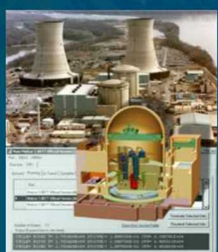
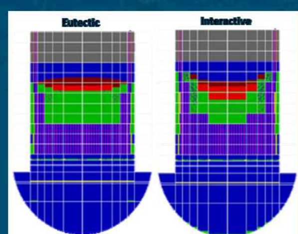
SAND2019-3572C

MELCOR Code Development Status
EMUG 2019

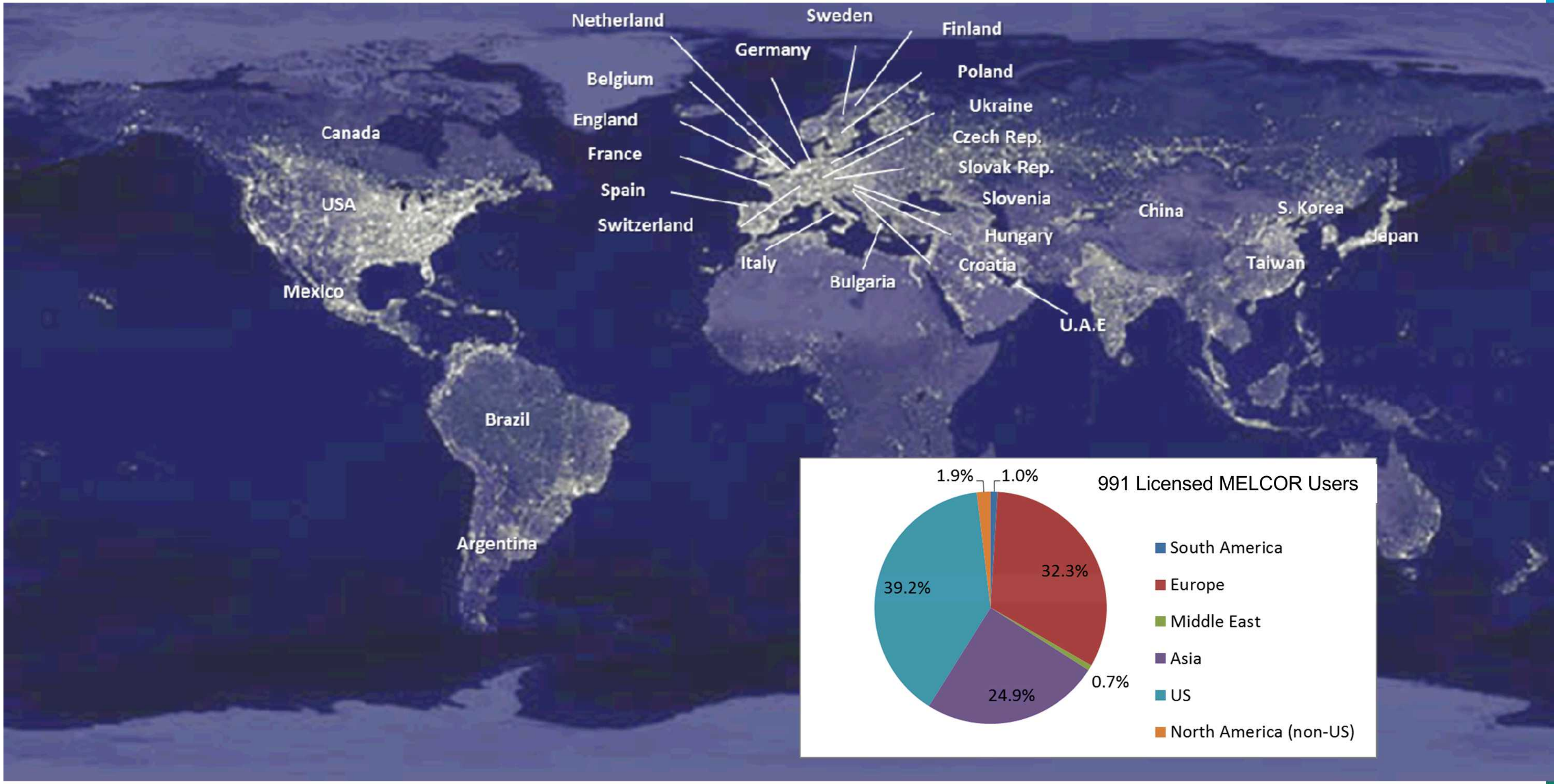




PRESENTED BY

Larry Humphries, Sandia National Laboratories

International Use of MELCOR

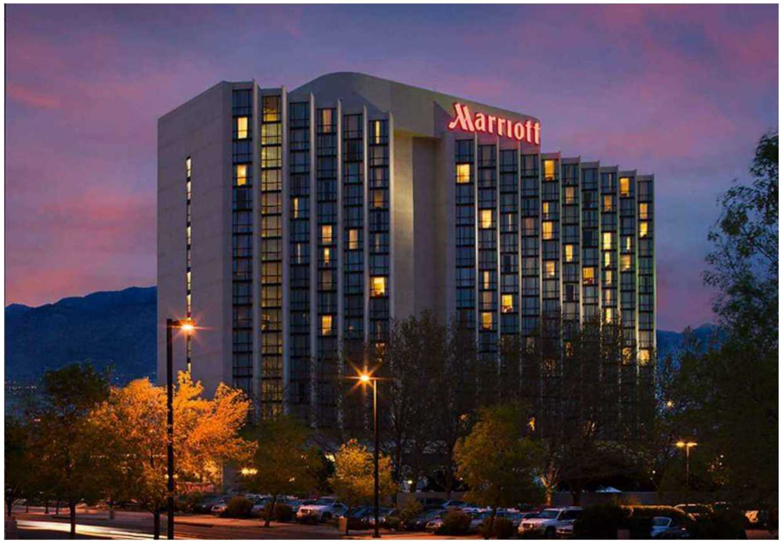


MELCOR Workshops & Meetings

2018 Asian MELCOR User Group (AMUG)
- Hosted by CRIEPI (Japan)
- August 2018
- MELCOR/MACCS Topics

2019 European MELCOR User Group (EMUG)
- Hosted by Paul-Scherrer Institute (PSI)
- Workshop on COR Package (April 3)
- April 4-5, 2019

2019 CSARP/MCAP/MELCOR Workshop
- CSARP (June 3-5), MCAP (June 5-6), Workshop (June 6 afternoon)
- Albuquerque, NM
- ½ day workshop with focused topics on ex-vessel corium modeling



MELCOR Fusion Applications

Multiple Attendees and Papers from Fusion Community at EMUG 2018

- Simulation of transients of a lithium loop with MELCOR fusion 1.8.6, Gianluca D'Ovidio, CIEMAT
- Accident analyses for the Cryostat-building interface components, Emili Martínez Saban, IDOM
- MELCOR-Fusion: Loss of Vacuum Accidents on JET, Samuel Ha, UK Atomic Energy Authority
- Xue Zhou Jin, KIT

Many arguments for implementing these models immediately

- Long-term maintenance of these models is assured.
- Would be smoother transition to transfer models to MELCOR 2.2 rather than MELCOR 3.
- Synergy between fusion models and non-LWR models
  - Model for condensation and freezing of fluid on surfaces already exists for fusion.

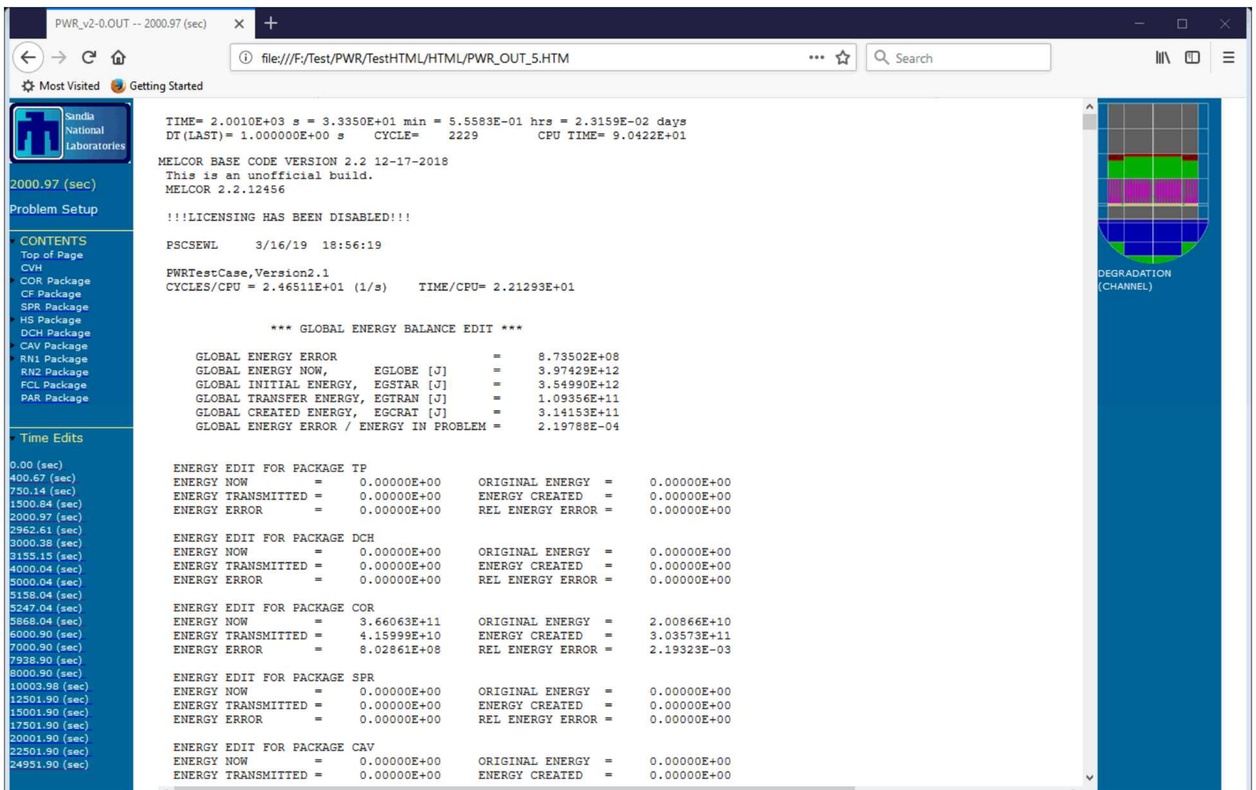
Proceeding forward with implementation of models

- Prioritized list of fusion modeling needs
- Obtained EOS libraries for Li-Pb, cryogenic helium, cryogenic N2
- INL currently adding models to MELCOR 2.2 branch
  - Status update on 2.2 for fusion at ISFNT-14 in Budapest this September

MELCOR HTML Output

HTML Output for MELCOR has been available for several years

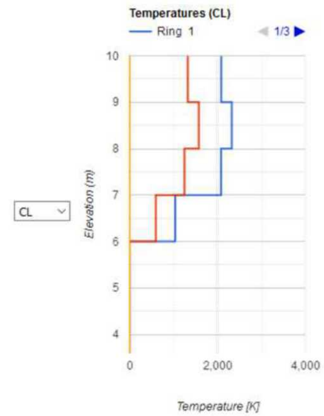
- Text output distributed among multiple files
  - File generated for each output time
  - Hyperlinks between files
  - Convenience in navigation.
- Graphical depiction of core degradation taken from PTFREAD coding several years back.
- Not often used by the general user community



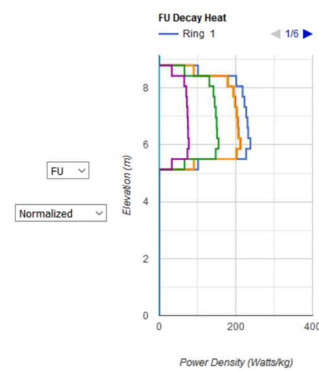
MELCOR HTML Output

Recent updates to HTML output

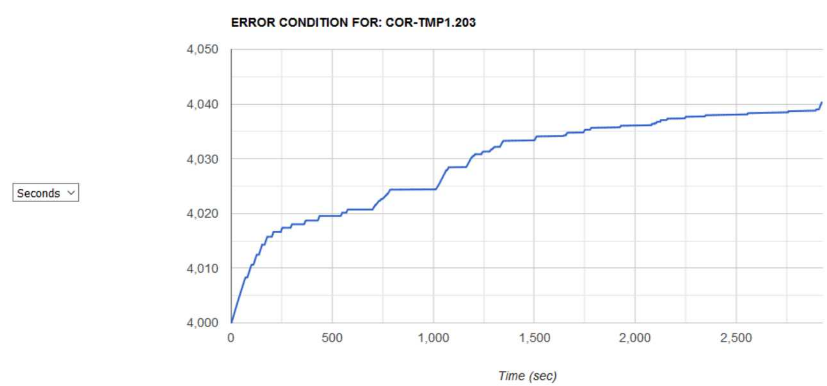
- Uses an ‘included’ file for time history
  - Speeds up MELCOR generation of HTML files
- Graphical depiction of output data recently added (hopefully next official code release)
  - Several data types for COR package added
    - Temperature profiles
    - Power profiles (decay, oxidation, convection,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



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



	Elevation [m]	Ring 1	Ring 2	Ring 3	Ring 4	Ring 5	Ring 6
1	0	0	0	0	0	0	0
2	0.93	0	0	0	0	0	0
3	1.42	0	0	0	0	0	0
4	1.91	0	0	0	0	0	0
5	2.4	0	0	0	0	0	0
6	4.59	0	0	0	0	0	0
7	5.13	101.8	90.92	90.1	66.41	33.41	0
8	5.5	226.8	202.5	200.6	147.7	74.04	0
9	5.86	238.1	212.6	210.7	155.1	77.73	0
10	6.23	232.3	207.4	205.5	151.3	75.82	0
11	6.6	230.5	205.8	203.9	150.2	75.24	0
12	6.96	227.1	202.8	201	148	74.16	0
13	7.33	222.5	198.7	196.9	145	72.65	0
14	7.69	217.7	194.4	192.6	141.8	71.08	0
15	8.06	201.1	179.5	177.9	131	65.68	0
16	8.42	101.5	90.64	89.82	66.21	33.31	0
17	8.79	0	0	0	0	0	0



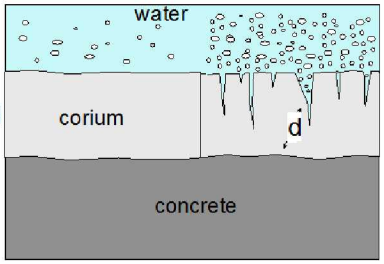
New Model Development Tasks (2014-2017)

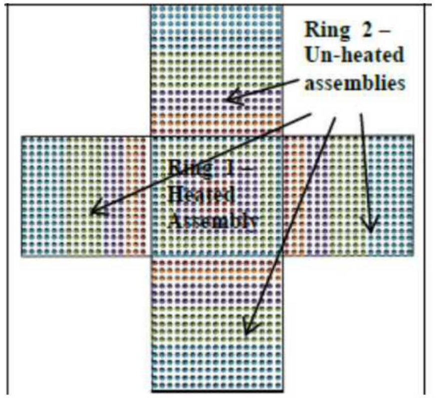
Completed

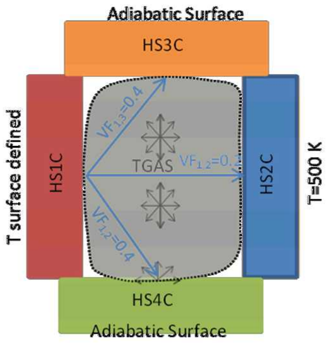
- Fuel Rod Collapse Model (NRC)
- Homologous pump model (NRC)
- Multi-HS radiation enclosure model
- Aerosol re-suspension model
- Zukauskas heat transfer coefficient (external cross-flow across a tube bundle)
- Core Catcher (multiple containment vessels)
- Multiple fuel rod types in a COR cell (NRC)
- 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

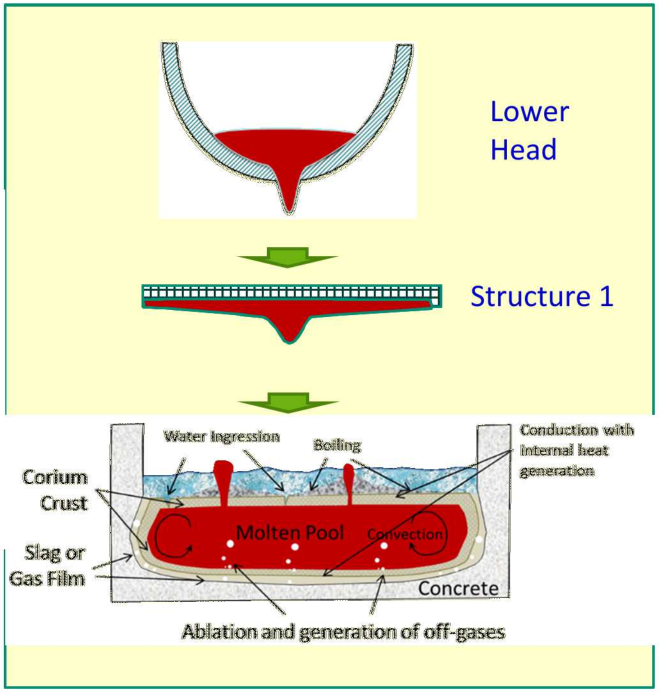
In Progress or future

- Vectorized Control Functions (NRC)
- CONTAIN/LMR models for liquid metal reactors
- CVH/FL Numerics (NRC)





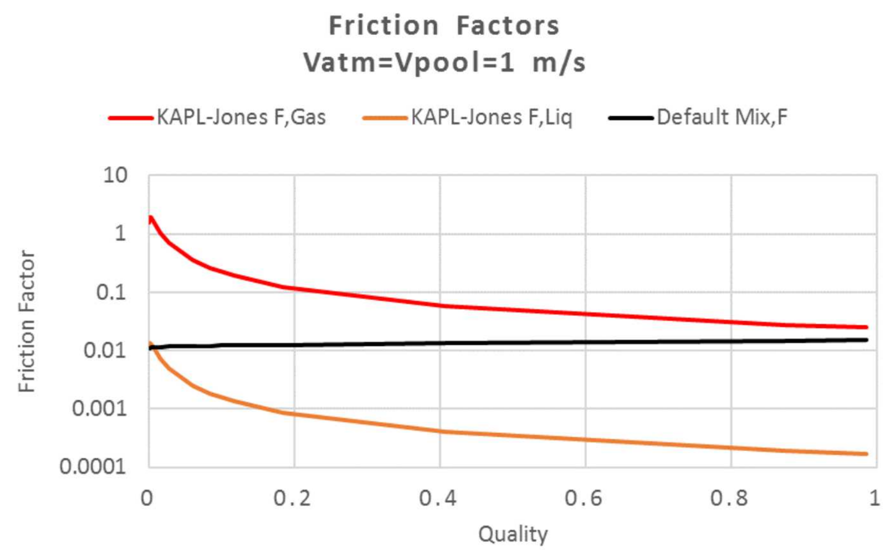


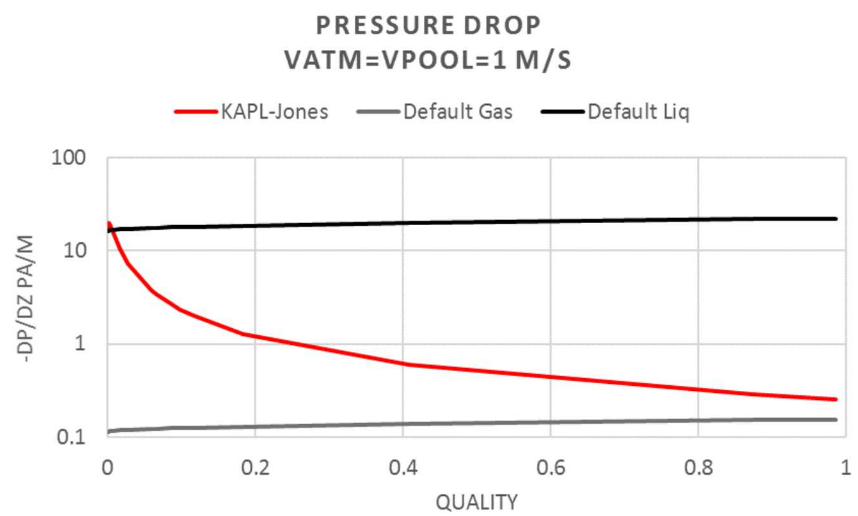


Two-Phase Friction Factor

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

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





MELCOR 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

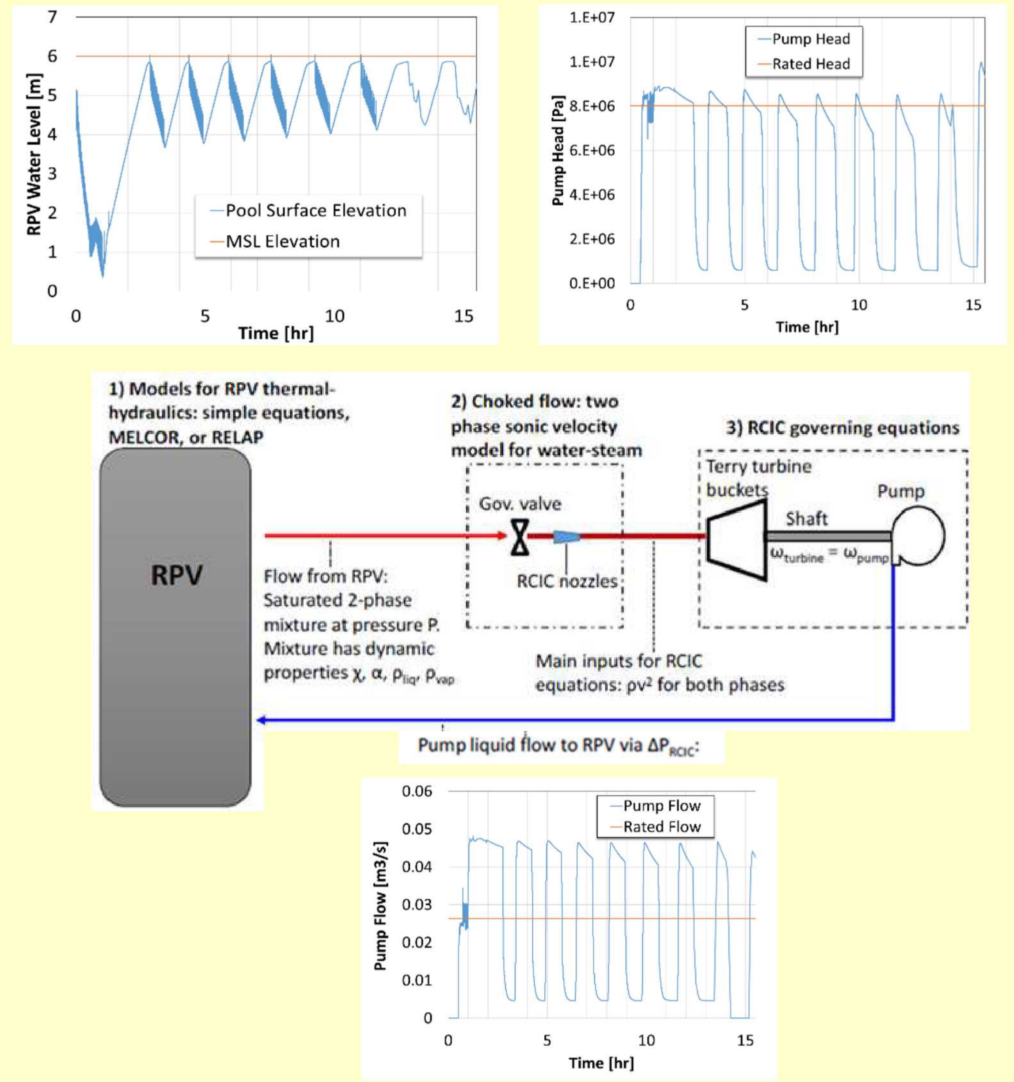
Terry turbine compound velocity-stage model (impulse of steam on turbine rotor)

- 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

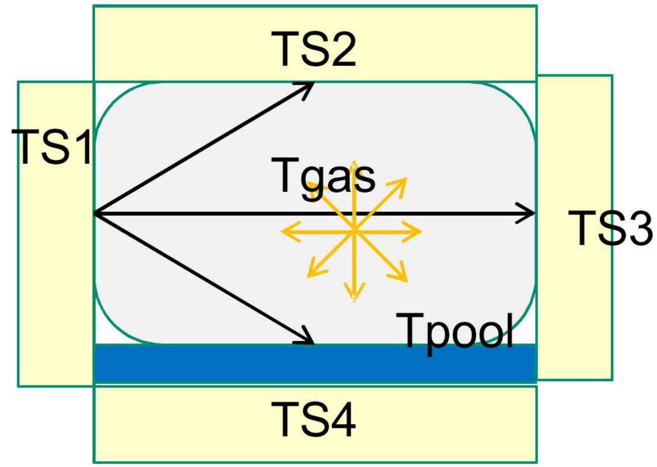
New models exercised on a pseudo-Fukushima RCIC.



Multi HS Radiation Enclosure Model

Recent model improvements

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




```
HS_Rad 4  NET3      !EM     BeamL    VF
  1  HS1C     RIGHT  EM1     0.5       0.0   0.2   0.4   &
                                        'MyLongNamedCF'
  2  HS2C     LEFT   EM2     0.5       0.2  0.0  0.3  0.5
  3  HS3C     LEFT    -      0.5       0.4  0.3  0.2  0.1
  4  HS4C     RIGHT   -      0.5       0.4   0.5  0.1  0.0
```

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

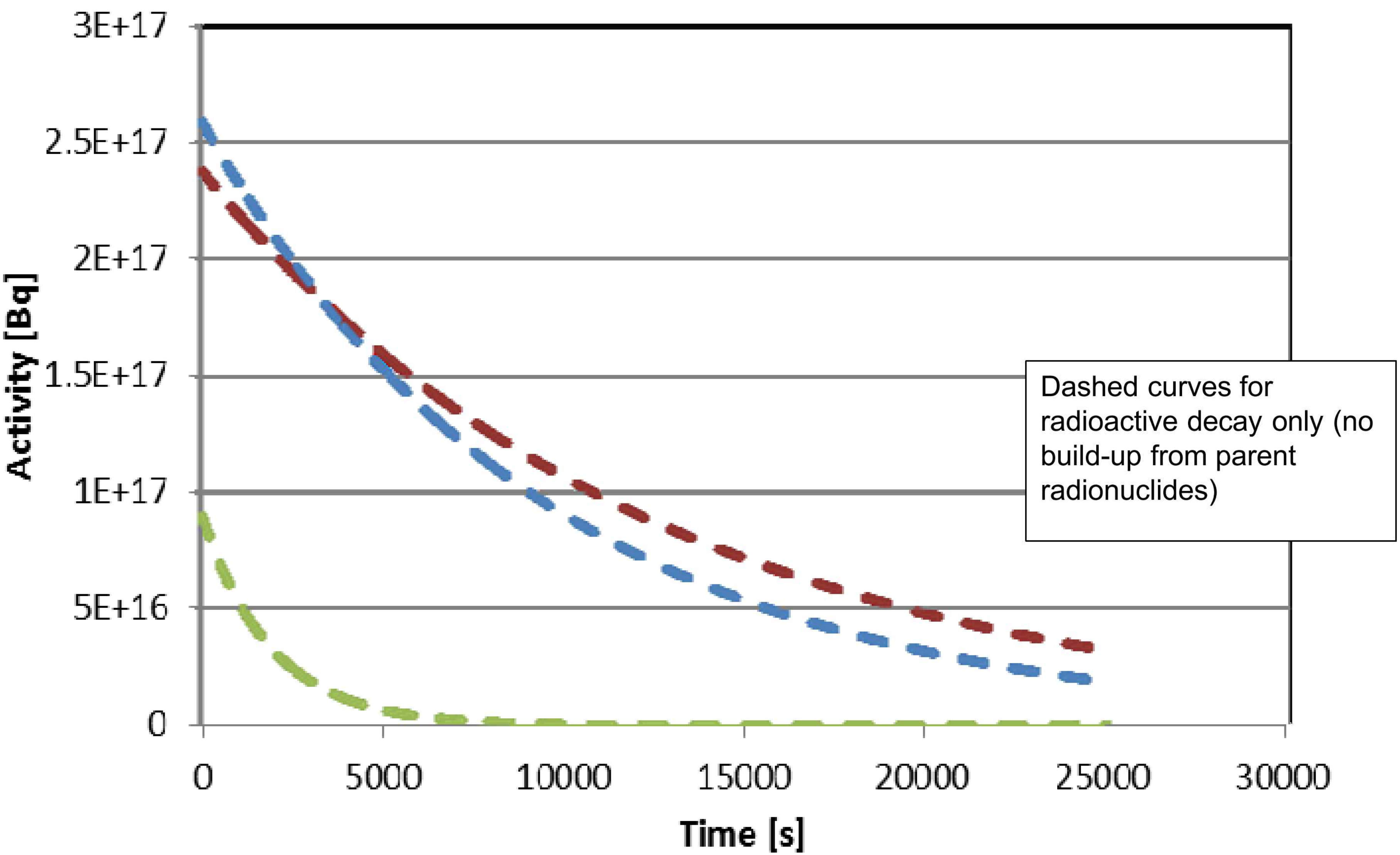
$$\frac{dN_i}{dt} = \sum_{j=1}^{i-1} \lambda_j N_j - \lambda_i N_i$$

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)



Dose Plot Variable

Plot variables for dose estimate recently added (April 2018)

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

Example

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

- Gamma energy from user files
  - 1^{st} uses gamma energy from FissProd.in file
  - Overwrites with any gamma energy on 3^{rd} 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 i^th isotope [Rad/hr]
- ϕ_i - gamma flux of the i^th isotope [1/(cm^2 s)]
- E_i - gamma energy of the i^th 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

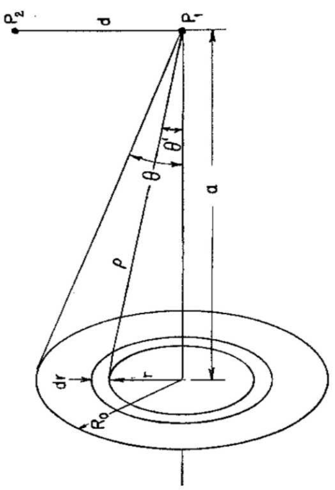
$$\phi_i = (3.7 \times 10^{10}) \frac{A_i}{V\rho_{air}\left(\frac{\mu_s}{\rho}\right)_{air}} \left(1 - e^{-\rho_{air} R \left(\frac{\mu_s}{\rho}\right)_{air}}\right)$$

- Where
  A_i = activity for the i^th isotope (Ci),
  R = equivalent spherical radius of volume V (cm³),
  ρ_{air} = density of air (g/cm³),
  $\left(\frac{\mu_s}{\rho_{air}}\right)$ = total attenuation coefficient of air at E_i (cm²/g),
  and V = volume of MELCOR control volume(s) of interest (cm³).
- **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 Temperature

UO2-INT/ZRO2-INT

Melt temperature for UO_2 & ZrO_2 is the same for intact materials as it is for conglomerate.

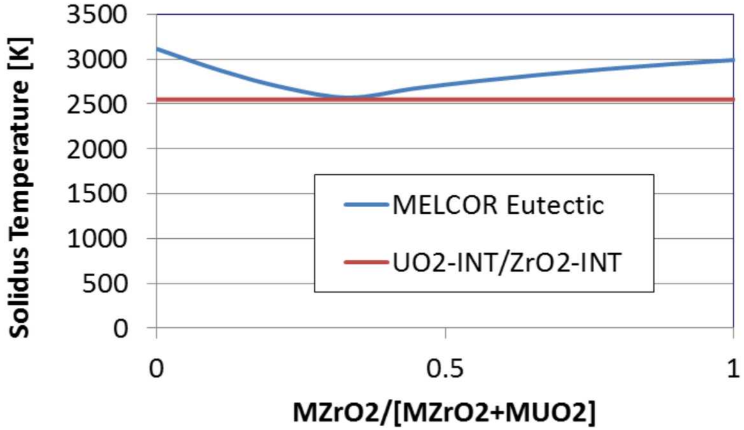
Does not depend on composition

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



Dissolution of solids by molten mixture

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

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

The solution is iterative

Component	Solids Dissolved by Mixture
Cladding	UO2 from intact fuel
	ZrO2 from intact cladding
Canister	ZrO2 from intact canister
	ZrO2 from intact cladding (A)
	UO2 from intact fuel
Other structure SS or NS (steel only)	steel oxide from the same other structure
Other structure NS (BWR control rod)	steel oxide from the same other structure
	ZrO2 from intact canister (A)
	Zr from intact canister (A)
Other structure NS (PWR control rod)	steel oxide from the same other structure (B)
	Zr from the same other structure
	ZrO2 from intact cladding (A)
	UO2 from intact fuel (A)
Particulate debris	UO2 from particulate debris
	ZrO2 from particulate debris
	ZrO2 from intact cladding
	UO2 from intact fuel
(A)	indicates solid is attacked only if there is no holdup of the mixture in the component.
(B)	indicates solid is attacked only if the mixture is being held up by the component

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

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

where

x_j^f = final mass fraction of material j,

x_j^i = initial mass fraction of material j,

Δt = timestep (s), and

$A_{ZrO2} = 1.47 \times 10^{14}$ $A_{UO2} = 1.02 \times 10^{15}$

$B_{ZrO2} = 8.01 \times 10^{4}$ $B_{UO2} = 8.14 \times 10^{4}$

Cross-walk and Model Uncertainty

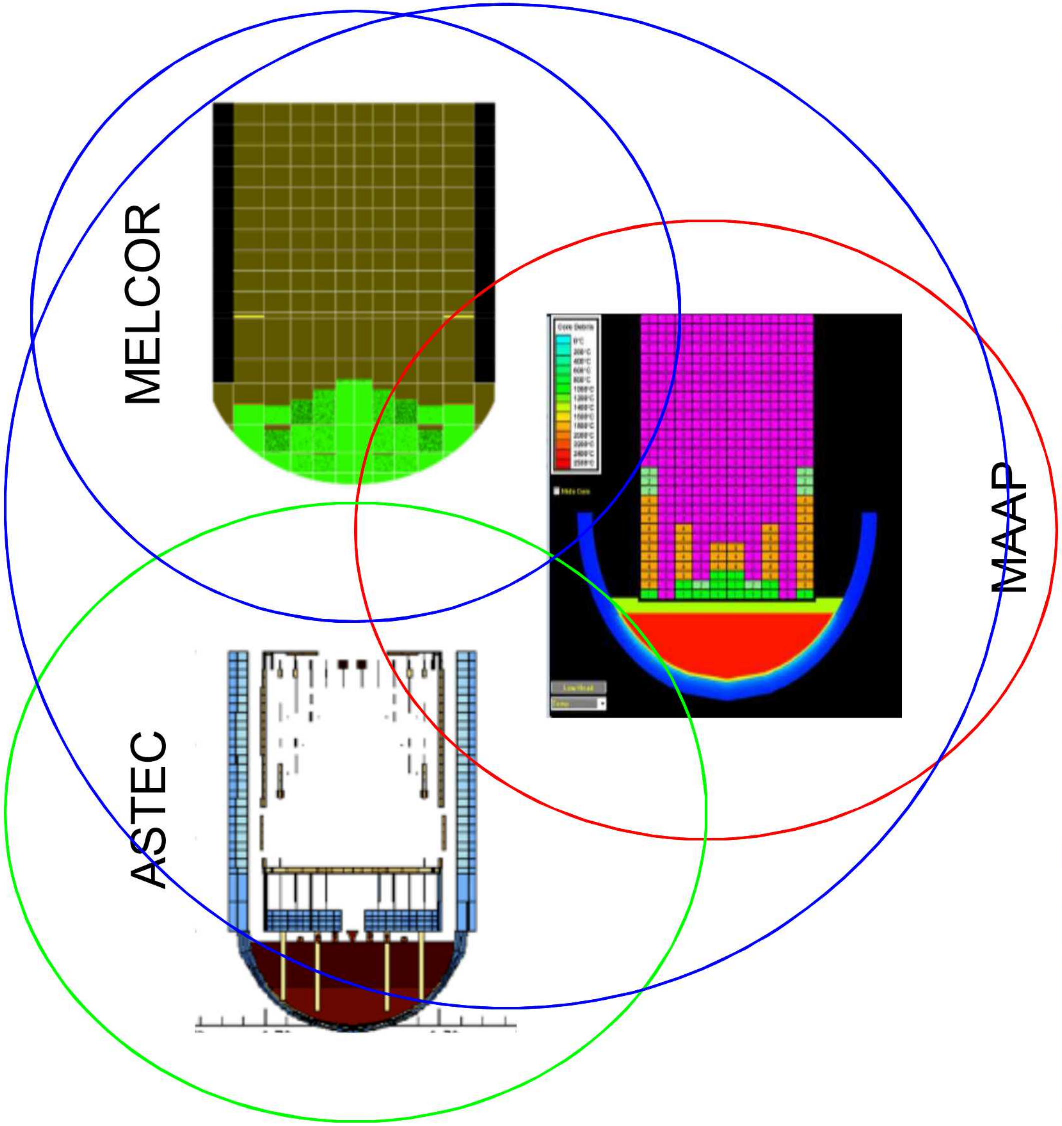
Where validation data exists, codes give reasonable agreement

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**

Non-LWR Reactor Applications

Advanced Technology Fuels (ATF)

Non-LWR Reactors

- HTGR
- Sodium
- Molten Salts

ATF Design Concepts

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

Accident Tolerant Fuel Modeling Needs

- New material properties (hard-coded, user defined)
  - Thermophysical
  - Mechanical
  - Emissivity
- New oxidation models (or modified oxidation kinetics parameters)
  - Arrhenius-type equation with user-specified coefficients
    - Maybe not entirely possible with sensitivity coefficients
  - Extension of models for multiple oxidation reactions (SiC)
    - Parabolic oxidation reaction

$$SiC(s) + 3H_2O(g) = SiO_2(s) + 3H_2(g) + CO(g)$$

    - Linear volatilization reaction

$$SiO_2(s) + 2H_2O(g) = Si(OH)_4(g)$$

    - Rate constant fit over two pressure ranges
    - Stochiometry of reactions
  - Code modifications should allow nitriding for air oxidation (SFP)
  - Oxidation chemistry
    - User specified parameters for moles of reactants and products and heat of reaction

Accident Tolerant Fuel Modeling Needs

- Modified fuel failure models (time at temperature)
- Possible modified ORNL-BOOTH fission product release models
- Allowances for new materials in in/ex-vessel phenomenological models
  - New core material eutectic formations
  - In-vessel core degradation like melting, candling, collapse, relocation, etc.
  - In-to-ex vessel transition (configure TP to track COR-LHC or COR-CAV relocations)
  - Ex-vessel phenomena (allow for new materials in LHC or CAV
- Effects that would require major changes
  - Thick protective layer with radically different properties could require layered clad
  - Not likely a concern
- Minor code changes
  - Bypassing (with source code modifications) the "zero clad thickness" issue that arises when zircaloy is absent from the CL component
  - Text and plot variable output

High Temperature Gas Reactor

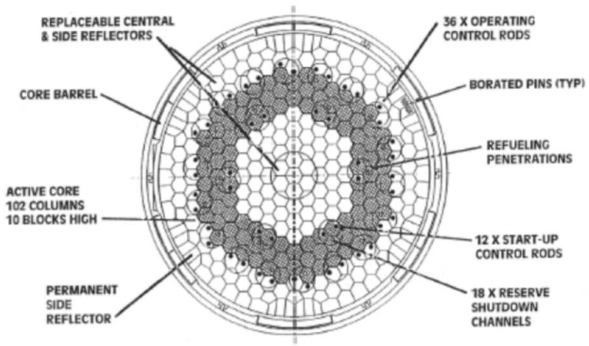
Reactor Components
- PBR Reactor components
- PMR Reactor Components

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

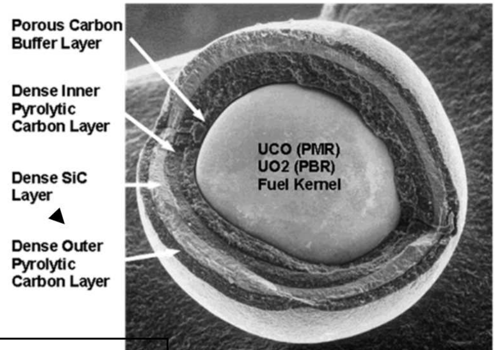
Graphite Dust Modeling
- Aerosol physics models
  - Turbulent Deposition
  - Resuspension

Point Kinetics Model

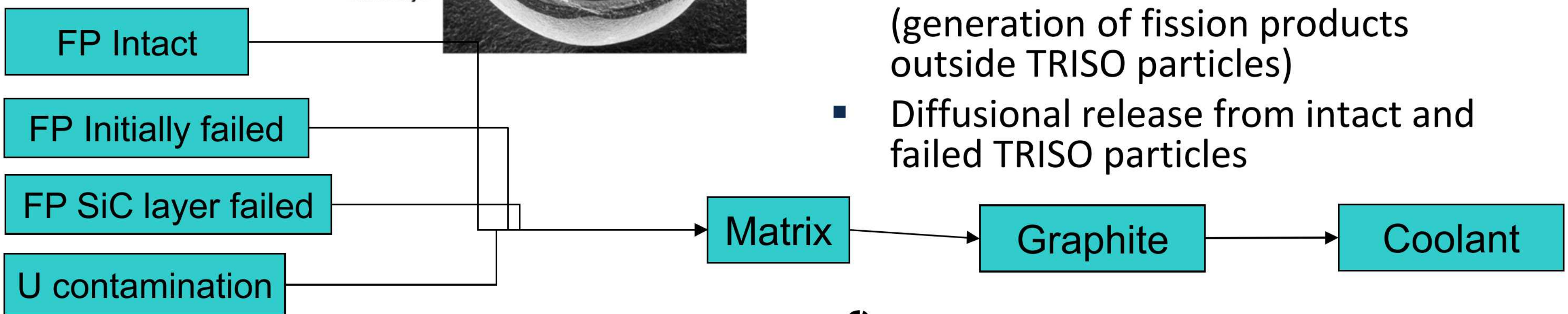
Steady state initialization and transient solution strategy



MELCOR FP Release Model



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



Particle Release

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

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

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

Diffusional Release

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

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

$$m = 2 \ (spherical)$$

C = Concentration (kmol/m^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

Simple Sample Problem

Point kinetics for operating reactor applications

- Model developed by UNM

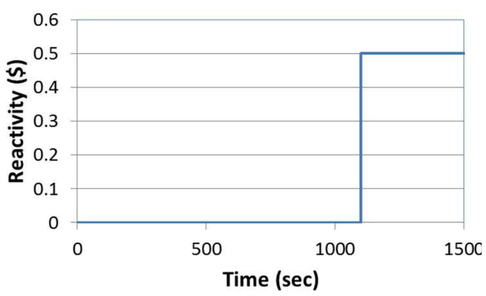
$$\frac{dn}{dt} = \frac{\rho - \beta}{\Lambda} n + \sum_{i=1}^{6} \lambda_i C_i + S_0$$

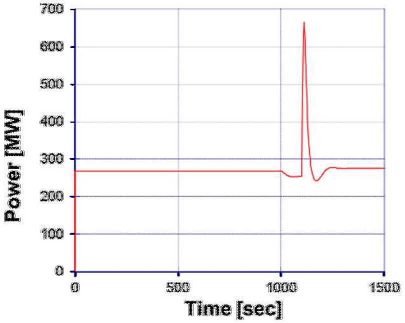
$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n - \lambda_i C_i$$

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

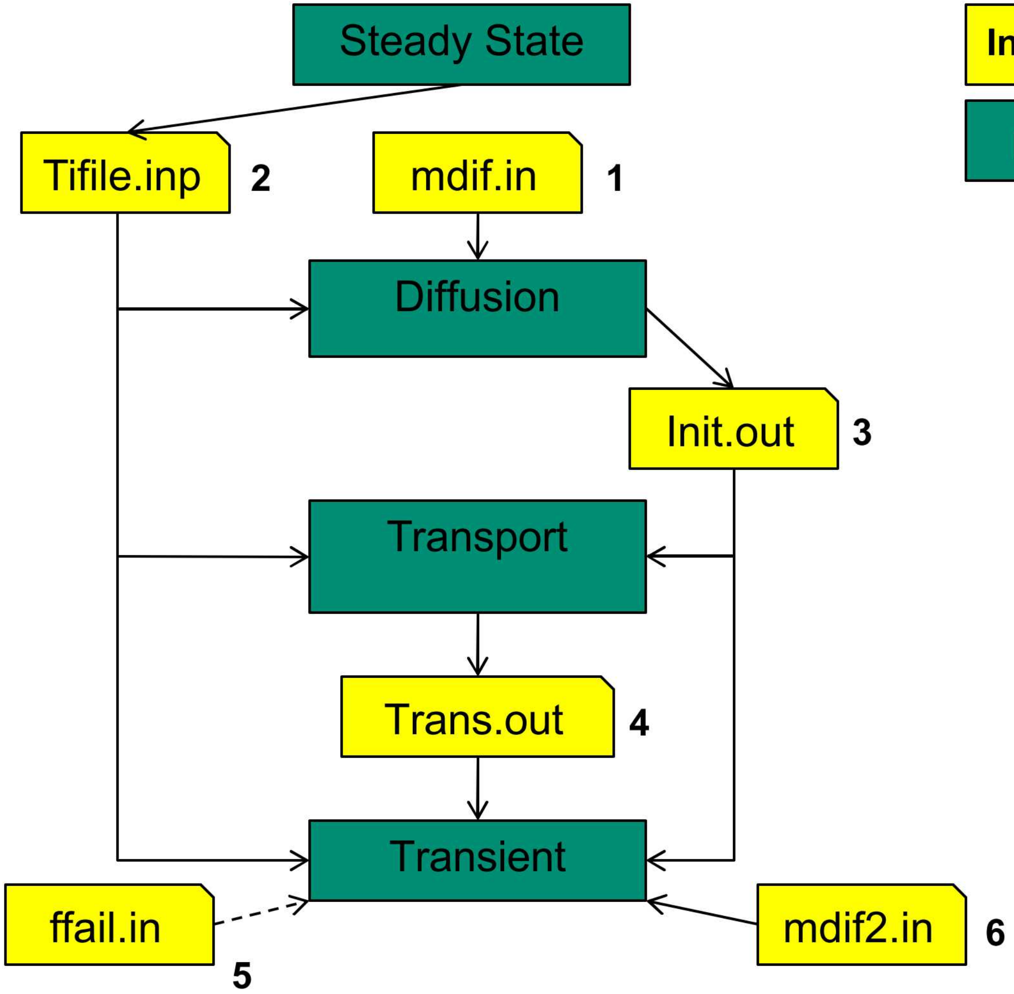
- Initial power level is 268 MW
- Control Function used to insert $0.50 reactivity step at 1100s
- Doppler feedback from fuel and moderator
- PK Model turned on at 1000 s
- Example Input:

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



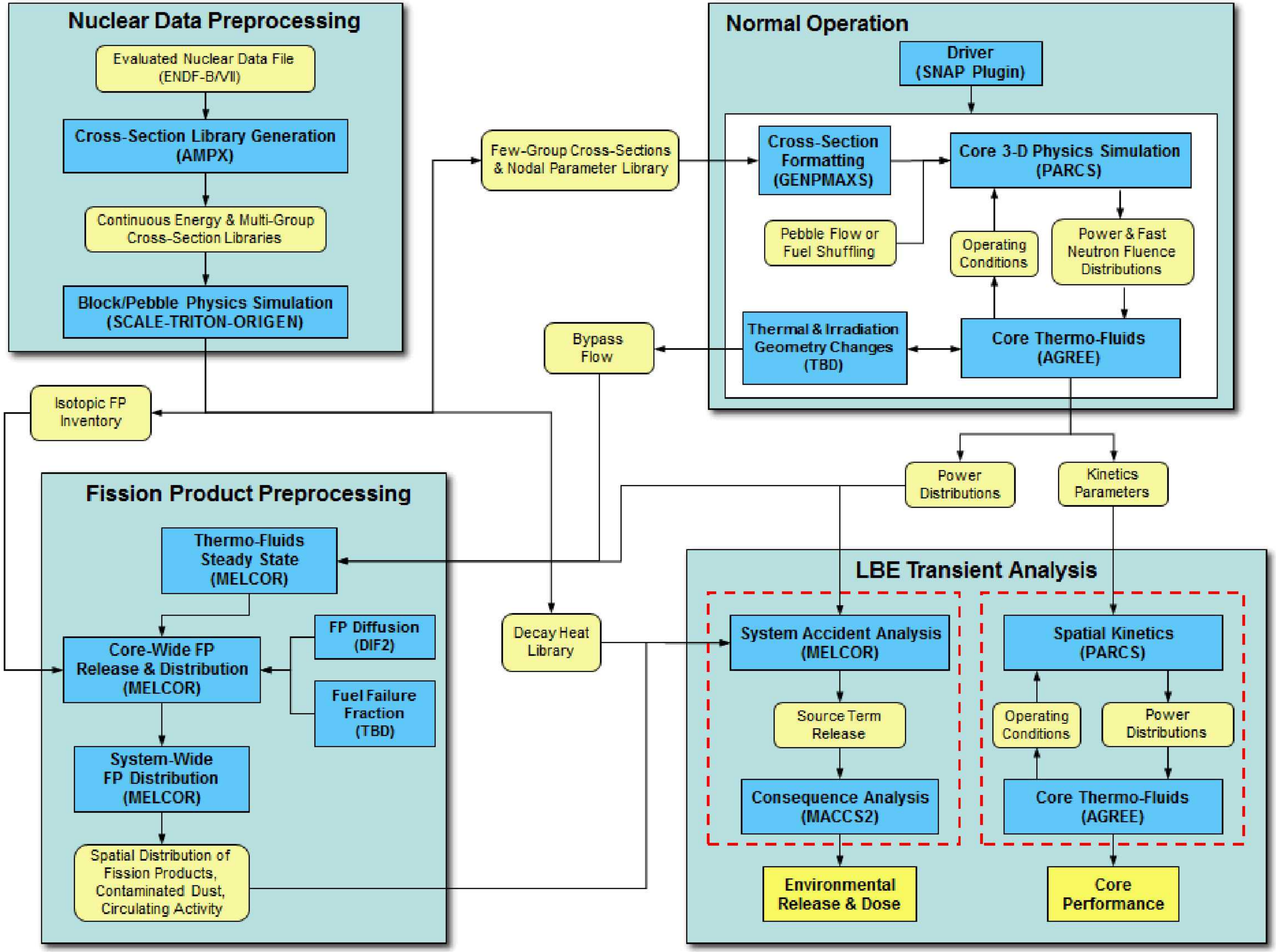


HTGR – Analysis Strategy



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

HTGR – Evaluation Model



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

High Temp Gas-Cooled Reactors

Existing Modeling Capabilities

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

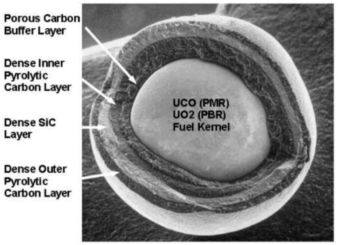
$$\frac{\partial C}{\partial t}=\frac{1}{r^m}\frac{\partial}{\partial r}\left(r^m D\frac{\partial C}{\partial r}\right)-\lambda C+S$$

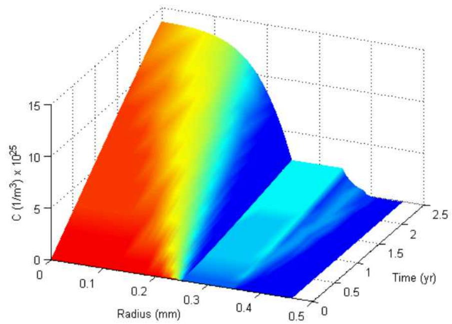
$m=1$ (*cylindrical*)

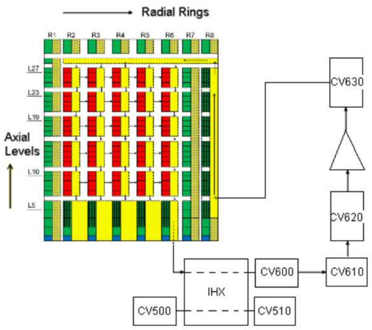
$m=2$ (*spherical*)

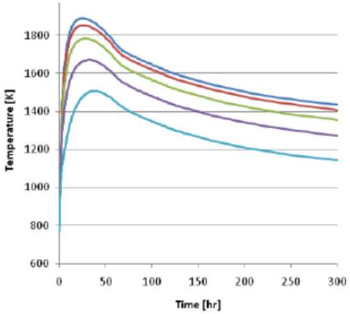
Existing Modeling Gaps

- 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

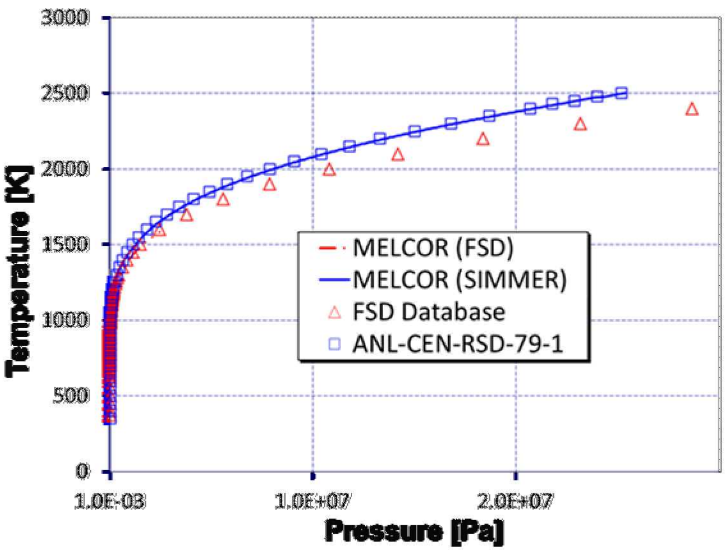
Two models implemented

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

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

Test problems have been created demonstrating model capability

Some improvement for FSD database were made last FY



Spray Fire Chemistry

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) $2\ Na + {}^{1}/_{2}\,O_2 \rightarrow Na_2O$,
  - (S2) $2\ Na + O_2 \rightarrow Na_2O_2$
- Fixed ratio of peroxide and monoxide

$$\frac{1.3478 \cdot F_{Na_2O_2}}{1.6957 - 0.3479 \cdot F_{Na_2O_2}}$$

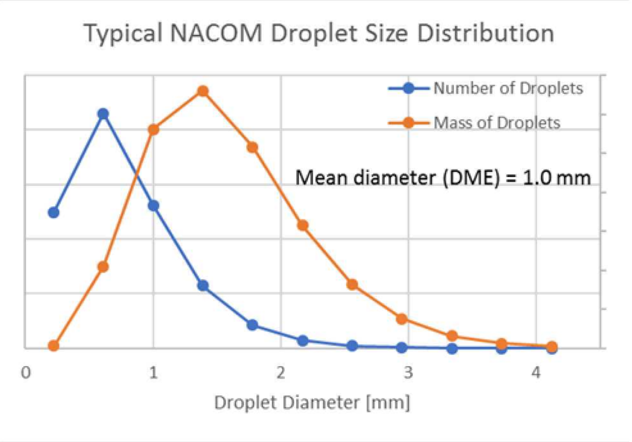
- Predicted quantities include:
  - Mass of Na (spray, burned, pool), O_2(consumed), Na_2O_2+ Na_2O(produced)
  - Energy of reactions

Enhancements

- Droplet acceleration model
- Pre-ignition burn rate
- Adjustment to heat of combustion to include heat of vaporization
  - Na_2O from 9.18 to 13.71 MJ/kg of sodium
  - Na_2O_2 from 10.46 to 15.88 MJ/kg of sodium

Missing from model

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



Pool Fire Model

Based on SOFIRE II code from ANL

- Reactions considered:
  - $2\,Na + O_2 \rightarrow Na_2O_2$, 10.97 MJ/kg
  - $4\,Na + O_2 \rightarrow 2\,Na_2O$, 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:

$$D = \frac{6.4315\times10^{-5}}{P} T^{1.823}$$

- 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

Predicted quantities:
- Mass of Na(pool, burned), O_2(consumed), Na_2O_2+Na_2O(produced)
- Energy of reactions

Model Extensions
- Radiation Heat Transfer Between Heat Structures and Pool Surface
- Heat Transfer Between Pool and Atmosphere

  - CONTAIN/LMR uses film temperature for evaluating many thermodynamic properties.
- User controllable pool surface area
  - User-specified surface area (control function)

Atmospheric Chemistry

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)

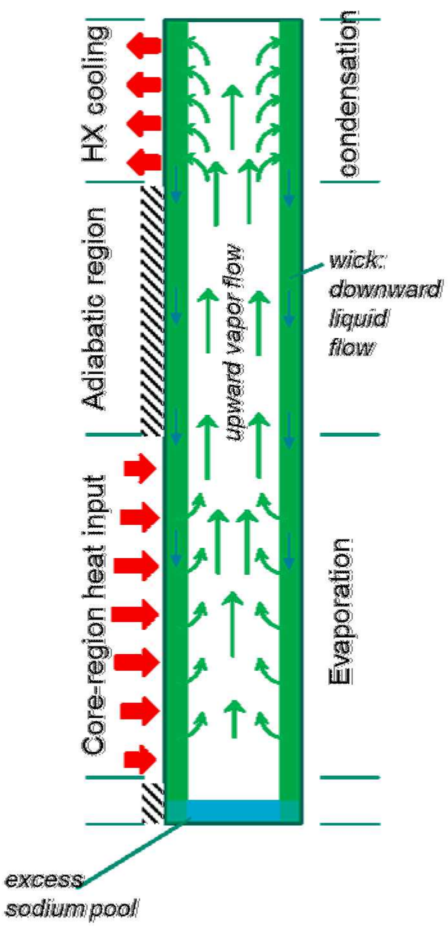
Outputs

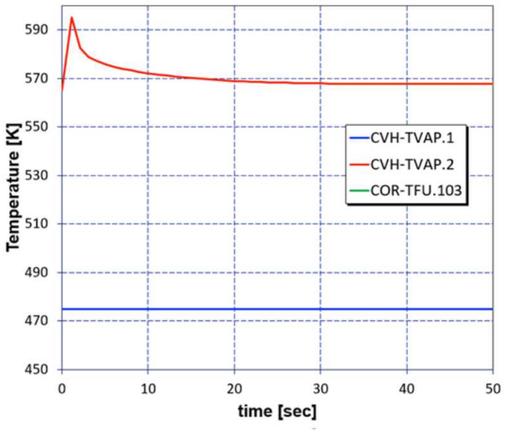
- Reaction number, reaction energy, byproducts (Na classes, H_2), gas and liquid consumed (Na, H_2O, O_2)

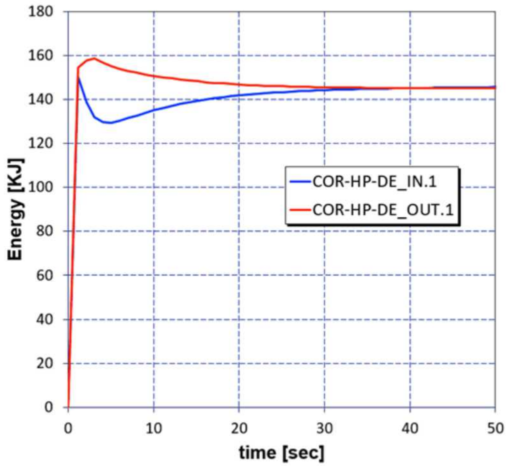
Heat Pipe Model (ongoing development)

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

A Generic Heat Pipe Illustration







Aerosol Radiation Model

Aerosol cloud emissivity derived per Pilat and Ensor

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

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

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

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

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

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

Radionuclide Transfer between Pool & Atmosphere

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

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

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

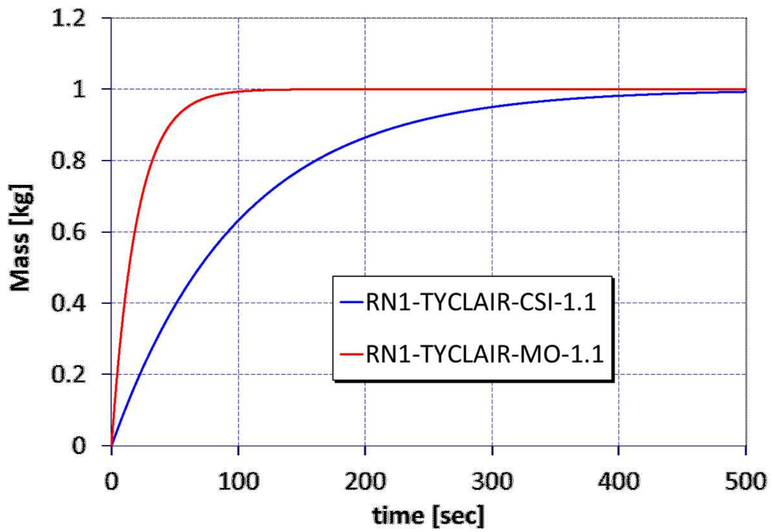
- User specifies table (for each CV) of radionuclides and CFs for calculating RN transfer

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

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

Example Input:

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



Example case:

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

Sodium Fast Reactors

Existing Modeling Capabilities

Sodium Properties
- Sodium Equation of State
- Sodium Thermo-mechanical properties

Containment Modeling
- Sodium pool fire model
- Sodium spray fire model
- Atmospheric chemistry model
- Sodium-concrete interaction model (in development)

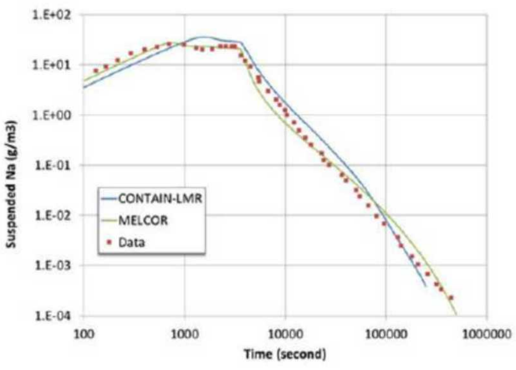


Figure 33. Suspended Na Aerosol Mass - AB1

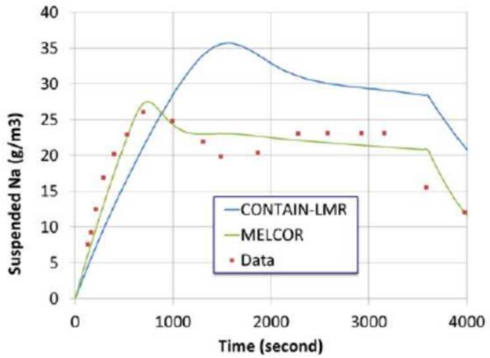


Figure 34. Suspended Na Aerosol Mass-AB1

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

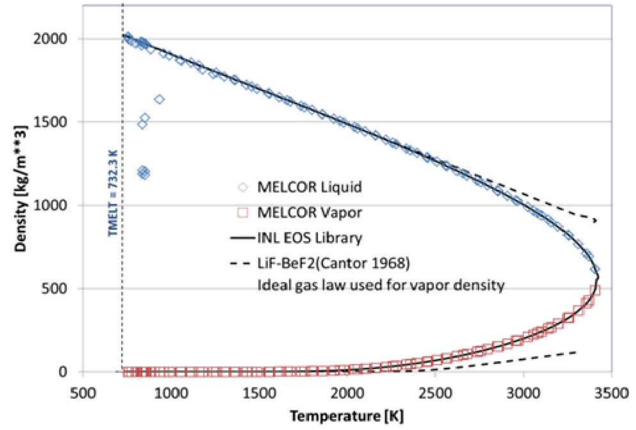
- Equation of State
  - Current capability
- Thermal-mechanical properties
  - Current capability
- EOS for other molten salt fluids would need to be developed
  - Minor modeling gap

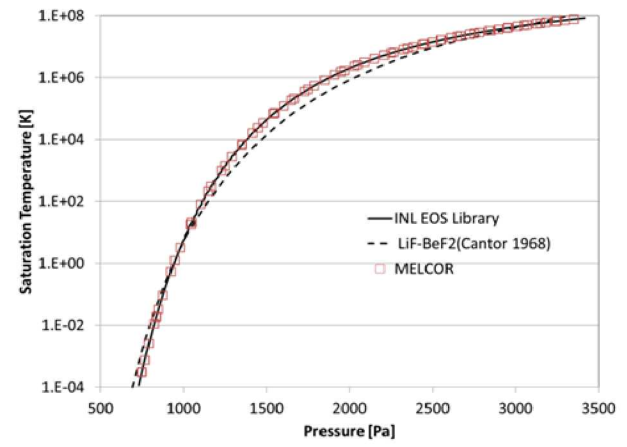
Fission product modeling

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

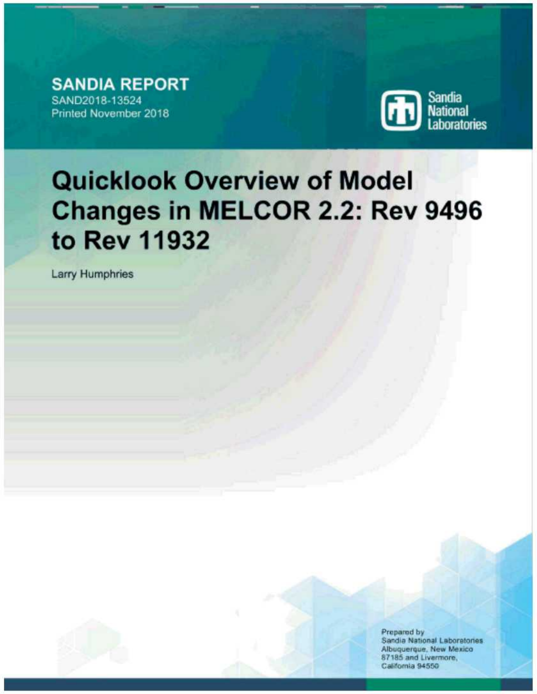
Two reactor types envisioned

- 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.





MELCOR 2.2.11932 Code Release (November 30, 2018)


SANDIA REPORT
SAND2018-13524
Printed November 2018

Sandia National Laboratories

Quicklook Overview of Model Changes in MELCOR 2.2: Rev 9496 to Rev 11932

Larry Humphries

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico
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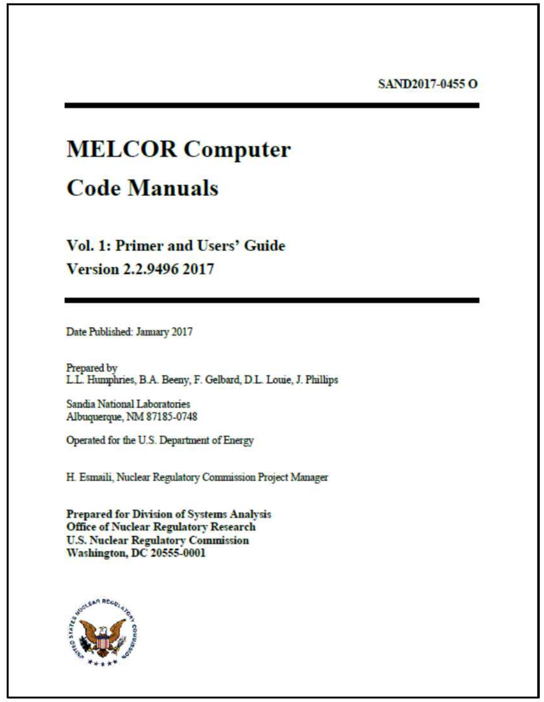
MELCOR 2.2 Quicklook Overview of Model Changes in MELCOR 2.2

SAND2018-13524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MELCOR Computer Code Manuals

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

Date Published: January 2017

Prepared by
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Operated for the U.S. Department of Energy

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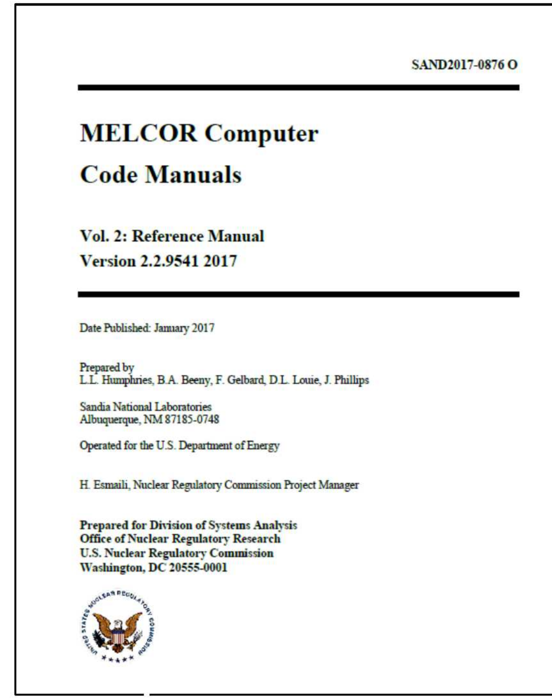
Prepared for Division of Systems Analysis
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001

Volume I: User Guide

SAND2018-13559 O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MELCOR Computer Code Manuals

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

Volume II: Reference Manual

SAND2018-13560 O

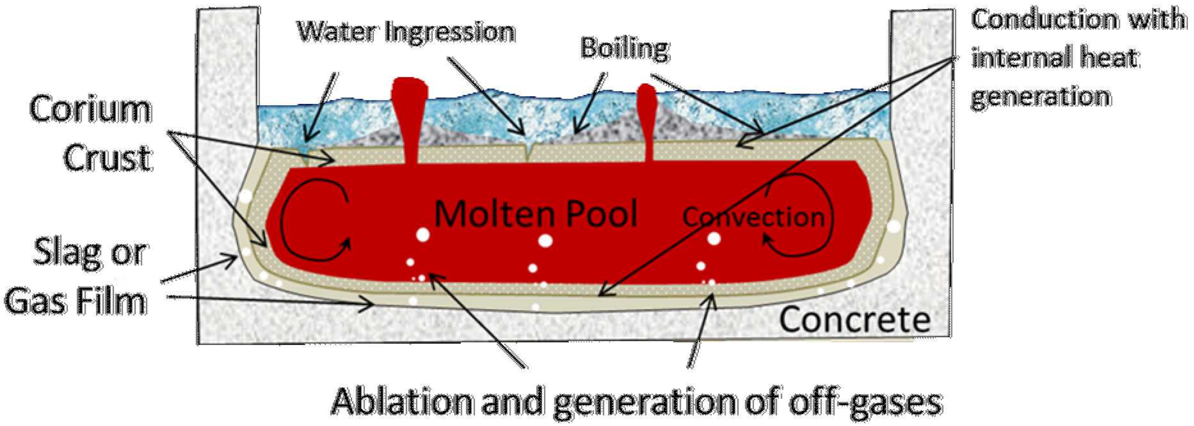
Cases in MELCOR Assessment Report - SAND2015-6693 R

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

MELCOR ASSESSMENTS AGAINST EXPERIMENTS
- Analysis of ABCOVE AB5 and AB6 Aerosol Experiments
- Analysis of ACE Pool Scrubbing Experiments
- Analysis of AHMED 1993 NaOH Experiments
- Analysis of the Bethsy 6.9c Experiment (ISP-38)
- Analysis of Containment System Experiment for Spray – A9 Test
- Analysis of the Cora 13 (ISP 31) Experiment
- Analysis of Aerosol Behavior from the Demona-B3 Experiment
- Analysis of Level Swell from the General Electric Large Vessel Blowdown and Level Swell Experiment – 5801-13
- Containment Analysis from the JAERI Spray Experiments
- Analysis of LACE LA-4 Experiment
- Analysis of LOFT LP-FP-2 Experiment
- Analysis of Critical Flow from the Marviken CFT-21 and JIT-1 Experiments
- Analysis of Marviken-V Aerosol Transport Test (ATT-4)
- Analysis of NTS Hydrogen Burn Combustion Tests
- Analysis of the Nuclear Power Engineering Corporation (NUPEC) Mixing Tests
- Analysis of the PHEBUS FPT-1 Experiment
- Analysis of the PHEBUS FPT-3 Experiment
- Analysis of the POSEIDON Integral Experiments under Hot Pool Conditions
- Analysis of STORM Aerosol Mechanical Deposition Tests
- Melt Coolability and Concrete Interaction Experiments
  - CCI-1, CCI-2, and CCI-3

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

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 and formation of voids

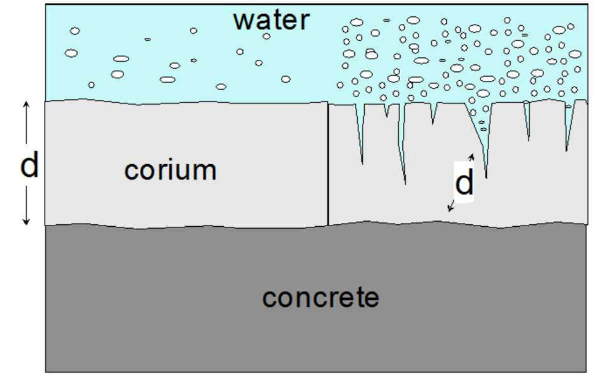
- Water ingression reduces conduction path to molten pool and increases surface area of contact

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

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

Pre 2015 MELCOR Best Practice

- Water 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

CORCON/CORQUENCH Model

Enhanced Conductivity (2010)

CAV_U 9

…

5 BOILING value 10.0

6 COND.OX mult 5.0

7 COND.MET mult 5.0

8 HTRINT multip 1.0

9 HTRSIDE multip 1.0

Modified Enhanced Conductivity (2012)

CAV_U 10

…

5 BOILING value 10.0

6 COND.OX mult 1.0

7 COND.MET mult 1.0

8 HTRINT multip 5.0

9 HTRSIDE STAND

10 COND.CRUST 3.0

Still current best practice

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

Not recommended in current release
Will be corrected in next release

Observations on Core Degradation from Fukushima

What we know from experiments

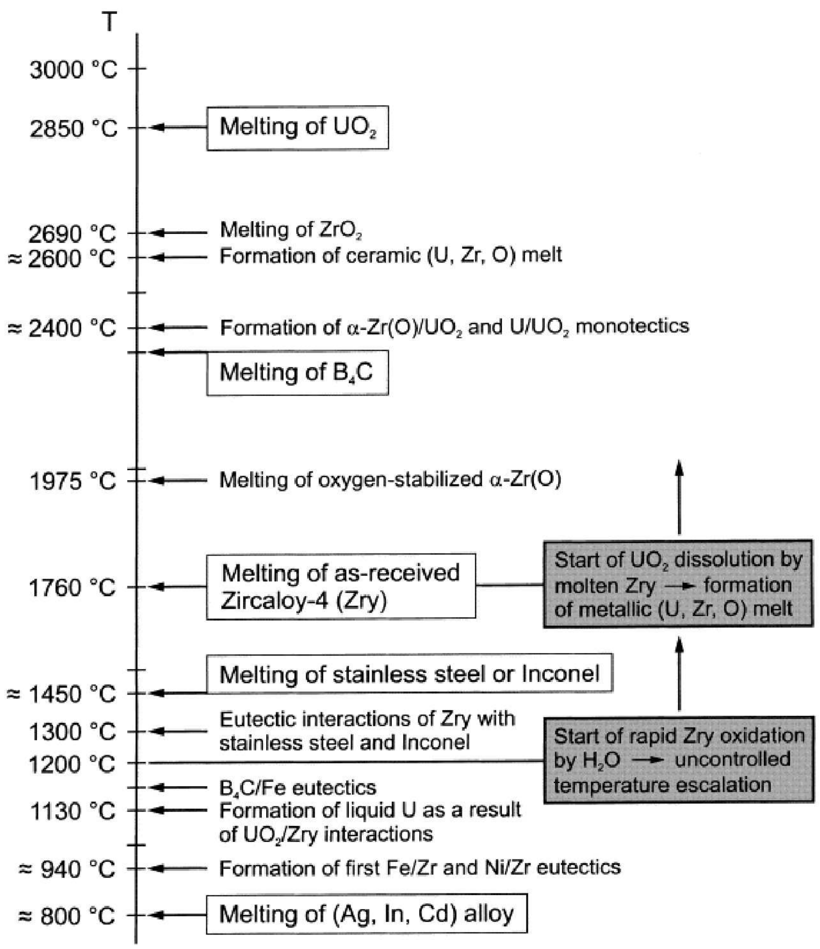
What is modeled in codes

Important materials interactions

Chronology of damage progression roughly follows in order of increasing melting/liquefaction temperatures

- Plausible sequence to explain 1F-2,3 robotic visual examinations
- Highlight MELCOR modeling observations
- Highlight potential decommissioning phase data collection needs

Important Material Interactions
(Hagen and Hoffman – KfK)



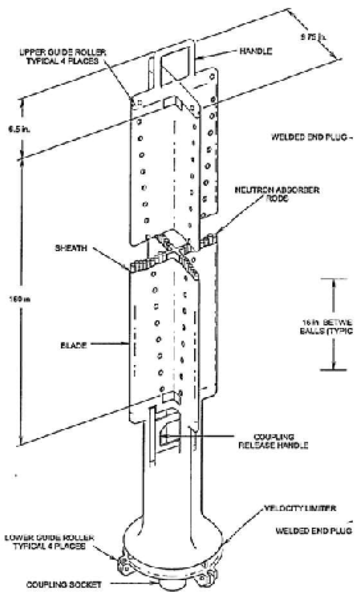
- View in 1980's (STCP) assumed fuel melts at 3200K
- Early experiments showed role of material interactions showed fuel "liquefied" at lower temperatures
  - 2400K up to 2880K
- DF-4 BWR Experiment showed B_4C/SS blades liquefy at ~1500K (compared to 1700K)
- Eutectics form between Zr/SS with liquefactions as low as 1200K to 1573K
- *Heat of mixing of Zr/Fe is exothermic and generally not treated*

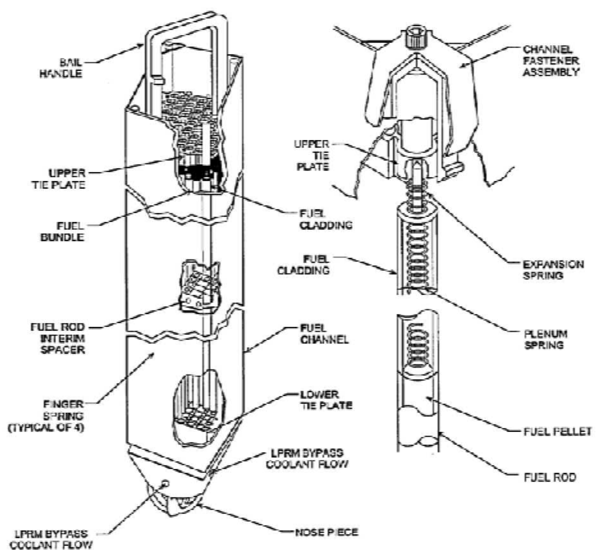
BWR Core Components

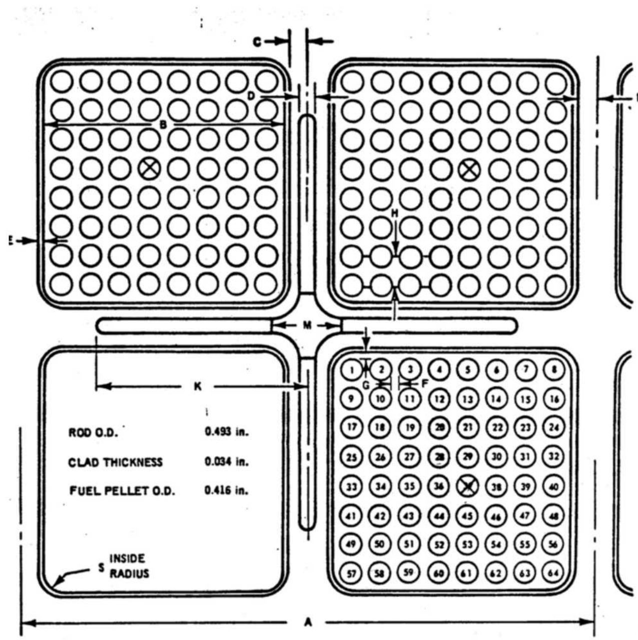
$UO_2/Zr(O)$ liquefactions → ~2400K

B_4C/SS liquefactions → ~1500K

$B_4C/SS/Zr$ liquefactions → ~1200K to 1500K







Differing Materials in close proximity

BWR Reactors Materials

15 m^3 UO_2

5 m^3 Zr Cladding

3.2 m^3 Zr Canisters

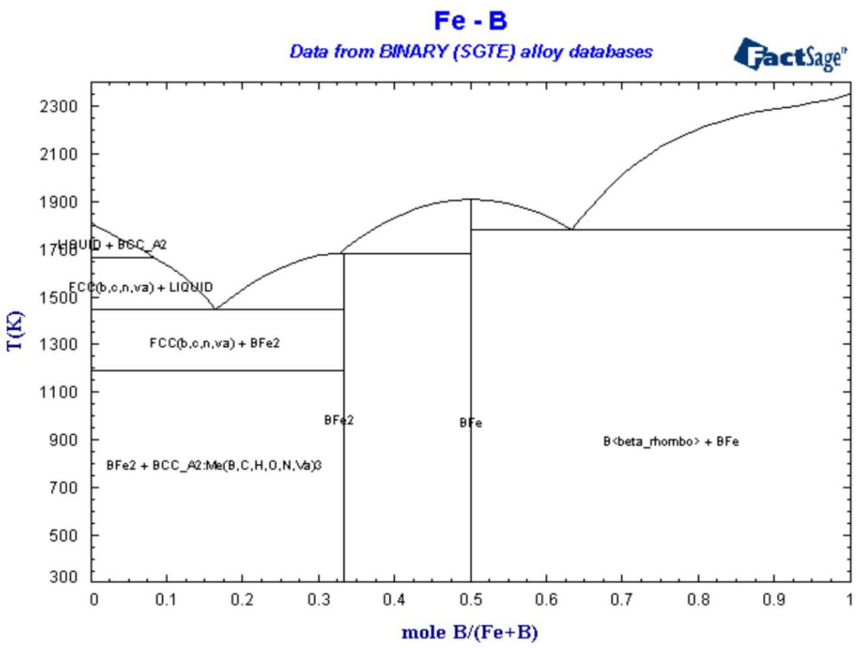
2.6 m^3 SS Blades

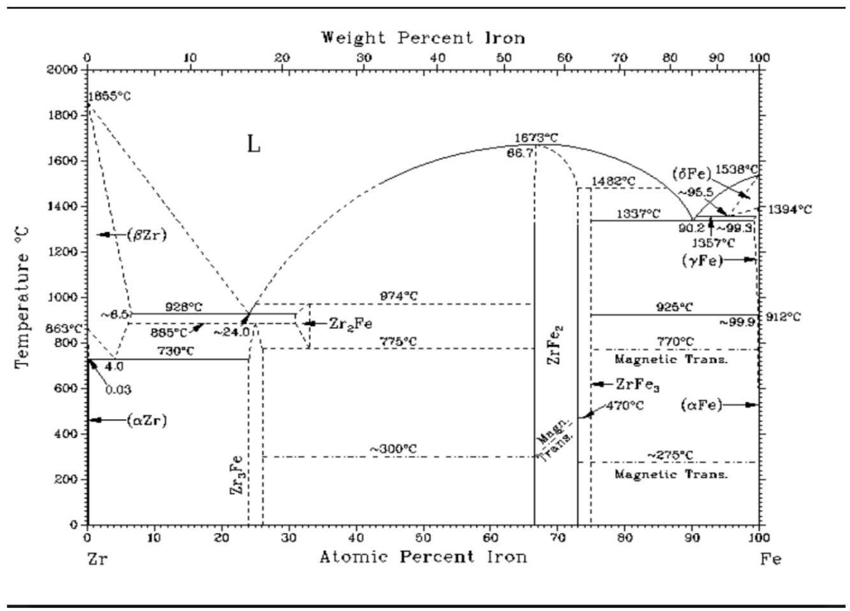
Typical amounts of fuel, zircaloy and other comparisons between comparably sized PWR and BWR reactor cores.**

Component	3411 MWth PWR	3579 MWth BWR
Fuel (UO_2)	118,000 kg	155,000 kg
Cladding	21,000 kg	33,800 kg
Fuel Canisters	N/A	21,600 kg
Total Zircaloy	21,000 kg	55,400 kg
Control Material	1,200 kg Ag/In/Cd	885 kg B_4C
Ratio Zr/UO_2 mass	0.18	0.36
Potential H_2 from Zr oxidation	923 kg or ~10,300 m^3	2435 kg or ~27,300 m^3

** Data compiled from reference 15.

Control Blade/B4C & SS/Zr Interactions

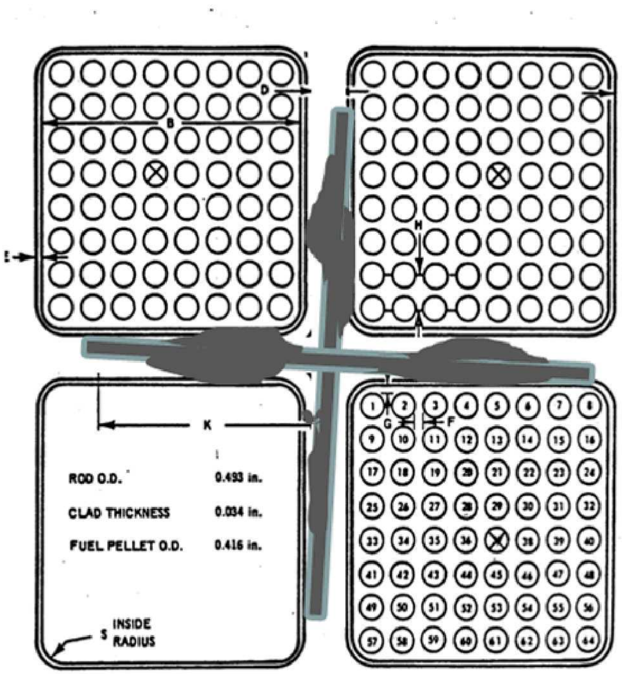




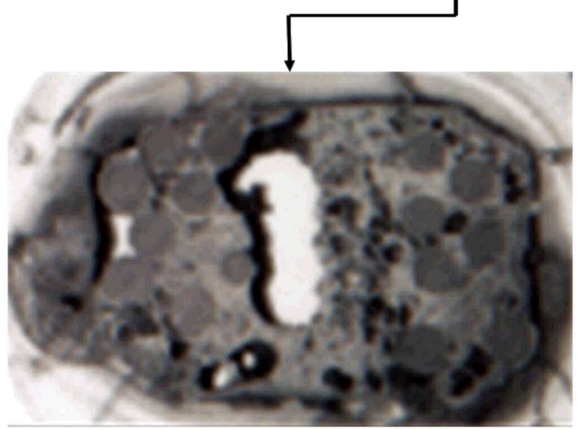
- Reaction rate seems very rapid based on experiments
- B_4C seems largely consumed into eutectic melt
- B_4C likely follows liquefied SS

- Blade distorts and melt contacts Zr channel box
- Channel box liquefied by Fe-Zr eutectic (1200K)
  - Channel box "unzips"
- Liquefied materials drain downward
  - Inside channel box and outside channel box

Attack of Channel Box (Zr) by Liquefied Blade Material (SS/B4C)



DF-4 BWR Experiment in ACRR (SNL)



- Channel and blade obliterated over most of length
  - Slight remnant at bottom
  - Blade material at bottom

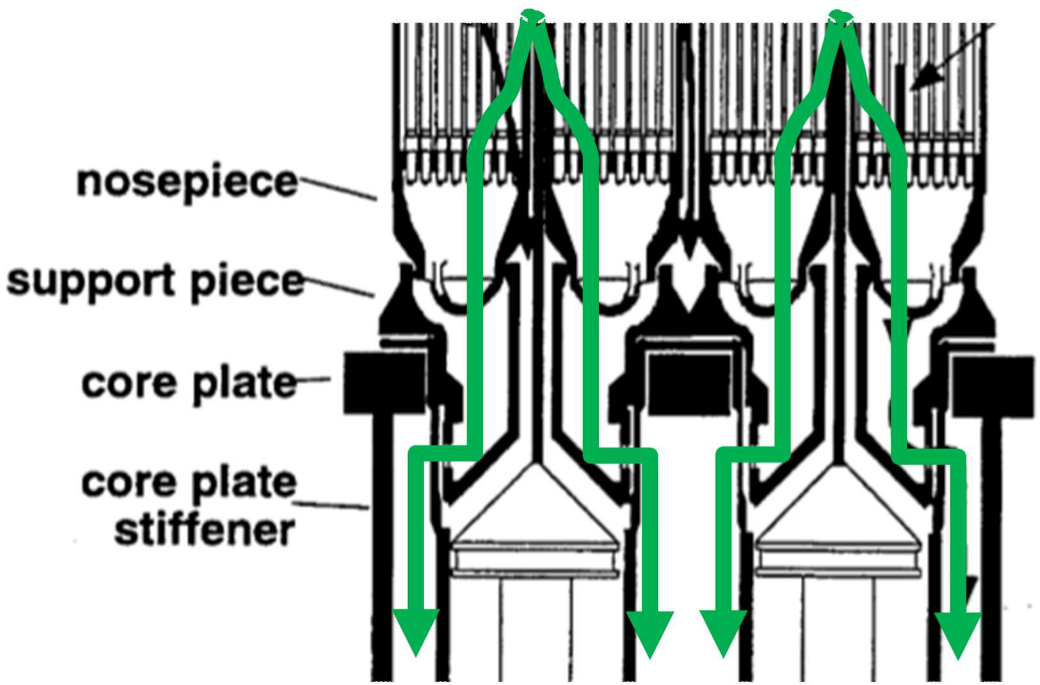
Blade/Canister Melt Draining Inside Fuel Canister

Liquefied Blade (SS) and Canister (Zr) can enter fuel rod canister

Drain into nose pieces and fuel support piece

Exit support piece through flow orifices

Drain down outside of guide tubes

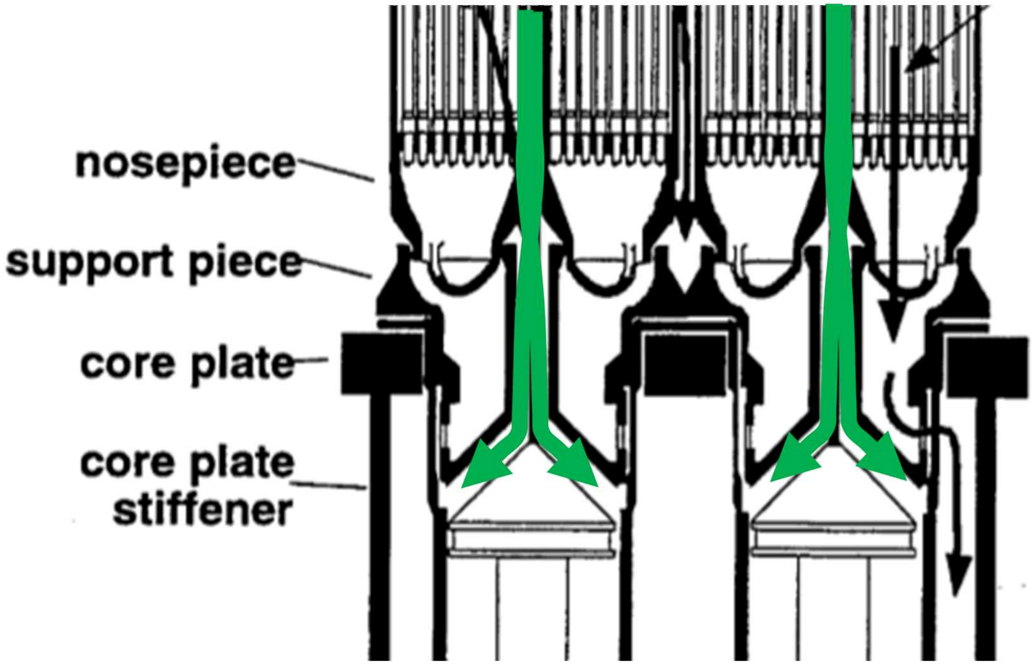


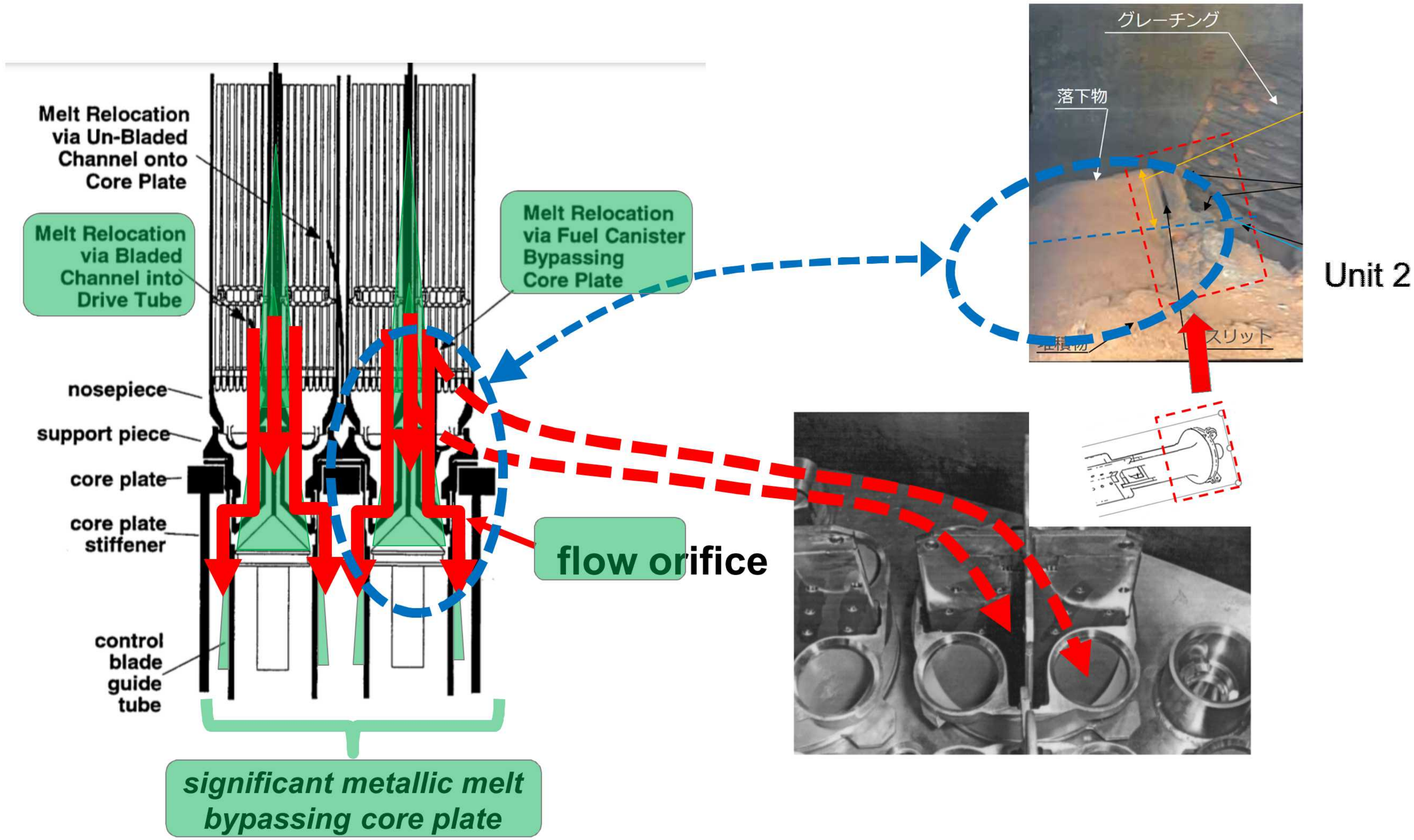
Blade/Canister Melt Draining Within Blade Region

Liquefied Blade (SS) and Canister (Zr) can also drain down the blade region

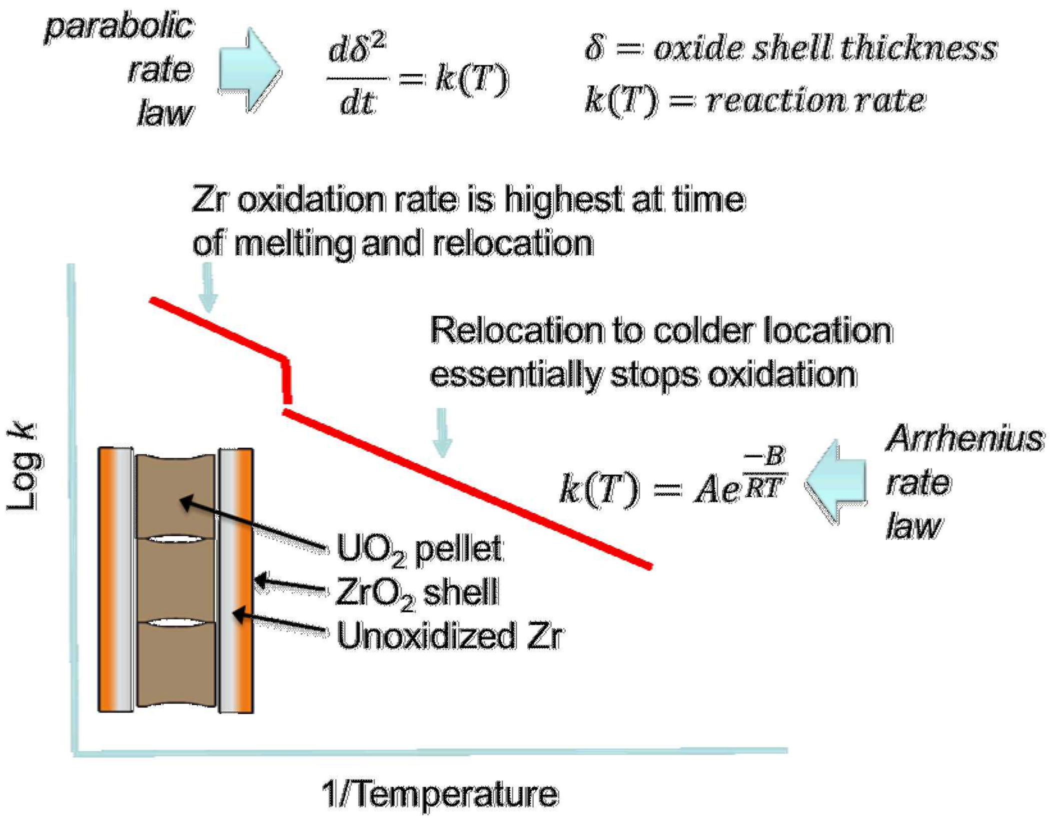
Drains into bladed region below core plate

Melt will accumulate on velocity limiter



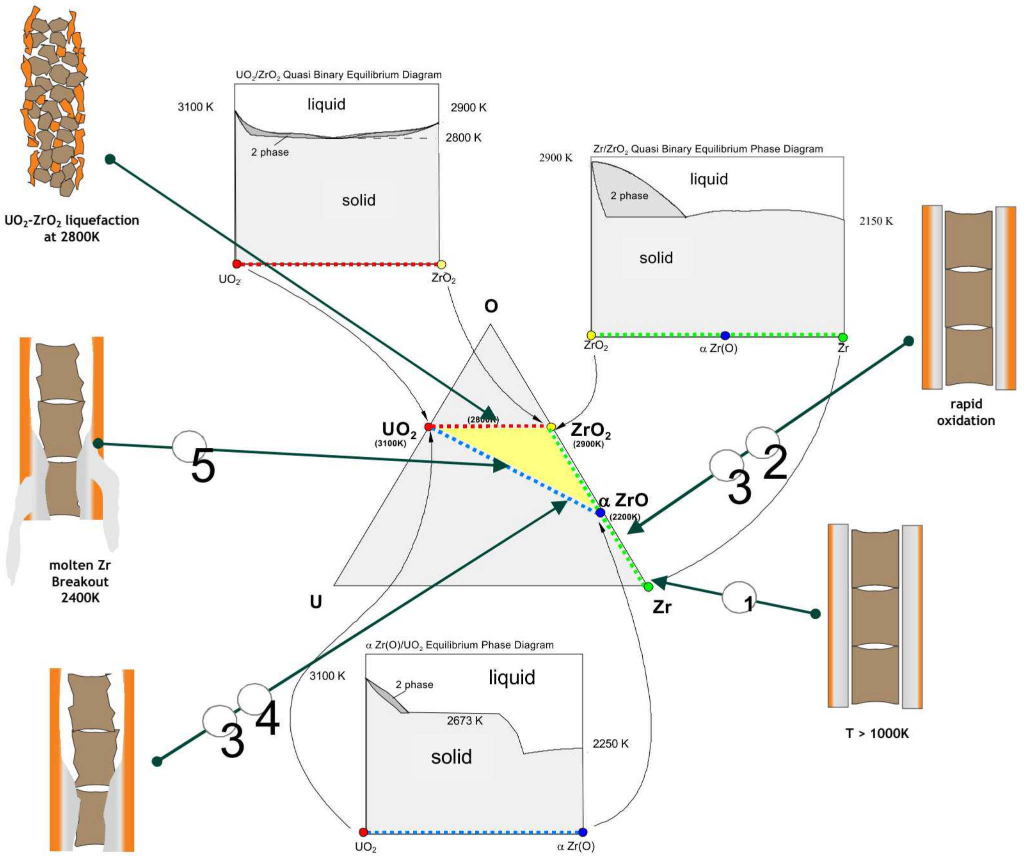

Melt Relocation via Un-Bladed Channel onto Core Plate
Melt Relocation via Bladed Channel into Drive Tube
Melt Relocation via Fuel Canister Bypassing Core Plate
nosepiece
support piece
core plate
core plate stiffener
control blade guide tube
flow orifice
significant metallic melt bypassing core plate
グレーチング
落下物
スリット
Unit 2

Exotherimc Reaction between Zr and Steam



- ❑ $Zr + 2H_2O \rightarrow ZrO_2 + 2H_2$ + energy
- ❑ Reaction rate is autocatalytic (accelerates with T)
- ❑ Decay power heatup rate ~1K/s
- ❑ Oxidation power heatup rate ~15K/s
- ❑ *Short time between start of oxidation and relocation of liquefied Zr*

U/Zr/O Material Interactions



1. Zr cladding begins to oxidize with steam at ~1000K
   - ZrO_2 outer shell forms
   - Underlying Zr-metal takes on dissolved oxygen
2. α Zr(O) melts at ~2100K confined under ZrO_2 shell
3. Molten α Zr(O) wets and interacts with cracked UO_2
   - UO_2 dissolved into α Zr(O) (U-Zr-O)
4. Equilibrium dissolution or rate limited ?
   - Parabolic interaction rate measured by Hoffman (MELCOR option)
5. ZrO_2 shell breaks at ~2400K releasing molten U-Zr-O
   - Metallic U-Zr-O segregates from oxidic UO_2/ZrO_2

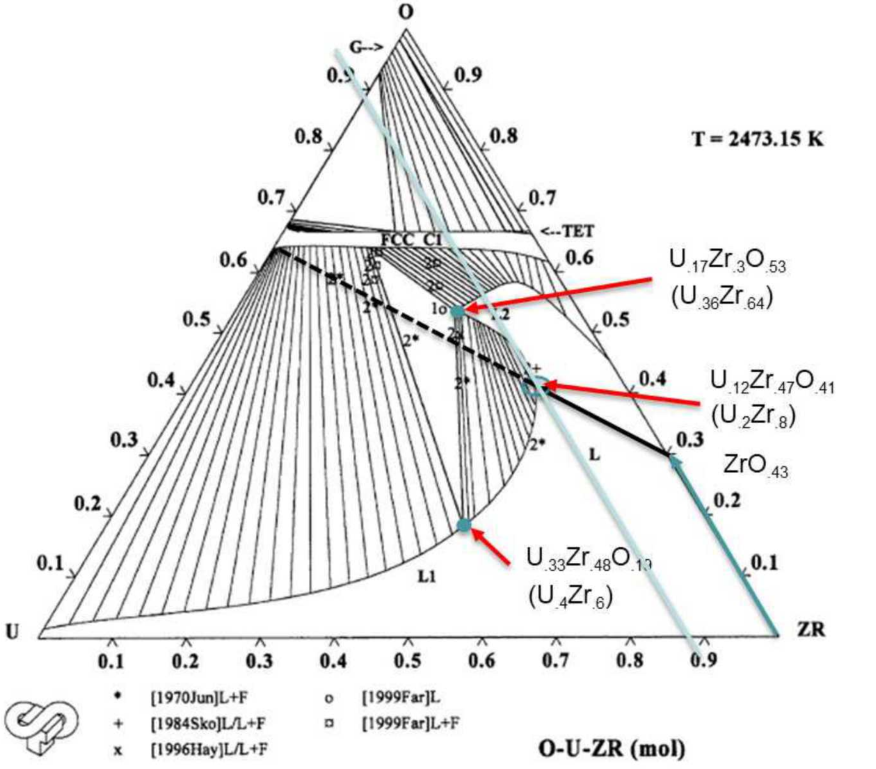


Fig. 12. Calculated O–U–Zr isothermal section at $T = 2473$ K compared to the selected experimental information.

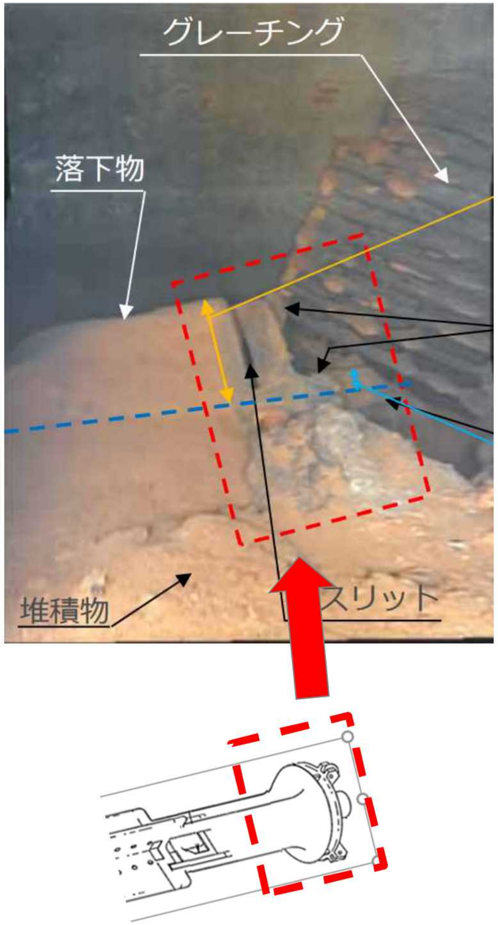
Steam oxidation
UO2/ZrO interaction
kinetics

Temperatures escalating – 10K/s

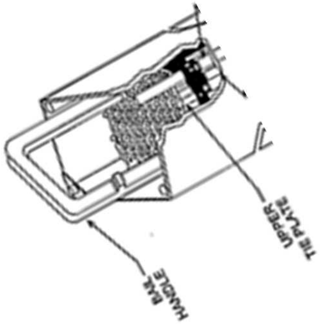
Melt release criteria ?

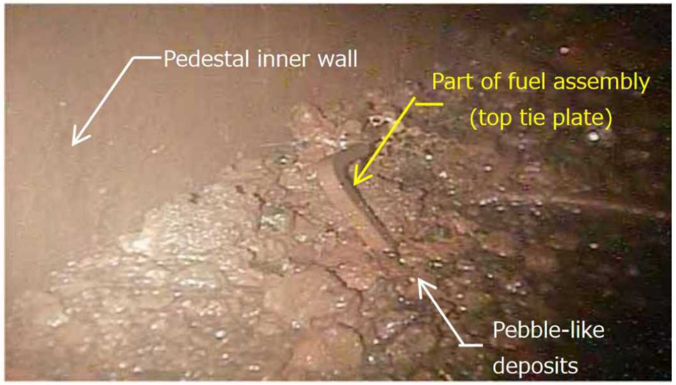
U/Zr mass ratio in liquid in range of 0.6 to 1.8

Unit 3

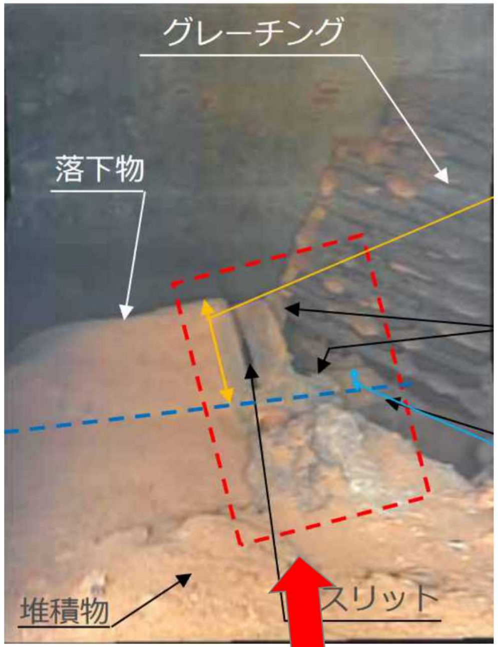


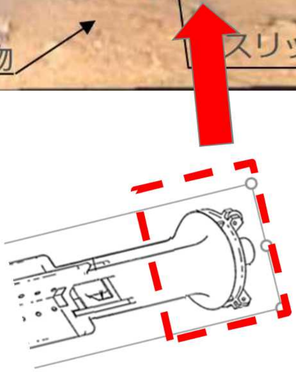
Unit 2


BAIL HANDLE
UPPER TIE PLATE

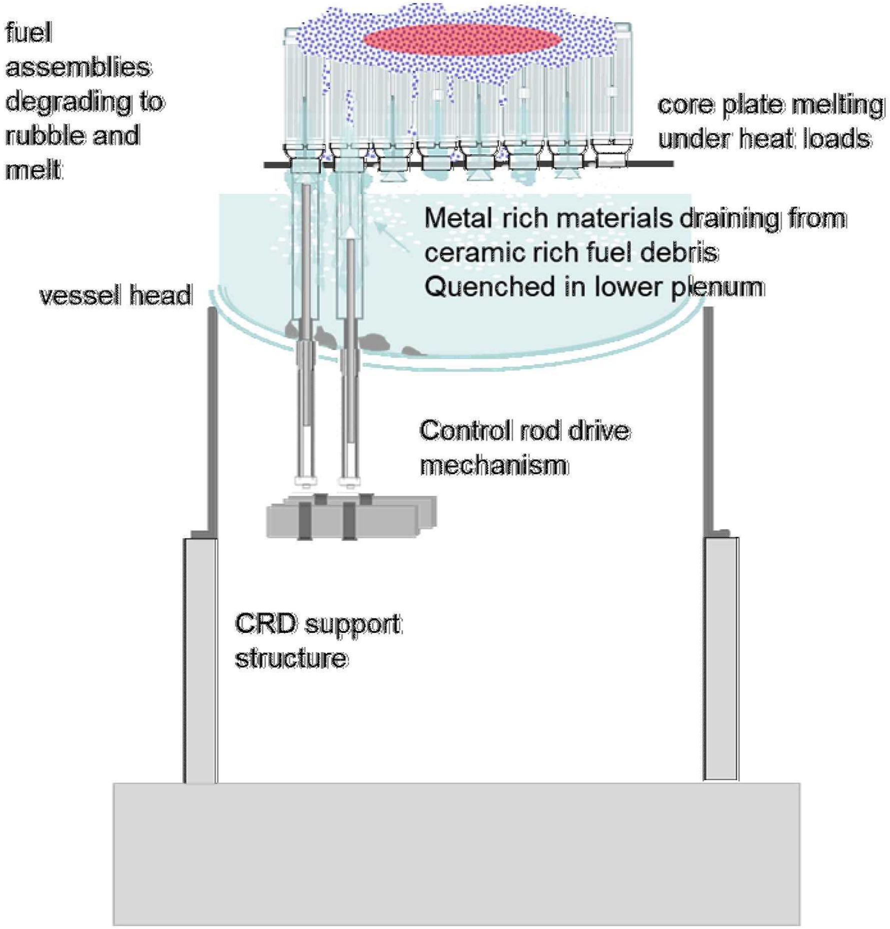

Pedestal inner wall
Part of fuel assembly (top tie plate)
Pebble-like deposits

Unit 2

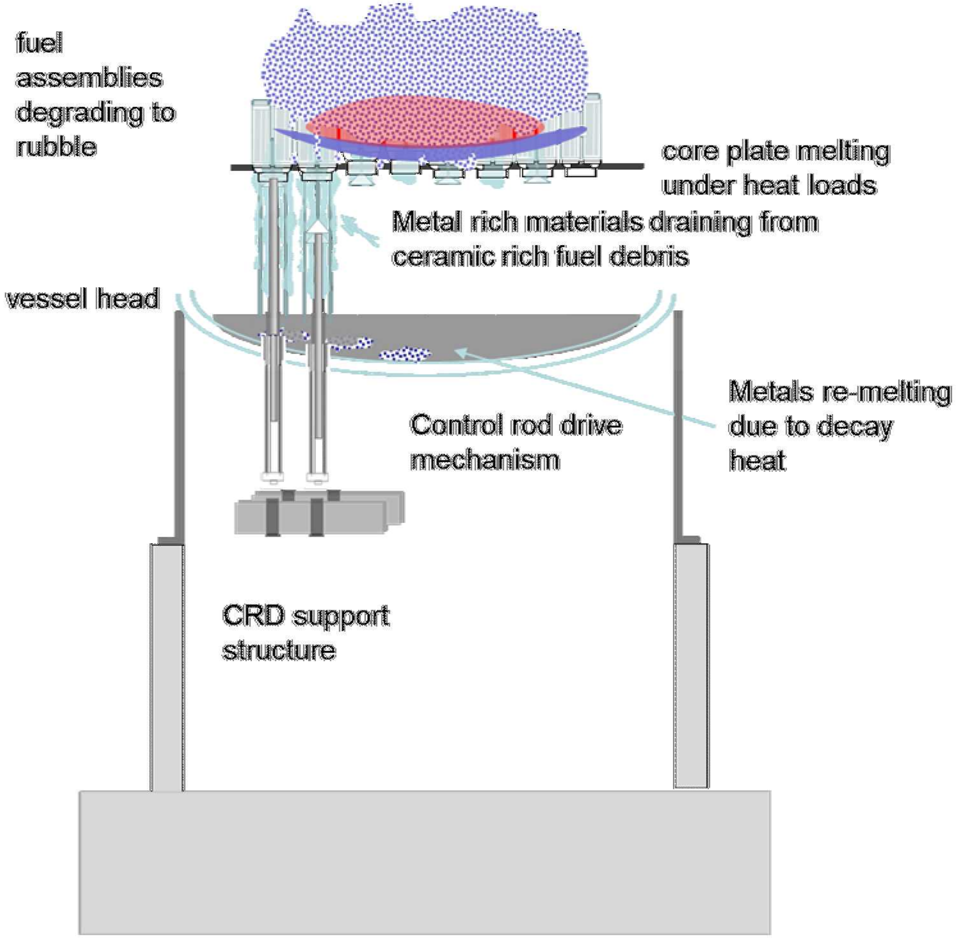

グレーチング
落下物
堆積物
スリット



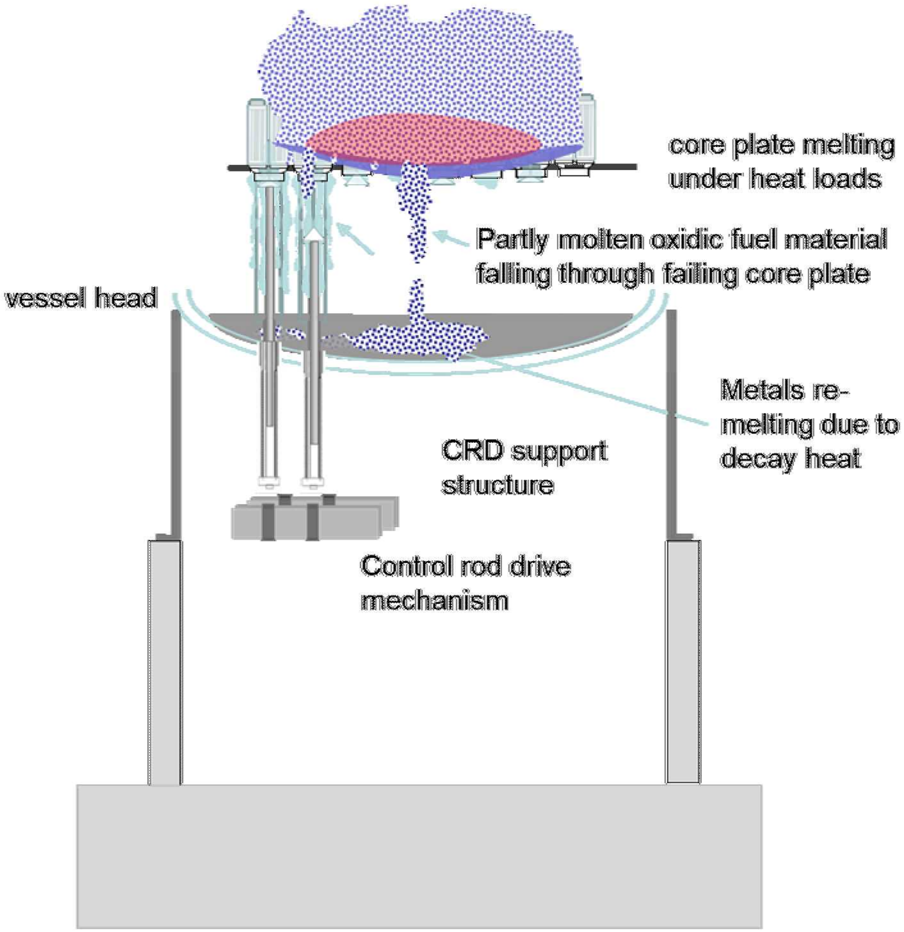
Unit 2



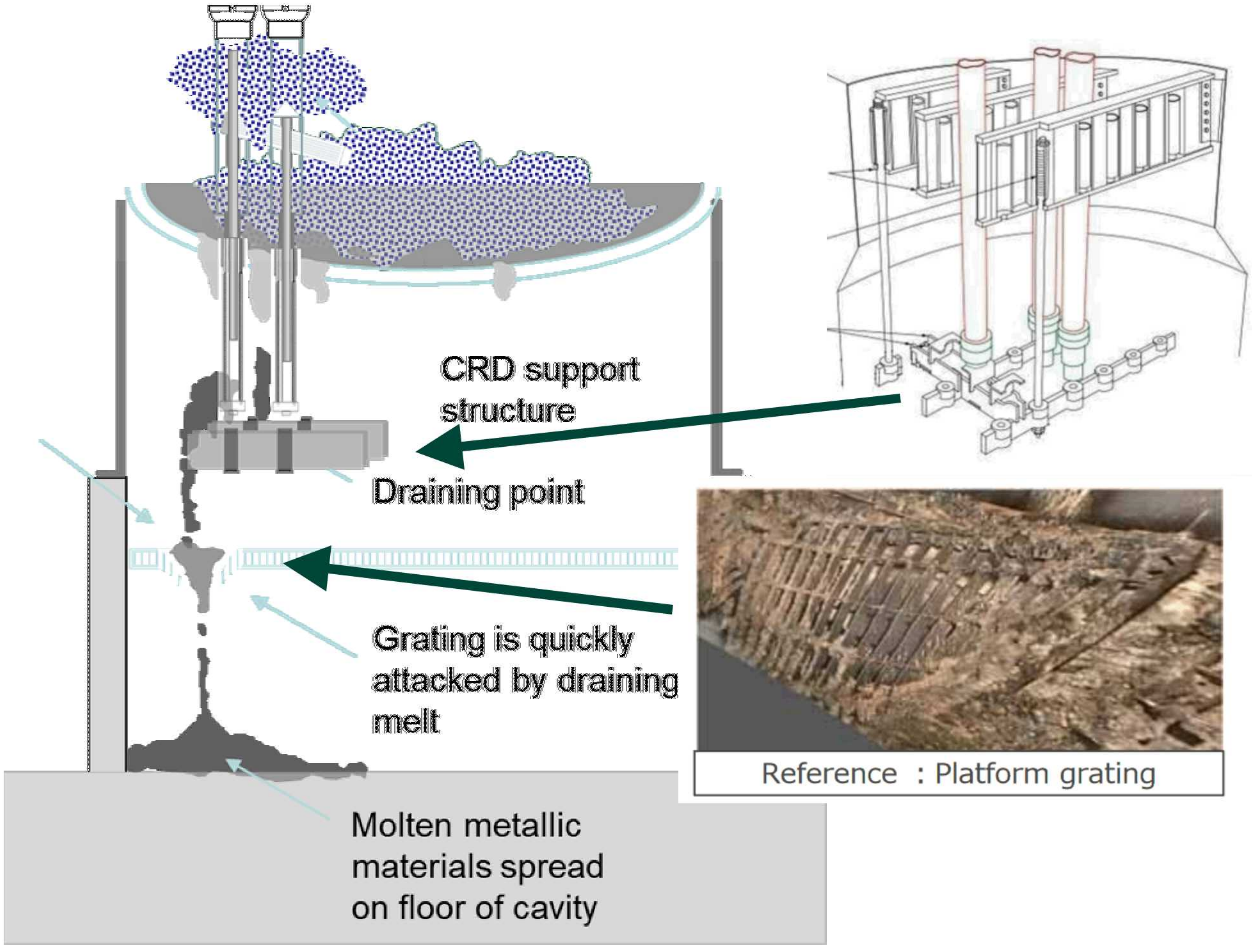
- ❑ Control blades melt first and drain away from fuel materials, falling through core plate and nose pieces DF4 and XR2-1.
- ❑ Interaction with and dissolution of Zr channel boxes are expected – <u>not considered by MELCOR without eutectics model</u>
- ❑ Metals drain to lower head and may quench in water
- ❑ Core debris region degrades as metallic are accumulating on lower head – a race



- Zr-cladding and channel boxes remnants oxidize
- Fuel rods degrade and slump, either
  - onto core plate, or
  - In-Core TMI-2 like crucible could also form
- Lower head water evaporates and metals (SS-Zr + U-Zr-O) accumulations heat and remelt
  - Dissolved UO2 content could will increase heat loads to lower head

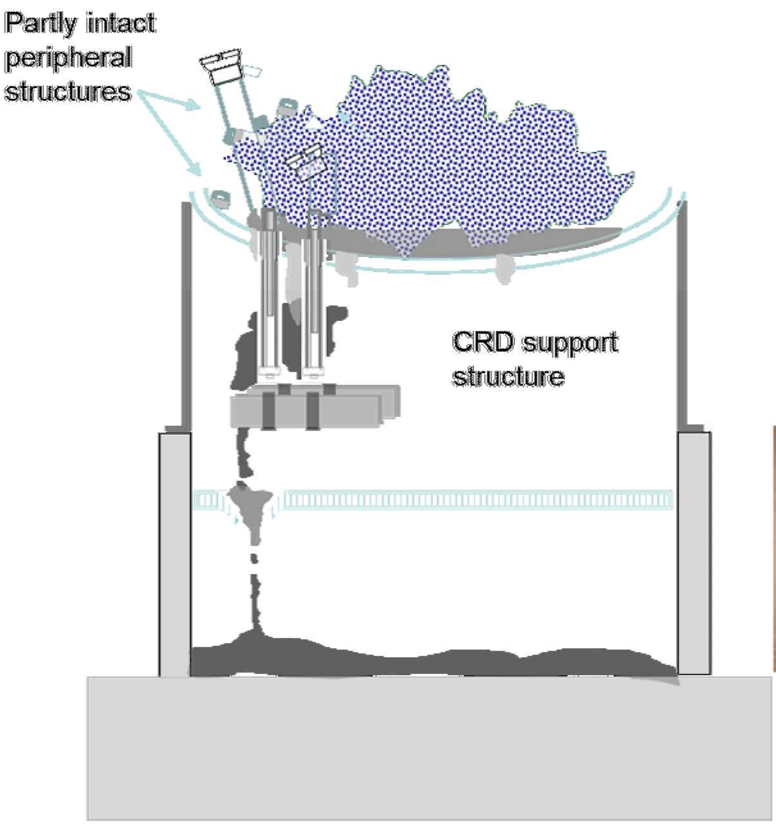


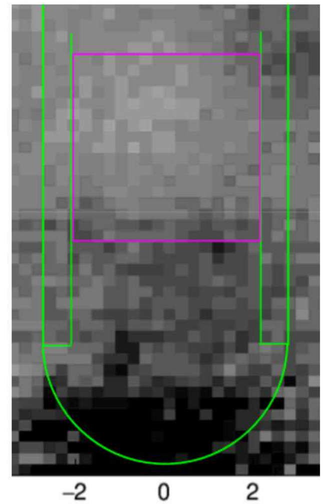
- Partly molten/partly solid fuel oxidic fuel materials heat metals above carbon steel melting temperature
- Configuration resembles “hot rocks in molten soup of Zr-SS metal”
- Heat conduction to vessel wall begins to melt wall
- Intermetallic reactions and heat of mixing (Fe-Zr) may be very exothermic and drive progressive attack of vessel wall
- Competition in collapse of core with failure of lower head

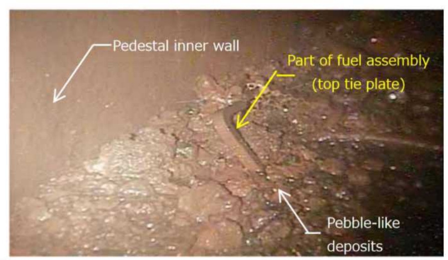


- Vessel wall melted or yielded away leaving drive tube remnants standing, supported by CDR support structure below vessel head
- Molten Fe-Zr-U-O metals drain from multiple holes in vessel head
- Accumulations form on CRD support structure and find draining point
- Underlying grating structures attacked by draining melt
- Vessel wall may be largely disintegrated leaving only CRD drive tubes and penetration nozzles supported by CRD support structure

Unit 2 End State

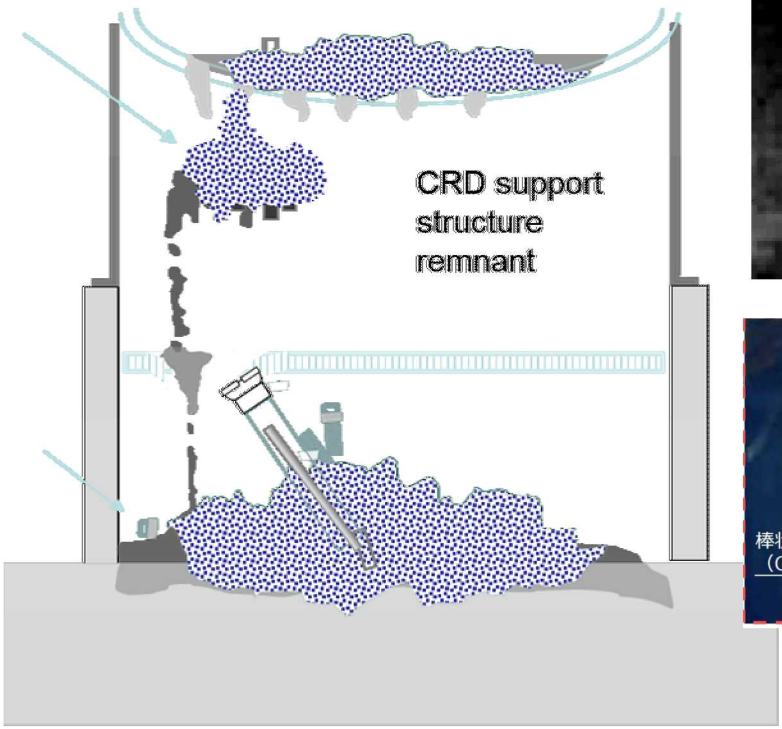


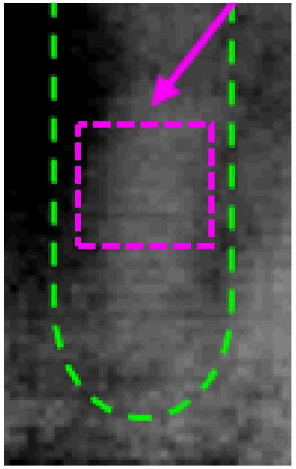




- Peripheral structures may be partly intact at edge of core and fall to lower head – MELCOR *could* capture this with code modifications
- Metallic melt spreads to walls of cavity – MELCOR can do
- 1F2 may have been arrested by this time leaving a mostly level metallic layer on cavity floor – 1F2
- Some intact parts apparently fell through largely disintegrated lower head – 1F3

Unit 3 End State





- ❑ Increasing melt release to C/R support structure fails structure, finally allowing dropping of in-core drive tube structures
- ❑ Lower head must be largely melted/slumped away allowing large in-core structures to fall to cavity floor

Summary

Material interactions potentially more significant in BWR melt progression compared to PWR

Control blade liquefaction by B4C interaction at 1500K

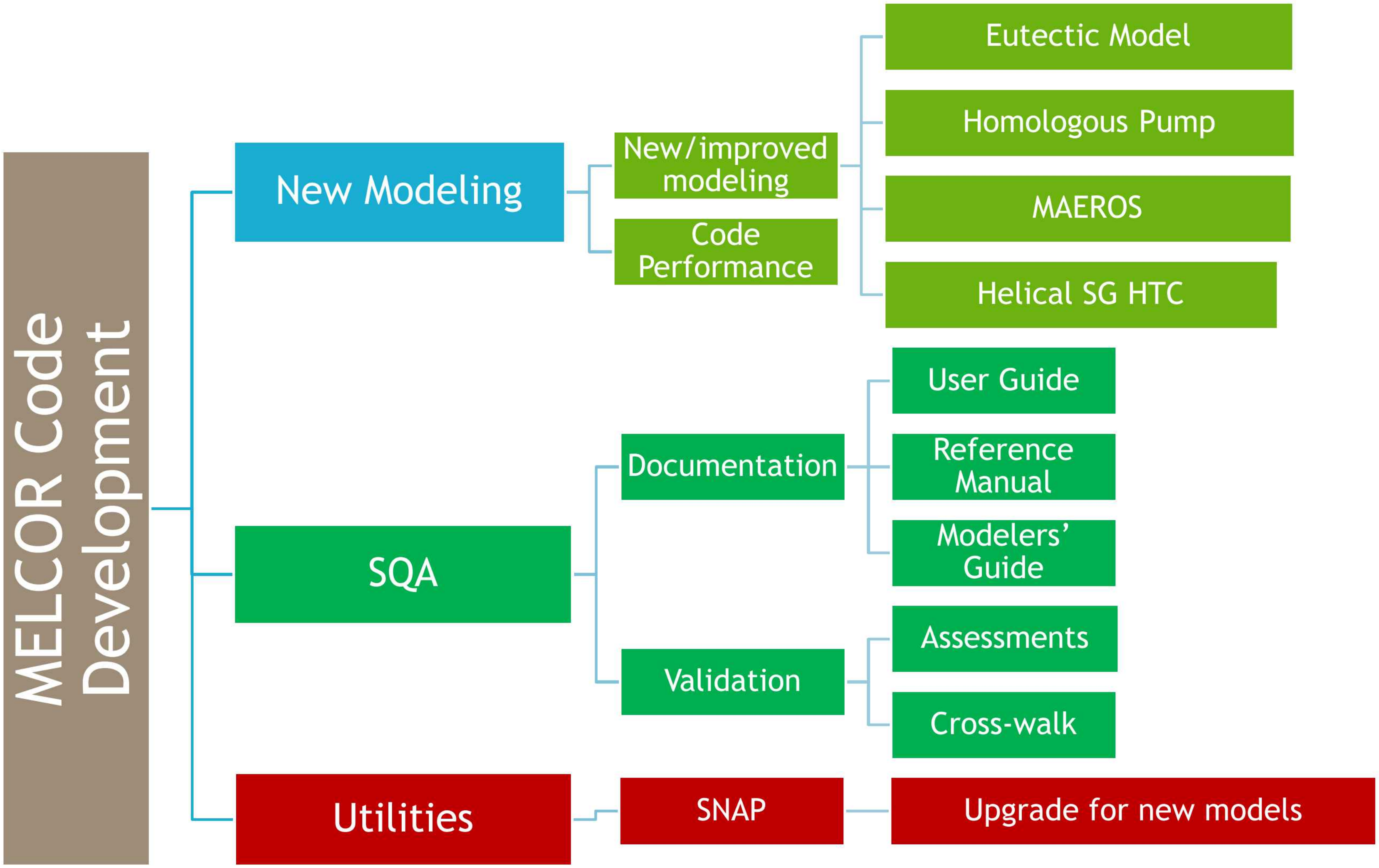
Model for channel box attack by molten control blade SS needed

UO2 dissolution by molten Zr creates lower temperature heat bearing molten phase – need kinetics model for dissolution

Metallic melts (SS/Zr) can segregate from core fuel and relocate to bottom head – models for head failure need attention

- Heat of mixing for Zr-Fe possible head failure phenomena

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