SAND2019-1661PE

MELCOR Code, Source Term Models, and Recent Updates

SAND2018-XXXX

PRESENTED BY

Larry Humphries

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Outline

MELCOR Overview

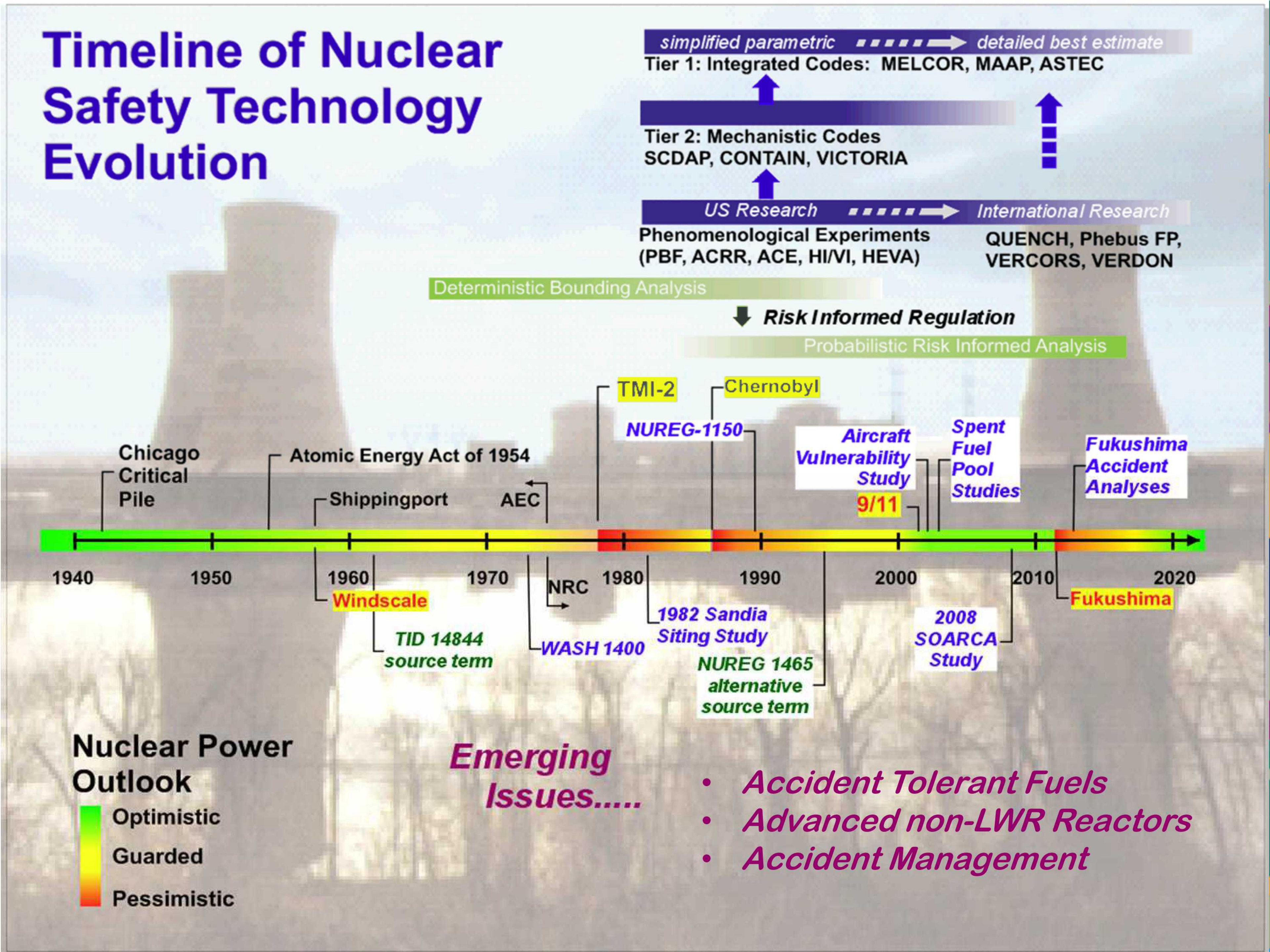
Detail Description of Source Term Model

New/Improved Models

Code Development Plans

X-Walk Insights to Severe Accident Modeling (time permitting)

MELCOR Overview


Timeline of Nuclear Safety Technology Evolution
simplified parametric
detailed best estimate
Tier 1: Integrated Codes: MELCOR, MAAP, ASTEC
Tier 2: Mechanistic Codes
SCDAP, CONTAIN, VICTORIA
US Research
International Research
Phenomenological Experiments
(PBF, ACRR, ACE, HI/VI, HEVA)
QUENCH, Phebus FP,
VERCORS, VERDON
Deterministic Bounding Analysis
Risk Informed Regulation
Probabilistic Risk Informed Analysis
TMI-2
Chernobyl
NUREG-1150
Aircraft Vulnerability Study
Spent Fuel Pool Studies
Fukushima Accident Analyses
Chicago Critical Pile
Atomic Energy Act of 1954
Shippingport
AEC
9/11
1940
1950
1960
1970
1980
1990
2000
2010
2020
NRC
Windscale
Fukushima
1982 Sandia Siting Study
2008 SOARCA Study
TID 14844 source term
WASH 1400
NUREG 1465 alternative source term
Nuclear Power Outlook
Optimistic
Guarded
Pessimistic
Emerging Issues.....
• Accident Tolerant Fuels
• Advanced non-LWR Reactors
• Accident Management

Requirements of an Integrated Severe Accident Code

Fully Integrated, multi-physics engineering-level code

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

Diverse Application

- Multiple 'CORE' designs
- User constructs models from basic constructs
- Adaptability to new or non-traditional reactor designs
  - ACR700, ATR, VVER, HTGR, …

Validated physical models

- ISPs, benchmarks, experiments, accidents

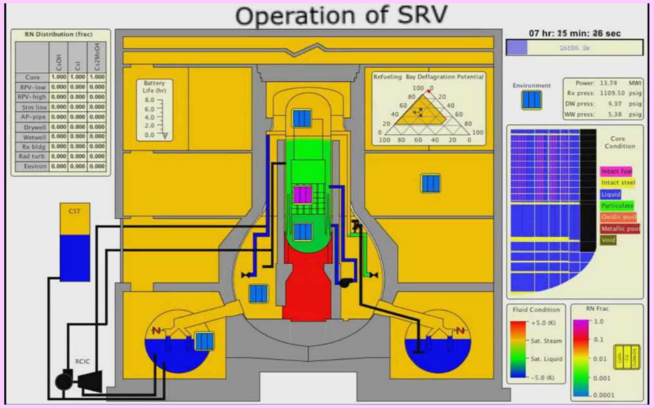
Uncertainty Analysis & Dynamic PRA

- Relatively fast-running
- Reliable code
- Access to modeling parameters

User Convenience

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

Multi- Physics

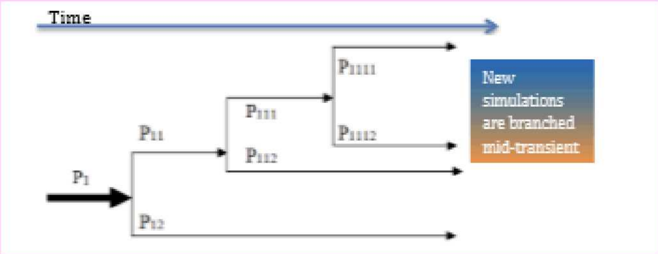


SOARCA LTSBO

Diverse Application

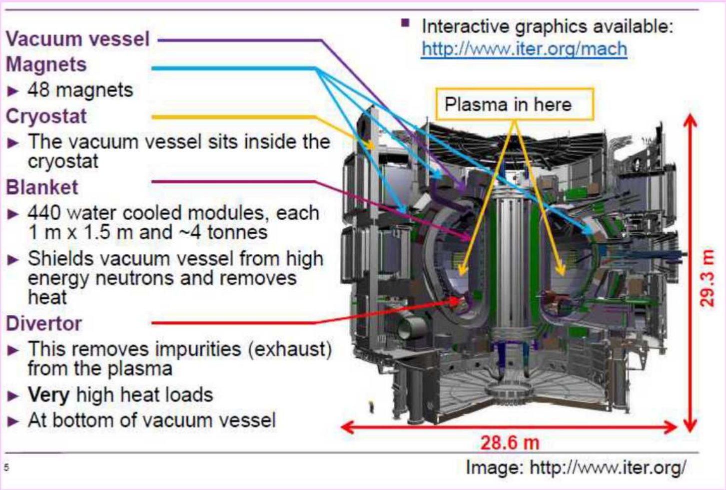
Advanced Test Reactor

Uncertainty & Dynamic PRA



Dynamic Event Tree

Non-Reactor Applications

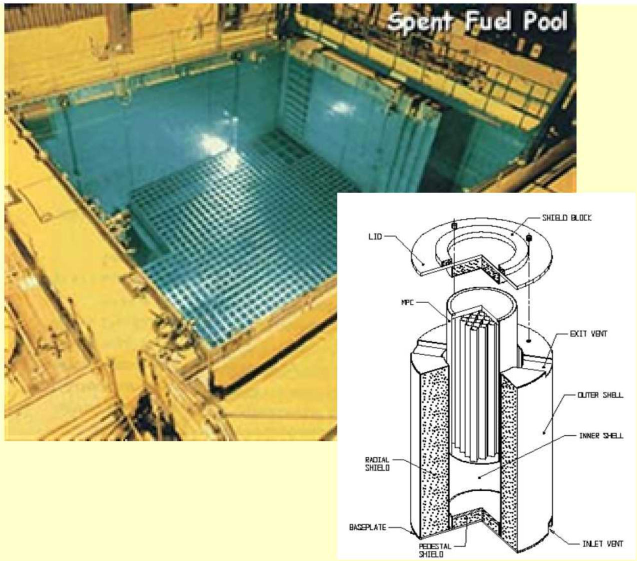


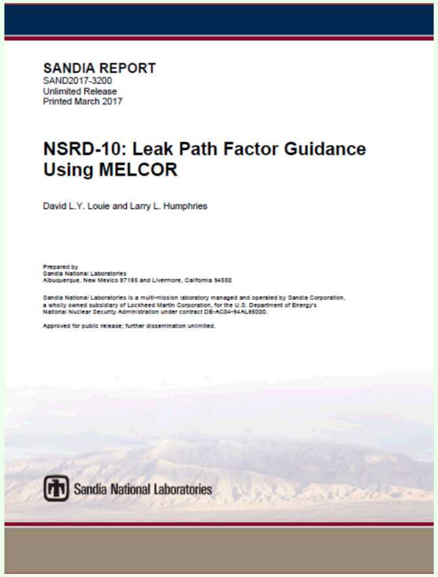
Fusion

- 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





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NSRD-10: Leak Path Factor Guidance Using MELCOR

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Sandia National Laboratories

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

Detailed Description of ST Models

Radionuclide Package

Tracks the release and transport of
- Fission product vapors & aerosols
- Non-radioactive masses such as water, concrete, etc.
- Traces hosted by other materials
  - Negligible volume and heat capacity

Aerosol physics
- MAEROS

Agglomeration of aerosols
- Several mechanisms cause collisions and sticking to produce larger particles
  - Brownian diffusion
  - Differential gravitational settling
  - Turbulent agglomerating by shear and inertial forces

Hygroscopic effects

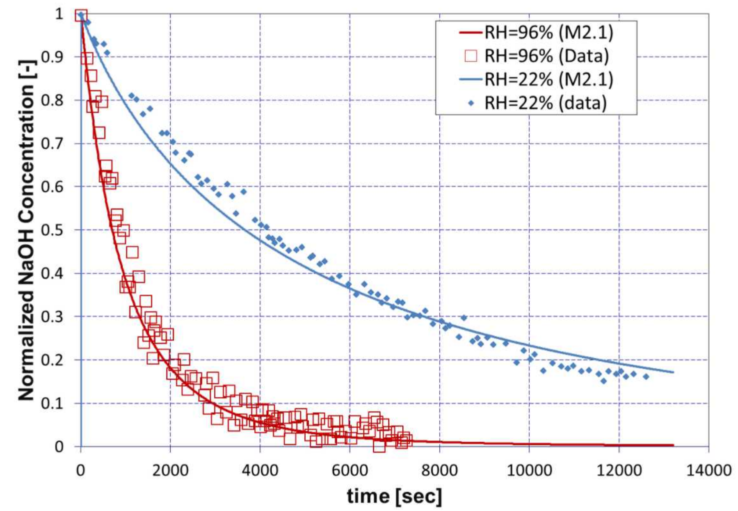
Condensation & evaporation
- TRAP-MELT

Deposition on surfaces
- Modeled as always sticking to surfaces contacted
- Several mechanisms drive aerosols to surfaces
  - Gravity
  - Brownian diffusion
  - Thermophoresis
  - Diffusiophoresis
  - Turbulent deposition

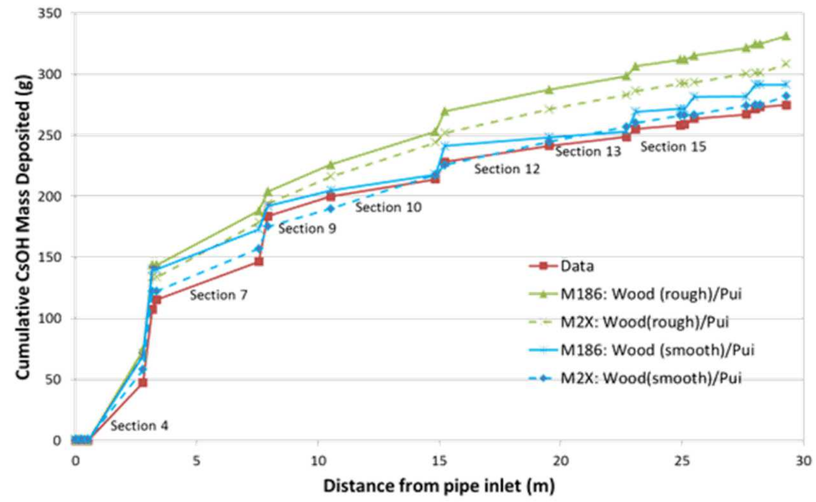
Pool Scrubbing
- SPARC

Iodine Pool Chemistry

AHMED – Hygroscopic Effects



LA3 – Turbulent Deposition



Initial Radionuclide Inventories

- RN Classes
  - species with similar chemical properties.
- Elemental inventories from tables of ORIGEN calculations
  - Can be user specified
- Spatial distributions
  - Fuel in the core
    - Radial & axial profiles
  - Fuel-cladding gap
  - Any initial cavity debris, and
  - Atmosphere and pool (of any control volume)
- Fuel FPs are transported with the fuel until released

Class	Name	Element	All Member Elements
1	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	Alkaline Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	Halogens	I	F, Cl, Br, I, At
5	Chalcogens	Te	O, S, Se, Te, Po
6	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	Early Transition	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, TC, Ta, V
8	Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Gd, Sm, Eu, Tb, Dy, Ho, Er, Tm, Yb, Cm, Lu, Am, Bk, Cf
10	Uranium	U	U
11	More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl,
12	Less Volatile Main Group	Sn	Ga, Ge, In, Sg, Ag
13	Boron	B	B, Si, P
14	Water	H2O	H2O
15	Concrete	–	-
16	Cesium	iodide	CsI-

Fission product release/transport is governed primarily by thermo-chemical characteristics of species, not their radioactive properties. Therefore, species with similar chemical properties are combined.

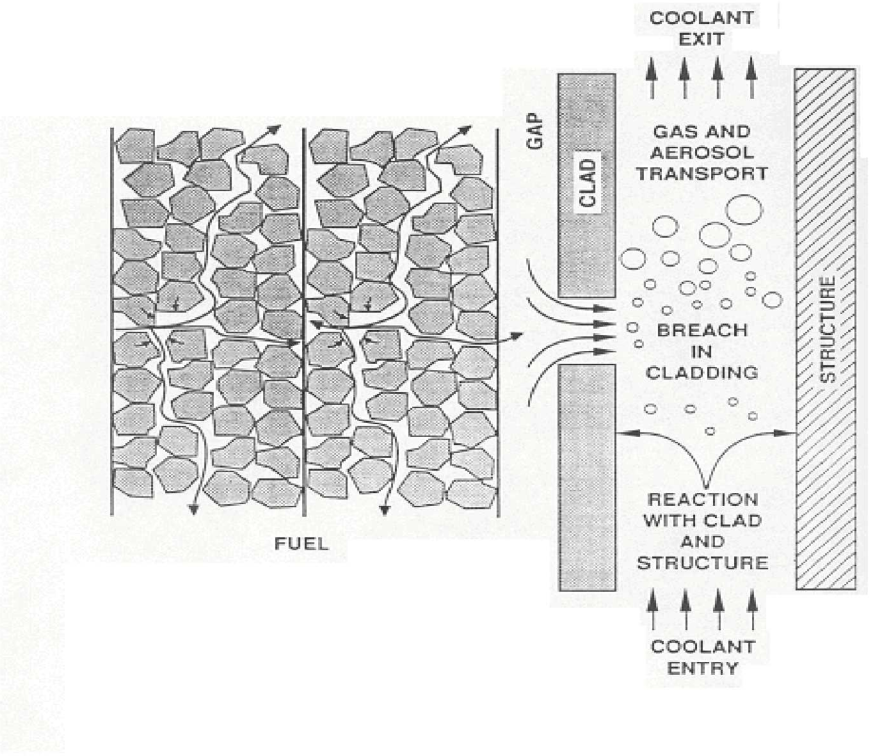
RN Release

Can occur from

- Fuel-cladding gap exceeding a failure temperature criterion (or losing intact geometry)
- Material in the core using the various CORSOR empirical release correlations [based on T_{fuel}]
- During core-concrete interactions in the reactor cavity using the VANESA release model

After release to a control volume, masses may exist as aerosols and/or vapors

- Depending on the vapor pressure of the radionuclide class and the volume temperature



Four basic release models, with options

- CORSOR

  $k = A \exp(B\,T) \qquad for\ T \ge T_i$ where k is the release rate

- CORSOR-M,

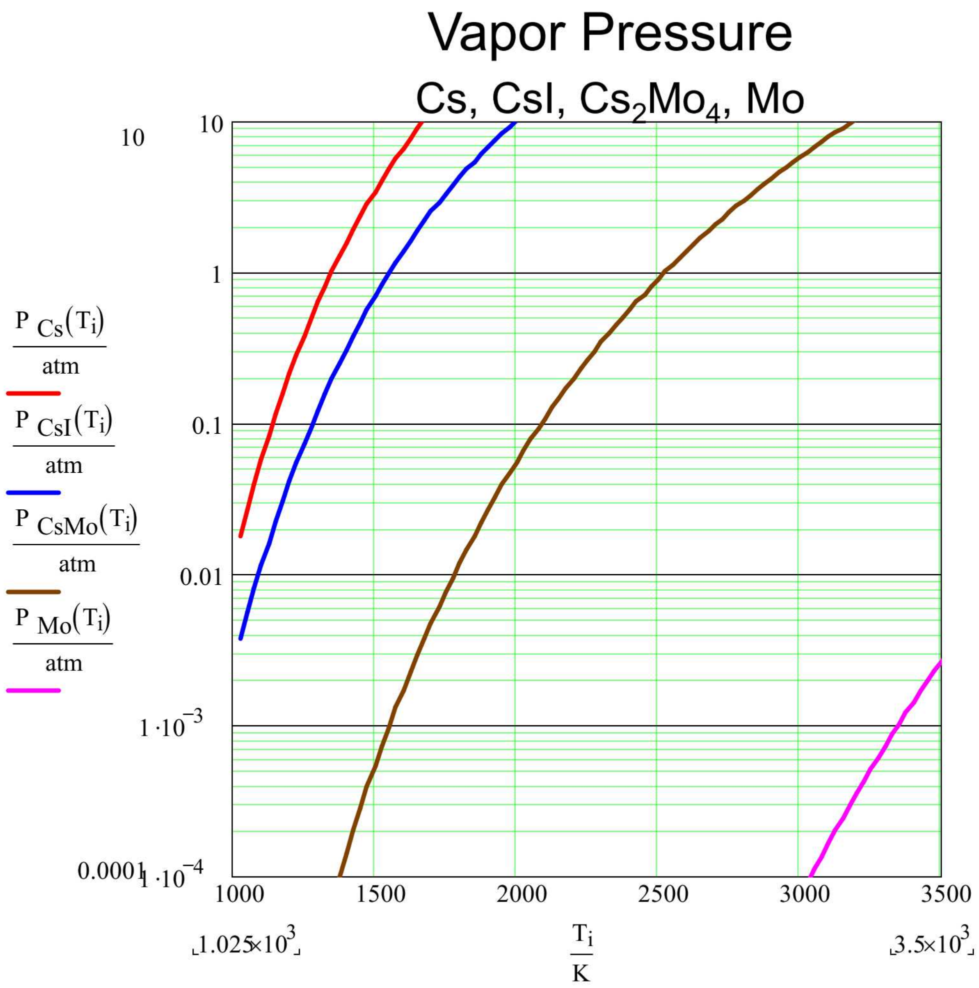
  $k = k_o \exp(-Q/RT)$

- CORSOR-Booth*,
  - Limited by mass transport in fuel
  - $D_0 \exp(-Q'/RT)$
  - Also limited by mass transfer through gas phase
  - Options for high- or low-burn-up fuel

MELCOR RN Release Models

Modified ORNL Booth
- Same equation set
  - Known Limitations
- Cs_2MoO_4 vapor pressure
- Modified scaling factors

Improved results
- FPT-1
  - Cs, I, Mo
- ORNL VI Tests
  - VI 2 (oxidizing)
  - VI 3 (oxidizing)
  - VI 5 (reducing)
- Vercors 4 (oxidizing)
  - Cs, I, Mo



Aerosol Component/Class Mapping

MELCOR uses CLASS grouping to represent FP species

- Common physical/chemical characteristics (e.g., volatility)

MAEROS recognizes and operates on the aerosol portions of these FP (radioactive and non-radioactive) classes

- Component ≡ a particular type of aerosol material

MELCOR allows the user to define aerosol ***Components*** which are groupings of one or more fission product ***Classes*** (the mapping between RN classes and MAEROS aerosol components)

- These components are allowed to have distinct size distributions
  - The size distributions are characterized by the amount of aerosol mass within a range of aerosol particle sizes
  - Size ranges are called ***Sections***

Aerosols: MAEROS

MAEROS sectional model of Fred Gelbard
- 10 sections [.1 - 50 μm]
- Condensed FP vapor sourced into smallest section

Particles grow in size
- Agglomeration
- Water condensation

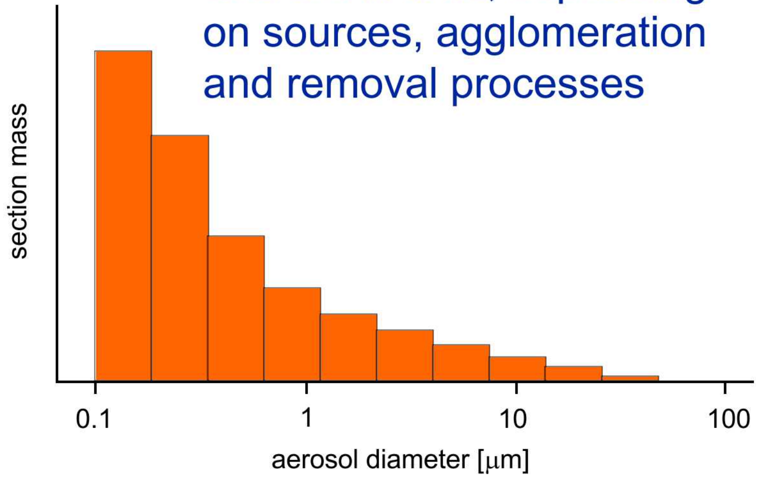
Particle fallout by gravitational settling

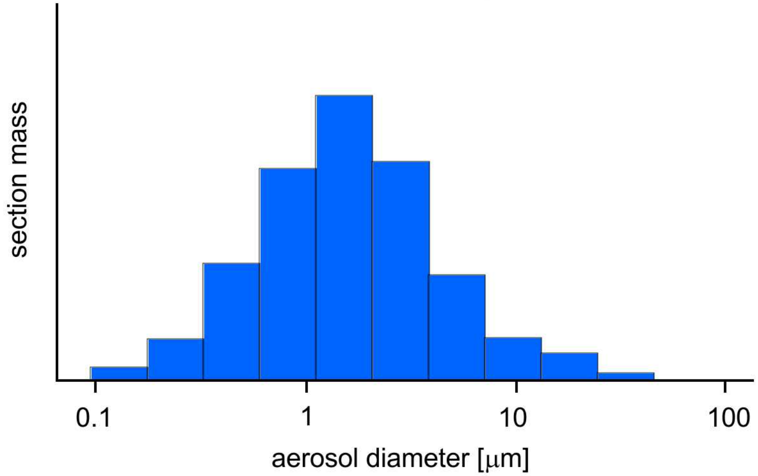
Particle deposition processes
- Thermophoresis
- Diffusiophoresis
- Brownian motion

PWR Ag aerosol release from control rods modeled
- Significant aerosol mass
- Affects agglomeration, growth and fallout

Cs chemisorption in RCS modeled
- Iodine from CsI revolatilizes when reheated

Aerosol size distribution evolves in time, depending on sources, agglomeration and removal processes

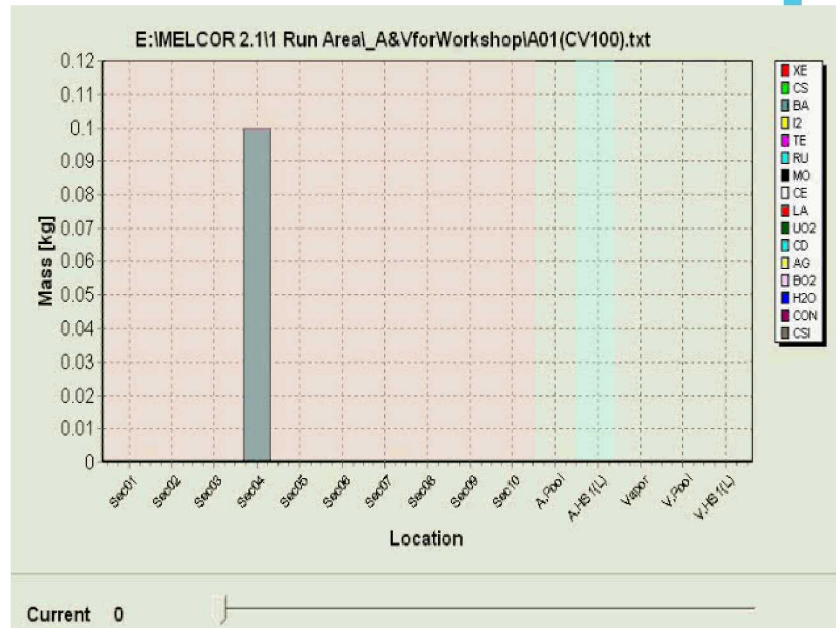


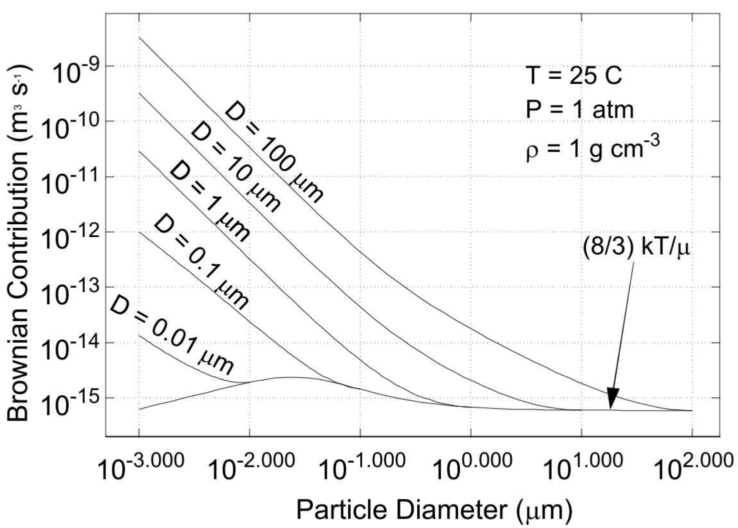


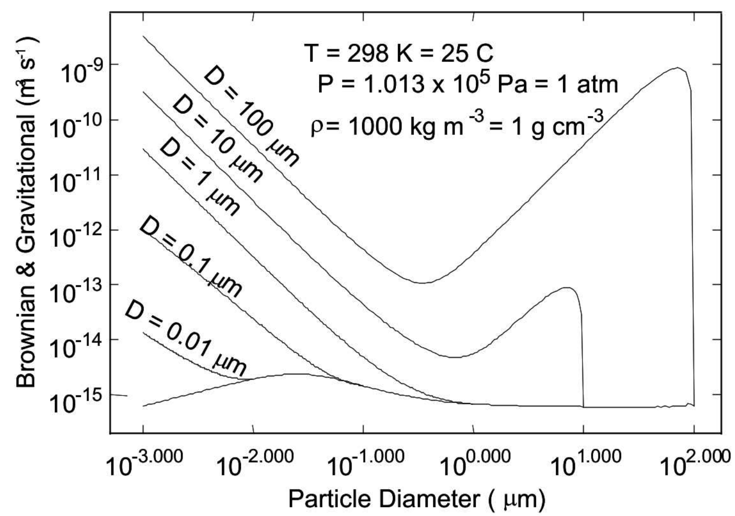
Agglomeration

Agglomeration becomes more significant for more concentrated aerosols

- Particles collide, stick, and become larger particles;
  Rate ~ $\beta N(D_i)\, N(D_j)$ where N is the number density (m^{-3})
- Brownian mechanism dominates for small particles, differential gravitational for large ones







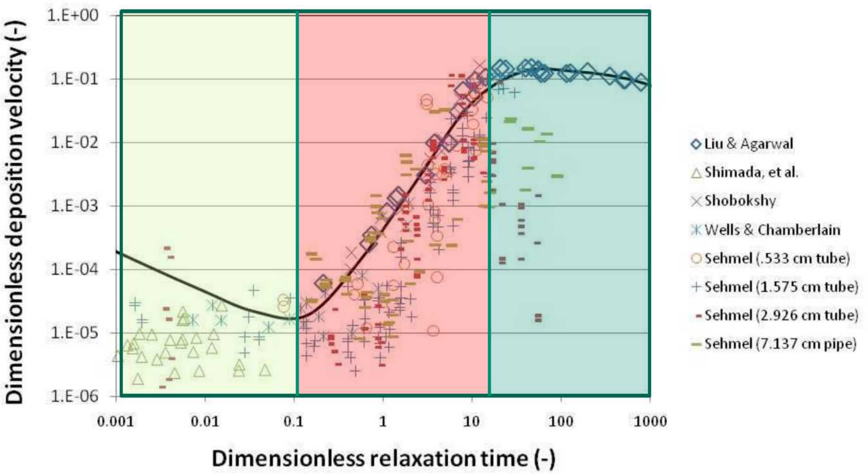
Validation against DEMONA tests

Turbulent Deposition Models

Turbulent deposition in pipe flow
- Wood's model for smooth pipes (default)
- Wood's model for rough pipes
- Sehmel's model for perfect particle sinks (VICTORIA)

Bend Impaction Models
- Pui bend model
- McFarland bend model
- Merril bend model

- Inertia moderated regime
- Eddy diffusion impaction regime
- Turbulent particle diffusion



Validation against LACE tests

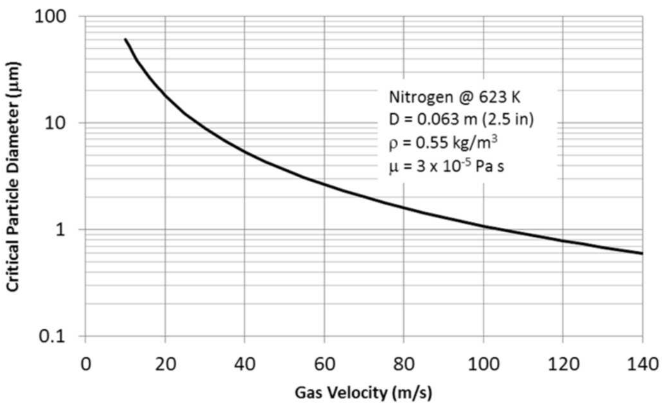
Re-suspension Model

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

$$D_{crit} = \frac{4\times10^{-5}}{\pi\tau_{wall}}\ (m), \qquad \tau_{wall} = \frac{f\rho v^2}{2}\ (N/m^2) \qquad f = \frac{0.0791}{Re^{0.25}}$$

- Does not account for possible changes in size distribution at the surface
- Assumes continually homogenous distribution of particle sizes
- Alternatively, 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

Reference

- "Liftoff Model for MELCOR," Mike Young
- SAND2015-6119

Validation against Tests

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

Condensation/evaporation

FPs & water can condense/evaporate onto/from

- Aerosols; heat structure surfaces; and/or water pools

Aerosol water ≡ fog (CVH pkg)

- Change in fog mass
  - Determined by thermodynamics
  - Distributed over aerosol sections

Water condensation/evaporation for heat structure and water pool surfaces

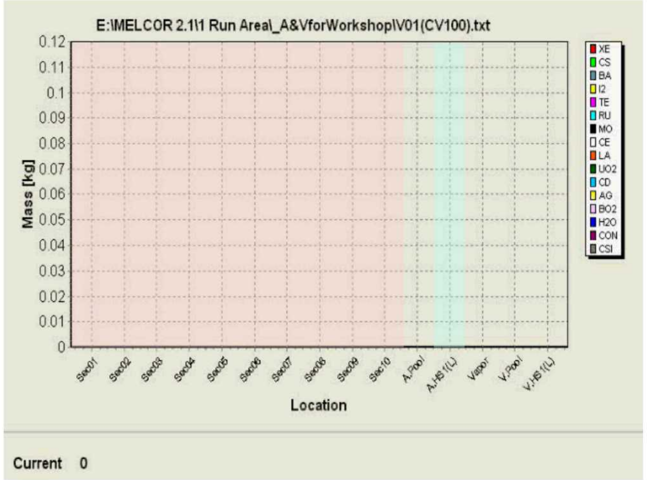
- Mason equation

Calculation of FP vapor condensation/evaporation

- TRAP-MELT2 rate equations based on
  - Surface areas, mass transfer coefficients, atmosphere concentration, and the saturation concentrations corresponding to the temperatures of the surfaces

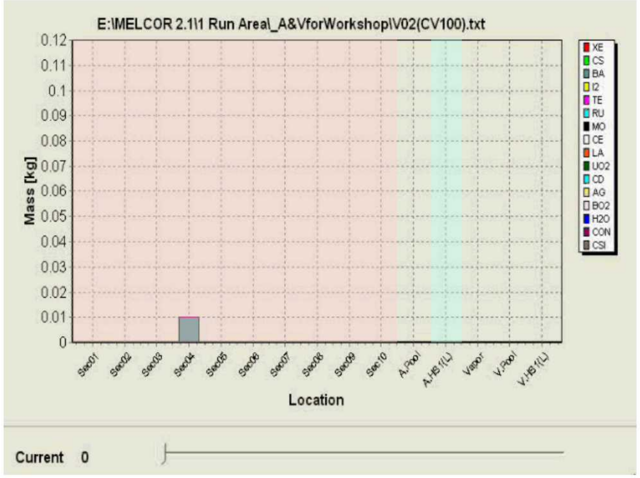
Case 1 No vapor, no aerosol

- Cs concentration rises to saturation
- First aerosols form in smallest section, then agglomerate rapidly
- Further condensation on existing aerosols



Case 2 No vapor, little aerosol

- Same rise to saturation
- Most early condensation on existing Ba aerosols



Decay Heat Distribution (CV)

All decay heat released by radionuclides in a control volume pool is assumed to be absorbed by that pool

Decay heat released by radionuclides in the control volume atmosphere and from those deposited on the various heat structure surfaces can be apportioned according to user specifications among the

- Volume atmosphere
- Surfaces of heat structures in that volume
- Pool surface (if a pool is present)

Decay Heat Distribution (FP)

Simulation of decay radiation transmitted through flow paths

- Specify the fraction going to the atmosphere and surfaces of other volumes

Decay heat generated as

- γ-radiation (~½) & β-radiation (~½)

Deposition of decay heat in a volume atmosphere results primarily from absorption of β-radiation

Pool Scrubbing

Adapted from SPARC-90 code

- Steam condensation at the pool entrance
- Aerosol deposition by Brownian diffusion, gravitational setting, and inertial impaction
- Subject also to evaporative forces, for the rising bubble

Aerosols and iodine vapor are removed

- Removal of other vapor species can be treated identically to iodine vapor

Model treats

- Regular flow paths that vent through pools,
- Gases generated by core-concrete interactions flowing through overlying pools

Decontamination factor calculated

Filter Trapping (1)

Some fraction of the transported RN materials may be removed by the action of filters in the flow paths

- Calculated by CVH: aerosols & vapors transported through flow paths with the bulk fluid flow of pool and/or atmosphere

Flow path can contain more than one filter

- Single filter can remove either, but not both, aerosol or fission product vapor

Filter efficiency, user-specified DFs per bin size or vapor

- By default, a DF (= 1) is applied to all RN classes except water

User-specified maximum loading

- Loading reached, no further RN materials are removed (i.e., DF = 1)

Filter Trapping (2)

Effect of filter loading on flow resistance of the associated flow path modeled through user input

- Requires construction of a CF to link the laminar loss coefficient for the flow path to the filter loading (see FL User's Guide)
- Filter loading may be obtained from one or more of the CF arguments (see RN User's Guide)

Decay heat energy from radionuclides deposited on filters is given to the downstream control volume according to the vapor flow direction

Spray Scrubbing (1)

Model, same as in HECTR code

Calculates the T-H behavior associated with spray systems

- Coupled to the RN pkg for the calculation of aerosol washout and atmosphere decontamination by the sprays
- SPR-RN interface may produce nonphysical results if the SPR pkg is required to make multiple passes through the same CV on a given timestep
  - Avoid by limiting the spray activity to a single drop size in each spray train
  - Restriction: only 1 spray train should pass through each CV

Spray Scrubbing (2)

Particulate removal by sprays is a mechanistic treatment of removal processes

- Modeled as a first-order rate process
- Different rate constants are used for vapors and aerosols because the removal processes are different
  - Vapor removal by adsorption is calculated using a stagnant film model for the adsorption efficiency
    - The vapor removal is calculated as an injection spray removal rate; no recirculation of spray liquid is considered

Limit on iodine adsorption by spray droplets (user specified) using a partition coefficient (equilibrium ratio of the iodine density in the liquid to its density in the gas)

- LWR accident conditions, iodine may exist as a vapor over relatively long time periods in containment pressure/ temperature conditions. Other materials have low vapor pressures at accident conditions that preclude their extended existence as vapors; that is, they condense to aerosol forms.

Spray Scrubbing (3)

Aerosol removal also included

- Inertial impaction and interception
  - Primary removal mechanisms as long as droplet radii are in the 10 – 100 micron size range
- Diffusiophoresis and diffusion effects
  - 1–10 μm diffusiophoresis becomes an important contributor
  - Diffusion only becomes important for droplets with radii , 0.1 μm
- Rate constant are a function of collection efficiency
  - Viscous and well as potential flow around a sphere are considered for both impaction and interception
  - Collection efficiencies for different processes are combined

No droplet interactions are considered

- Chemistry effects can be simulated in MELCOR through the use of class reaction and class transfer processes
  - class reaction process uses a first-order reaction equation with forward and reverse paths
  - class transfer process
    - can change material class or location of a radionuclide mass (caution: use feature carefully)
    - can be used to simulate fast chemical reactions
- With these two processes (reversible & irreversible reactions) phenomena including adsorption, chemisorption, & chemical reactions can be simulated
- Only FP vapors are considered in the chemistry models
  - Only fission product vapors can react with surfaces and only vapors and ions produced from them can undergo chemical transformations in the pool

FP Chemistry: Example

Consider the adsorption of CsI on a surface with a known deposition velocity which is then transformed immediately to CsOH plus HI when adsorbed water is present. After the transformation, the revaporization of CsOH is delayed until the surface temperature reaches T_1 while the HI revaporization is simply mass transfer limited. In this case, CsI, CsOH, and HI are separate material classes.

$$CsI(\text{gaseous}) \rightarrow CsI(\text{adsorbed})$$

$$\downarrow H_2O$$

$$CsOH\ (\text{gaseous}) \leftrightarrow CsOH\ (\text{adsorbed})$$

$$+\ (\text{depends on } T_1)$$

$$HI(\text{gaseous}) \leftrightarrow HI(\text{solid})$$

Chemisorption

Forms chemical bond with surface

Currently can only be done on materials in the MELCOR database & does not function for user-defined materials

Chemisorption Transport	
CsOH	Stainless steel
CsOH	Inconel*
CsI	Stainless steel
CsI	Inconel*
I_2	Stainless steel
HI	Stainless steel
Te	Stainless steel
Te	Inconel*

*not in database

Hygroscopic Models

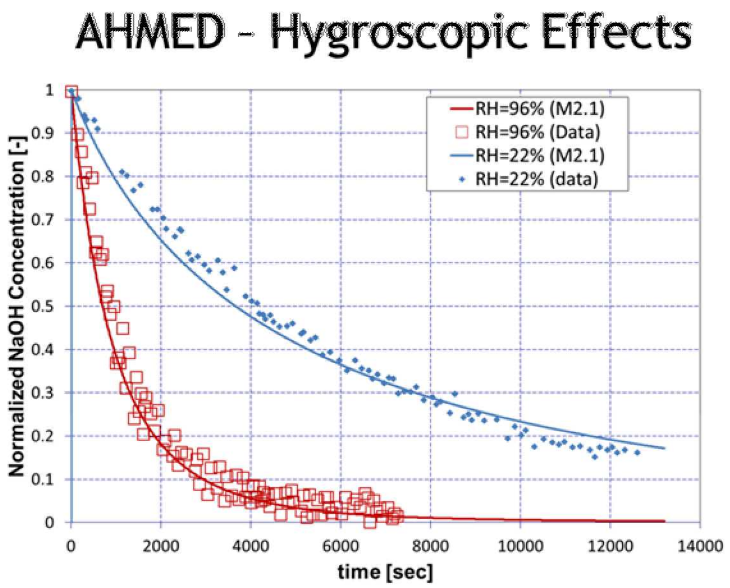
Mason Equation

Model describes diffusion of water vapor molecules to the surface of an aerosol particle, and the conduction of the latent heat of vaporization away from the particle and to the bulk atmosphere

- Solubility effect: hygroscopic
- Kelvin effect: surface tension
- Free molecule effects: noncontinuum

Aerosol particles that are soluble in water exhibit hygroscopic properties such that they can absorb moisture from an atmosphere with relative humidity less than 100%

- Effect leads to particle size growth as water vapor condenses onto the soluble particle
- Consequence:
  - Increase in gravitational settling rate
  - Subsequent depletion of airborne FP aerosols

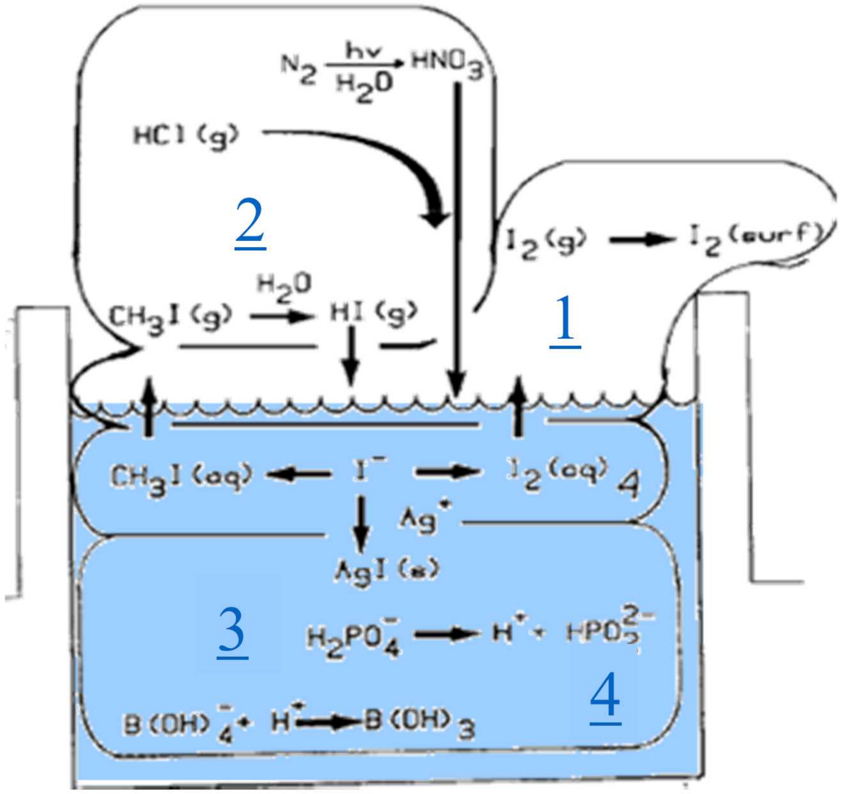


Amount of iodine released is reduced by controlling atmospheric iodine concentration

- Iodine can be confined in aqueous forms in pools and sumps, but
  - radioactive iodine may not remain trapped in water because of its relatively dynamic chemical behavior
    - There are important processes that can regenerate gaseous forms of iodine that release into the containment atmosphere from the water, thus becoming available for release to the environment for long times after the accident initiation
    - Chemical and radiolytic oxidation of iodine in the pool can lead to the formation of a variety of chemical forms of iodine, such as elemental iodine and volatile organic iodides
  - Formation of volatile forms of iodine in solution depends on
    - Dose rate to aqueous phase; temperature; pH; and total iodine concentration

Iodine Transformations Considered

Seven sub-models



- Acid generation and transport models (walls & pools)
- Pool pH calculation
- Silver iodine model
- Iodine aqueous pool chemistry (276 equation set)
- Pool atmosphere mass transfer
- Iodine atmospheric radiolysis and recombination
- Iodine atmosphere wall deposition

MELCOR Activity Calculations (BONUS) Bateman Equations

General Radioactive Decay Chain

$$N_1 \rightarrow N_2 \rightarrow N_3 \rightarrow \cdots N_j \rightarrow \cdots N_i$$

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 β and γ decays of fission products are considered

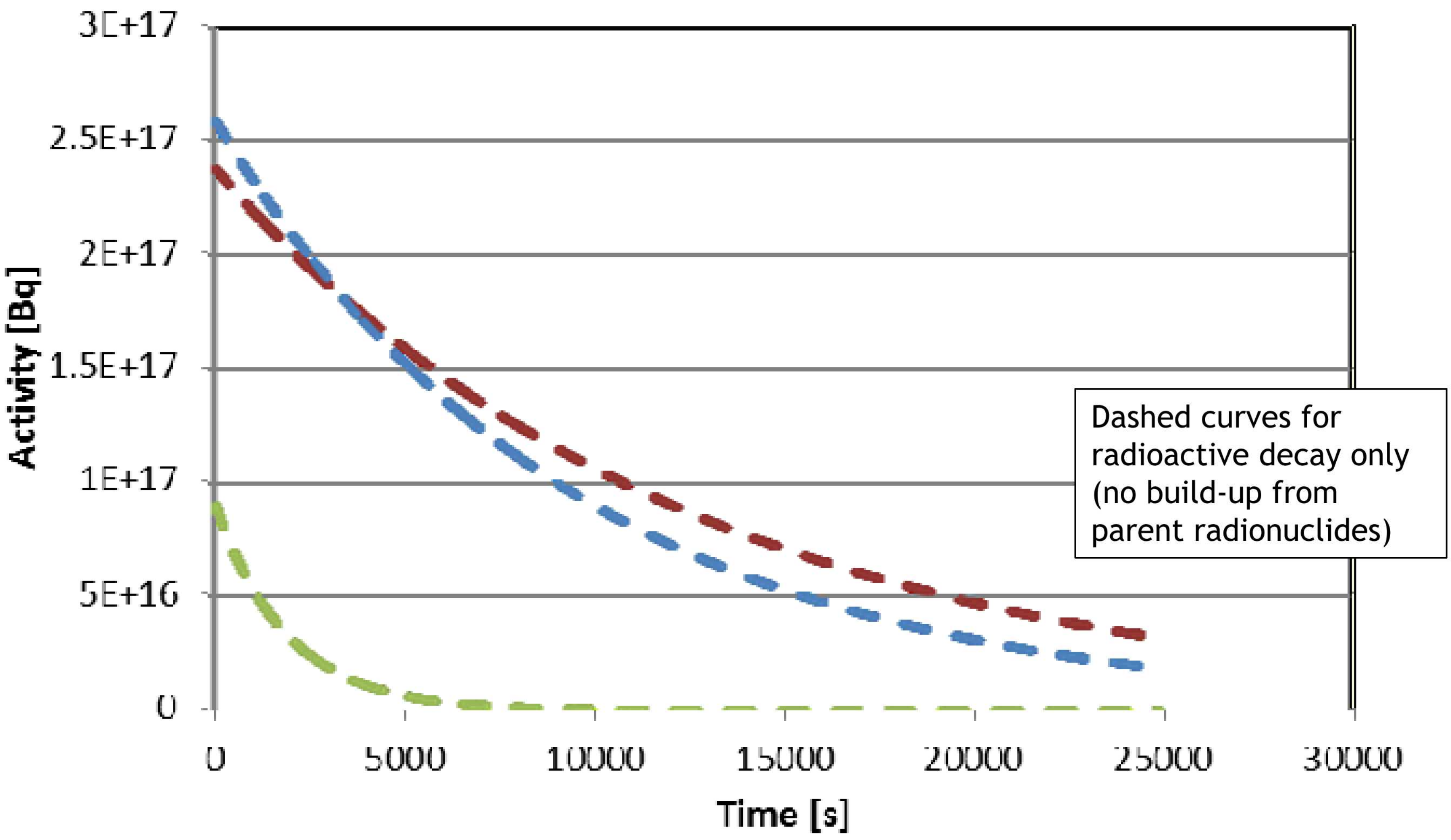
Thermal neutron capture also taken into account

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)

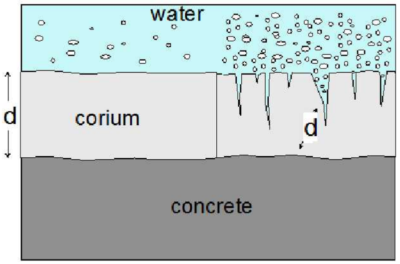


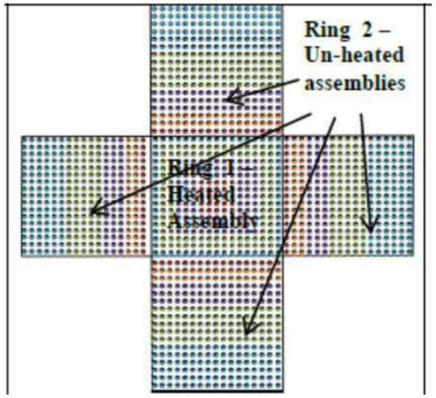
New or Improved Modeling

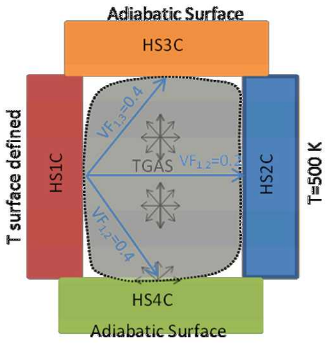
New Model Development Tasks (2014-2017)

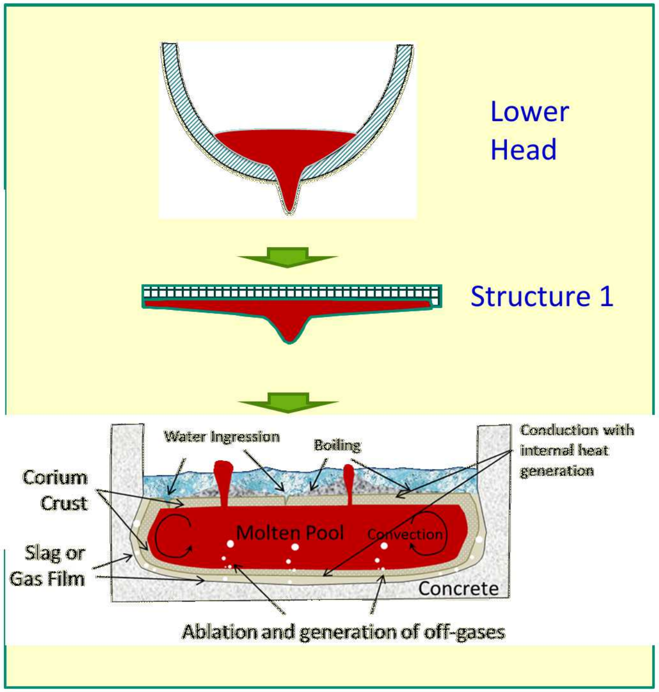
Completed

- 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)
- Vectorized Control Functions (NRC)
- CONTAIN/LMR models for liquid metal reactors
- Miscellaneous models and code improvements (NRC)
  - LAG CF
  - MACCS Multi-Ring Release
  - Valve Flow Coefficient
  - Non-dimensional parameters









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, 4th 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
  - 1st uses gamma energy from FissProd.in file
  - Overwrites with any gamma energy on 3rd field in inventory file.

Estimate dose given MELCOR-supplied activities throughout plant *One possible method*

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 ith isotope [Rad/hr]
- ϕ_i - gamma flux of the ith isotope [1/(cm^2 s)]
- E_i - gamma energy of the ith isotope [MeV]
- $\left(\frac{\mu_a}{\rho}\right)_{air}$ - mass absorption coefficient for air at E_i [cm^2/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

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 ith isotope (Ci),

R = equivalent spherical radius of volume V (cm^3),

ρ_{air} = density of air (g/cm^3),

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

and V = volume of MELCOR control volume(s) of interest (cm^3).

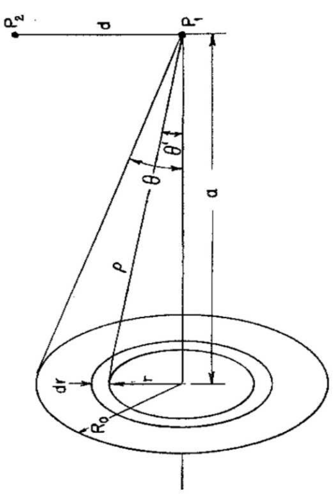
Assumptions:

- 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.

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

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



MELCOR Eutectic Model Overview

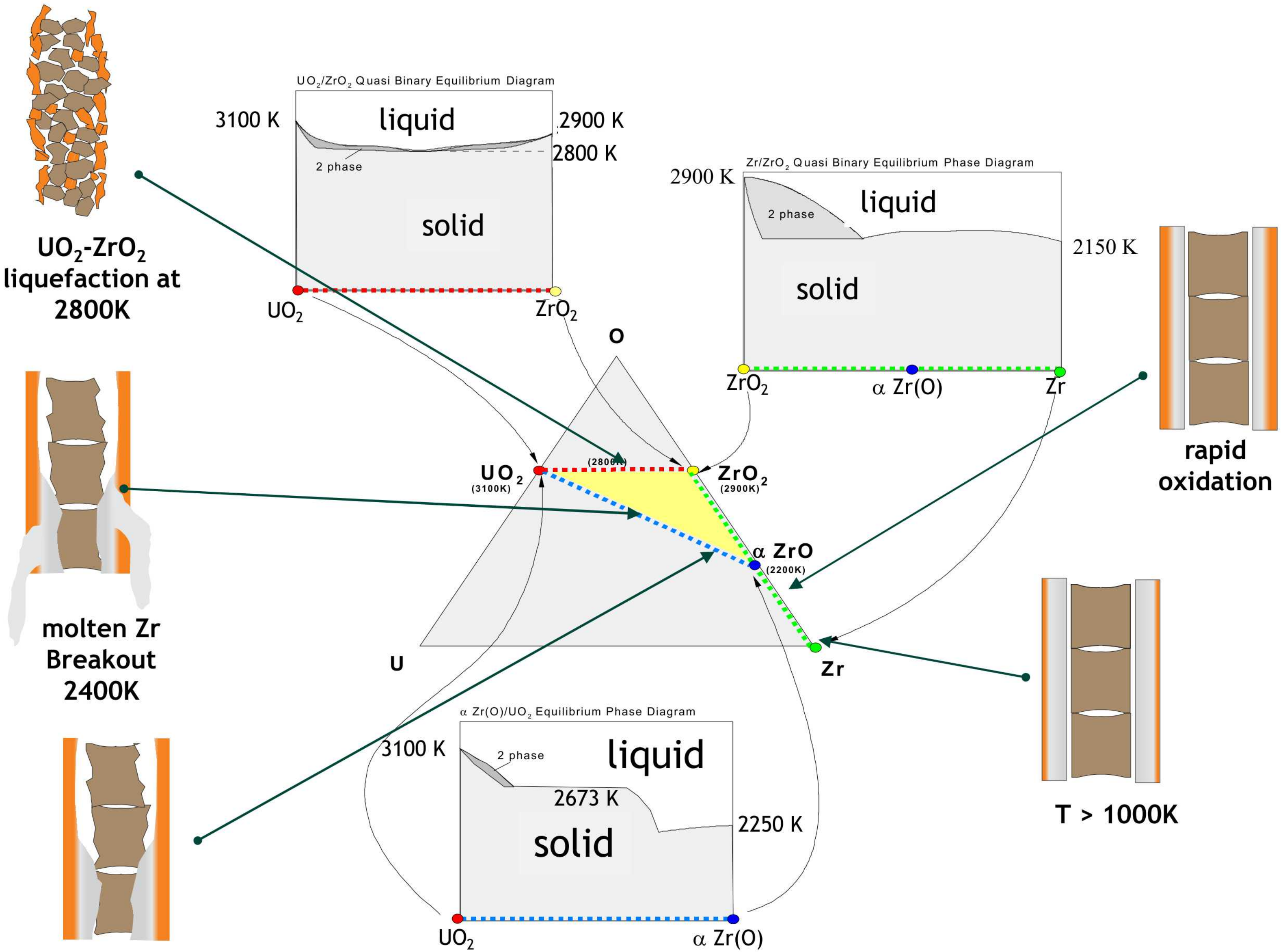
Eutectics model has been in the code since M1.8.2

- 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 almost ready for beta testing
  - Passes all mass energy conservation tests

U/Zr/O Ternary Phase Diagrams

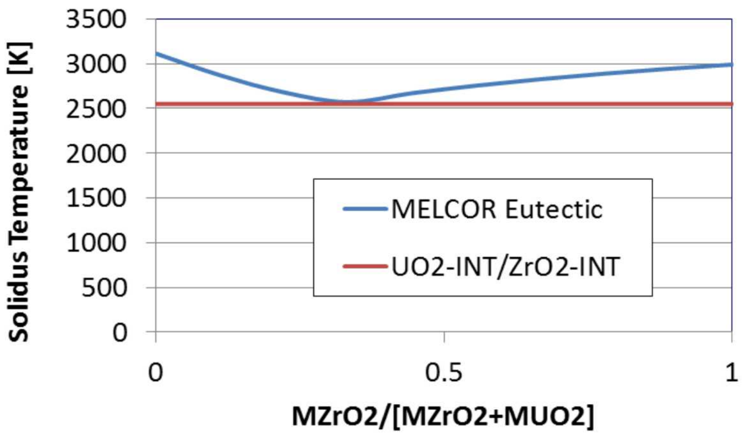


MELCOR Eutectic Temperature

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

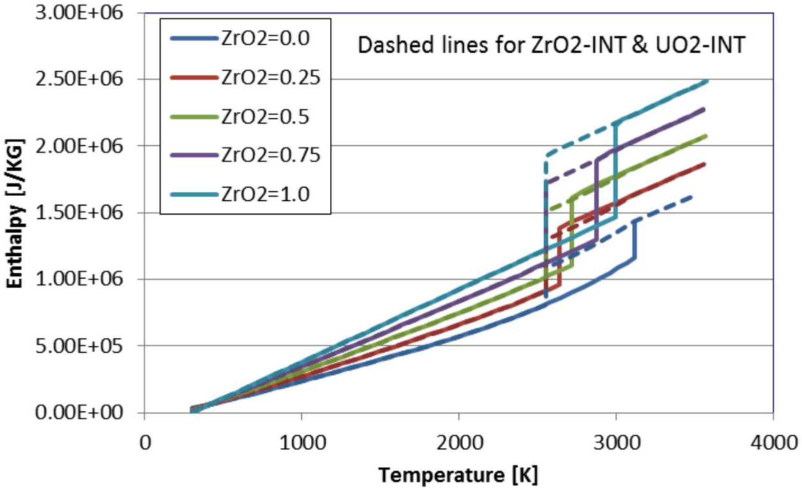


Eutectic Model

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



Eutectic Model Input

N

```
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

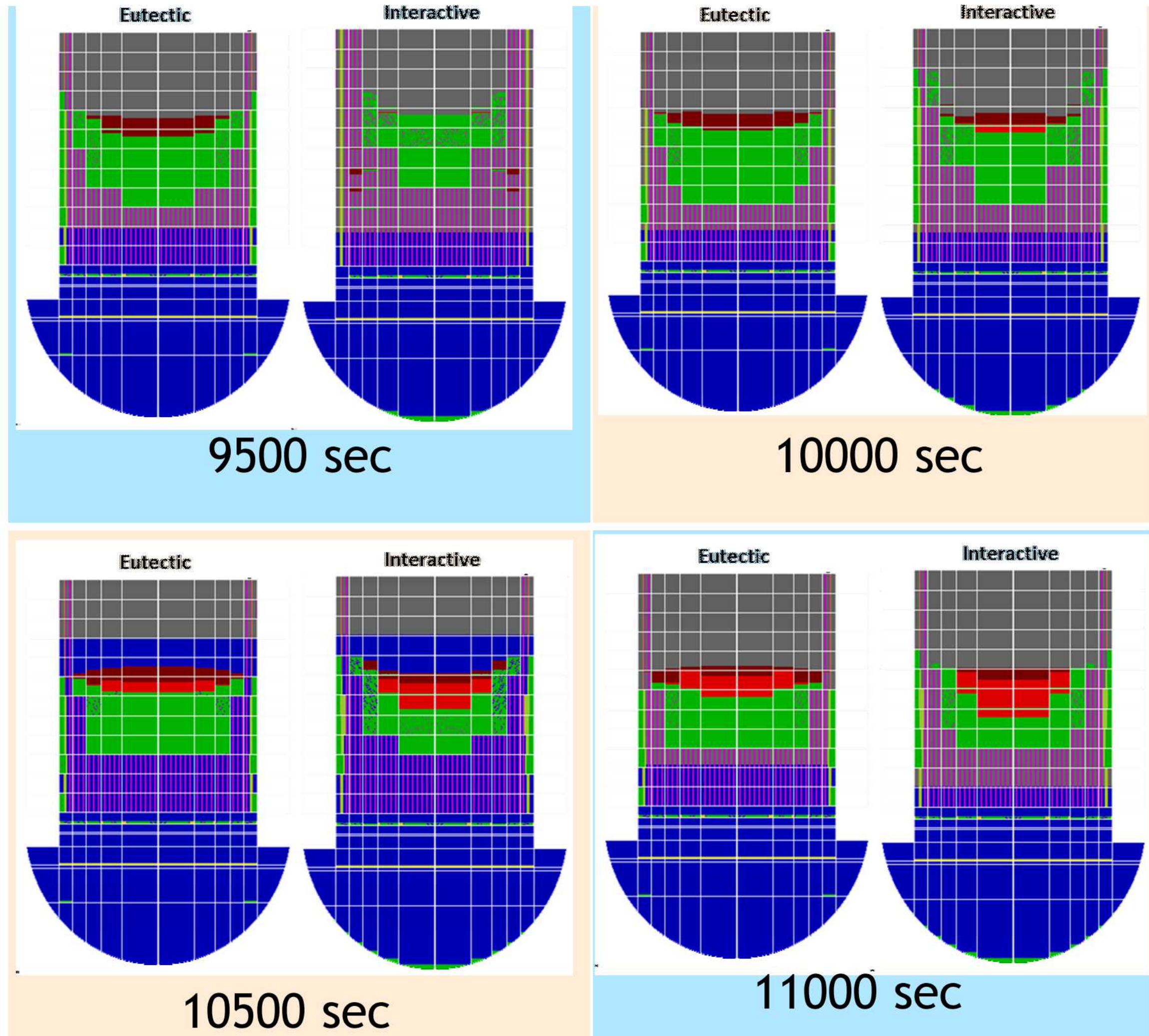
Interactive materials should not be used along with the eutectic model

```
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'
```

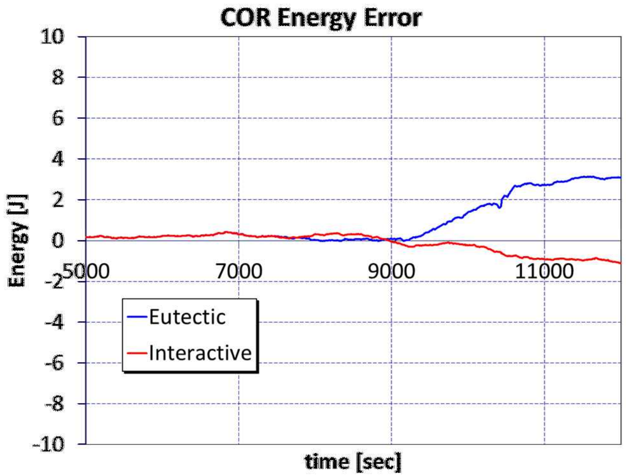
These records should be removed from input

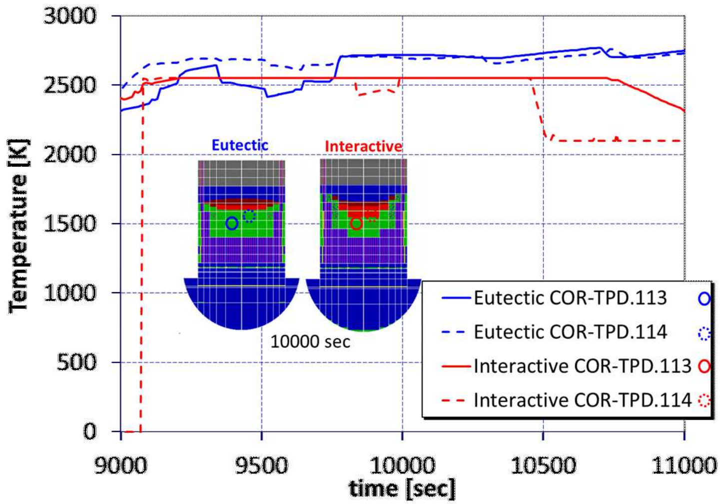
TMI Melt Progression –Preliminary Results

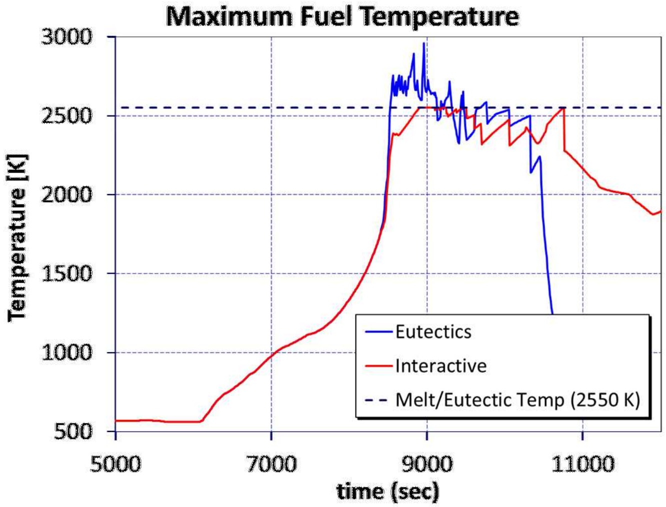
- Compare two TMI-2 test cases
  - Eutectics point = 2550 K
  - Interactive UO2-INT/ZRO2-INT 2550 K
- Similarities but notable differences
  - Core damage
    - Greater for eutectics
  - Size of Molten pool
    - Early: Greater for interactive
    - Later: Greater for eutectics
  - Material relocating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

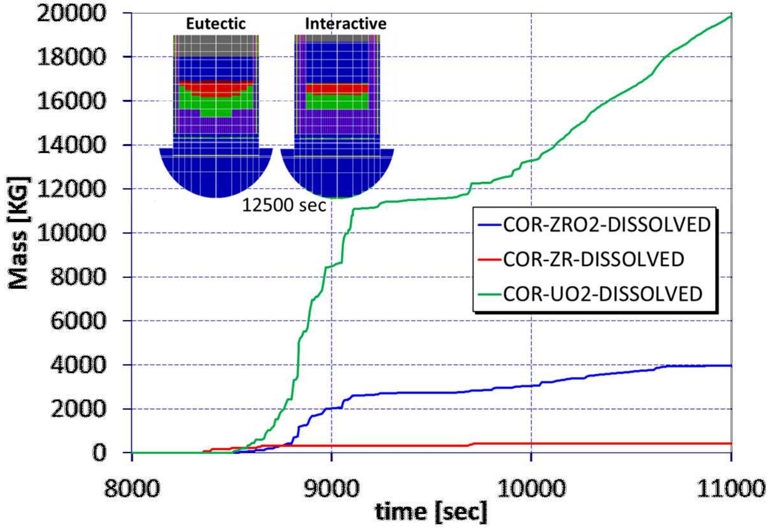


TMI Melt Progression –Preliminary Results









Code Development Plans

MELCOR Emerging Capabilities

High Temperature Gas Reactors

Sodium Fast Reactor

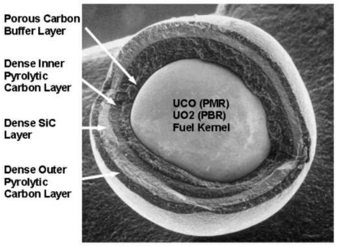
Molten Salt Reactor

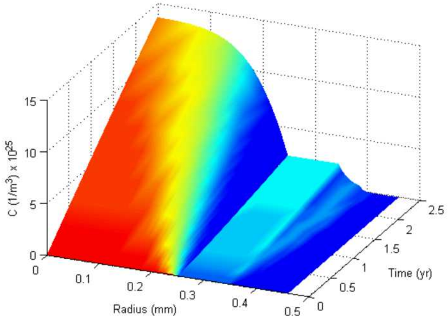
Developer	Design	Power	Technology
Oklo Inc.	Oklo	~ 7 MWt	Compact fast reactor
Transatomic power	Transatomic	Small scale	Molten Salt Reactor
Terrestrial Energy	Integral molten salt reactor	400 MWt	Molten Salt Reactor
X-Energy	Xe-100	200 MWt	Modular High Temperature Gas Cooled
Terrapower	Molten chloride fast reactor (MCFR(	~2000 MWt	Molten Salt Reactor

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

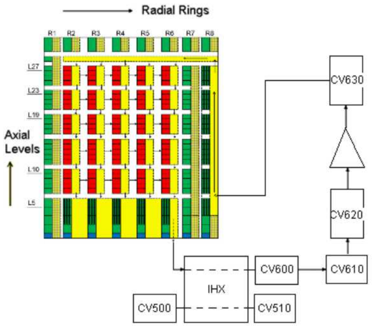
$$\frac{\partial C}{\partial t} = \frac{1}{r^m}\frac{\partial}{\partial r}\left(r^m D \frac{\partial C}{\partial r}\right) - \lambda C + S$$

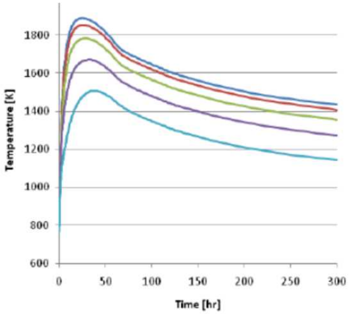




Existing Modeling Gaps

- 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





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

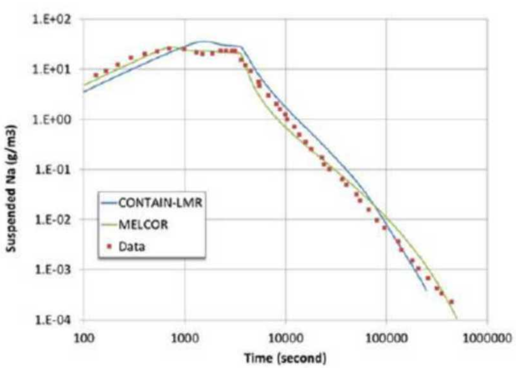


Figure 33. Suspended Na Aerosol Mass - AB1

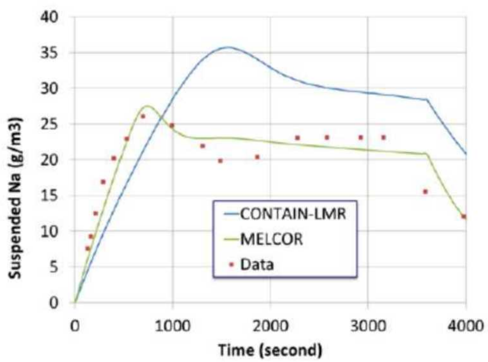


Figure 34. Suspended Na Aerosol Mass-AB1

Existing Modeling Gaps

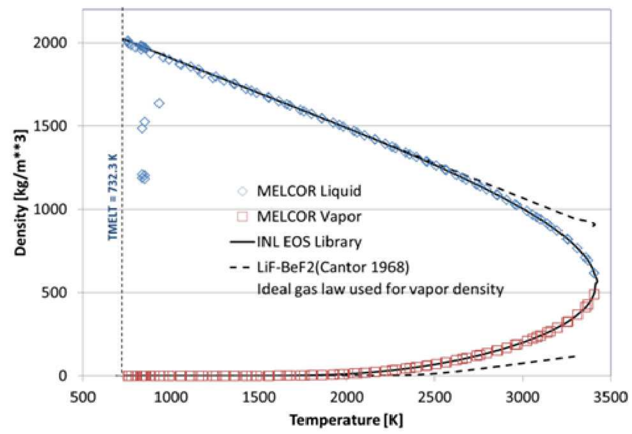
SFR Core modeling
- Fuel thermal-mechanical properties
- Fuel fission product release
- Fission product transport modeling
  - FP speciation & chemistry
  - Bubble transport through a sodium pool
- Core degradation models
  - SASS4A surrogate model

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
- Sodium-concrete interaction model (in development)

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

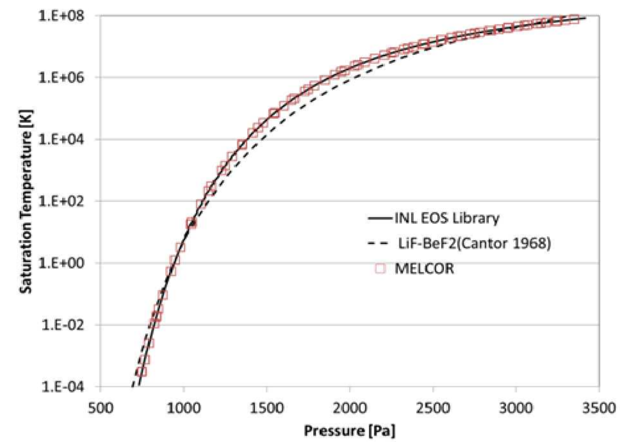


Fission product modeling

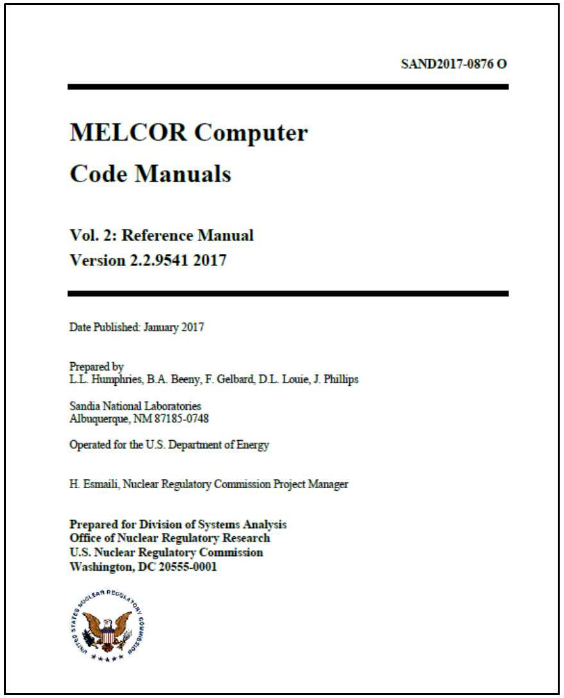
- Fission product interaction with coolant, speciation, vaporization, and chemistry

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.



Verification & Validation of Models



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MELCOR Computer Code Manuals

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Volume II: Reference Manual

R&A Complete
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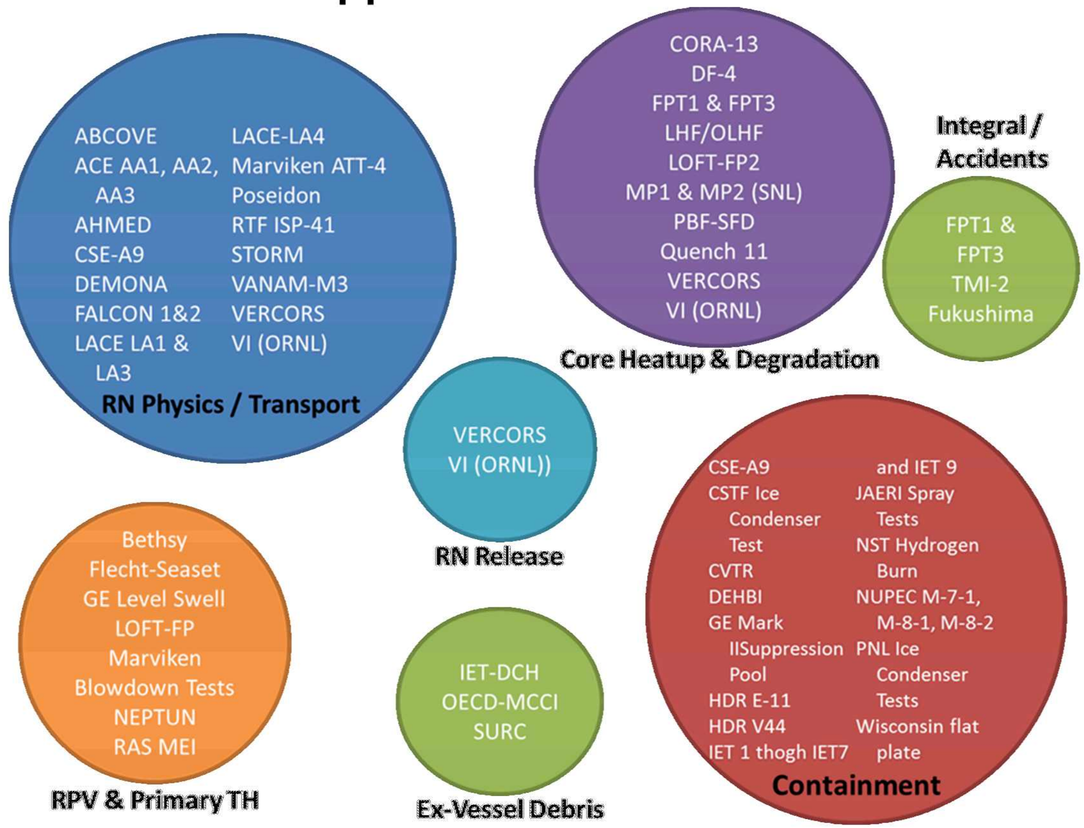
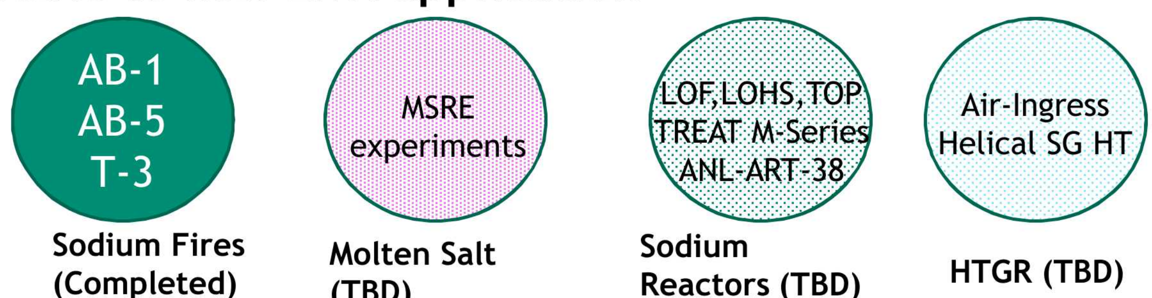
LWR & non-LWR applications



Specific to non-LWR application



Questions?

X-Walk Insights to Severe Accident Modeling

Cross-walk and Model Uncertainty

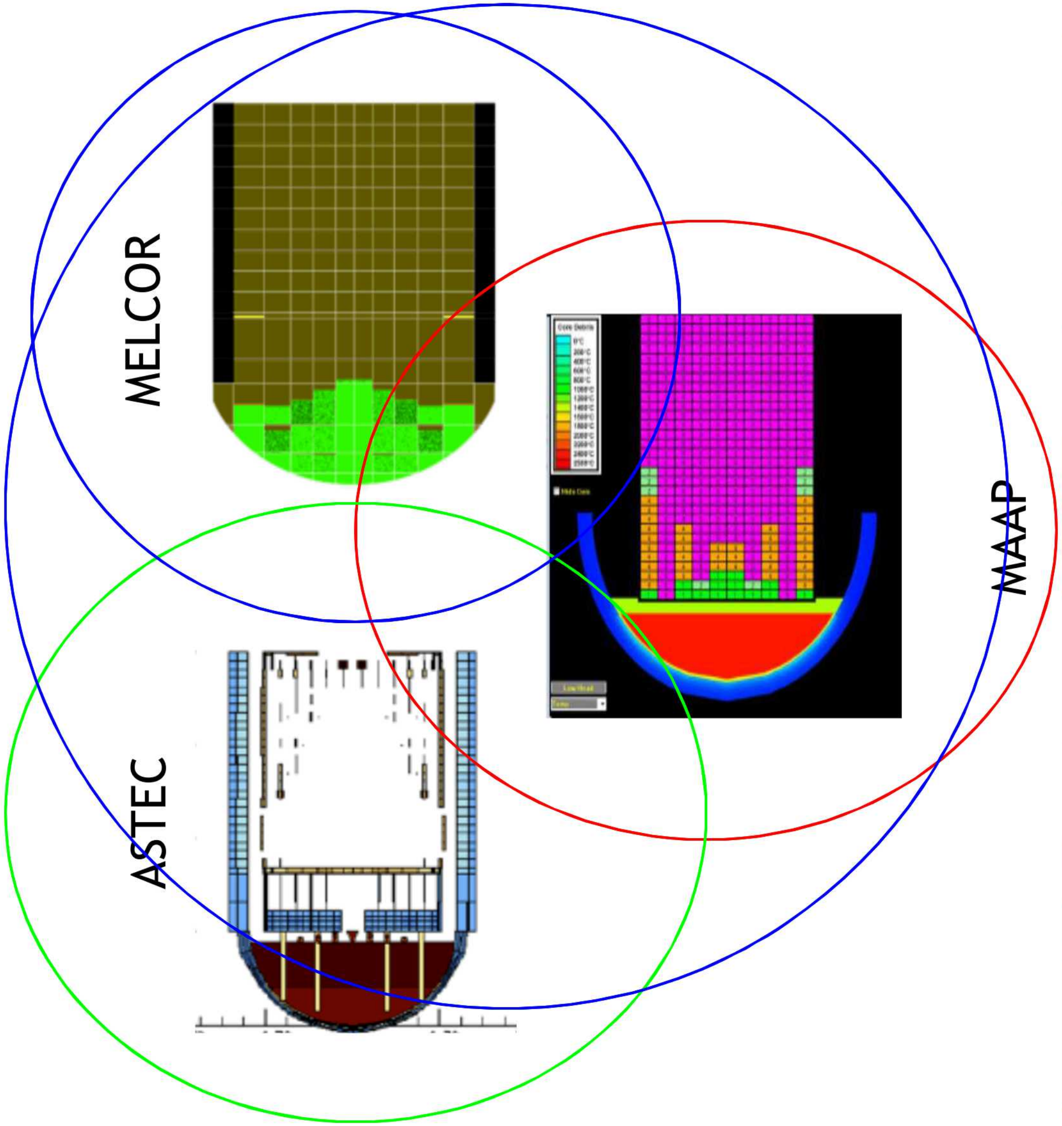
Where validation data exists, codes give reasonable agreement

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**

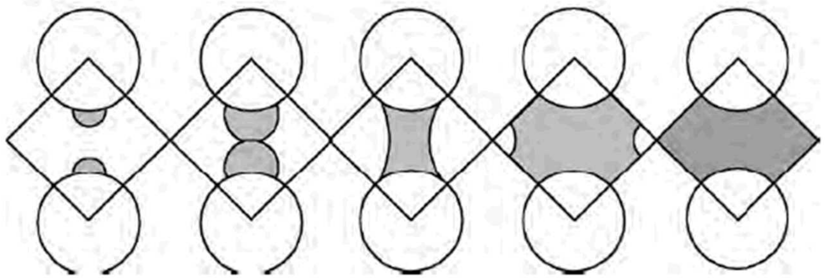
MELCOR- MAAP Cross-Walk Conclusions

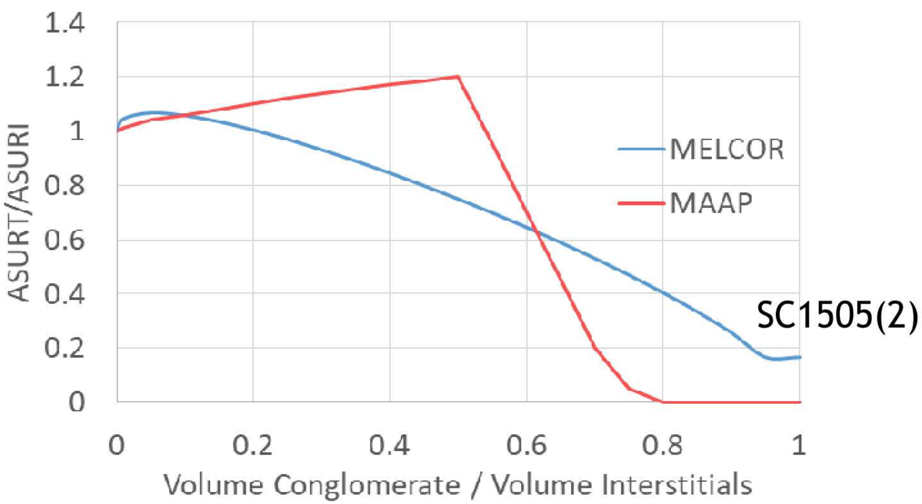
Cross-walk concluded that heat transfer degradation does not occur in MELCOR with decreasing debris bed porosity. This is wrong!

- 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

Flow Blockage Modeling

Code problems occur as control volumes are blocked

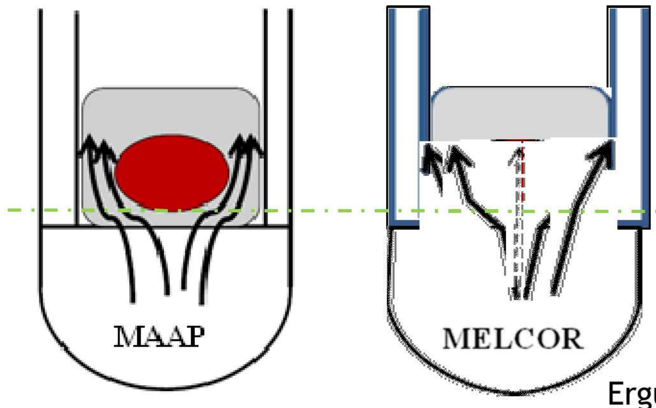
- Fluid volume can become small and subject to Courant limits
  - Vogtle SFP
- Pressure variations can become large as relocating core material reduces volumes
  - Can lead to time step issues with flow paths
  - Large pressures if CV is isolated and flow paths are removed

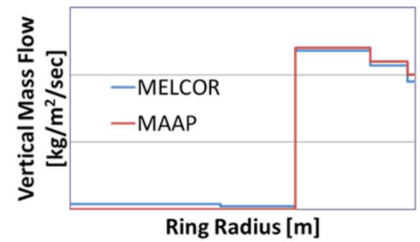
Current approach is to allow flow for small porosity

- SC1505(1) - Minimum porosity to be used in calculating the flow resistance (flow blockage model)
- SC1505(2) - Minimum porosity to be used in calculating the area for heat transfer to fluid.
- SC1505(3) – Fraction of volume reserved for CVH
- SC4414(1) Minimum Hydrodynamic Volume Fraction

- Default values for minimum porosities were increased based on recommendations from analysis

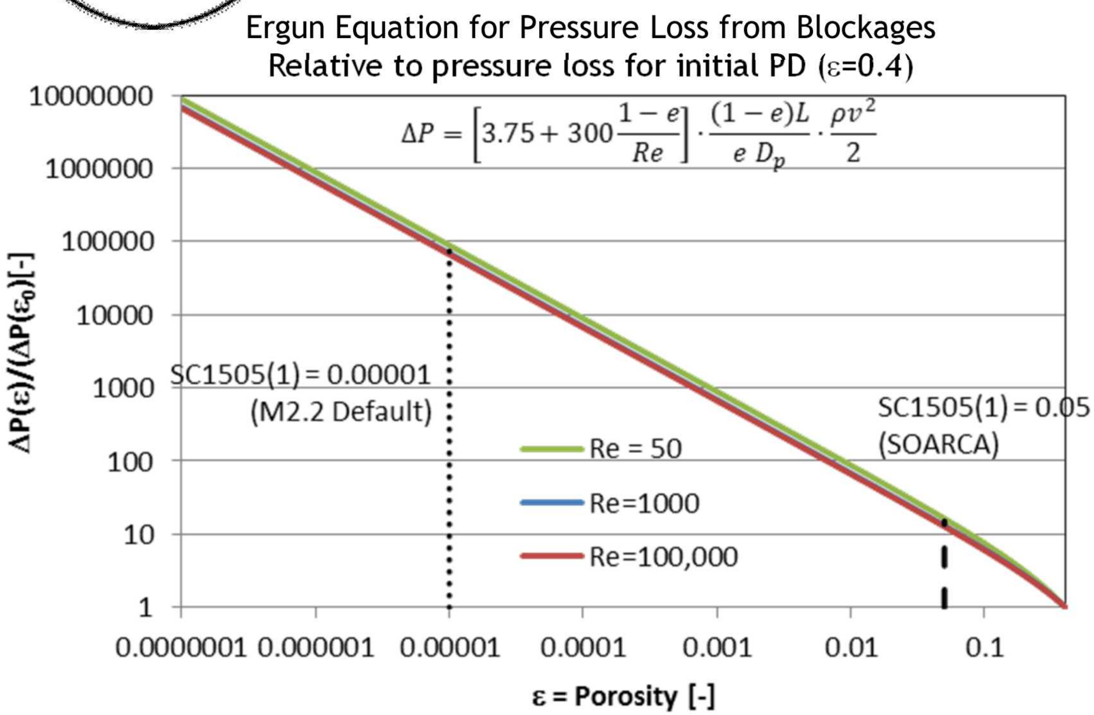
MELCOR- MAAP Cross-Walk Flow Resistance





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)



Real Differences in Code Modeling

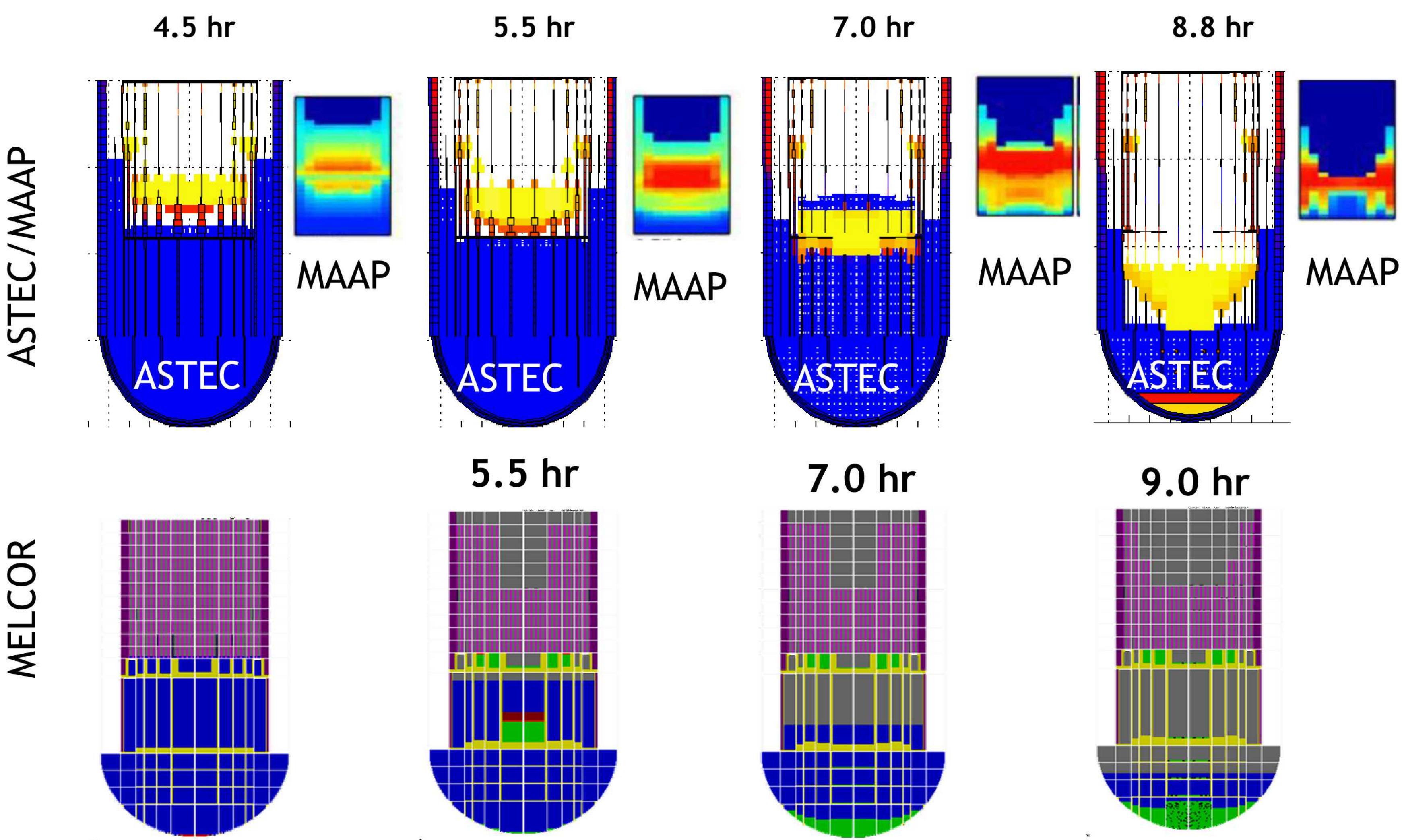
MELCOR cross-walk calculation assumed an effective UO2/ZRO2 melting temperature of 2800 K.

- User specified parameter ('SOARCA Best Practice' = Inertia)
  - Leads to much smaller blockages
  - Not consistent with conclusions from Phebus, TMI, or ATMI
- Eutectic temperature would be much lower leading to more extensive blockages
- It was impossible to enforce lower melting temperature through default in source code
  - Eutectics model did not work
  - User was required to modify UO2-INT and ZRO2-INT melt temperatures

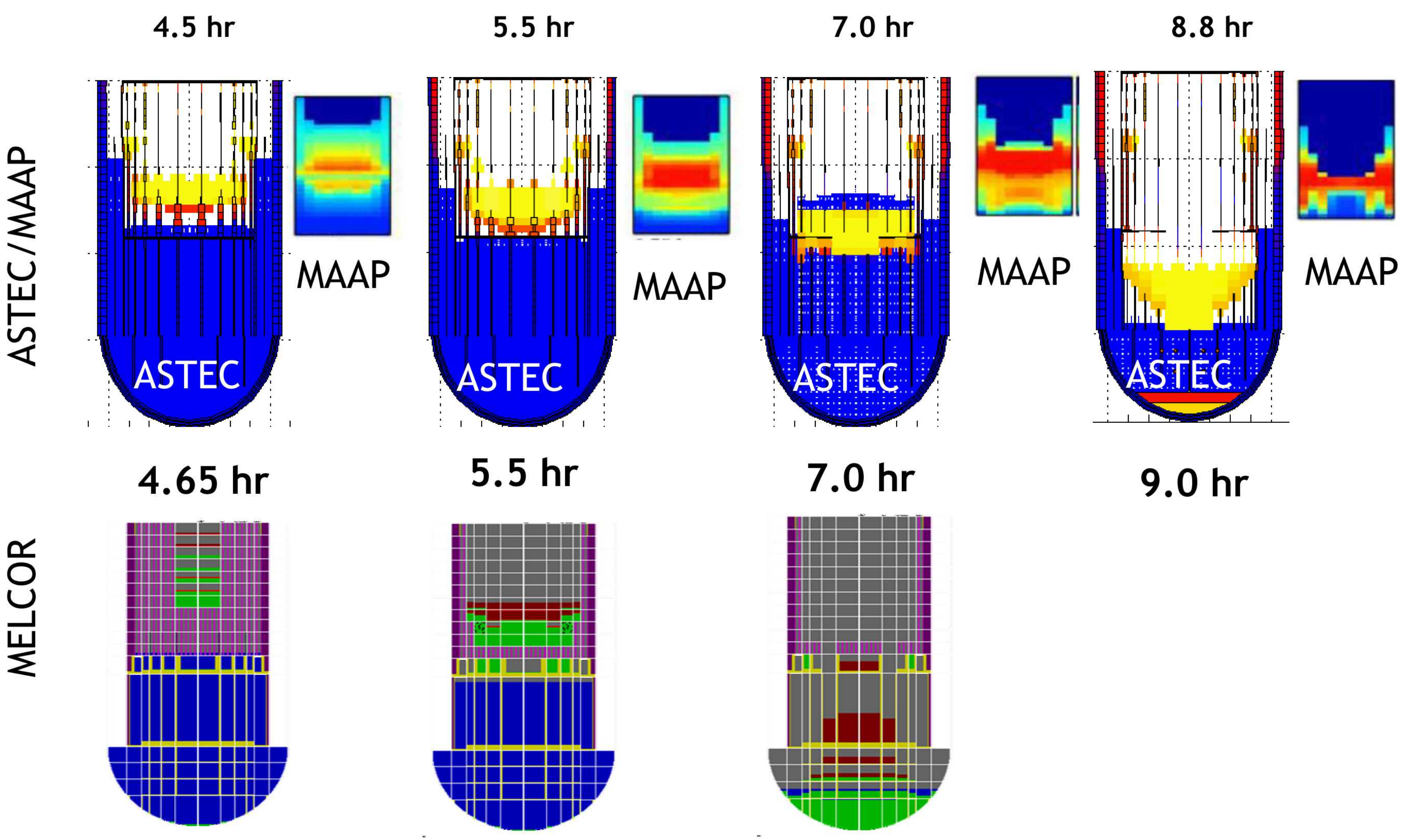
Bypass Modeling

- ASTEC does not model a bypass region for core relocation and it is also doubtful that MAAP does
- MELCOR relocates rubble bed through the bypass region to the core support plate and then to the lower plenum
- Molten pool transfers from cell to cell through the bypass and does not candle on surfaces

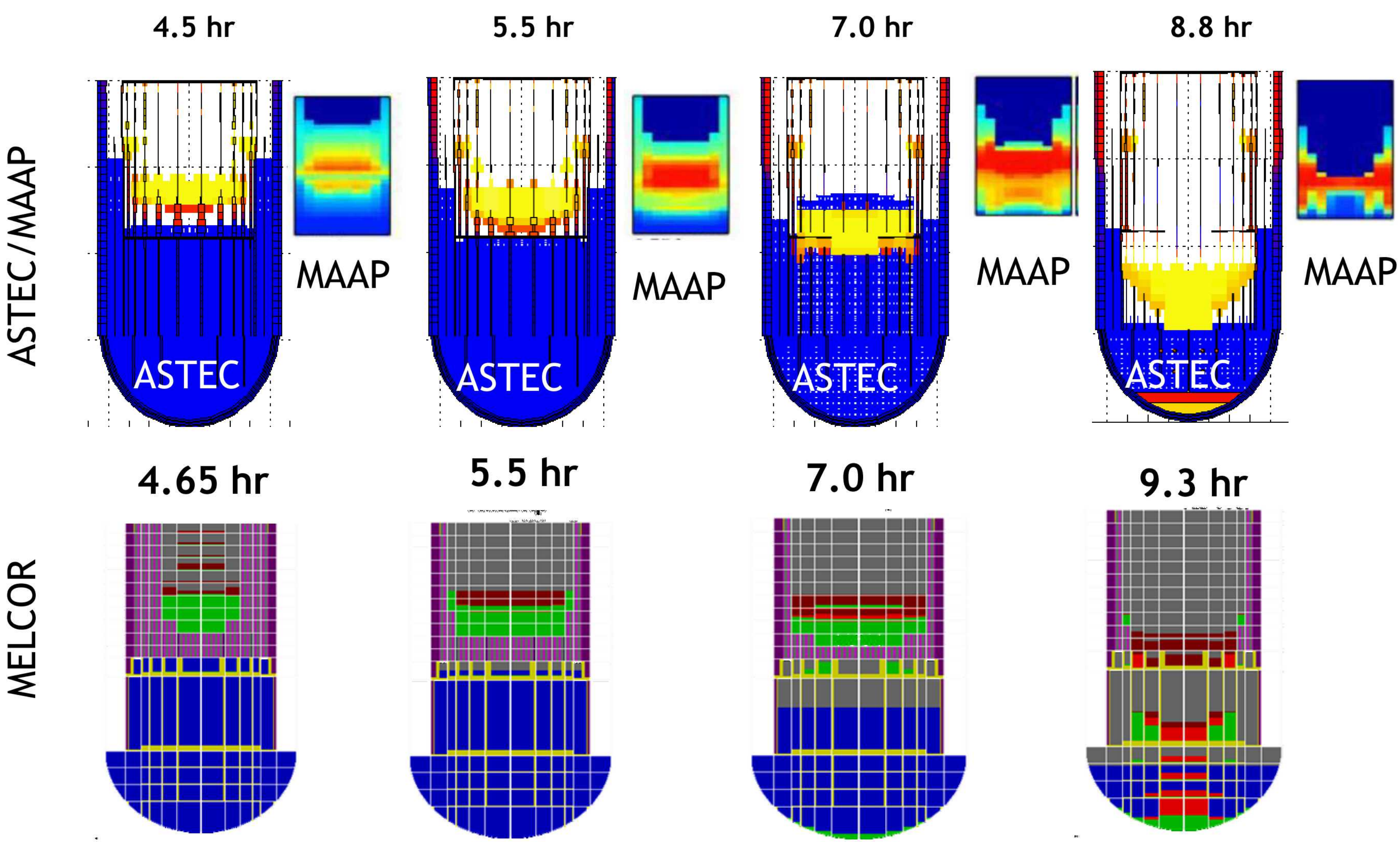
XWALK- MELCOR (Original)



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

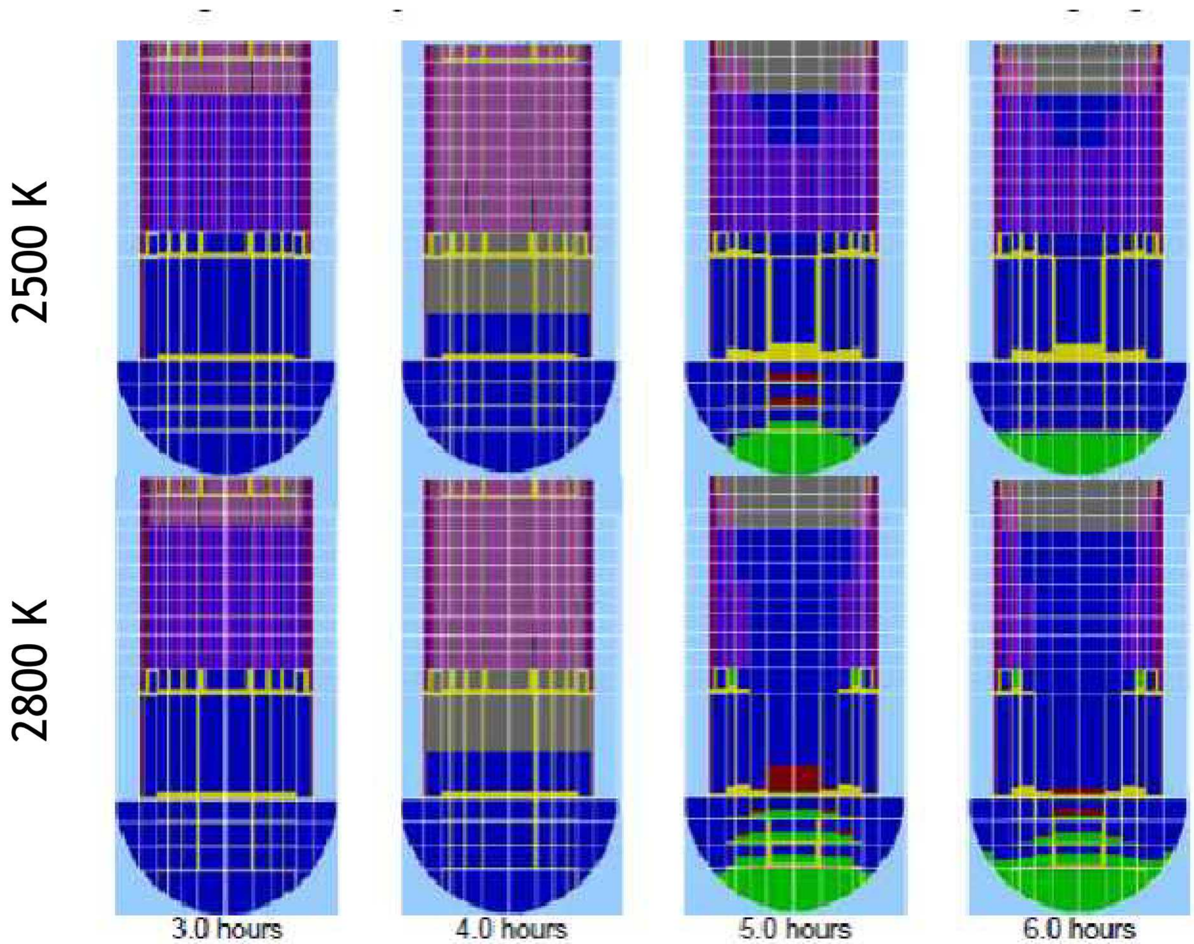


XWALK- MELCOR (Modified)



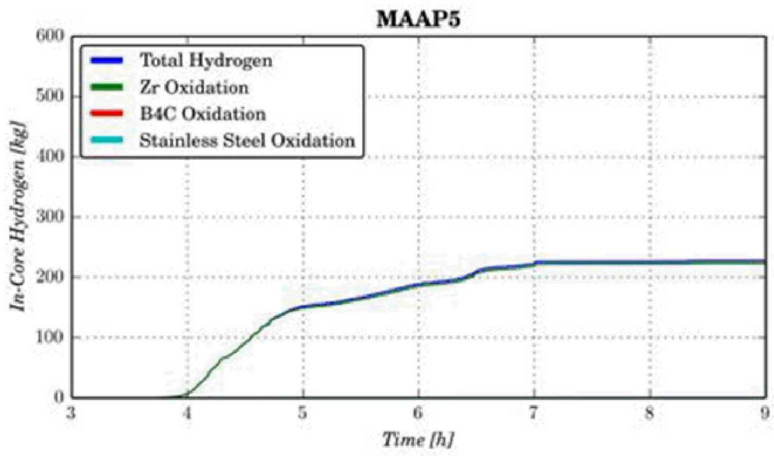
MELCOR Degradation

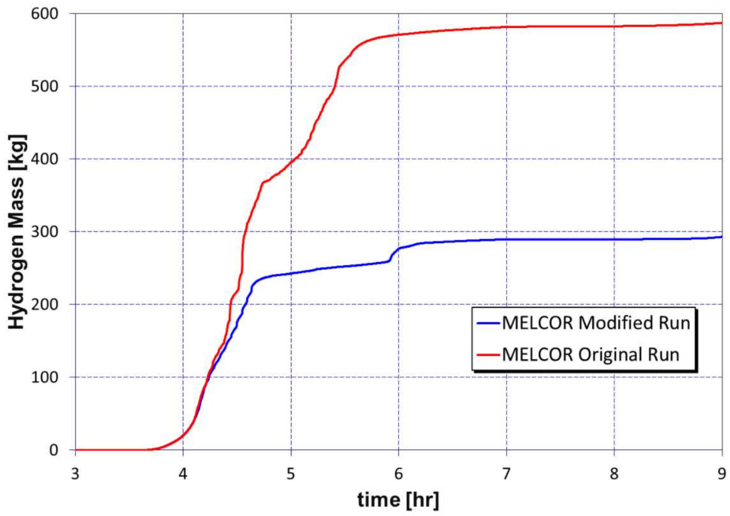
Phase II MELCOR/ MAAP Cross-Walk Report



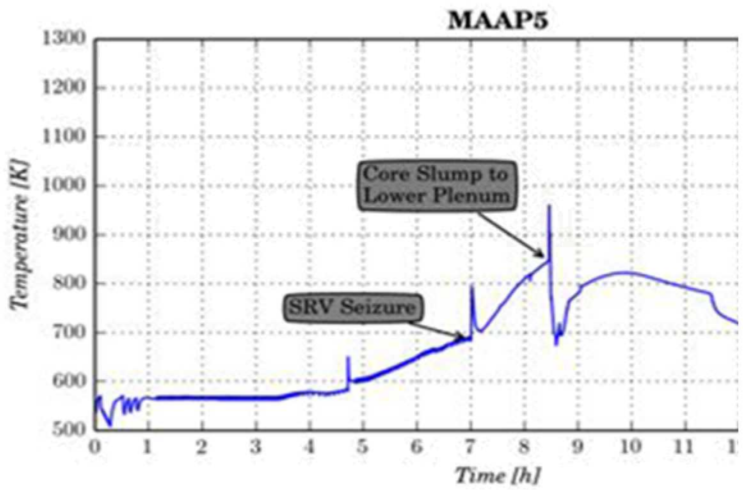
XWALK Steam Dome Temperature

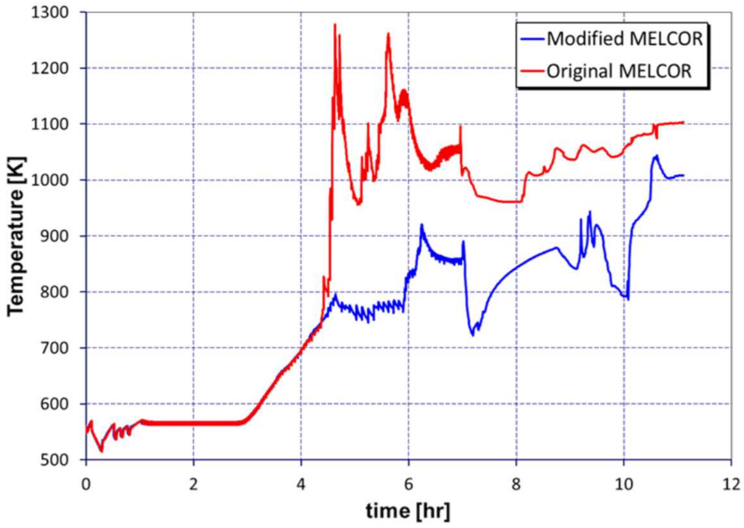
Hydrogen Generation





Steam Dome Temperature





Cross-walk and Model Uncertainty