SAND2019-13342PE

MELCOR Eutectics Model



PRESENTED BY

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MELCOR Eutectic Model Overview

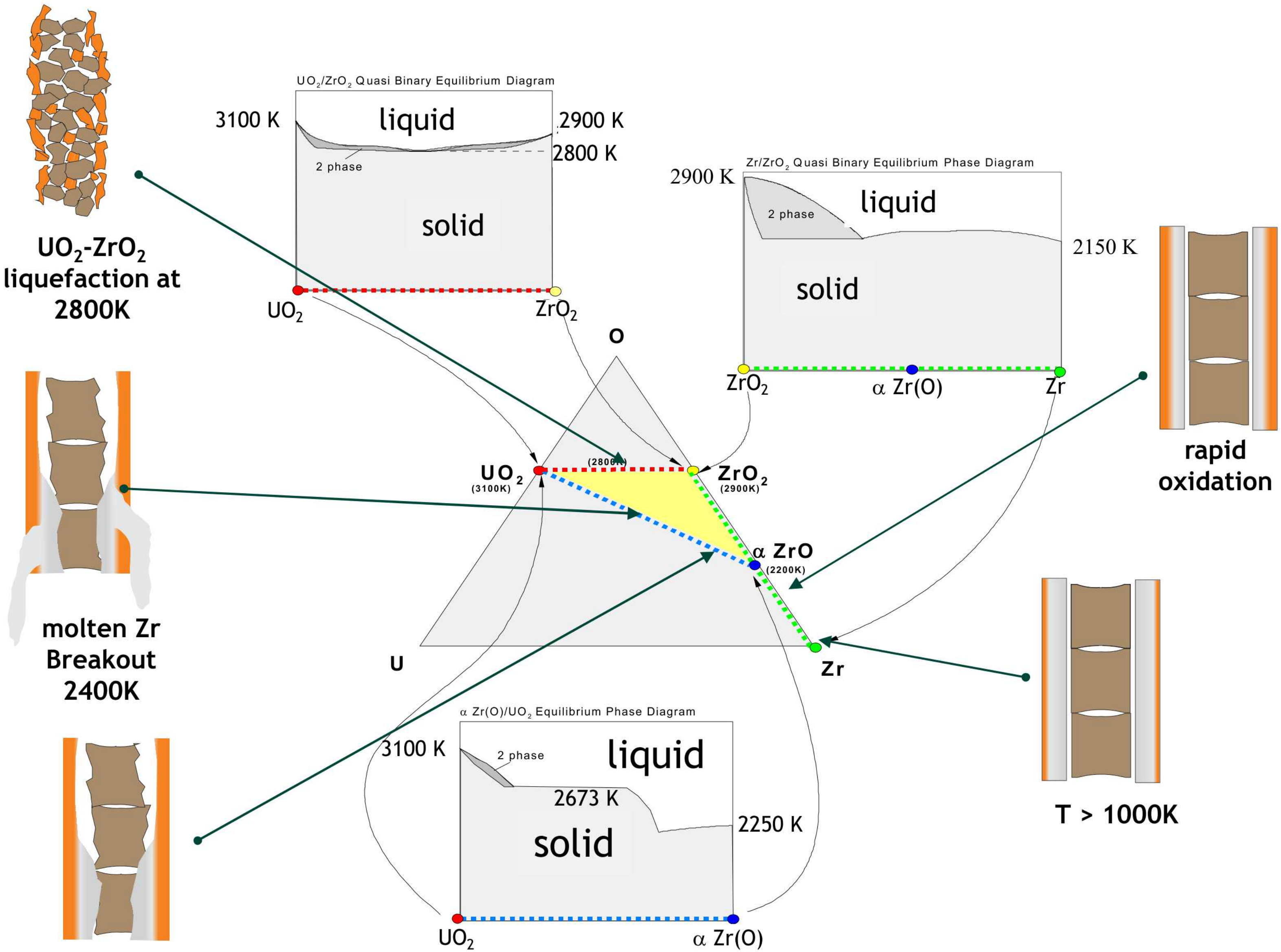
Eutectics model has been in the code since M1.8.2

- 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 ready for general use

U/Zr/O Ternary Phase Diagrams



Eutectic Model Input

New Input for the Eutectic model

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

COR_EUT ON enables the model & uses defaults
COR_EUT OFF disables the eutectics model

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
If not, you will see a warning in the diagnostic file and the eutectics model is essentially disabled.

Eutectic Mixtures

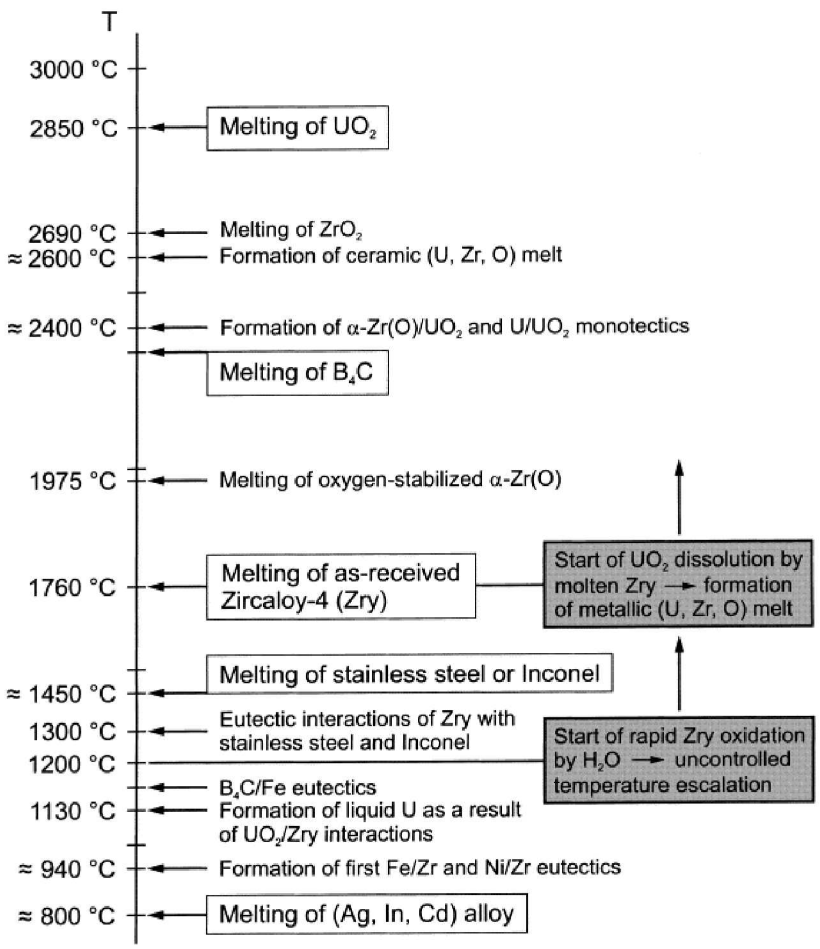
Eutectic mixture composition

- Conglomerate debris materials associated with any component are treated as part of a coherent mixture.
  - Some materials are treated as mutually miscible
  - Others are considered mutually immiscible
    - Melt and relocate independently of one another.
- As currently implemented, when the model is active all materials are part of the miscible mixture.

Formation of eutectic mixtures

- Normal liquid formed when an intact solid reaches its melting point
- Eutectic reaction product formed when two intact solids in mechanical contact within a core component reach their eutectic temperature
- Dissolution of an intact solid by an existing liquid mixture in the same core cell
  - Example: the dissolution of UO2 fuel by the liquid mixture associated with the cladding in the same core cell as the fuel.
  - At most two distinct solids
  - Hierarchy for dissolution

Important Material Interactions
(Hagen and Hoffman – KfK)



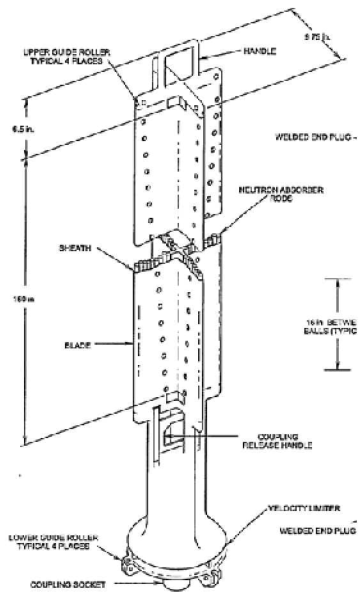
- View in 1980's (STCP) assumed fuel melts at 3200K
- Early experiments showed role of material interactions showed fuel "liquefied" at lower temperatures
  - 2400K up to 2880K
- DF-4 BWR Experiment showed B_4C/SS blades liquefy at ~1500K (compared to 1700K)
- Eutectics form between Zr/SS with liquefactions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

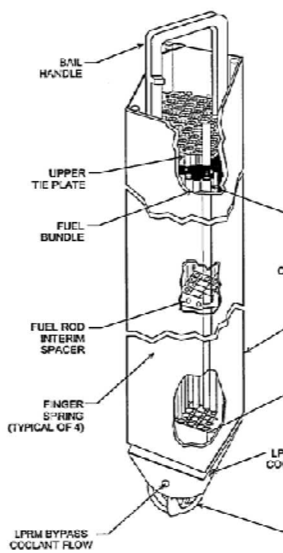
BWR Core Components

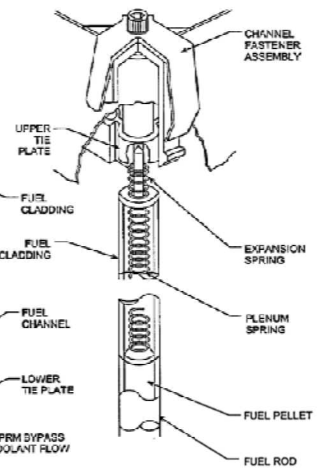
UO_2/Zr(O) liquefactions → ~2400K

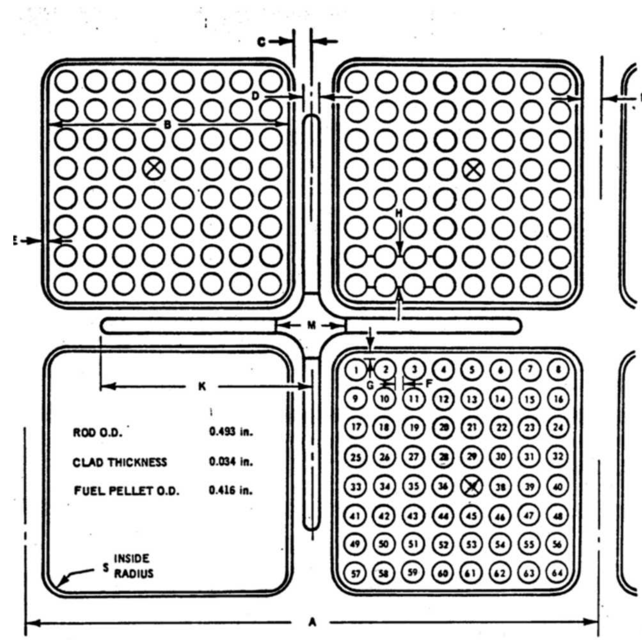
B_4C/SS liquefactions → ~1500K

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









Differing Materials in close proximity

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.

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
	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
	Zr from intact canister
Other structure NS (PWR control rod)	steel oxide from the same other structure
	Zr from the same other structure
	ZrO2 from intact cladding
	UO2 from intact fuel
Particulate debris	UO2 from particulate debris
	ZrO2 from particulate debris
	ZrO2 from intact cladding
	UO2 from intact fuel

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

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

where

x_j^f = final mass fraction of material j,

x_j^i = initial mass fraction of material j,

Δt = timestep (s), and

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

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

MELCOR Effective Melt 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

With this model it was impossible to enforce lower effective melting temperature through default in source code

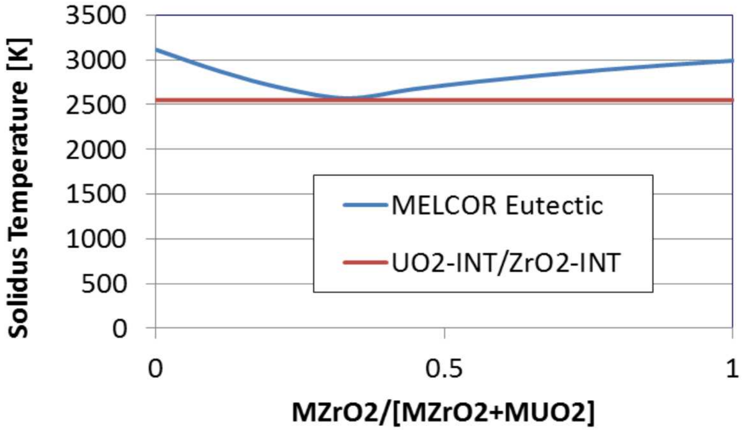
- User was required to modify UO2-INT and ZRO2-INT melt temperatures through input

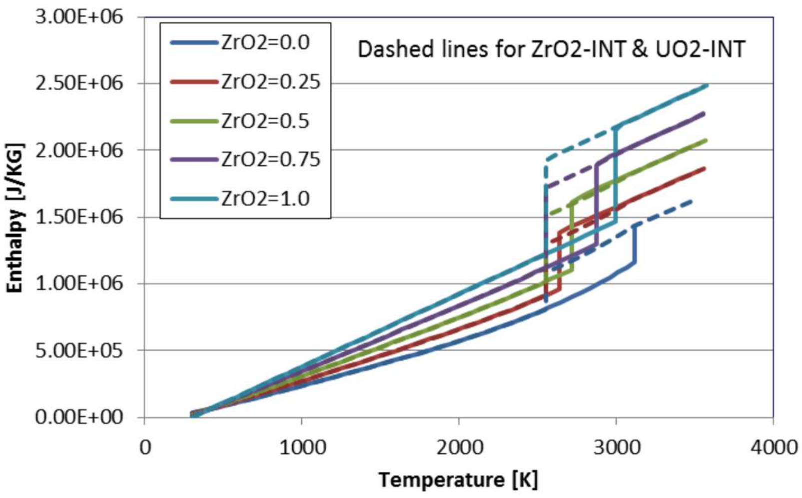
Eutectic Model

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





Calculation of the Solidus/Liquidus Temperatures of a Mixture

Determined by considering every binary combination of material pairs in the mixture (molar weighted combination of solidus temperatures

$$TS_{mix} = \frac{\sum_{j}\sum_{i \neq j} f_i \quad f_j \quad TS_{ij}}{\sum_{j}\sum_{i \neq j} f_i \quad f_j}$$

- *Eutectic pairs*
  - Lever Rule
    - The solidus temperature is given by the mole-weighted average of the eutectic temperature and solidus temperature of the component present in excess of the eutectic molar composition.

Material Pairs		Molar Ratio	Eutectic Temperature
Zr	Inconel	0.76 / 0.24	1210
Zr	steel	0.76 / 0.24	1210
ZrO_2	UO_2	0.50 / 0.50	2800
Zr	B_4C	0.43 / 0.57	1900
Steel	B_4C	0.69 / 0.31	1420
Zr	Ag-In-Cd	0.67 / 0.33	1470

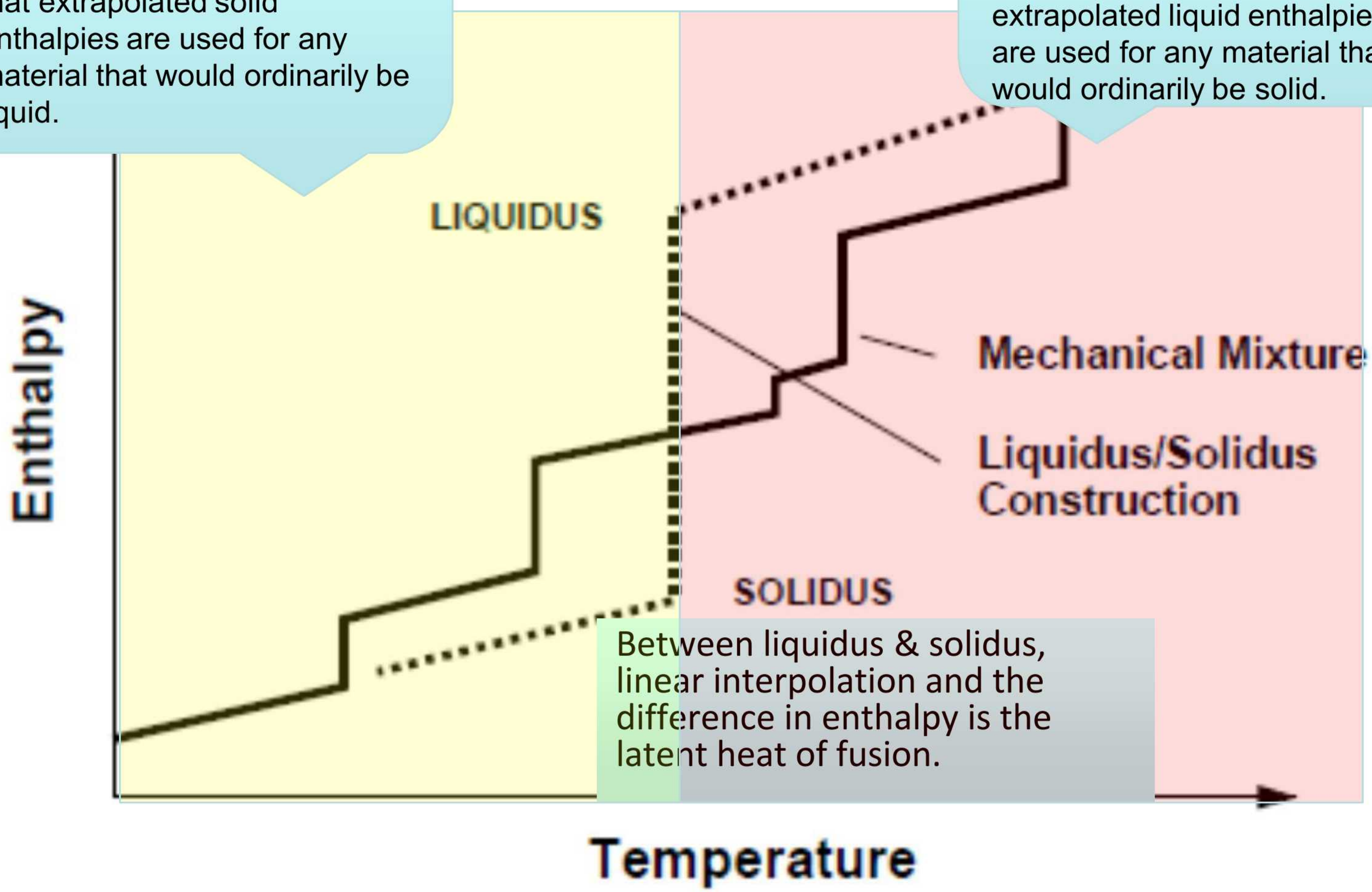
- *Non-Eutectic Pairs*
  - TS_{ij} is given by the mole-weighted average of the two solidus temperatures.

The liquidus temperature is set equal to the solidus temperature plus 0.01 K

Enthalpy of Eutectic Mixture

For temperatures less than the calculated solidus, the mass-weighted individual enthalpies are summed with the exception that extrapolated solid enthalpies are used for any material that would ordinarily be liquid.

For temperatures greater than the calculated liquidus, the mass-weighted individual enthalpies are summed with the exception that extrapolated liquid enthalpies are used for any material that would ordinarily be solid.



Between liquidus & solidus, linear interpolation and the difference in enthalpy is the latent heat of fusion.

Secondary Candling Model

- Eutectics model off
  - Simple model to allow transport of unmolten secondary materials
    - ZrO_2, UO_2, steel oxide, control poison
    - Dissolution of UO_2 by molten Zr or breaking off of pieces of thin oxide shells
  - Fraction of secondary material carried with candling molten material
    - Input fraction F1 of the molten mass

$$\Delta M_s = F_1 \, \Delta M_m$$

    - Fractional proportion to existing fraction within a component

$$\Delta M_s = F_2 \, \frac{M_{s,total}}{M_{m,total}} \, \Delta M_m$$

- Eutectic model on
  - Secondary candling is inactive
  - Material interactions predicted by eutectics model

Holdup Behind ZrO2 layer

Molten material is held up within a component

- if the oxide thickness is greater than a critical value Δr_{hold}
- if the component temperature is less than a critical value T_{breach}
- if no candling from the component in that cell has yet taken place.

Eutectic model protects materials from dissolution when they are behind an oxide layer

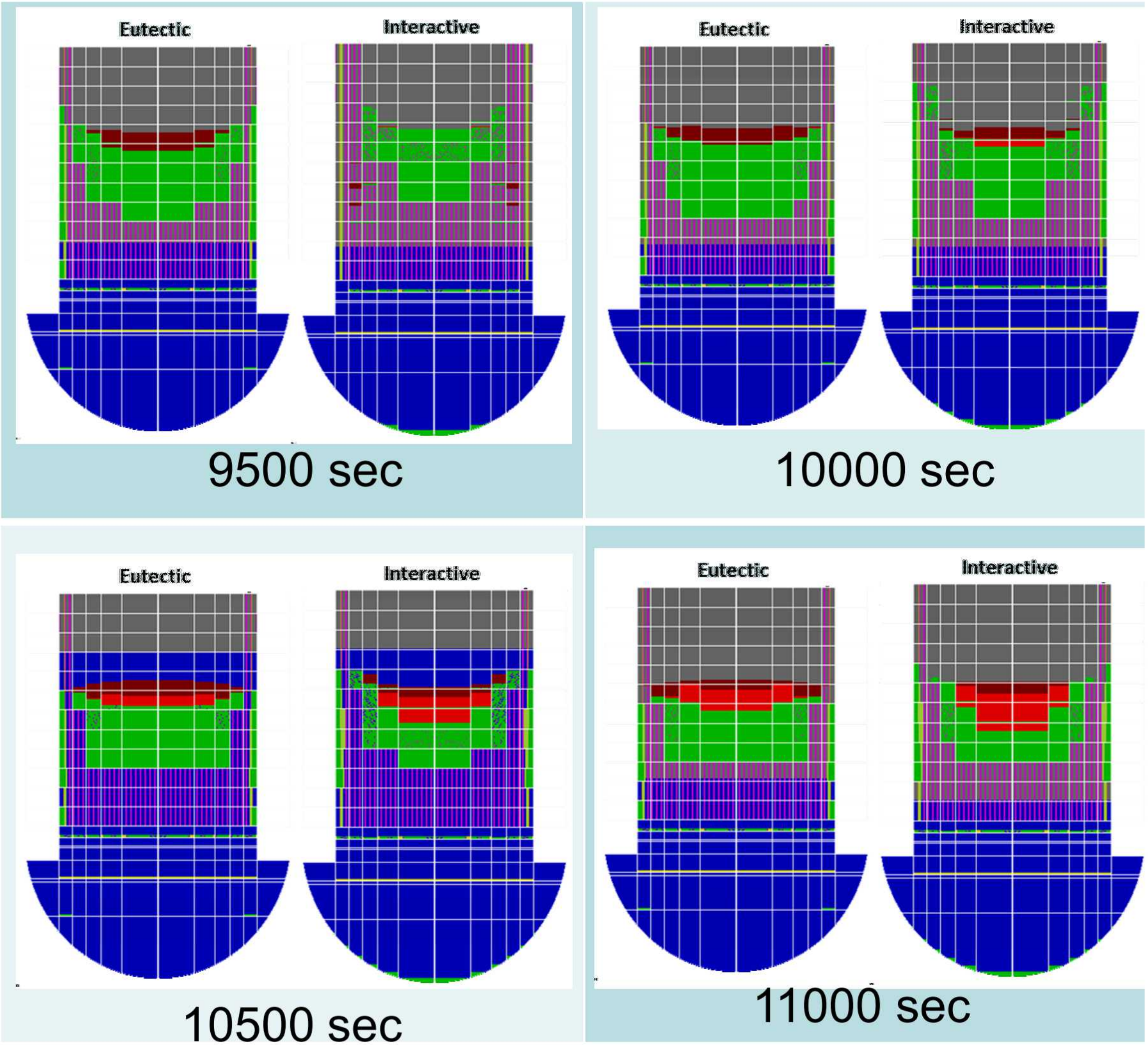
Component	Solids Dissolved Effected by Oxide Layer
Canister	ZrO2 from intact cladding (A)
Other structure NS (BWR control rod)	ZrO2 from intact canister (A) Zr from intact canister (A)
Other structure NS (PWR control rod)	Steel oxide from the same other structure (B) ZrO2 from intact cladding (A) UO2 from intact fuel (A)

A. solid is attacked only if there is no holdup of the mixture in the component.

B. solid is attacked only if the mixture is being held up by the component

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



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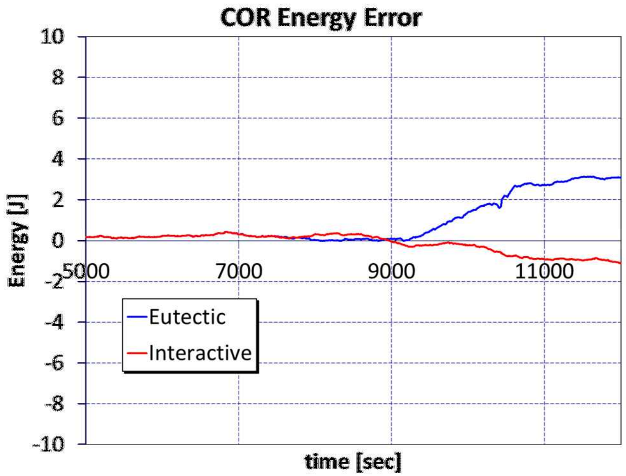

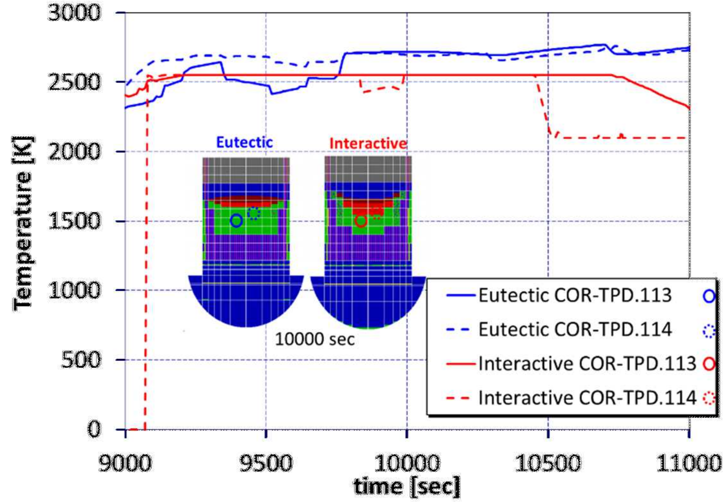

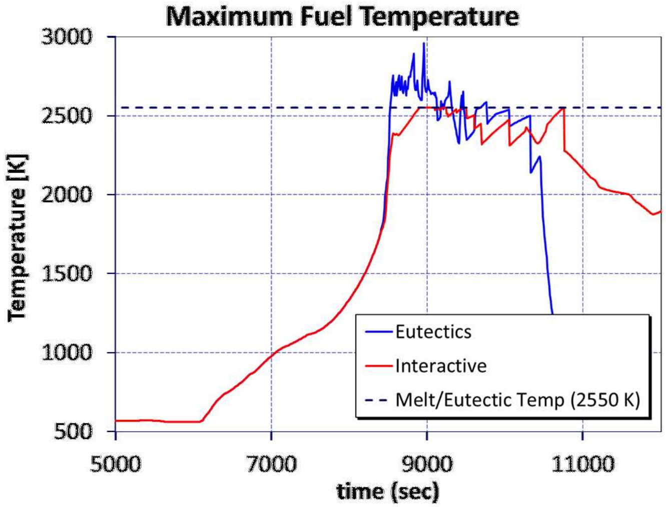

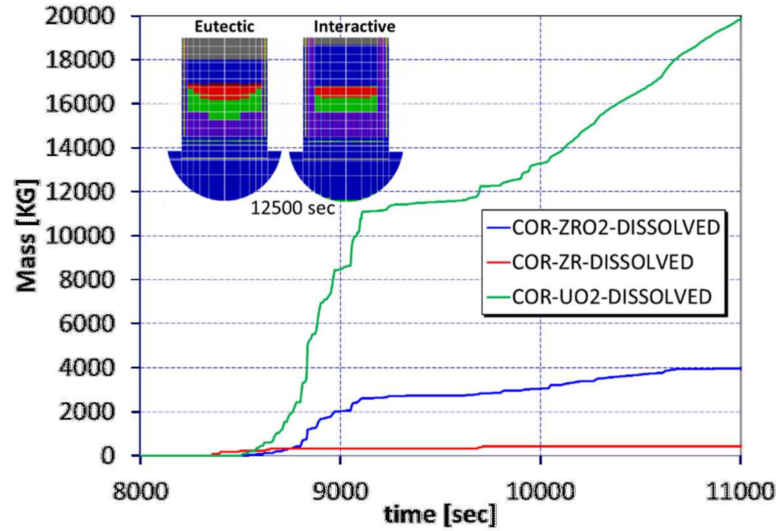

Eutectics Exercise

Input

- Remove any COR-INT, ZRO2-INT records
  - Look at both MP and COR input
- Check MP input for any alterations to UO2 or ZRO2 enthalpy or any alterations to melt temperature.
- Add COR_EUT record with effective eutectic melt temperature of 2600 K at a UO2 mole fraction of 0.5

Output

- Enable plots of dissolved masses
- Inspect EUTECTIC solidus temperature table in text output.
  - Note that input was in molar fraction
- Plot UO2, ZrO2, and Zr dissolved
- Create AVI showing degradation

```
THE EUTECTIC/DISSOLUTION MODEL WITH CONGRUENT MELT

 UO2MOLEFRACT  UO2MASSFRACT    TSOLIDUS[K]
         1.00          1.00        3113.00
         0.90          0.95        3020.40
         0.80          0.90        2927.80
         0.70          0.84        2835.20
         0.60          0.77        2742.60
         0.50          0.69        2650.00
         0.40          0.59        2718.00
         0.30          0.48        2786.00
         0.20          0.35        2854.00
         0.10          0.20        2922.00
         0.00          0.00        2990.00

    ZIRCONIUM DISSOLUTION MODEL ACTIVE
    STEEL DISSOLUTION MODEL ACTIVE
```