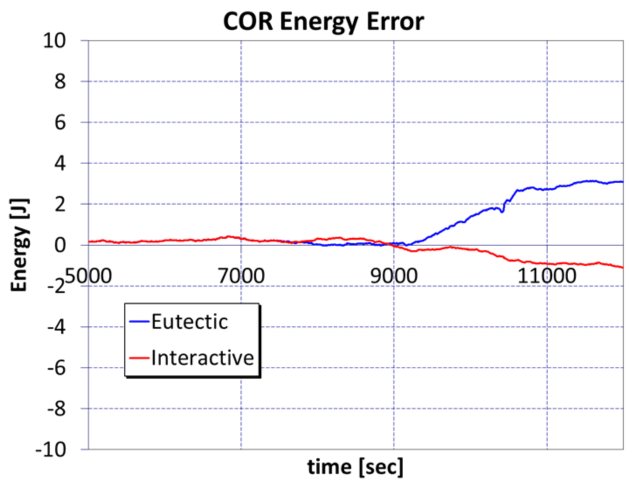
These records should be removed from input

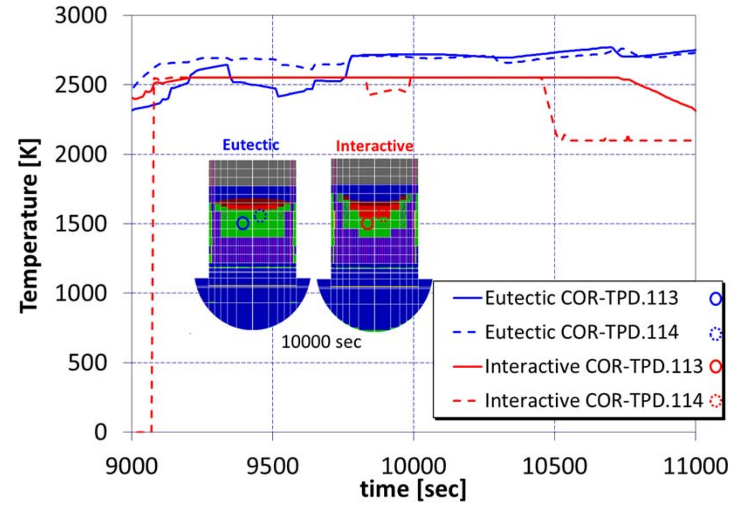
TMI Melt Progression – Preliminary Results

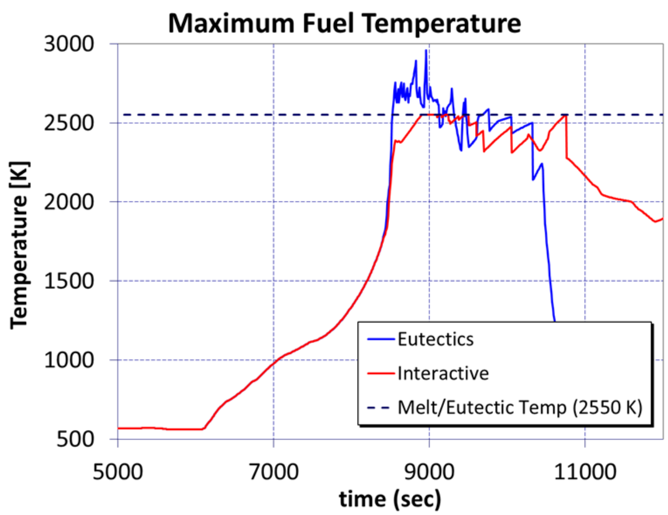
- Compare two TMI-2 test cases
  - Eutectics point = 2550 K
  - Interactive UO2-INT/ZRO2-INT 2550 K
- Similarities but notable differences
  - Core damage
    - Greater for eutectics
  - Size of Molten pool
    - Early: Greater for interactive
    - Later: Greater for eutectics
  - Material relocating to lower plenum
    - Greater for interactive
- Results are preliminary

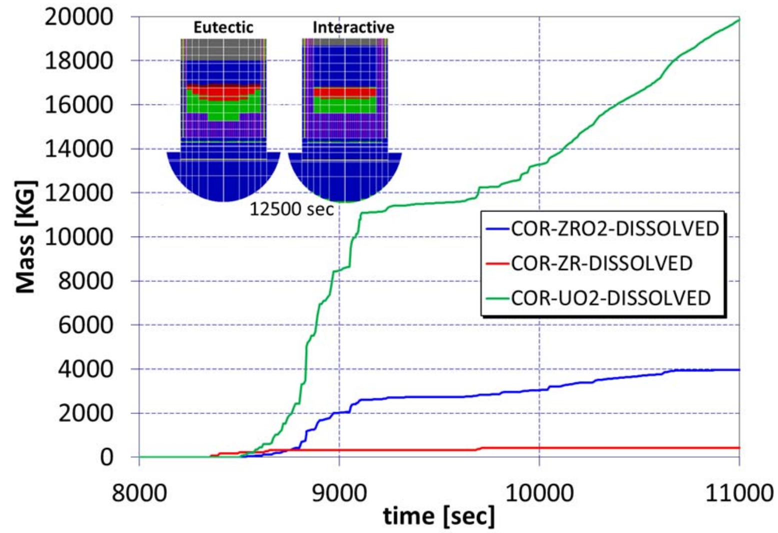


TMI Melt Progression – Preliminary Results



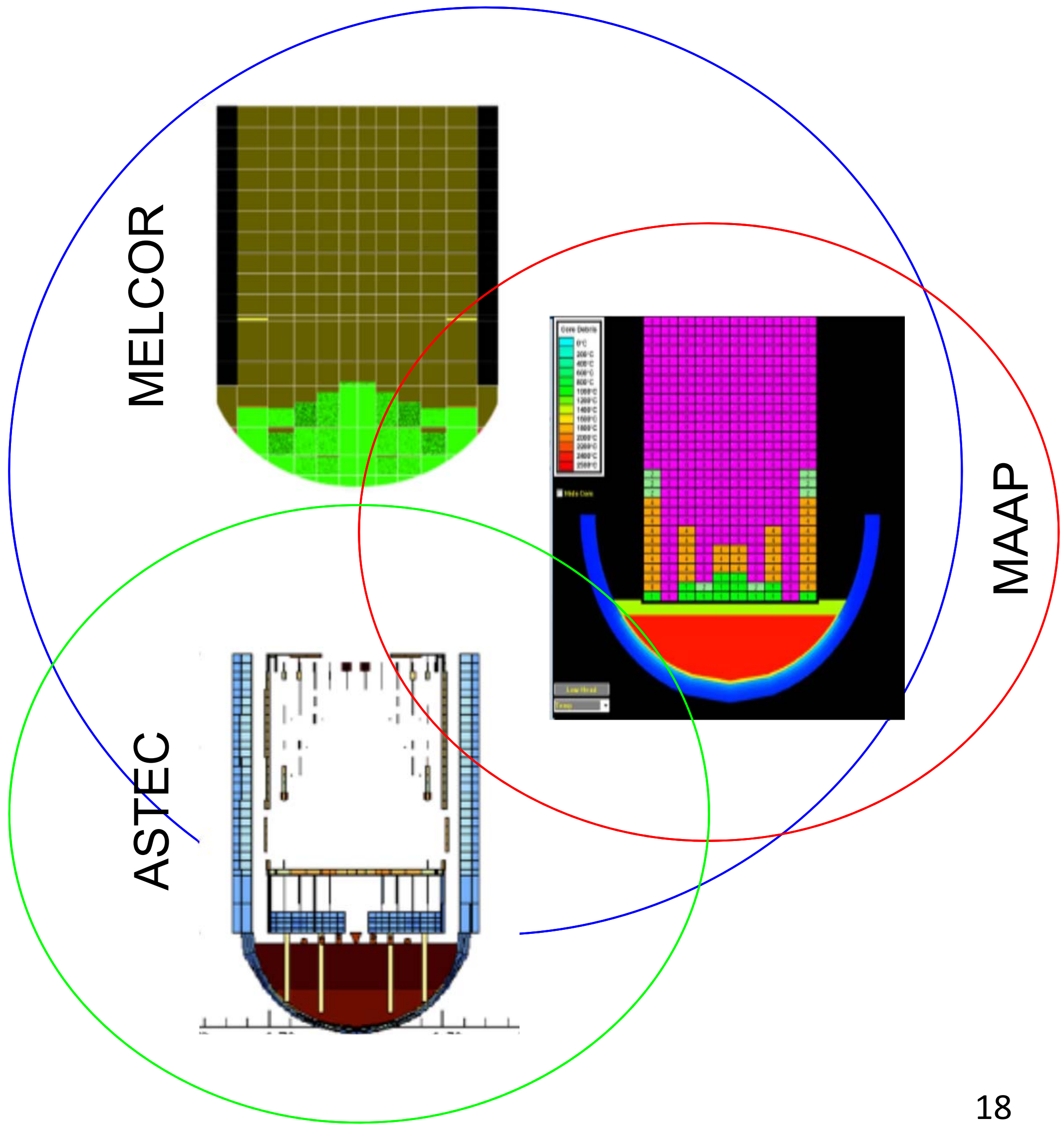






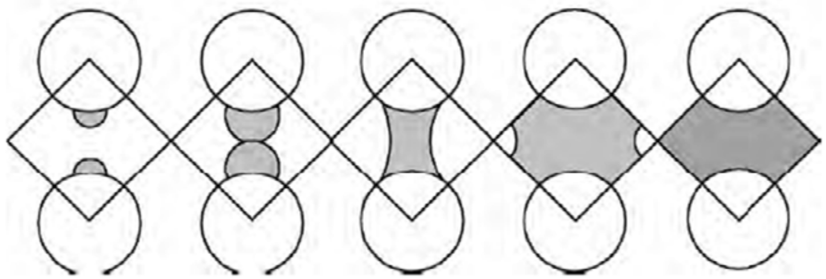
Cross-walk and Model Uncertainty

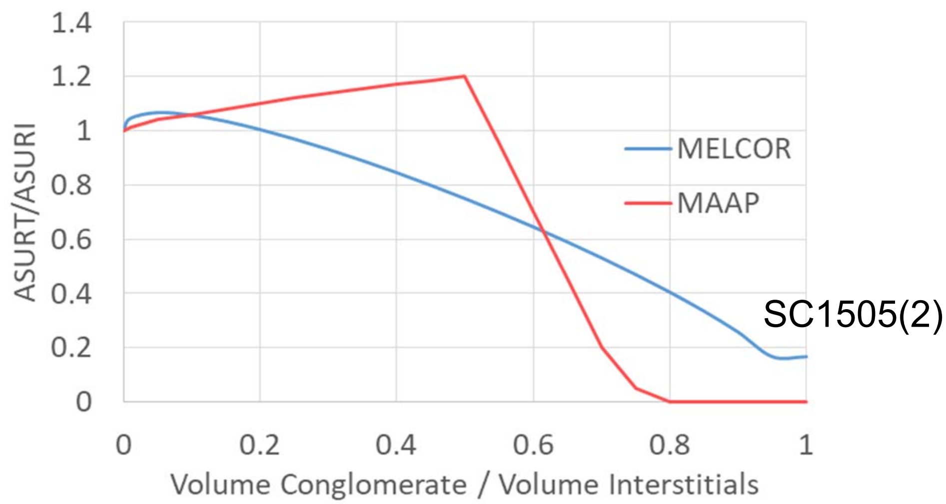
- Where validation data exists, codes give reasonable agreement
- During core degradation, codes diverge
  - Distinct core degradation models
    - ASTEC – Melting only
    - MELCOR – minimum porosity
    - MAAP – molten-pool crust
- What can code development gain from this activity?
  - Potential reduction 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



MELCOR- MAAP Cross-Walk Conclusions

- Cross-walk concluded that heat transfer degradation does not occur in MELCOR with decreasing debris bed porosity. This is wrong!
  - Erroneous statement from report: *"MELCOR represents a particulate debris bed in terms of fixed diameter particles – additional debris does not accumulate within open volume and limit the heat transfer surface area"*
- The MELCOR candling model calculates modified surface areas used for both oxidation and heat transfer
  - Similar to rodded geometry but modified for spheres
  - Oxidation and convective heat transfer use reduced surface areas:
    - ASURC - Conglomerate
    - ASURY - exposed intact surface area
  - Sensitivity coefficient used to set minimum surface area
    - SC1505(2) = 0.05 SOARCA Best Practice
    - Was 0.001 in M186
    - Currently 0.001 for M2.2 default



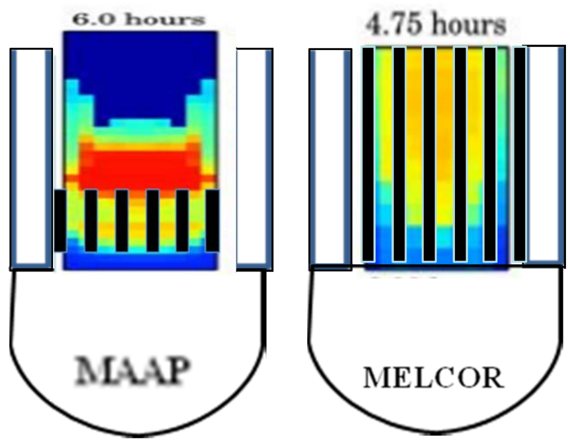


How Are they Used

- ASURT - Convective Heat Transfer
- ASURI - Radiation
- ASURI - Intact component area
- ASURC, ASURY – Oxidation

ASURT=ASURC+ASURY

MELCOR- MAAP Cross-Walk Blockages/Crucible



- MAAP predicts large coherent blockage across core that occur almost instantaneous
- MELCOR predicts local blockages by ring due to candling and refreezing
- MELCOR predicts much smaller molten pool
- What causes such divergence?

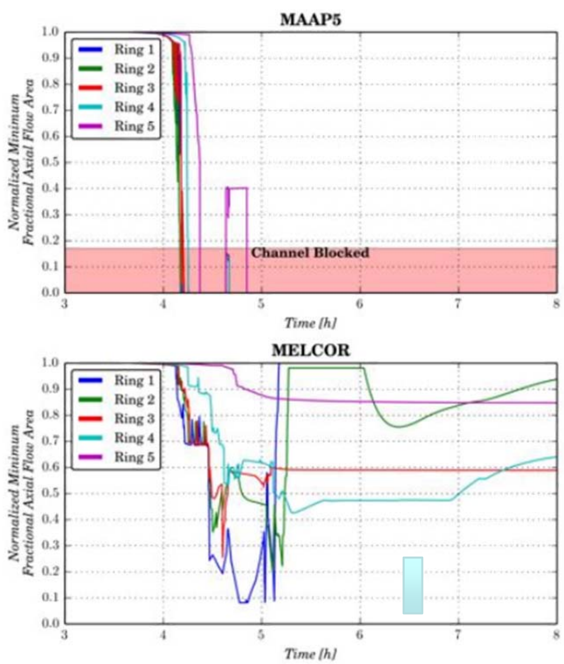
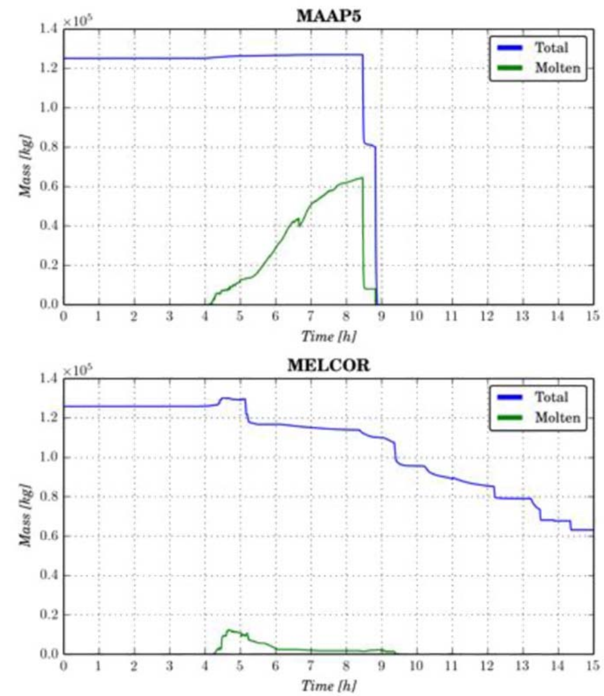
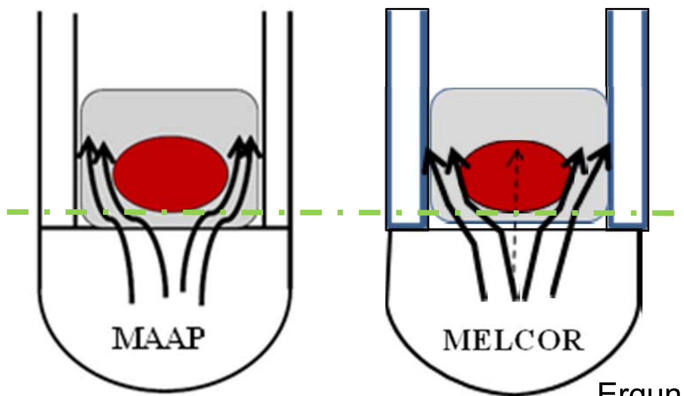
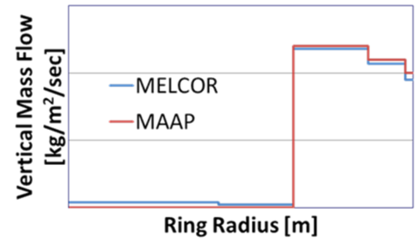


Figure B-18
Comparison of Minimum Vertical Flow Area through Fuel Assemblies across the Radial Extent of Core

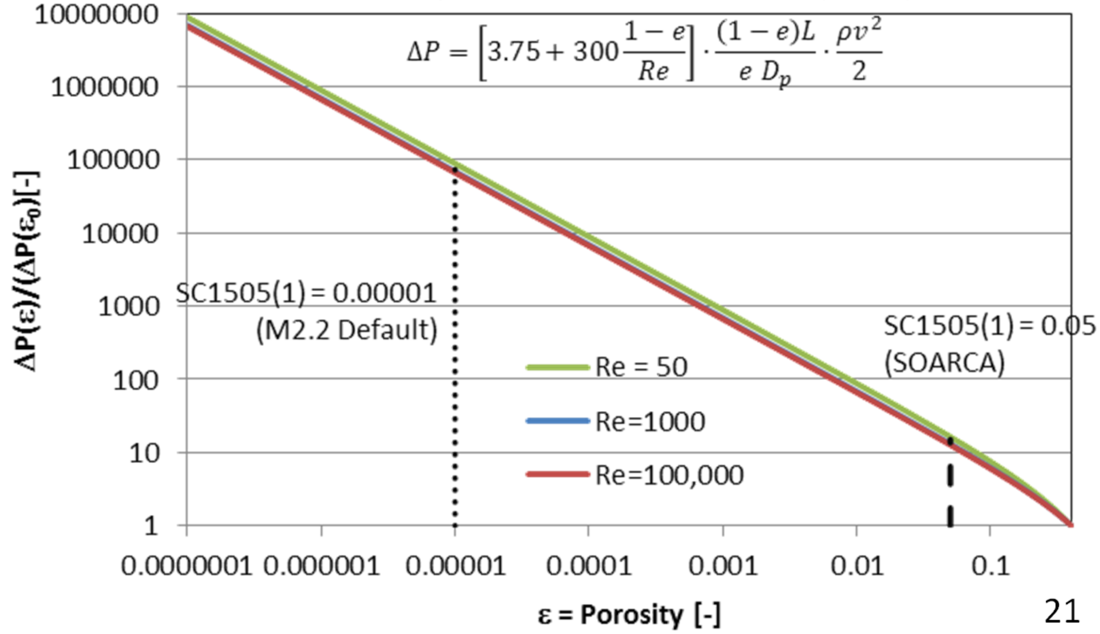


MELCOR- MAAP Cross-Walk Flow Resistance

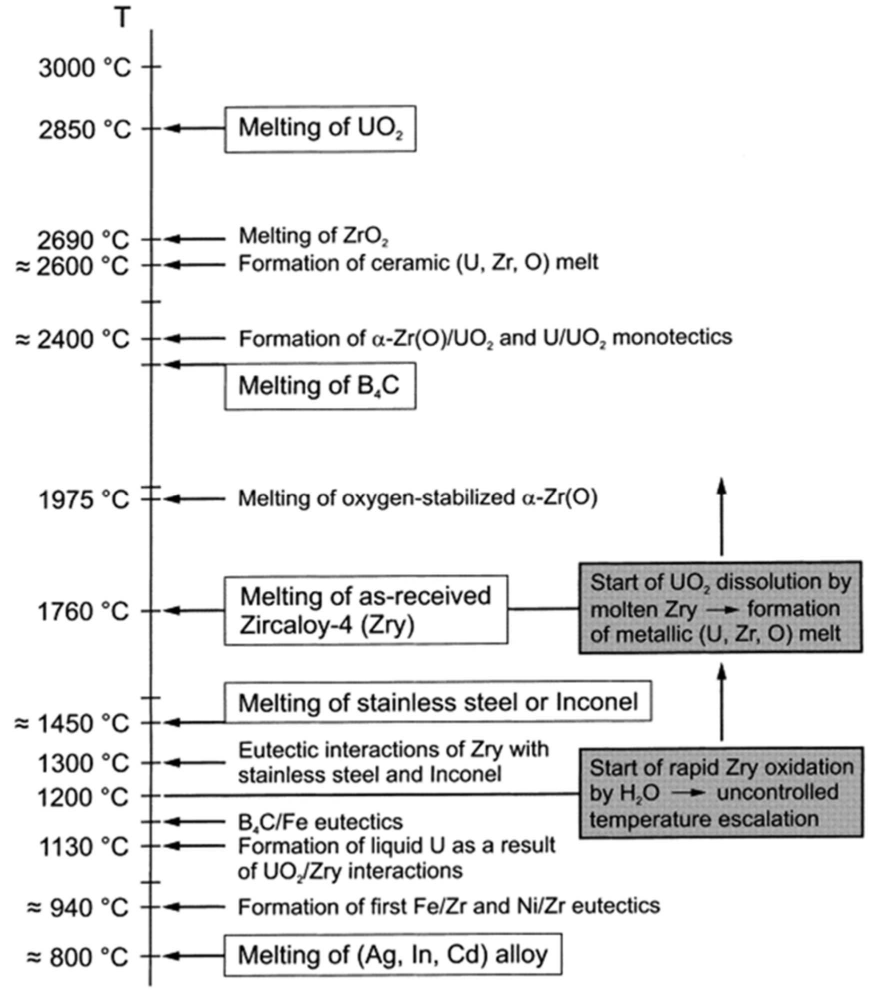




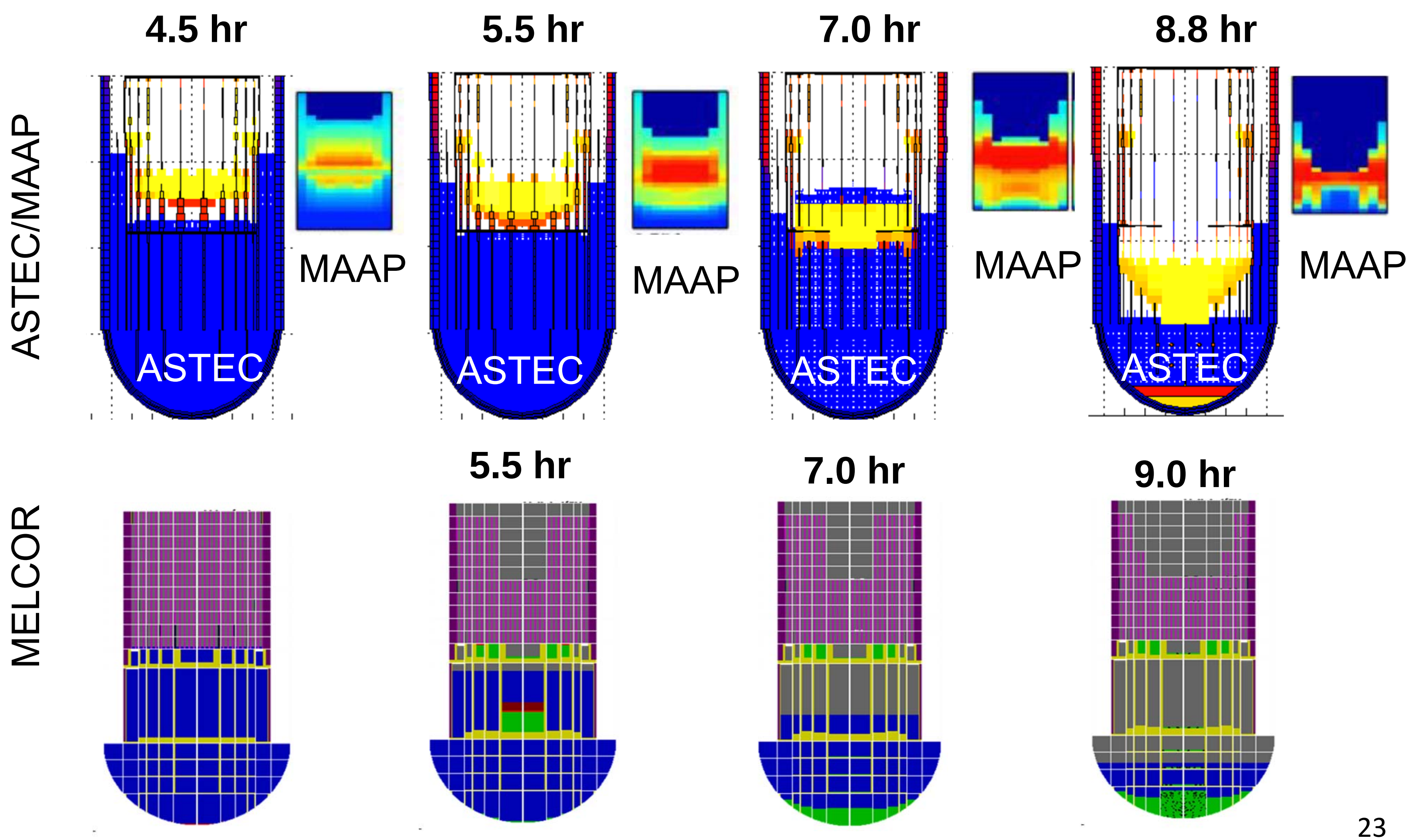
- A lot of attention was focused on the fact that MELCOR does not completely block fluid flow where MAAP does
  - However, for blockages, large pressure drop result in greatly reduced flow
  - MELCOR sensitivity coefficients for flow blockage SC1505(1)
    - 0.05 for SOARCA Best Practice
    - 1e-5 for M2.2 default
  - Recent sensitivity studies demonstrated that this is a second order effect on results (little impact on melt mass)



- Bigger difference: MELCOR cross-walk calculation assumed an effective UO2/ZRO2 melting temperature of 2800 K.
  - User specified parameter ‘SOARCA Best Practice’
    - Leads to much smaller blockages
  - Eutectic temperature would be much lower leading to more extensive blockages



XWALK- MELCOR (Original)



XWALK- MELCOR (UO2-INT/ZRO2-INT = 2550 K)

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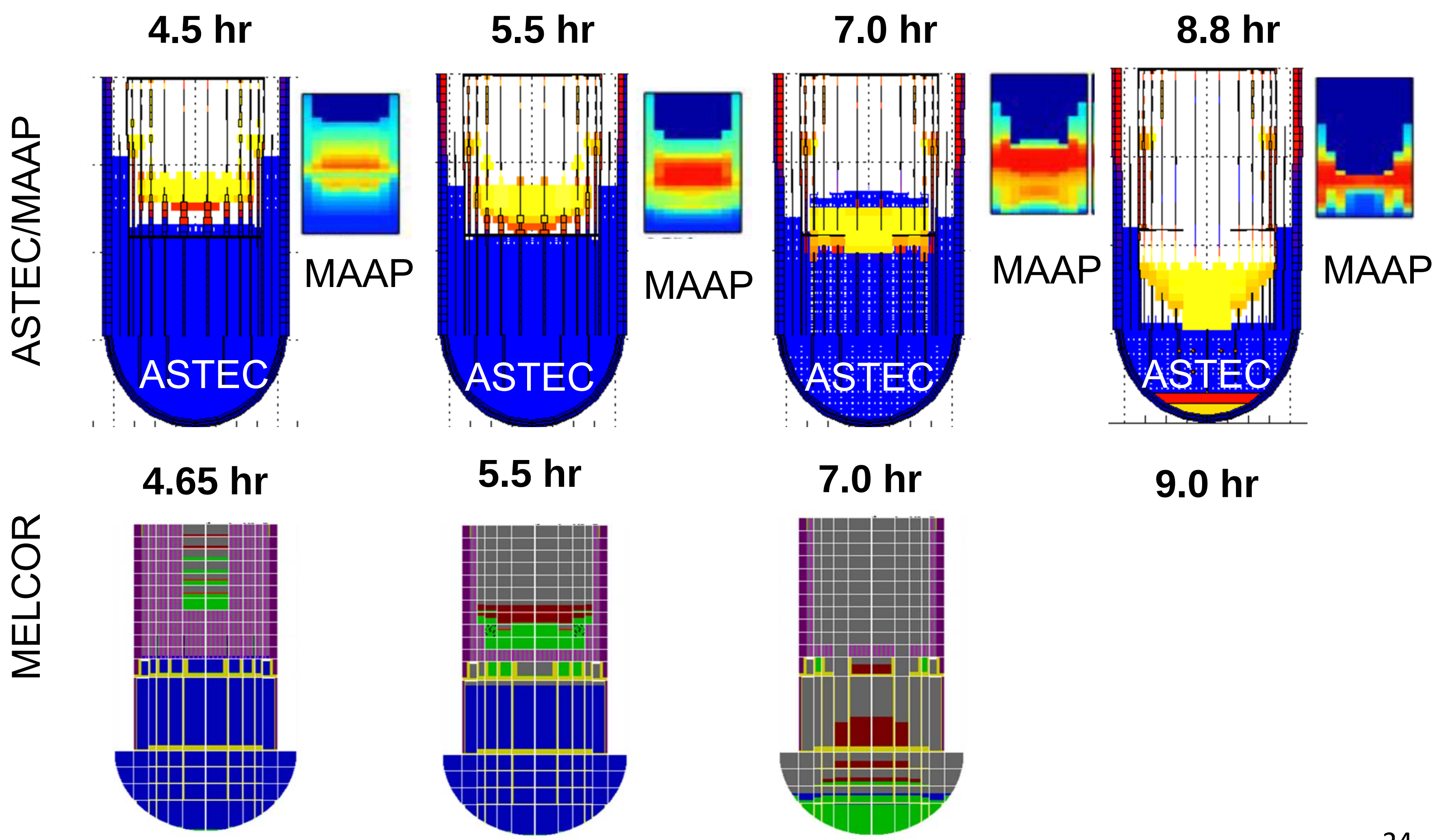
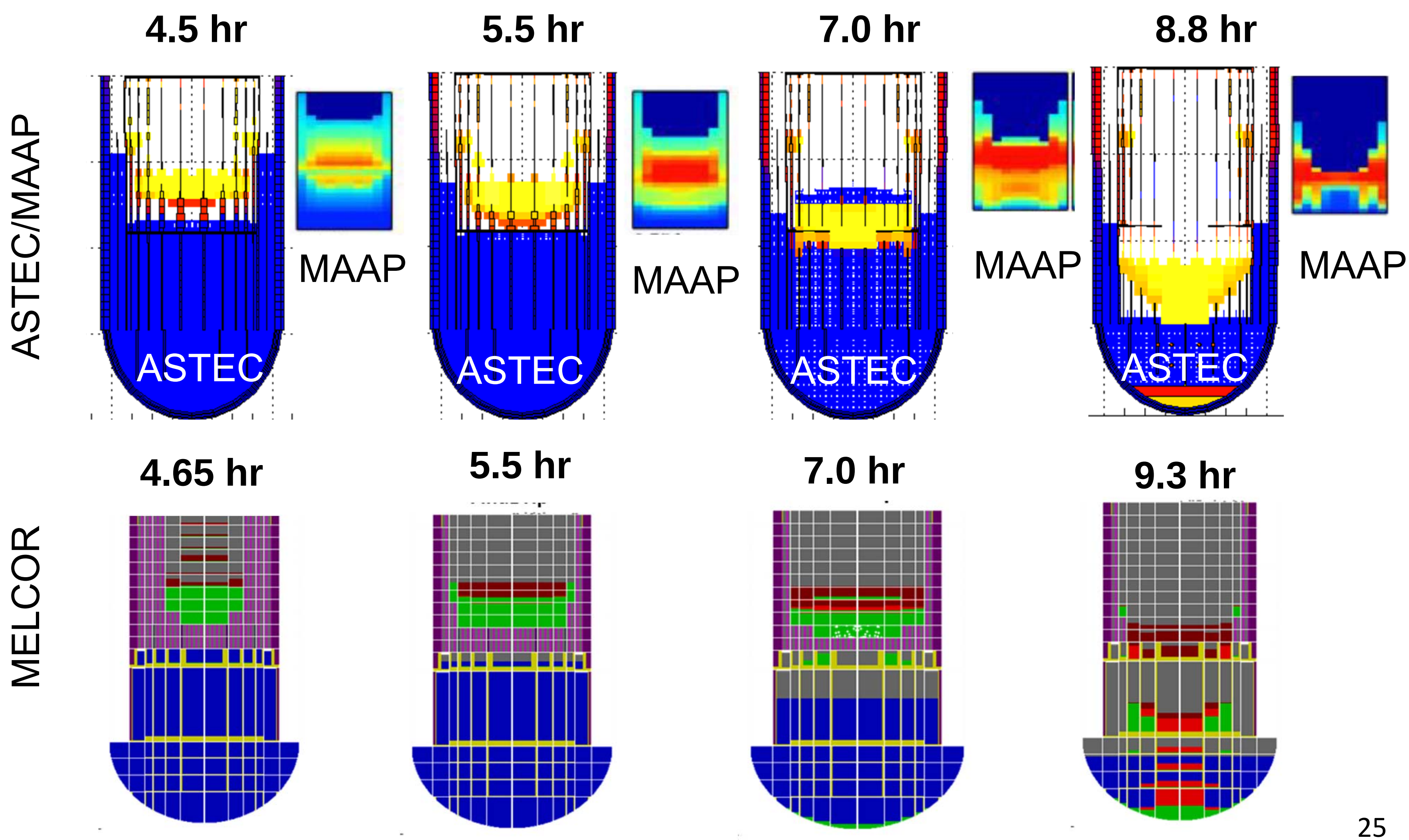


XWALK- MELCOR (Modified)



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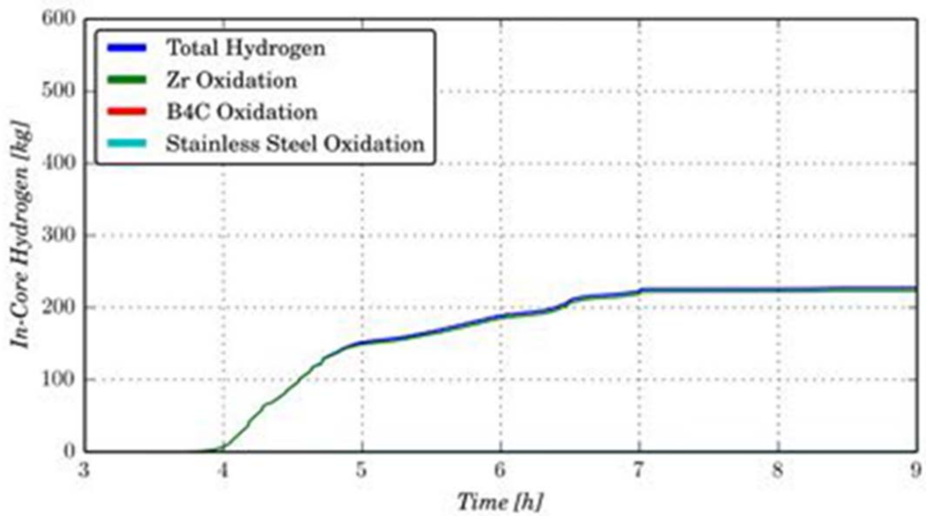
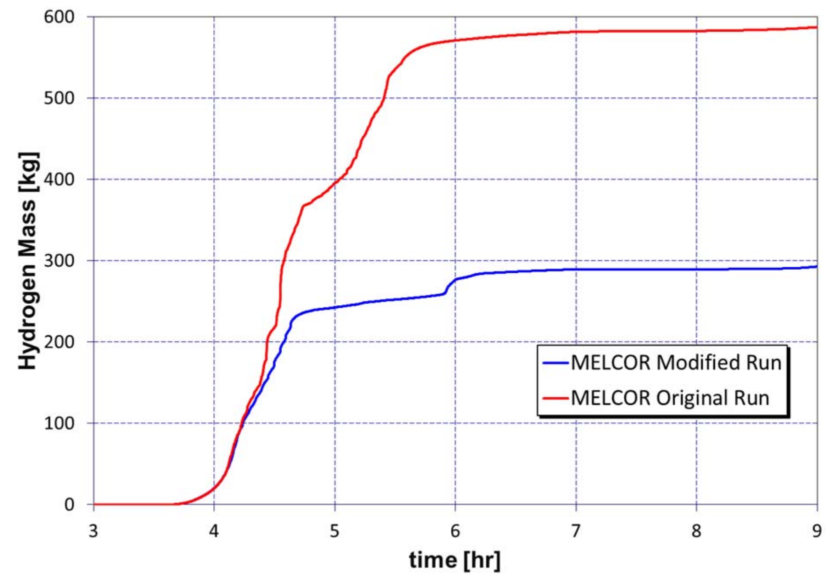
XWALK Hydrogen Generation Predicted

MAAP



MELCOR



MELCOR

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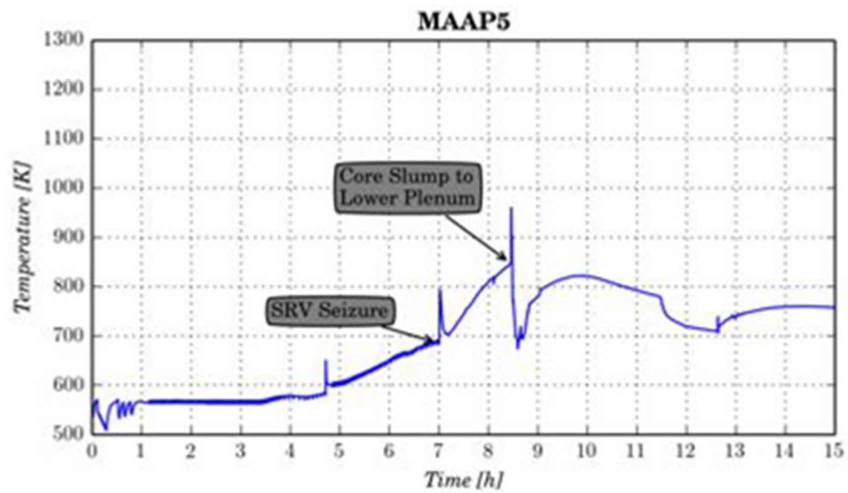
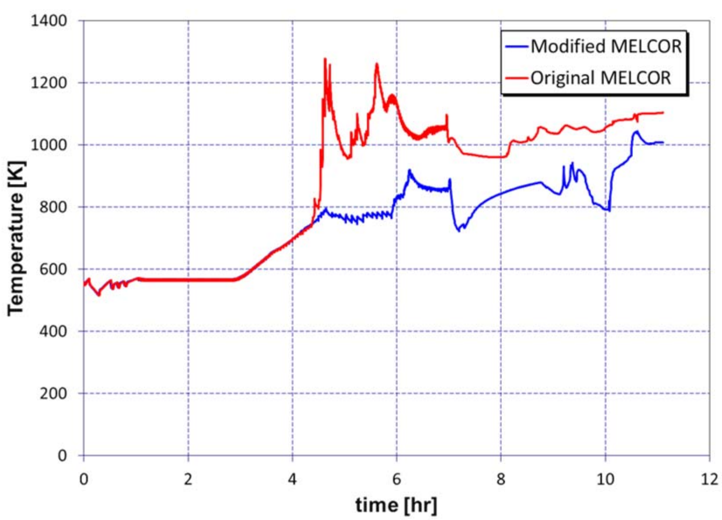
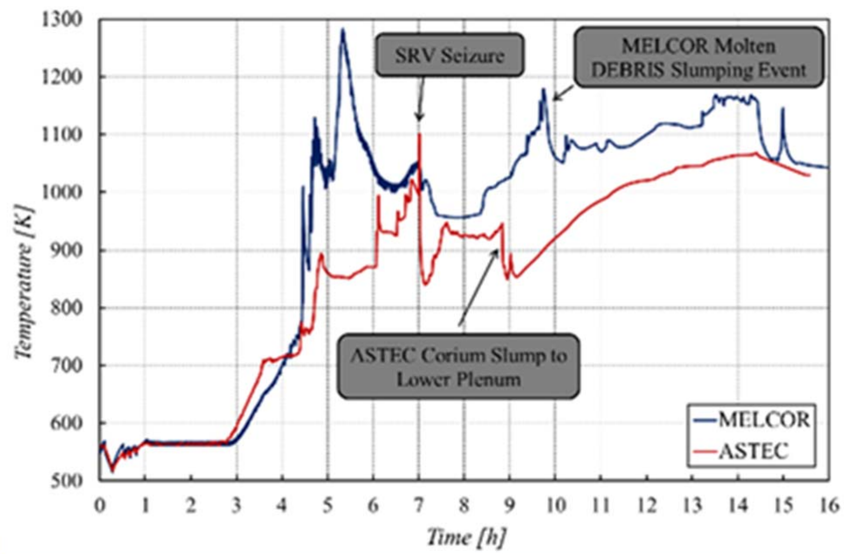
XWALK Steam Dome Temperature

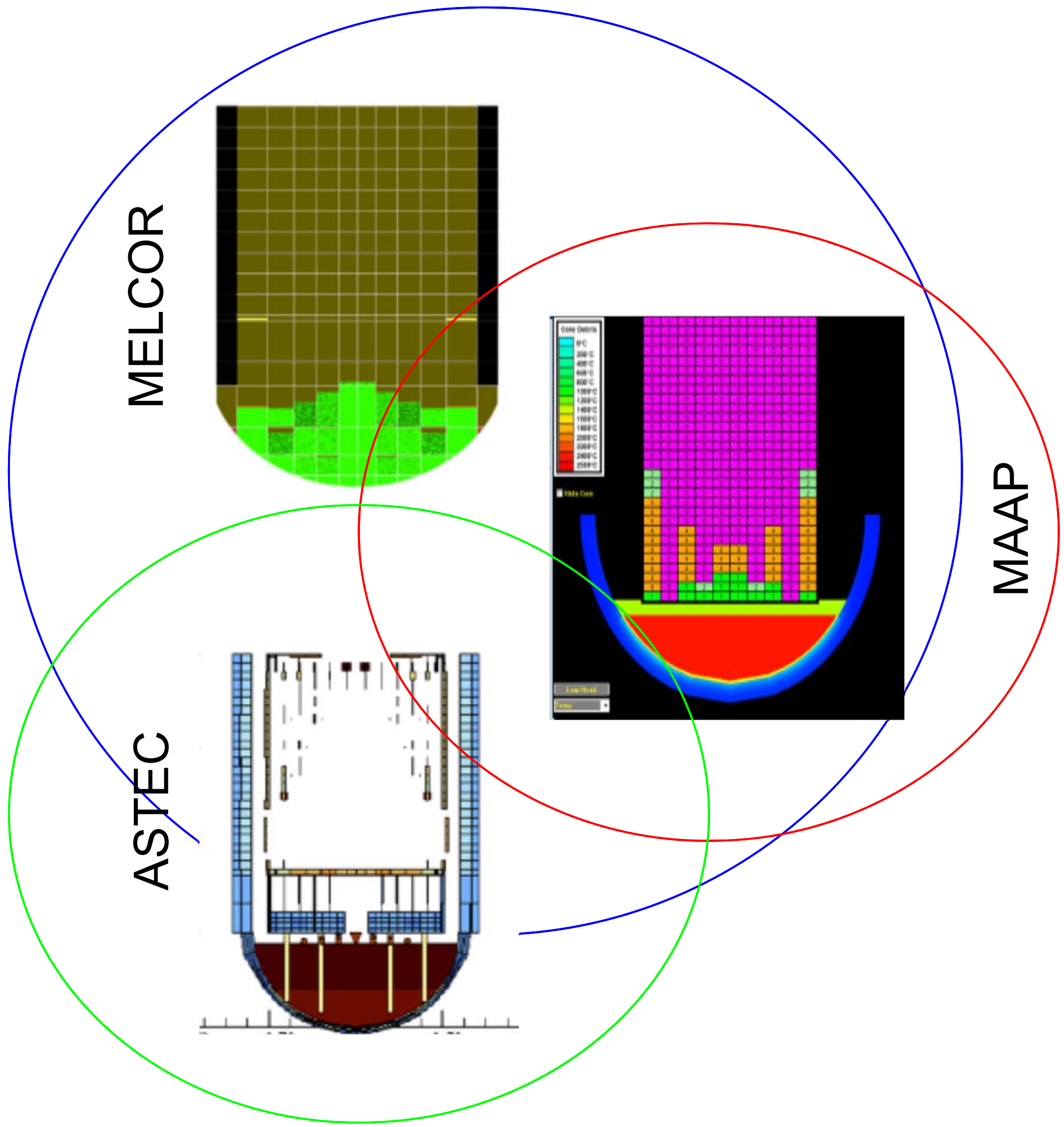
- Previously, MELCOR predicted much higher temperature in steam dome
  - Higher energy advected to MSL
    - Energy ‘bottled up’ in the crucible/pool.
  - More likely to fail the MSL







Uncertainty Domain



Non-LWR Reactor Applications

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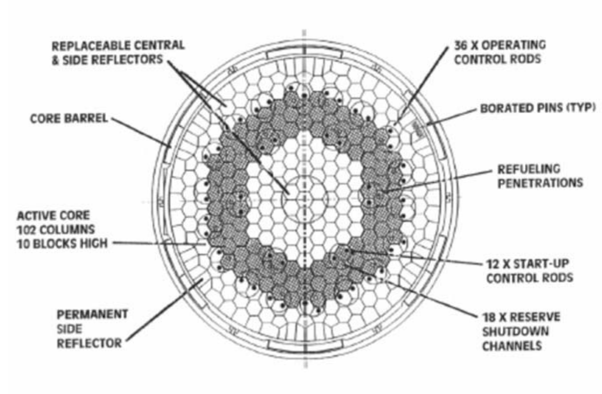
- Advanced Technology Fuels (ATF)
- Non-LWR Reactors
  - HTGR
  - Sodium
  - Molten Salts

High Temperature Gas Reactor

- 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



HTGR Reactor Components

Pebble Bed Reactors (PBR)

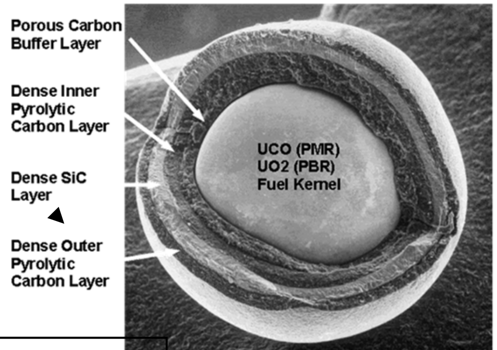
- A component representing the fueled part of a pebble fuel element, which includes UO_2 as the fuel material and graphite as the "extra fuel material"
- A two-sided, graphite reflector component.
- A radial fuel temperature profile (notions of peak and surface fuel temperature)
- Radial cell-to-cell conduction/radiation models in the core region (effective bed conductivity)
- Packed-bed flow correlations for friction factors, convection heat transfer through the pebble bed

Prismatic Reactors (PMR

- A component representing the fueled part of a fuel compact element, including UO_2 as the fuel material and graphite as the "extra fuel material"
- A two-sided, graphite reflector component
- A component representing the graphite hex blocks that are "associated" with fuel channels in block
- A logarithmic radial temperature profile associated with the hex blocks
- Radial cell-to-cell conduction/radiation heat transfer, account for hex block gas gap

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



FP Intact

FP Initially failed

FP SiC layer failed

U contamination

→ Matrix → Graphite → Coolant

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^3)
λ = Decay constant (1/s)
S = Source term (kmol/m^3-s)
D = Effective Diffusion coefficient (m^2/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)

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

- Maximum rates limited by gaseous diffusion to surface
- Reaction Products
  - The air reaction produces CO/CO_2
  - Steam reaction produces CO and H_2
  - The CO/CO_2 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

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

  - Eddy Diffusion –Impaction Regime

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

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

  - Inertia Moderated Regime
    - Deposition velocity is either constant

$$V_d^* = \sqrt{\frac{f}{2}} \qquad 10 \le \tau_* < 270$$

    - Or may decrease with increasing dimensionless relaxation time

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

- PUI Model for deposition in bends
  - Pui bend model
  - Merril'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

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

- 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

Sandia National Laboratories

- Point kinetics for operating reactor applications
  - Model developed by UNM

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

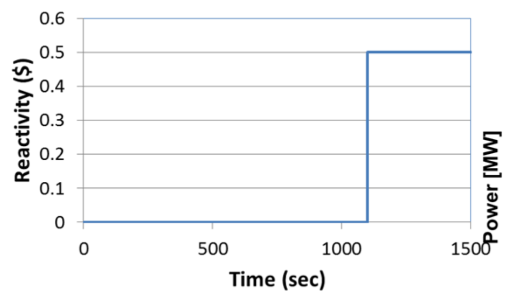
$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n - \lambda_i C_i$$

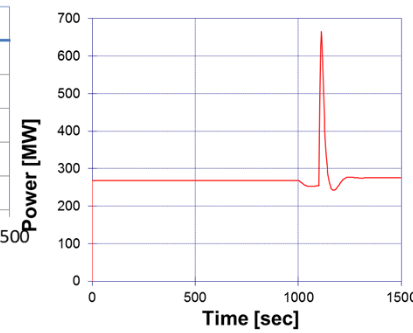
    - Unconditionally stable over wide range of timesteps
      - Exponential matrix approximated with a 7th order Pade(3,3) function
  - Temperature-dependent reactivity feedback from COR components
    - Fuel/Moderator/Reflector generalized weighting for spatially averaged feedback
  - External reactivity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

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:

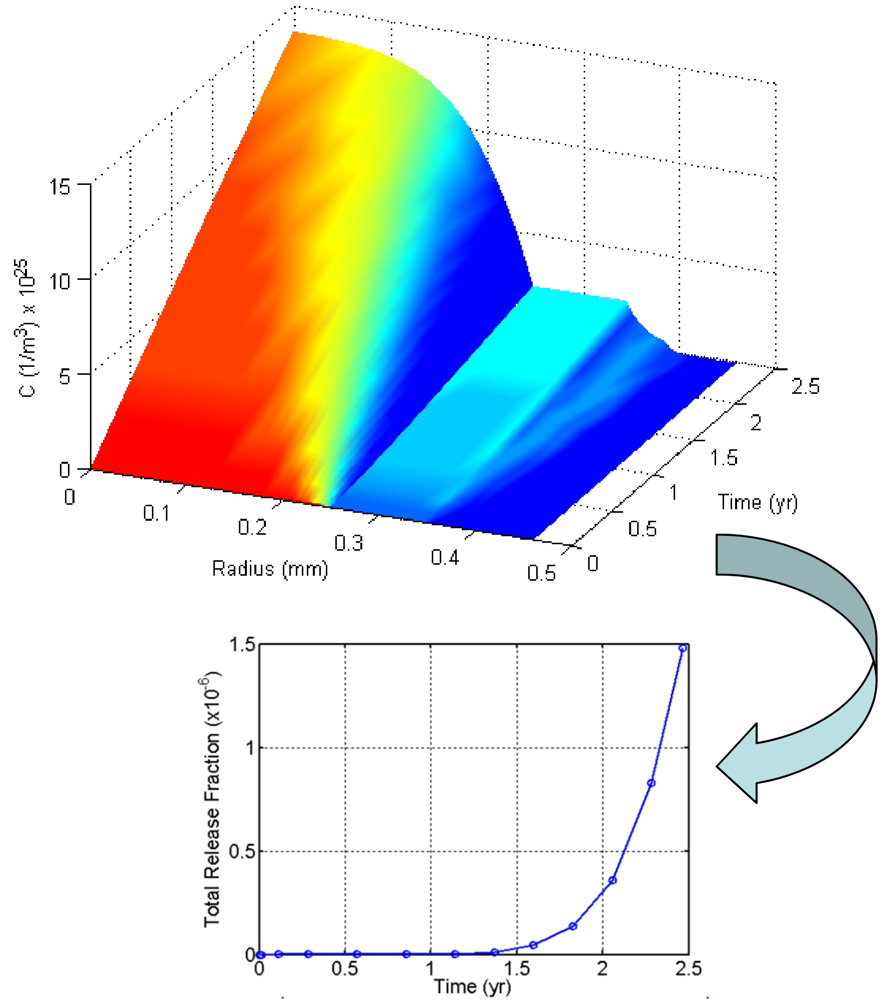
```
– !         NTPCOR   RNTPCOR   ICFGAP   ICFFIS   CFNAME
– COR_TP  NO       NO        NO       NO
– ! trigger PK on at 1000s
– !           TINIT    QINIT    FUEL   MODERATOR
– COR_PKM01   1000.0   2.68e8   UO2    GRAPH
– !           EXTREACCF            NEUSRCECF
– COR_PKM02   'Reactivity'
```





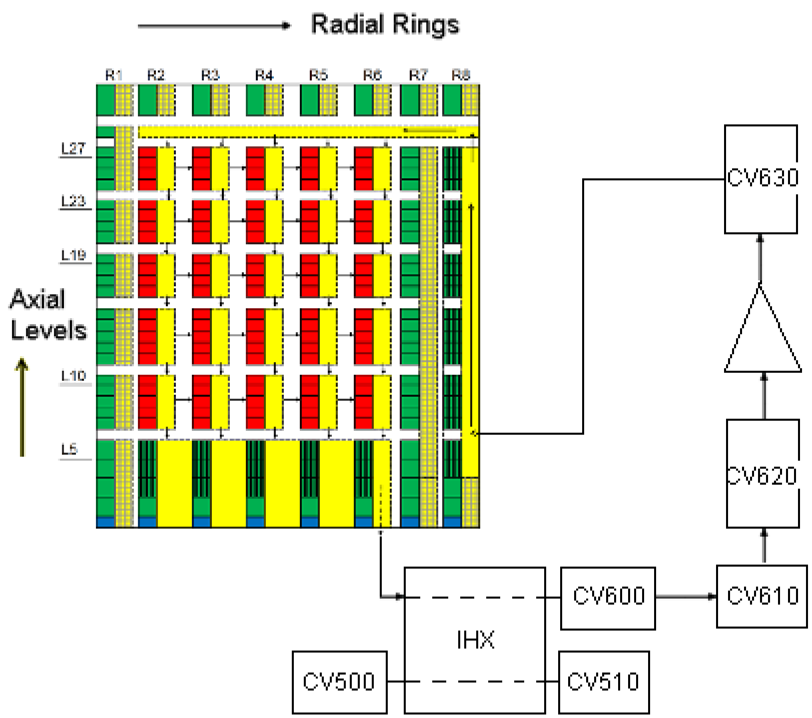
"Accelerated" Normal Operation (1)

- System Thermal Hydraulic
- Solve Diffusion Equation
  - Solve the diffusion equation using core cell component temperatures (temperature dependent diffusion coefficients)
  - Finite difference solver (DIF2) integrated into MELCOR
  - Track intact and failed particles
  - Output of the diffusion calculation is spatial distribution in the particles (kernel/buffer), graphite, and relative amounts released to the primary system (for each isotope from each core cell)
  - FP distribution and release rates are ultimately scaled using ORIGEN results for burnup (more accurate in terms of actual isotope inventory)



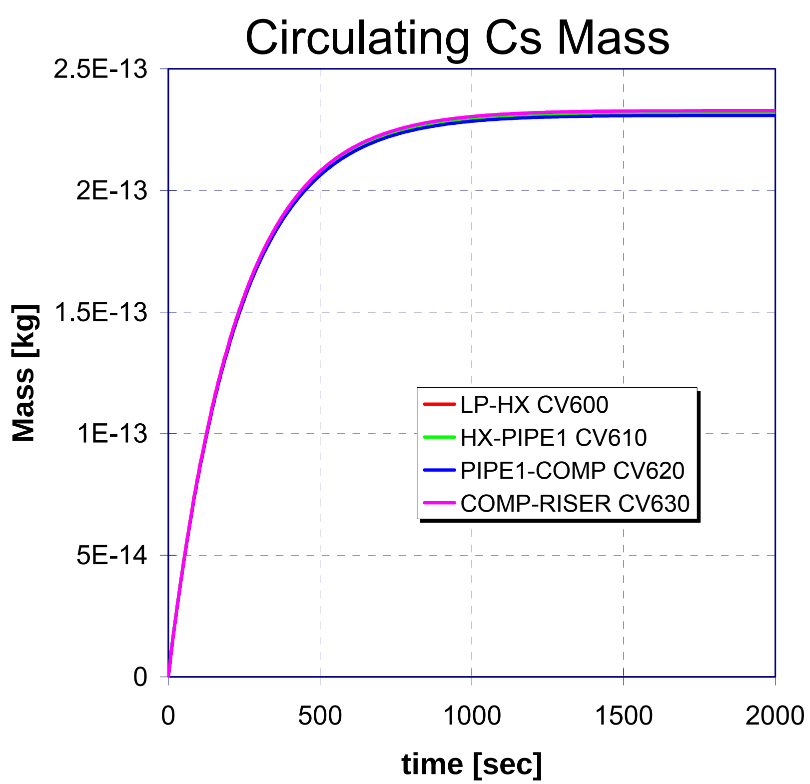
"Accelerated" Normal Operation (2)

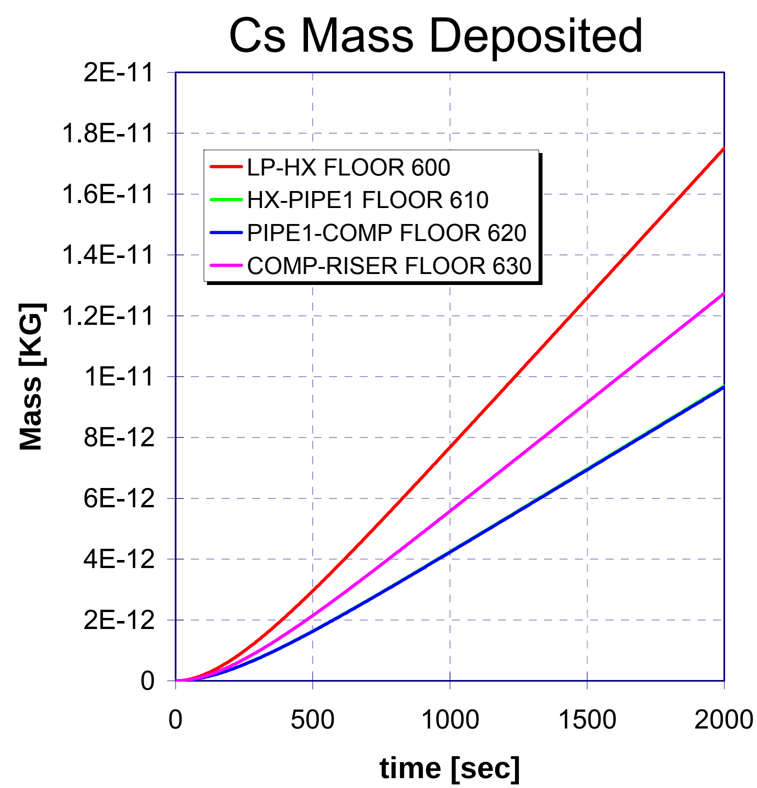
- FP/Dust Distribution in Primary System
  - MELCOR run for some problem time to establish distribution rates and patterns in the primary system (input is release to the coolant from previous step)
  - Dust deposition is also done at this stage



"Accelerated" Normal Operation (3)

- Example PBR400 Cs Distribution in Primary System
  - Scale to desired operating time
  - Use as initial condition for accident



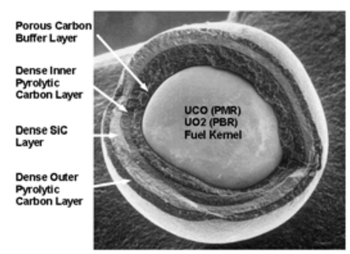


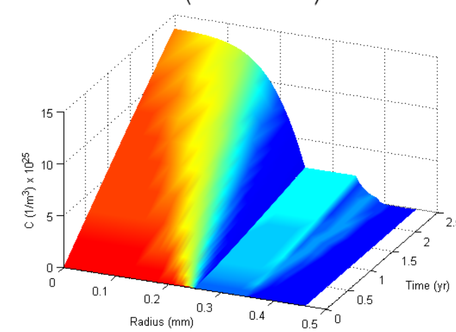
High Temp Gas-Cooled Reactors

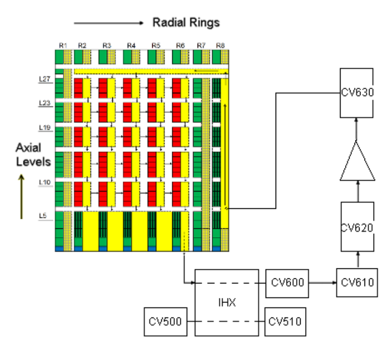
Existing Modeling Capabilities

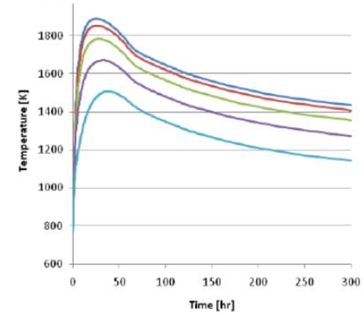
- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- Modified clad (CL) component (PMR/PBR)
- Core conduction
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure
- Graphite dust transport
  - Turbulent deposition, Resuspension
- Basic balance-of-plant models (Turbomachinery, Heat exchangers)
- Momentum exchange between adjacent flow paths (lock-exchange air ingress)
- Graphite oxidation

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









Existing Modeling Gaps

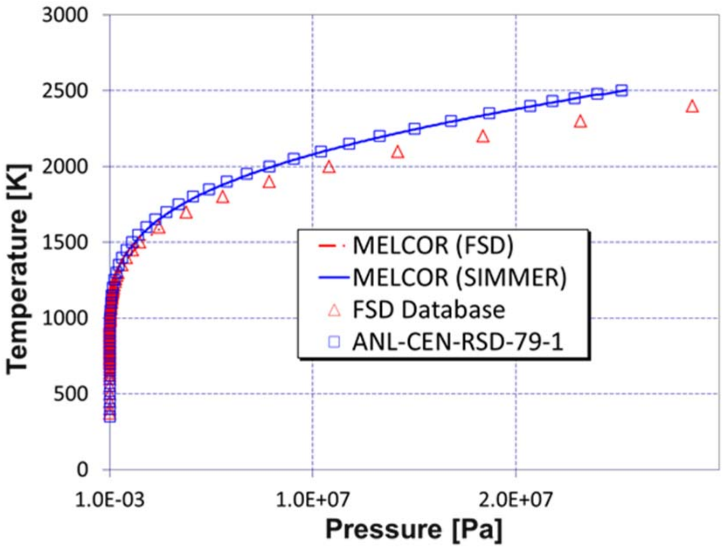
- Graphite structure/surface interactions with aerosols and fission products
- New designs use UC_x fuels rather than UO_2
- Mechanistic, specific balance-of-plant models

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

- Sodium Working fluid
  - Implement Sodium Equations of State (EOS)
  - Implement Sodium thermal-mechanical properties
- Two models implemented
  - Fusion safety database (FSD)
  - 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 in the past FY

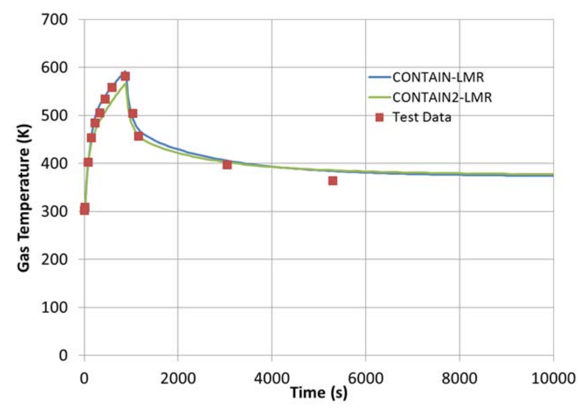


CONTAIN2-LMR Development

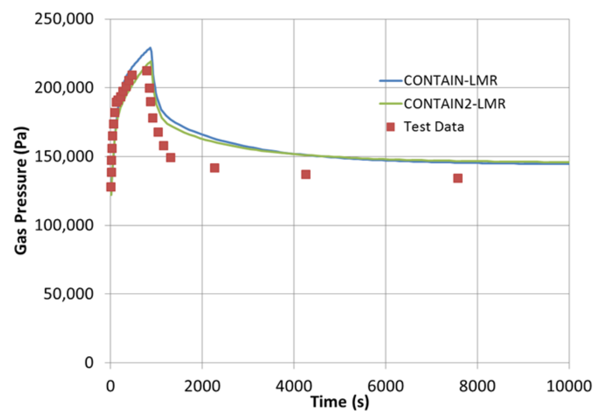
- CONTAIN2 is last version of CONTAIN development
  - Significant improvements over CONTAIN-LMR
  - CONTAIN-LMR only works for sodium problems
  - Available standard test sets for LWR applications
- Development of CONTAIN2-LMR
  - Port all sodium models from CONTAIN-LMR
  - Allows to run both LWR and sodium reactor problems
- Verification – same sets as in CONTAIN-LMR
  - Two condensable option and atmospheric chemistry model test problems
  - Experiments for pool and spray fires –AB5
  - Sandia SLAM experiments for sodium-concrete interactions (TBD)

ABCOVE AB5

Temperature

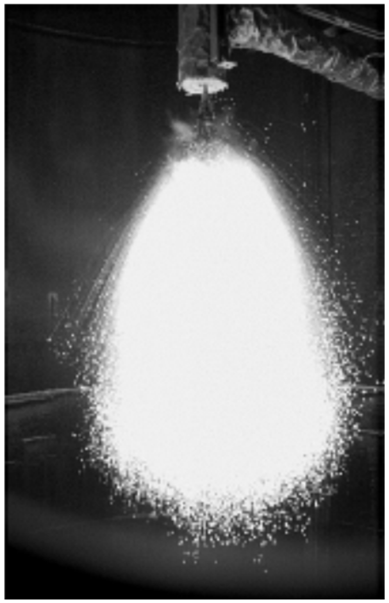


Pressure



Spray Fire Chemistry

- 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) $2\ \mathrm{Na} + {}^{1}/_{2}\,\mathrm{O_2} \rightarrow \mathrm{Na_2O}$,
    - (S2) $2\ \mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$
  - Fixed ratio of peroxide and monoxide $\left(\frac{1.3478 \cdot \mathrm{F}_{Na_2O_2}}{1.6957 - 0.3479 \cdot \mathrm{F}_{Na_2O_2}}\right)$
  - Tracked quantities include:
    - Mass of Na (spray, burned, pool), O_2(consumed), Na_2O_2+ Na_2O(produced)
    - Energy of reactions
- Plot Variables
  - NAC-SPR-NASM [KG] - Total mass of sodium introduced into the cell,
  - NAC-SPR-NABM [KG] - Total mass of sodium burned,
  - NAC-SPR-O2M [KG] - Total mass of oxygen removed,
  - NAC-SPR-NA2O2 [KG] - Total mass of aerosol Na202 added,
  - NAC-SPR-NA20 [KG] - Total mass of aerosol Na20 added,
  - NAC-SPR-MP [KG] - Total mass of sodium added to the pool,
  - NAC-SPR-EA [J] - Total energy released to the atmosphere, and
  - NAC-SPR-EP [J] Total energy added to the pool.



Sodium Spray Fire Model

NAC_SPRAY – Sodium Spray Fire Model

Optional

This model enables the modeling of the sodium spray fire in a given control volume if the sodium spray source is given.

(1) NUM The number of control volumes to include this model
(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC Table row index.
(type = integer, default = none, units = none)

(2) CVHNAME The name of the CVH volume.
(type = character, default = none, units = none)

(3) HITE Fall height of sodium spray. Default is CVH height.
(type = real, default = CVH volume height, units = m)

Used to determine droplet terminal velocity

(4) DME Mean sodium droplet diameter.
(type = real, default = 0.001, units = m)

(5) FNA2O2 Fraction of sodium peroxide produced by the spray fire.
(type = real, default = 1.0, units = m)

(6) SOU-TYPE Sodium spray source type: TF or CF. Default is TF. Note that two tables are expected: mass and temperature/enthalpy
(type = character, default = TF, units = none)

(7) MASS-NAME Name of the TF or CF for the mass source.
(type = character, default = none, units = kg/s)

(8) THERM-NAME Name of the TF or CF for the temperature of the source.
(type = character, default = none, units = temperature)

Pool Fire Chemistry

- Based on SOFIRE II code from ANL
  - Reactions considered:
    - $2\,\mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$, 10.97 MJ/kg
    - $4\,\mathrm{Na} + \mathrm{O_2} \rightarrow 2\,\mathrm{Na_2O}$, 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: $\mathrm{D} = \frac{6.4315\times10^{-5}}{\mathrm{P}}\mathrm{T}^{1.823}$
  - Input requirement:
    - F1 – fraction of 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
- Tracked quantities:
  - Mass of Na(pool, burned), O_2(consumed), Na_2O_2+Na_2O(produced)
  - Energy of reactions
- Plot Variables

NAC-PFI-O2MC [kg] cumulative O_2 consumed
NAC-PFI-NABMC [kg]: cumulative Na consumed
NAC-PFI-NA2O2MC [kg: Cumulative Na_2O_2 produced
NAC-PFI-NA2OMC [kg]: Cumulative Na_2O produced
NAC-PFI-EAC [J]: Cumulative energy to atmosphere
NAC-PFI-EPC [J]: Cumulative energy to pool

NAC-PFI-O2M [kg/s] rate of O_2 consumed
NAC-PFI-NABM [kg/s]: rate of Na consumed
NAC-PFI-NA2O2M [kg/s]: rate of Na_2O_2 produced
NAC-PFI-NA2OM [kg/s]: rate of Na_2O produced
NAC-PFI-EA [W]: rate of energy to atmosphere
NAC-PFI-EP [J]: rate of energy to pool

Sodium Pool Fire

NAC_PFIRE – Sodium Pool Fire Model

Optional

This model allows the modeling of the sodium pool fire in a given control volume. A number of fraction inputs can be specified.

(1) NUM The number of control volumes to include this model

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

The following data are input as a table with length NUM:

(1) NC Table row index.

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

(2) CVHNAME The name of the CVH volume.

(type = character, default = none, units = none)

(3) FO2 Fraction of the oxygen consumed that reacts to form monoxide. 1-FO2 is the remaining oxygen fraction for the reaction to form peroxide.

(type = real, default = 0.5, units = none)

(4) FHEAT Fraction of the sensible heat from the reactions to be added to the pool. The balance will go to the atmosphere.

(type = real, default = 1.0, units = none)

(5) FNA2O Fraction of the Na_2O remaining in the pool. The balance will be applied to the atmosphere as aerosols.

(type = real, default = 1.0, units = none)

(6) FNA2O2 Fraction of the Na_2O_2 remaining in the pool. The balance will be applied to the atmosphere as aerosols.

(type = real, default = 0.0, units = none)

Atmospheric Chemistry

- A number of reactions have been considered:
  - $Na(l) + H_2O\ (l) \rightarrow NaOH(a) + \frac{1}{2}H_2$
  - $2\ Na(g, l) + H_2O\ (g, l) \rightarrow Na_2O(a) + H_2$
  - $2\ Na(g, l, a) + \frac{1}{2}O_2$ or $O_2 \rightarrow Na_2O(a)$ or $Na_2O_2(a)$
  - $Na_2O_2(a) + 2\ Na(g, l) \rightarrow 2\ Na_2O(a)$
  - $Na_2O(a) + H_2O\ (g, l) \rightarrow 2NaOH(a)$
  - $Na_2O_2(a) + H_2O\ (g, l) \rightarrow 2NaOH(a) + 0.5O_2$
- Kinetics of atmosphere gases are not explicitly modeled.
- All these reactions are assumed to occur in hierarchal order:
  - In the order listed above
  - By location of reactions
    - Atmosphere(g), aerosol, surfaces (i.e., HS)
- Outputs
  - Reaction number, reaction energy, byproducts (Na classes, H_2), gas and liquid consumed (Na, H_2O, O_2)

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

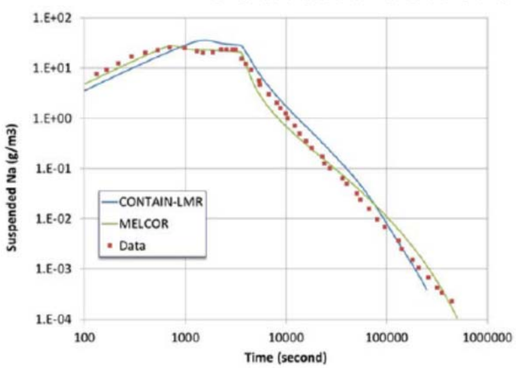


Figure 33. Suspended Na Aerosol Mass - AB1

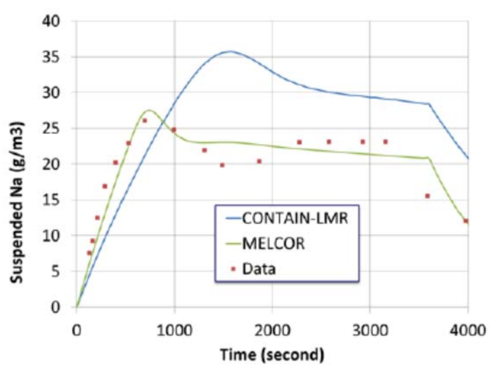


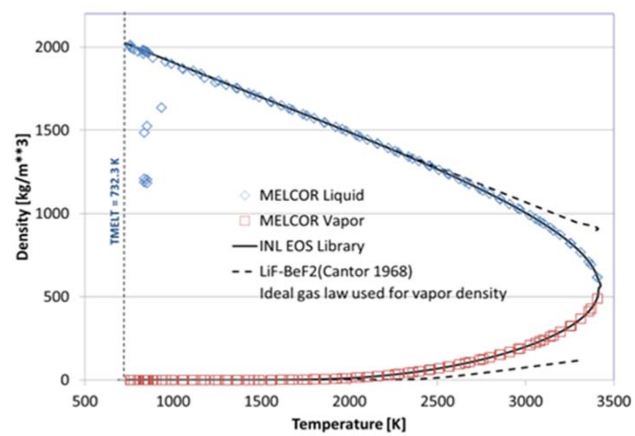
Figure 34. Suspended Na Aerosol Mass-AB1

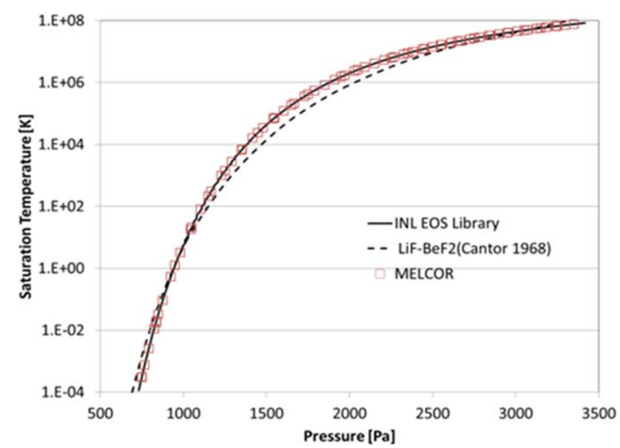
Existing Modeling Gaps

- 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-BeF2 have been added
  - Equation of State
    - Current capability
  - Thermal-mechanical properties
    - Current capability
  - EOS for other molten salt fluids would need to be developed
    - 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.

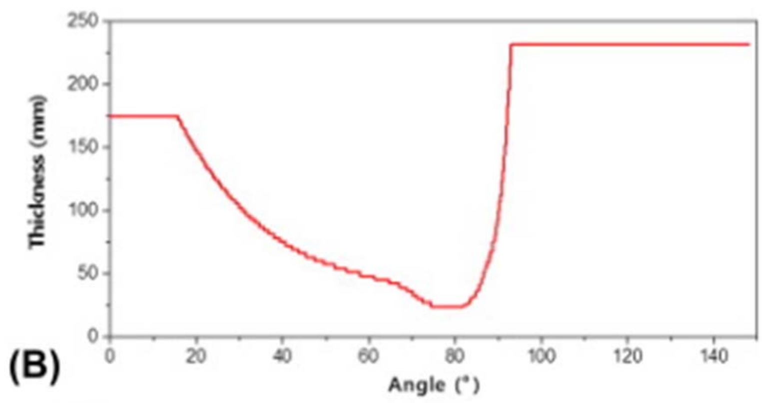




Future In-Vessel Retention Code Improvements

MELCOR: New Modeling | SQA | Utilities

- Melting Lower Head
  - Addition of molten steel to debris
    - Similar to HS degassing model
    - Impact on focusing effect
    - Steel relocates to CAV for MCCI
  - Modify lower head thermal model for moving melt boundary
    - Adaptive vs fixed grid
    - Thinning of vessel wall
    - Effect on local stress
  - Improved diagnostics
- Control Rod Guide Tubes
  - Cooling effects
  - Penetration Failure Model
    - Review of LHF experiments and add strain-based model
  - Heavy Metal Layer?



Thickness of the reactor vessel wall SBO

Evaluation of heat-flux distribution at the inner and outer reactor vessel walls under the in-vessel retention through external reactor vessel cooling condition
Jaehoon Jung, KAERI, January 2015

MELCOR

New Modeling

SQA

Utilities

MELCOR 2.2 Code Release

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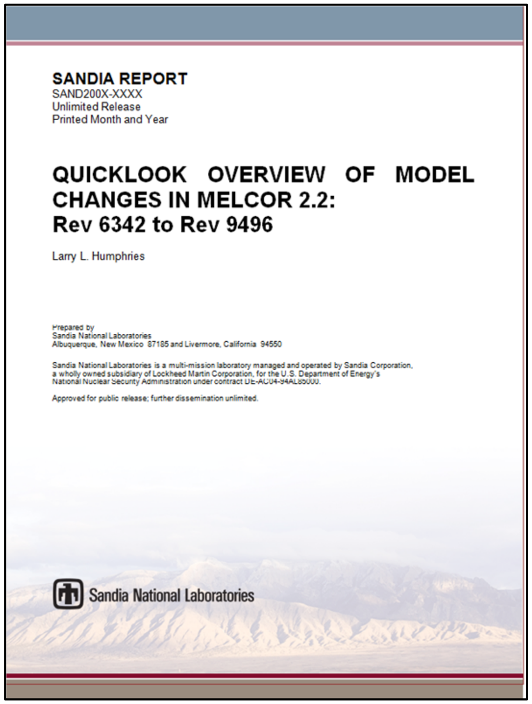

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QUICKLOOK OVERVIEW OF MODEL CHANGES IN MELCOR 2.2:
Rev 6342 to Rev 9496

Larry L. Humphries

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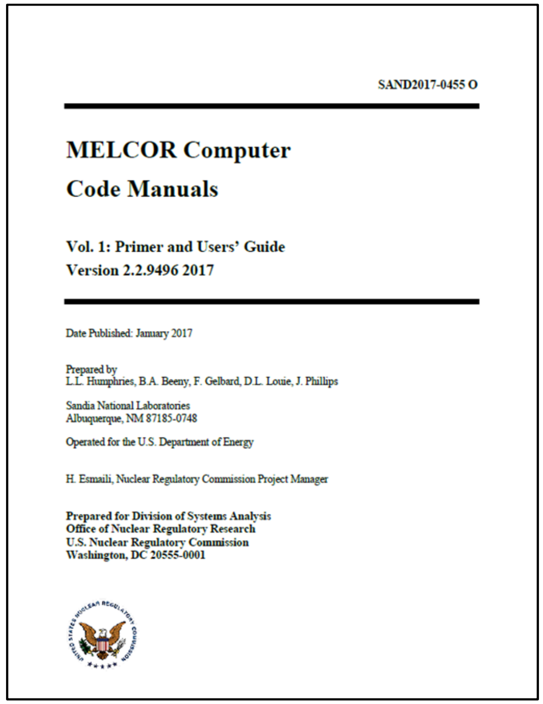

SAND2017-0455 O

MELCOR Computer
Code Manuals

Vol. 1: Primer and Users' Guide
Version 2.2.9496 2017

Date Published: January 2017

Prepared by
L.L. Humphries, B.A. Beeny, F. Gelbard, D.L. Louie, J. Phillips

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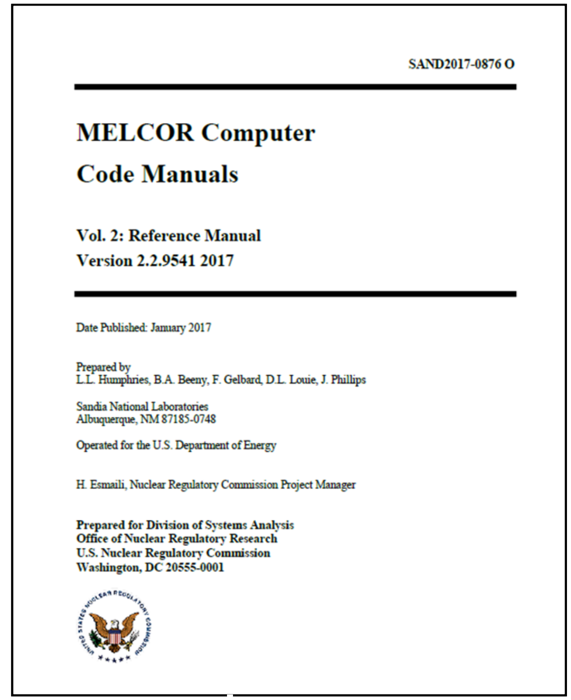
Operated for the U.S. Department of Energy

H. Esmaili, Nuclear Regulatory Commission Project Manager

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



SAND2017-0876 O

MELCOR Computer
Code Manuals

Vol. 2: Reference Manual
Version 2.2.9541 2017

Date Published: January 2017

Prepared by
L.L. Humphries, B.A. Beeny, F. Gelbard, D.L. Louie, J. Phillips

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MELCOR 2.2 Quicklook Overview of Model Changes in MELCOR 2.2

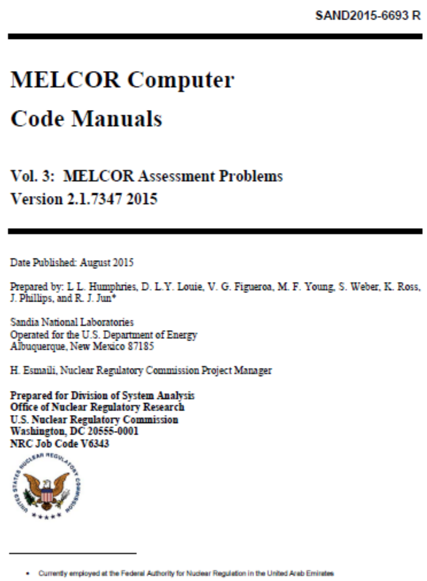
Volume I: User Guide

R&A Complete
SAND2017-0445 O

Volume II: Reference Manual

R&A Complete
SAND2017- 0876 O

Future MELCOR Manual Updates



SAND2015-6693 R

MELCOR Computer Code Manuals

Vol. 3: MELCOR Assessment Problems
Version 2.1.7347 2015

Date Published: August 2015

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

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Volume III: Assessments

R&A Complete
SAND2015-6693 R

By September 2018
- Demo PWR plant deck
- Demo BWR plant deck
- COR/CVH Nodalization
- Containment DBA
- Numerical Variance
- Steady State Initialization

By September 2019
- FL/CVH Modeling
- Uncertainty Analysis
- Spent Fuel Pool Modeling
- Radionuclide Class Modeling
- MELCOR/MACCS Integration
- Troubleshooting MELCOR runtime issues
- Lower Head Modeling
- Heat Structure Modeling
- Cavity Related Modeling

Volume IV: Modeling Guide

Objectives for Modeling Guide

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

MELCOR

- New Modeling
- SQA
- Utilities

Cases in MELCOR Assessment Report - SAND2015-6693 R

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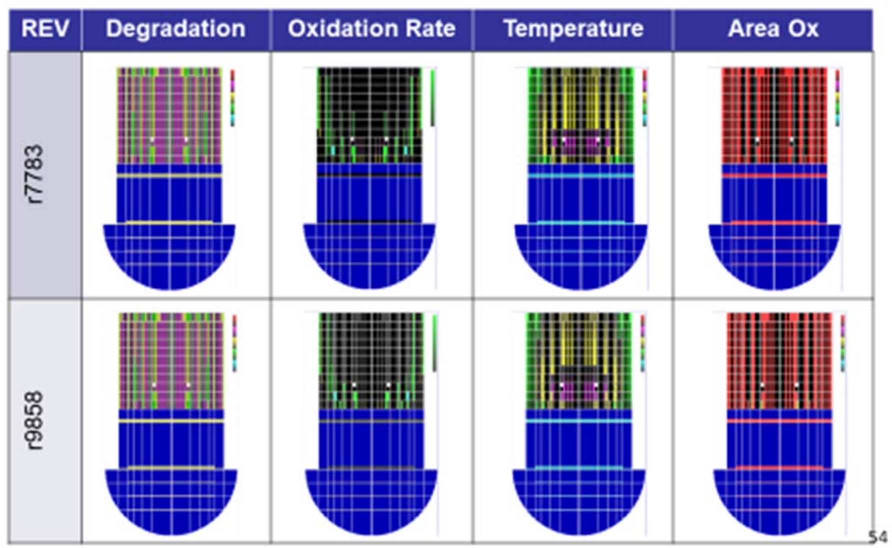
- **MELCOR ANALYTIC ASSESSMENT**
  - Saturated Liquid Depressurization
  - Adiabatic Expansion of Hydrogen
  - Transient Heat Flow in a Semi-Infinite Heat Slab
  - Cooling of Heat Structures in a Fluid
  - Radial Heat Conduction in Annular Structures
  - Establishment of Flow
- **MELCOR ASSESSMENTS AGAINST 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)

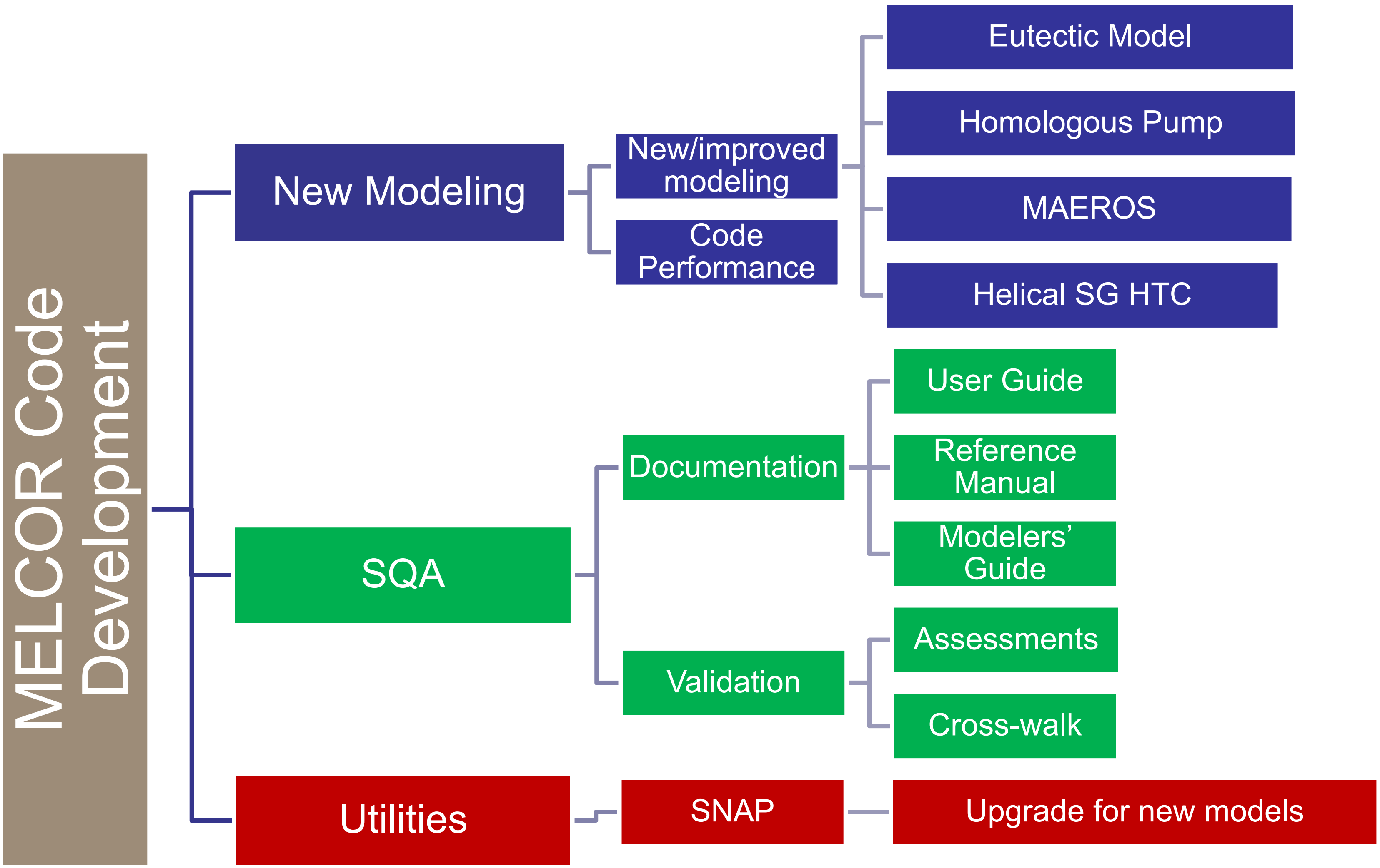
SNAP Upgrade (Upcoming)

- Input Processing
  - Support input for new models
    - Recent update to UG would be a good start but we should review again for missing input
    - Some features may be difficult to implement – vector CFs
  - Review nomenclature used
  - Possible reorganization of interface
    - COR package input is inefficient

- Post-processing
  - Remove idiosyncrasies -
    - Requirement to load a med file in order to inherent COR dimensions
  - Improve interface
    - Adding a profile plot is extremely laborious
  - Extending graphical output
    - Update COR bean to show more than just component degradation
      - temperature, oxidation rate, Zr mass, flow, etc.
    - Update MELCOR & PTFREAD for BWR first



Questions?



MELCOR Code Development
New Modeling
New/improved modeling
Code Performance
Eutectic Model
Homologous Pump
MAEROS
Helical SG HTC
SQA
Documentation
User Guide
Reference Manual
Modelers' Guide
Validation
Assessments
Cross-walk
Utilities
SNAP
Upgrade for new models

Backup Slides