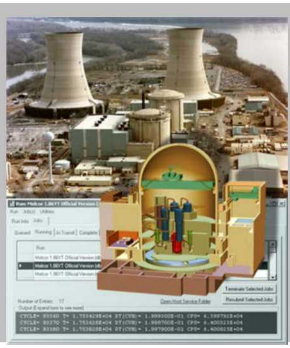
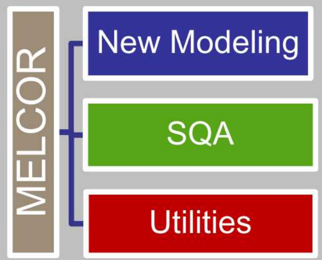
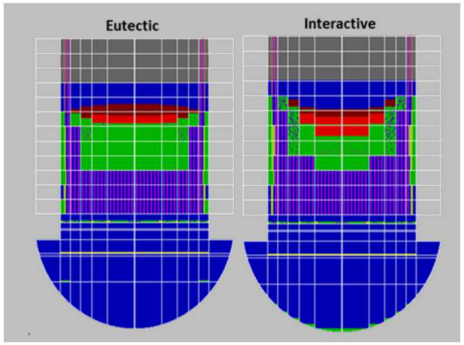
SAND2018-6906PE

Exceptional service in the national interest

Sandia National Laboratories







MELCOR Eutectics Model

Presented by Larry Humphries

June, 2018

U.S. DEPARTMENT OF ENERGY

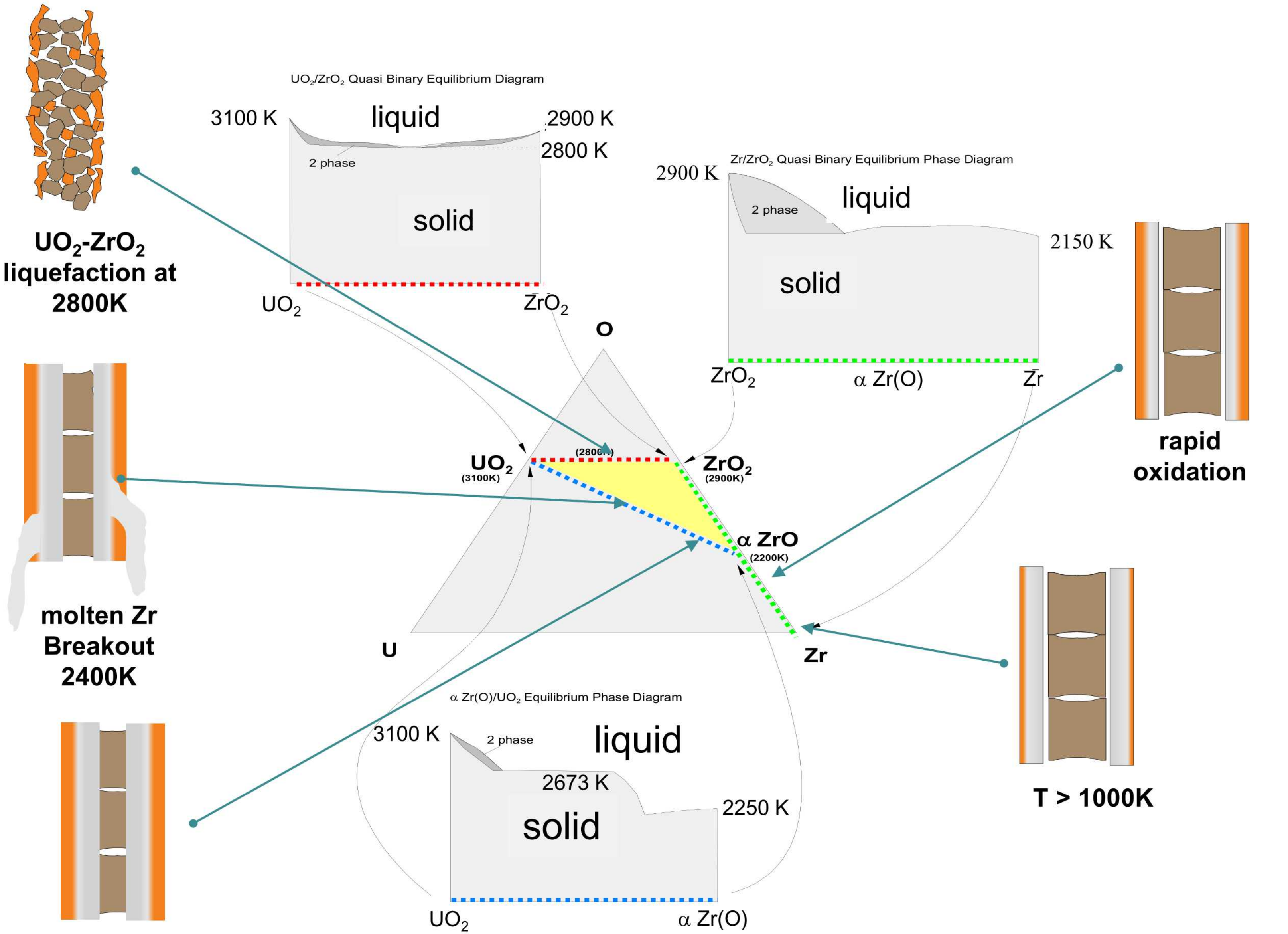
NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525

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



Eutectic Model Input

- New Input for the Eutectic model

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

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

PairMelt can be one of the following:

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

TM is the Solidus temperature for the eutectic pair

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

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

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

These records should be removed from input

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
      - treated as they are when the model is inactive (i.e. they melt and relocate independently of one another).
  - As currently implemented, when the model is active all the 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

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

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

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

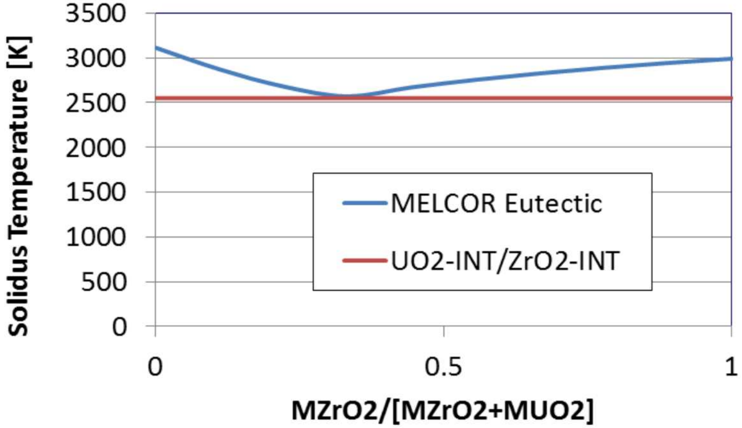
MELCOR Effective Melt Temperature

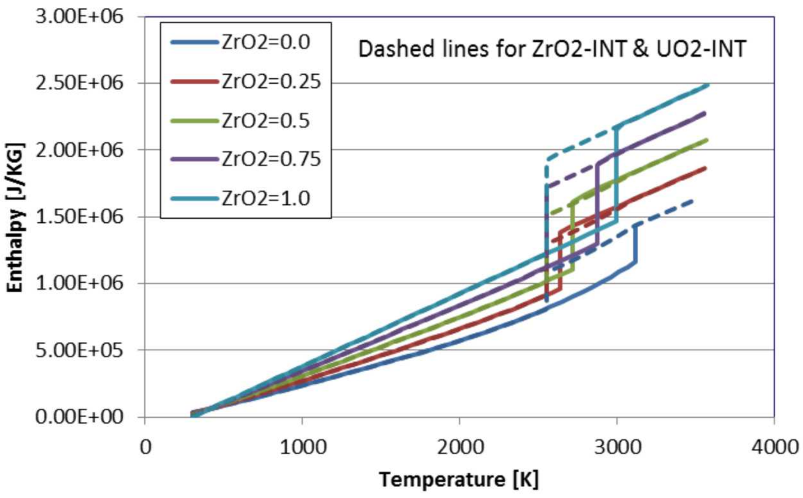
UO2-INT/ZRO2-INT

- 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

Sandia National Laboratories

- *Determined by considering every binary combination of material pairs in the mixture (molar withged 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*
    - 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

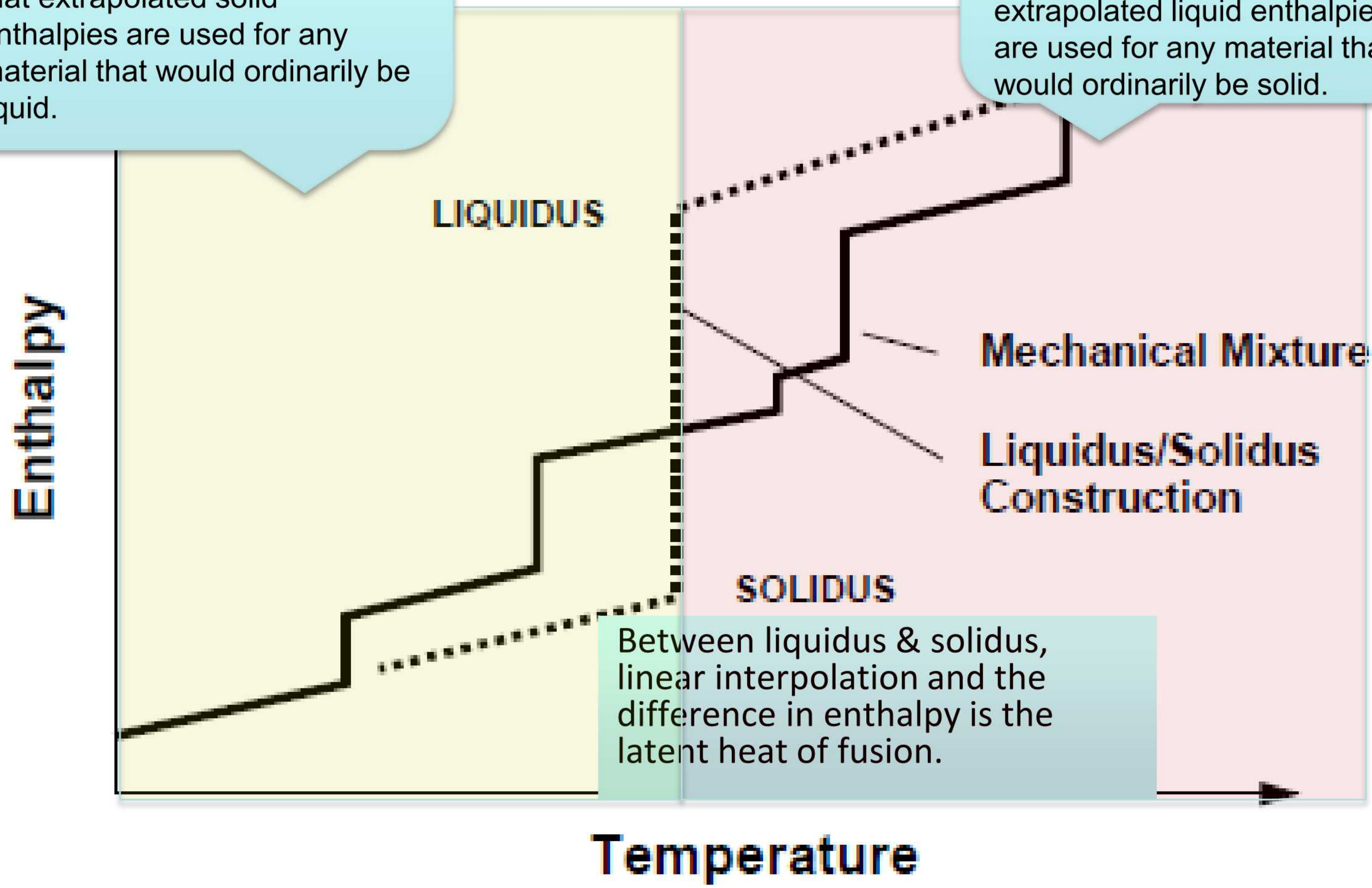
  - *Non-Eutectic Pairs*
    - TS_{ij} is given by the mole-weighted average of the two solidus temperatures.

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.

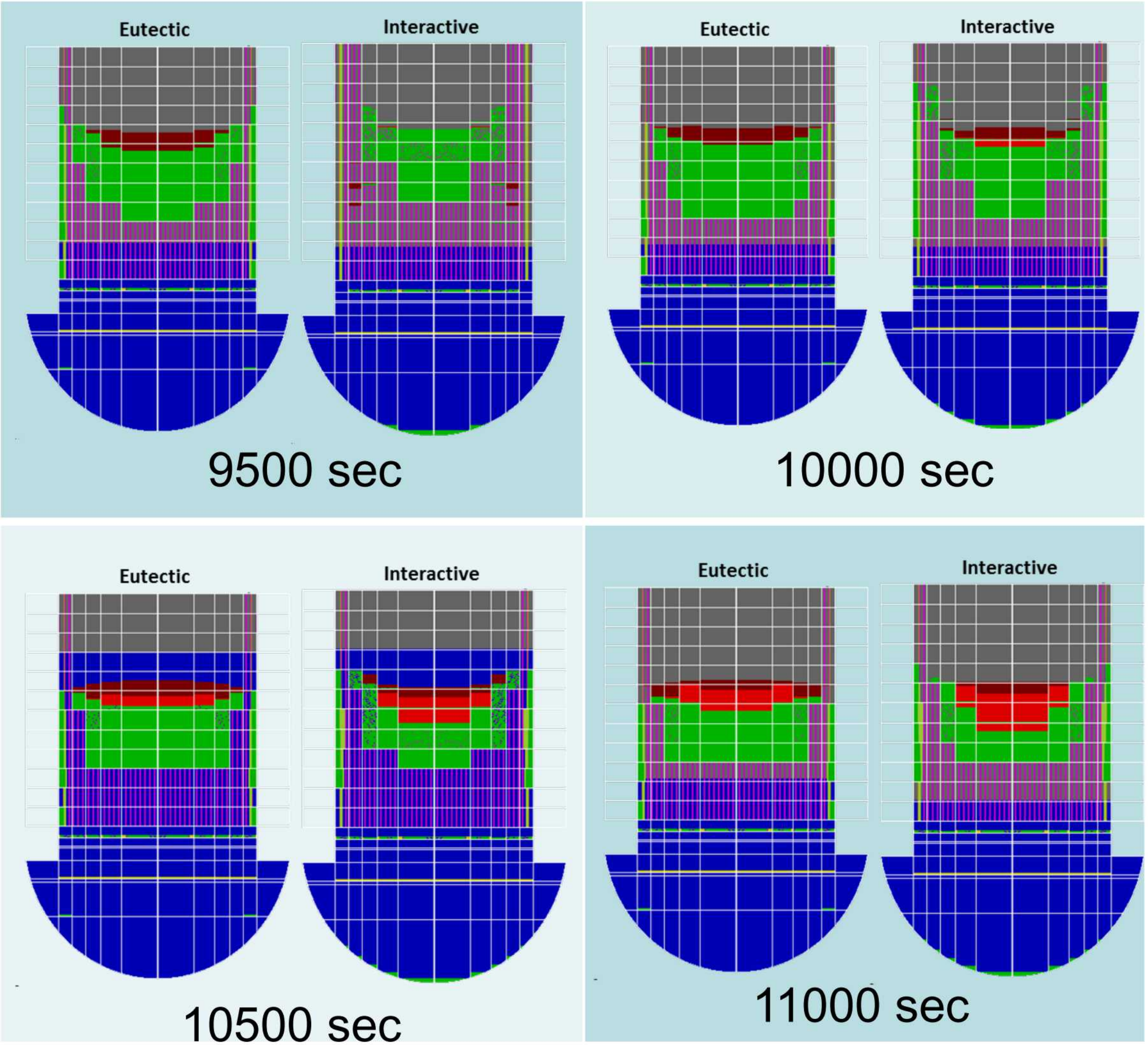
For temperatures greater than the calculated liquidus, the mass-weighted individual enthalpies are summed with the exception that extrapolated liquid enthalpies are used for any material that would ordinarily be solid.



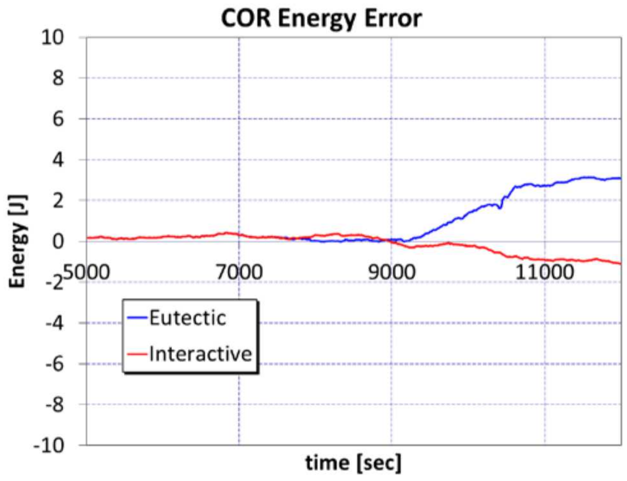
Between liquidus & solidus, linear interpolation and the difference in enthalpy is the latent heat of fusion.

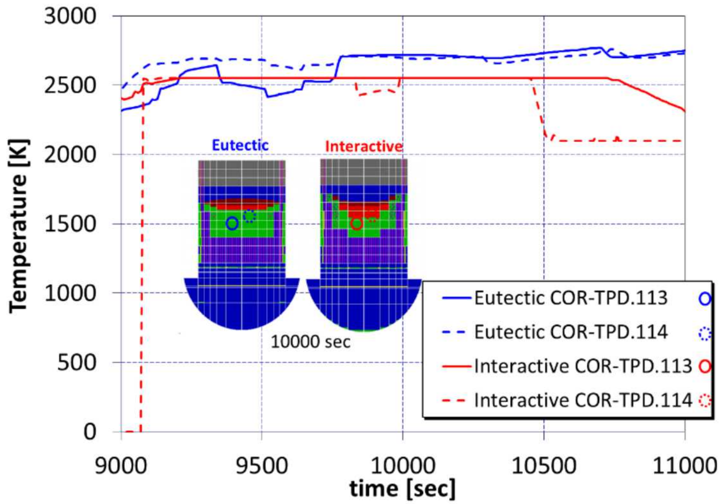
TMI Melt Progression –Preliminary Results

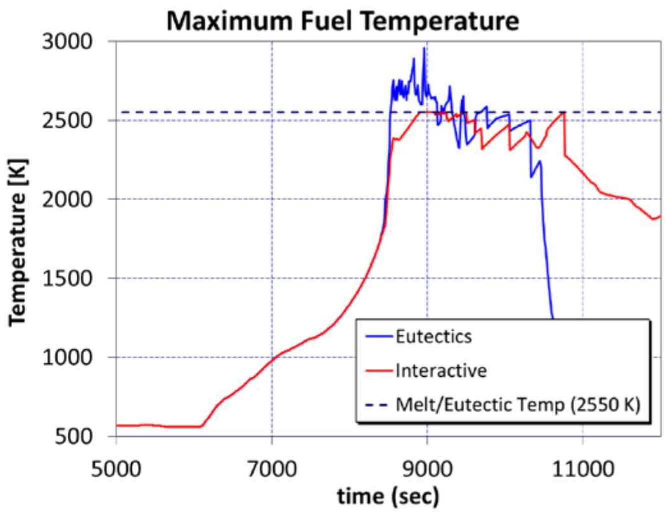
- Compare two TMI-2 test cases
  - Eutectics point = 2550 K
  - Interactive UO2-INT/ZRO2-INT 2550 K
- Similarities but notable differences
  - Core damage
    - Greater for eutectics
  - Size of Molten pool
    - Early: Greater for interactive
    - Later: Greater for eutectics
  - Material relocating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

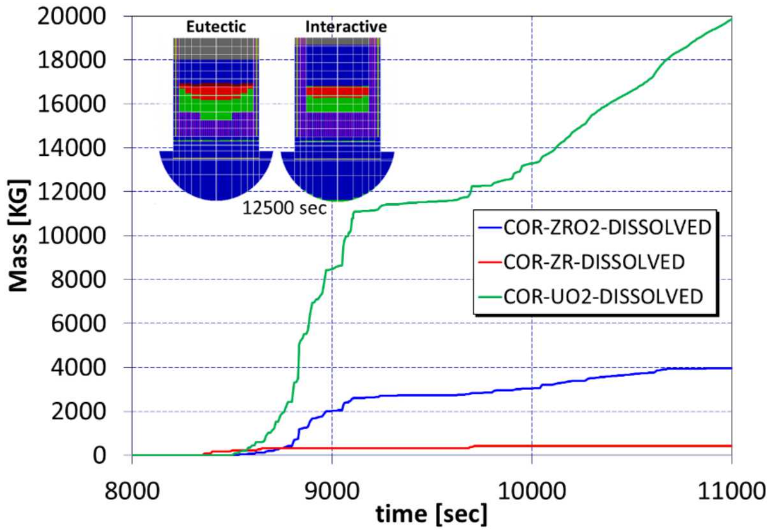


TMI Melt Progression –Preliminary Results









Eutectics Exercise

- Open input file and 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

```
COR_EUT 1
 1 'UO2/ZRO2' 2550.0 0.5
```

- Enable plots of dissolved masses

```
COR_PLOTS 1
 1 COR-DISSOLVED ON
```

- 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
```