

#### **New 'Best Practice' Default Values for MELCOR 2.1**

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#### Change in MELCOR Defaults Based on MELCOR Best Practices

- Default values for sensitivity coefficients should represent the best available value for general application
  - Recognize that there is uncertainty in each value and the default represents something like the mean in a probability distribution
- Recent changes in default values based on SNL'Best Practices'
  - Many proposed by Scott Ashbaugh, and Randy Gauntt, Mark Leonard, and K.C. Wagner
    - Some were based on MELCOR 1.8.5 experience only
  - Many sensitivity coefficients were typically overridden by users and it was desired to make the changes more generally available
  - Default values changed in MELCOR 2.1 (Sept 2008)
    - User can revert to original default values through input
      - CORDEFAULT 1.8.6
      - CAVDEFAULT 1.8.6
      - RN1DEFAULT 1.8.6
      - HSDEFAULT 1.8.6
      - CVHDEFAULT 1.8.6
  - New defaults and best practices presented at 2008 Workshop
    - "New and Improved MELCOR Models," Joonyub Jun
    - "Best Practices," K.C. Wagner



# Review of Several Modified Sensitivity Coefficients

#### **Heat Transfer**

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- **COR Heat Transfer** 
  - Candling Heat Transfer
  - COR radiant view factors
  - Lower head and penetration heat transfer coefficients.
  - Falling Debris Quench Model
- CAV Package
  - Multipliers for heat transfer
- Numerical Stability Parameters
  - Criteria for Solving the Flow Equations in Sparse Form
  - HS Error Tolerance for Transient Conduction
  - Flow Blockage Friction Parameter
  - COR Package Min. Porosity for Flow & Heat Transfer
- As part of this work, we enhanced testing capabilities to expose sensitivity coefficients as command line arguments
  - Values can be overwritten at runtime without hand editing input decks
  - Using existing test harness, able to test effects on large number of test calculations
  - All comparison calculations were performed with MELCOR 2.1
- User meetings such as this will provide additional insights into appropriate default values





#### COR00005 (1.8.6) or COR\_CHT (2.1)

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- Refreezing heat transfer coefficients to be used in the candling model
  - Specified for each molten core material.
- Old default values were order-of-magnitude estimates that appeared to produce plausible simulations of relocation phenomena
  - should be varied in sensitivity studies to determine their impact on overall melt progression behavior.

Material	Old Default (W/m <sup>2</sup> -K)	New Default (W/m <sup>2</sup> -K)
UO2	1000	7500
Zr	1000	7500
SS	1000	2500
ZrO2	1000	7500
SSX	1000	2500
СР	1000	2500



#### Candling Heat Transfer Coefficient Estimates Based on Conduction Analogy

- From conduction analogy, appropriate for slow moving melt:  $Q = -k \frac{dT}{dx} A \Delta t \cong h A (T_{melt} - T_{surf}) \Delta t$
- The heat transfer coefficient can then be reasonably estimated from

$$h_{cond} \approx k / dx$$

• The estimate of the conduction length can be approximated from

$$dx \approx ((\sqrt{2} \ pitch - diameter) / 2) \approx .005m$$

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#### **Candling Heat Transfer Coefficient**

Material	Old Default (W/m <sup>2</sup> -K)	Thermal Conductivity (W/m-K)	Calculated (W/m <sup>2</sup> -K)	New Default (W/m <sup>2</sup> -K)	High Values (W/m <sup>2</sup> -K)
UO <sub>2</sub>	1000	3.96	800	7500	1000
Zr	1000	58.4	10000	7500	10000
SS	1000	34.5	7000	2500	7000
ZrO <sub>2</sub>	1000	2.49	500	7500	1000
SSOX	1000	20	4000	2500	4000
СР	1000	48	10000	2500	10000





# Uncertainty Distribution in Zr Heat Transfer Correlation

- Values calculated for Zr may be as large as 10,000 W/m<sup>2</sup>-K
- Value selected was biased low to avoid large changes from old defaults
- Sampling distribution chosen is a log-normal form to assure that half of the cases use values between 5,000 and 10,000 W/m<sup>2</sup>-K and the mean is the current default value.
- Note, use of a high heat transfer coefficient does not result in complete blockage unless sufficient heat sink is available







#### Candling Heat Transfer Coefficient Time of Vessel Failure

Test Case	Old Defaults	New Defaults	High Defaults
BWR Demo (2 rings)	6693(sec)	5892(sec)	6300 (sec)
	7152 (cycle)	6465 (cycle)	6926 (cycle)
PWR Demo(2 rings)	5297 (sec)	6559 (sec)	5916 (sec)
	5505 (cycle)	6783 (cycle)	6224 (cycle)
PWR – 6 radial 19 radial	24300 (sec)	22785 (sec)	22092 (sec)
(SBO)	94243 (cycle)	138568 (cycle)	94326 (cycle)
BWR -6 radial 17 axial (SBO)	21,822 (sec)	24,993 (sec)	25,927 (sec)
	123456 (cycle)	121500(cycle)	134559(cycle)
BWR2 -6 radial 17 axial (SBO)	Still running	Still running	21,242 (sec) 101618 (cycle)



#### Candling Heat Transfer Coefficient Core Degradation Progression (PWR)

#### 14900 sec

15200 sec

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#### Candling Heat Transfer Coefficient Hydrogen Generation (PWR)



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#### COR Package Radiation Heat Transfer Parameters

- COR00003 Record
  - FCELR: COR package radial radiation heat transfer parameter
    - 0.25 (Old Default)
    - 0.1 (New Default)
  - FCELA: COR package axial radiation heat transfer parameter
    - 0.25 (Old Default)
    - 0.1 (New Default)

#### • From User Guide

"These values should be based on standard expressions for simple geometries, where possible, or on experimental data or detailed radiation calculations for complicated geometries involving intervening surfaces, such as for radiation between "representative" structures in cells containing a number of similar structures (e.g., fuel rod bundles). In the absence of any information to aid in selection of view factors, they should be used as arbitrarily varied parameters to examine the effects of radiation on the course of a calculation.."





# MELCOR Radiant Heat Transfer in COR Package

#### MELCOR radiation model is extremely simple

- Only five user input "view factors "(FCNCL, FSSCN, FCELR, FCELA, FLPUP)
- "View factors "do not depend on time (except for debris)
- Little guidance given users in selecting values
- Values are problem dependent
- Rod surfaces more than a few rod diameters from the cell boundary have small visibility (view factor) from the boundary
  - **1.** The appropriate radiation area is the cell boundary area for very large cells and the rod surface area (axially) or perhaps half of it (radially) for very small cells;
  - 2. The appropriate difference in  $T^4$  for radiation across the boundary is much less than  $(T_1^4 T_2^4)$  for large cells.

#### **Continuum Model for Estimating View Factor** as a Function of Depth

First consider a simple 1-D "continuum" model with some qualitative relationship to the "real" world (ignore rod geometry). Assume that the combination of distance between differential surfaces (the factor of r<sup>-2</sup> in the solid angle subtended) and the obscuring of line of sight by intervening surfaces may together be approximated by a simple exponential. That is, we assume that the fraction of unobscured solid angle remaining visible from a differential surface at depth x is  $e^{-\alpha x}$ . In consequence, the rate at which solid angle *becomes* obscured—i.e. is intercepted by other differential surface—is  $\alpha e^{-\alpha x} dx$ .



#### **Simple "Continuum" View Factor Derivation**

• The view factor between a cell of length (perpendicular to the cell boundary) of  $L_1$  and one of length  $L_2$  may be calculated as

$$A_{1}F_{12} = \int_{-L_{1}}^{0} dx_{1}A_{cell} \left(\frac{A}{V}\right)_{1} e^{-\alpha_{1}x_{1}} \int_{0}^{L_{2}} dx_{2}\alpha_{2}e^{-\alpha_{e}x_{2}}$$

• In terms of dimensionless variables:

$$A_{1}F_{12} = A_{cell} \left(\frac{A}{\alpha V}\right)_{1} \int_{-\alpha_{1}L_{1}}^{0} dy_{1} e^{y_{1}} \int_{-\alpha_{2}L_{2}}^{0} dy_{2} e^{y_{2}} = A_{cell} \left(\frac{A}{\alpha V}\right)_{1} \left(1 - e^{-\alpha_{1}L_{1}}\right) \left(1 - e^{-\alpha_{2}L_{2}}\right)$$

• And by reciprocity:

• Where 
$$\kappa = \left(\frac{A}{\alpha V}\right)_1 = \left(\frac{A}{\alpha V}\right)_2$$
 and since  $\mathbf{V}_{\mathbf{i}} = \mathbf{A}_{\text{cell}} \mathbf{L}_{\mathbf{i}}^{\mathbf{i}}$ :  $\alpha_i L_i = \frac{A_i}{KA_{cell}}$ 

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$$A_2 F_{21} = A_1 F_{12} = AF = A_{cell} F_0 = A_{cell} K \left( 1 - e^{-\alpha_1 L_1} \right) \left( 1 - e^{-\alpha_2 L_2} \right)$$

- Limits for the equation:
- $AF \rightarrow A_{cell}K$  for both cells large (K=1 gives the correct behavior)
  - for cell 1 small and cell 2 large
- $AF \rightarrow \frac{A_1A_2}{KA_{mil}}$  for both cells small

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•  $AF \rightarrow A_1$ 





#### Effect of Rod Geometry on View Factor Monte Carlo Simulation

- Monte Carlo calculation of "View Factor "
  - Calculate view factor as function of diameter
    - Surface to volume density varied while maintaining mass (pitch to diameter ratio)
    - Calculated values are +/-1%
  - Continuum model predicts larger F0 because surface to volume ratio is larger

$$F_0 = \frac{A_2}{A_{cell}} F_{21} = \frac{A_1}{A_{cell}} F_{12}$$



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#### **Effective View Factor Derivation**

The "effective" view factor that accounts for the restricted temperature difference is modeled as

 $(AF)_{eff} = -A_{cell}K \int_{-\alpha_{1}L_{1}}^{0} dy_{1}e^{y_{1}} \int_{-\alpha_{2}L_{2}}^{0} dy_{2}e^{y_{2}} \frac{2(y_{1} + y_{2})}{\alpha_{1}L_{1} + \alpha_{2}L_{2}}$ 

where the fraction in the integrand is the fraction of the average difference in  $T^4$  between point 1 and point 2.

– We have assumed that  $T^4$  is linear in  $\alpha x$ 

Thus,

$$\left(AF\right)_{eff} = -2\frac{A_{cell}K}{\alpha_1L_1 + \alpha_2L_2}\int_{-\alpha_1L_1}^{0} dy_1 e^{y_1}\int_{-\alpha_2L_2}^{0} dy_2 e^{y_2} \left(y_1 + y_2\right)$$

Using previous relation between K and alpha:

$$\left(AF\right)_{eff} = 2\frac{\left(A_{cell}K\right)^{2}}{A_{1} + A_{2}} = \left\{ \left[1 - \left(1 + \alpha_{1}L_{1}\right)e^{-\alpha_{1}L_{1}}\right] \left(1 - e^{-\alpha_{2}L_{2}}\right) + \left(1 - e^{-\alpha_{1}L_{1}}\right) \left[1 - \left(1 + \alpha_{2}L_{2}\right)e^{-\alpha_{2}L_{2}}\right] \right\}$$

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- $\left(AF\right)_{eff} = 2\frac{\left(A_{cell}K\right)^{2}}{A_{1} + A_{2}} = \left\{ \left[1 \left(1 + \alpha_{1}L_{1}\right)e^{-\alpha_{1}L_{1}}\right]\left(1 e^{-\alpha_{2}L_{2}}\right) + \left(1 e^{-\alpha_{1}L_{1}}\right)\left[1 \left(1 + \alpha_{2}L_{2}\right)e^{-\alpha_{2}L_{2}}\right] \right\}$
- Limits:

# • $(AF)_{eff} \rightarrow 4 \frac{(A_{cell}K)^2}{A_1 + A_2}$ for both cells large • $(AF)_{eff} \rightarrow K \frac{A_1 A_{cell}}{A_1 + A_2}$ for cell 1 small and cell 2 large • $(AF)_{eff} \rightarrow \frac{1}{2} \frac{A_1^2 + A_2^2}{A_1 + A_2}$ for both cells small

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## Sensitivity of Calculations to FCELR Zion SBO (6 rings)

	FCELR		
Event	0.25	0.1	
Gap Release	12,610 s	12,576 s	
Core support failure	14,355s	14,122 s	
Vessel Failure	24,729 s	21,720 s	





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# COR Package Min. Porosity for Flow & Heat Transfer

- SC1505(1) and SC1505(2)
- These coefficients specify the geometric parameters affecting core flow resistance and heat transfer under conditions of flow blockage.
- SC1505(1): Used to determine the maximum pressure drop for blocked flows

$$(\Delta P)_{powrousbed} = \frac{1}{2} \rho j^2 \frac{L}{D_p} \left( \frac{1-\varepsilon}{\varepsilon^3} \right) \left[ C_1 + C_2 \left( \frac{1-\varepsilon}{\text{Re}} \right) + C_3 \left( \frac{1-\varepsilon}{\text{Re}} \right)^{C_4} \right]$$

- 0.001 (Old Default)
- 0.05 (New Default)
- SC1505(2): To avoid overheating a vanishing CVH fluid, the sum of the surface areas of the intact component and its associated conglomerate debris, which constitutes the total effective surface area for heat transfer to CVH, cannot exceed

$$A_{tot,\max} = \max(V_{CVH}R_{SVR}, \varepsilon_{\min}V_{COR})$$

- 0.001 (Old Default)
- 0.05 (New Default)

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#### COR Package Min. Porosity for Flow & Heat Time of Vessel Failure

	New Defaults		Old Defaults	
Test Case	Runtime seconds	LHF time seconds	Runtime seconds	LHF time seconds
BWR	-	-	35:27	6,693
PWR	10:29	6,157	12:54	5,297
Test_lnew	18:19	6,700	21:04	6,888
PWR – 6 radial 19 radial (SBO)	Still running	24,015	10:28:33	24,015
BWR -6 radial 17 axial (SBO)	Still running	>18,701	16:03:39	24,778
Grand Gulf	Still Running	21,822.	Calculation Failed	





## Debris to Penetration/Lower Head Heat Transfer Coefficient

# • COR00009 (MELCOR 1.8.6) COR\_LHF (MELCOR 2.1)

- HDBPN: Heat transfer coefficient from debris to penetrations
  - 1000.0 w/m<sup>2</sup>/s (Old Default)
  - 100.0 w/m<sup>2</sup>/s (New Default)
- HDBLH: Heat transfer coefficient from debris to lower head
  - 1000.0 m/s (Old Default
  - 100.0 m/s (New Default)
- TPFAIL: Failure Temperature of the penetrations
  - 1273.15 K (Old Default)
  - 9999. K (New Default)





### **MELCOR Modeling of Penetration**

• Penetration failure is not modeled as a mechanism for vessel failure.

- In the SNL LHF tests it was observed that gross creep rupture of the lower head was the most likely mechanism for vessel failure.
- Penetration ejection was highly unlikely.
- Penetration failure occurred at relatively large strains
  - Weld failure due to strain
- MELCOR penetration model lacks sufficient resolution to adequately model multi-dimensional heat transfer
  - Lumped capacitance
  - No possibility of modeling replugging
  - Typically predicted failure long before the vessel strains observed in LHF





# Debris to Penetration/Lower Head Heat Transfer Time of Vessel Failure

	New Defaults		Old Defaults	
Test Case	seconds	Failure mode	seconds	Failure mode
PWR – 6 radial 19 radial with penetrations (SBO)	23,980	vessel	Calculation did not complete	
BWR -6 radial 17 axial with penetrations (SBO)	25,890	vessel	10,815	penetration



# **Debris to Lower Heat Heat Transfer Coefficient Calculated from Debris Thermal Conductivity**

- Heat transfer from particulate debris to lower head doesn't need to be defined as a heat transfer coefficient
  - Was probably implemented as a heat transfer coefficient when there was no separate field for molten mass
  - Possible to use control function
- User can request internal conduction calculation from debris to lower head
  - User specifies 'model' on input field and code calculates effective heat transfer coefficient from thermal conductivity of debris
  - HTC = K<sub>debris</sub> / Zeff<sub>i</sub>
    - Zeff<sub>i</sub> = half the height of debris in cell adjacent to lower head
  - Doesn't account for any gap between debris and lower head
  - Undocumented feature
  - Hasn't been reviewed
  - Will rerun test cases using this value



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## In-Vessel Falling Debris Quench Model Parameters

- COR00012 (MELCOR 1.8.6) COR\_LP (MELCOR 2.1)
  - HDBH2O: Heat transfer coefficient from in-vessel falling debris to pool
    - 100.0 w/m<sup>2</sup>/s (Old Default)
    - 2000.0 w/m<sup>2</sup>/s (New Default)
  - VFALL: Velocity of falling debris
    - 1.0 m/s (Old Default
    - 0.01 m/s (New Default)



# In-Vessel Falling Debris Quench Model Parameters Estimation from FARO data

- The heat transfer for a single spherical particle falling through a fluid can be obtained from the following correlation.
- Using values for water and corium, the curve at right shows the dependency of the HTC on particle size.
- Interference from other particles would lead to a reduced heat transfer.
- Review of FARO data shows that for fragmented particle sizes on the order of 0.005 m, the HTC may be 1000 W/m^2-K
- This would indicate that the ideal heat transfer was reduced by 5%
- We assume particle sizes of 0.002 m in the lower head





# **Observations From BWR Calculations**

- Many BWR calculations showed debris relocating to the lower head and quickly failing the lower head, even though there was more than a meter of water above.
  - Experiments showed that the distance a molten jet must travel to fully quench was between 20 & 50 jet diameters (no unoxidized metals) and 10 to 20 diameters for melts with unoxidized metals.
  - Using a jet diameter of ~ 10 cm (unit cell of a fuel assembly) quenching qould be achieved in 2 to 5 m (oxidic melts) or 1 to 2 m (metallic melts)
- It was assumed that if a sufficient pool exists, the falling debris would quench
  - Debris hydraulic diameter corresponds to average end-state conditions observed in the FARO tests
  - 'fall velocity' was set to a value that caused the temperature of falling debris to decrease by an amount that ensured debris temperatures in the lower head were below the film boiling limit.
  - The one-dimensional counter-current flow limitation (CCFL) limitation was removed from the overlying debris heat transfer model to represent water penetration into the debris bed, perhaps through 2- or 3-dimensional circulation flow patterns.



#### **Vessel Falling Debris Quench Model Parameters Comparison of Representative Calculations**

	New Defaults		Old Defaults	
Test Case	LHF mode	LHF time seconds	LHF mode	LHF time seconds
BWR	yielding	6693	yielding	5956
PWR	yielding	5297	yielding	4919
Test_lnew	yielding	6888	yielding	7006
PWR – 6 radial 19 radial (SBO)	Creep rupture (ring 6)	20,770.	Creep rupture (ring 1)	24,015.
BWR -6 radial 17 axial (SBO)	Penetration 1	21,240	Penetration 2	21,822

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## Criteria for Solving the Flow Equations in Sparse Form: SC4415(1)

• SC4415(1)

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- The maximum fraction of nonzero coefficients for use of the sparse form.
  - A value of 0.0 ensures that the direct solution will always be used, while a
  - value of 1.0 ensures that the iterative solution will always be used.
- CVH/FL maximum iteration criterion
  - 0.5 (Old Default)
  - 1.0 (New Default)
- It should be noted that we are currently reviewing the flow equations solver for MELCOR 2.1. These recommendations may be changed.





#### SC4415(1) Performance Comparison

	New Defaults		Old Defaults	
Test Case	Runtime seconds	LHF time seconds	Runtime seconds	LHF time seconds
BWR	18:00	6693	35:27	6693
PWR	17:37	5297	12:54	5297
Test_lnew	23:11	6888	21:04	6888
LOFT	10:36	-	12:38	-
Falcon1	19:45	-	15:24	-
PWR – 6 radial 17 axial (LOCA depressurization)	6:32:31	-	7:01:57	-
PWR – 6 radial 19 radial (SBO)	10:58:07	24015	10:28:33	24015
BWR -6 radial 17 axial (SBO)	12:56:51	24778	16:03:39	24778



#### HS Error Tolerance for Transient Conduction SC4055(2)

- SC4055(2)
  - Desired relative error tolerance for transient conduction calculations; NOTE: the conduction calculation is declared converged when the maximum relative error in the temperature profile within the structure is less than this value, normally.
  - However, if degassing or mass transfer (condensation/ evaporation) is occurring, then the iteration continues until the maximum relative error in the temperature profile (including the film surfaces) is less than the value specified by C4055(6). If the relative error is still larger than C4055(6) but smaller than C4055(2) after XITMAX iterations, then the solution is accepted as converged.
  - Default Values
    - 5.0e-4 (Old Default
    - 0.5 (New Default)



## SC4055(1) Performance Comparison

	New Defaults		Old Defaults		SC4055(1)=0.05	
Test Case	Runtime seconds	LHF time	Runtime seconds	LHF time seconds	Runtime seconds	LHF time seconds
BWR	24:02	6693	35:27	6693	19:27	6693
PWR	18:12	5297	12:54	5297	18:56	5297
Test_lnew	14:17	6888	21:04	6888	20:20	6888
LOFT	11:57	-	12:38	-	10:46	-
Falcon1	15:44	-	15:24	-	22:05	-
PWR – 6 radial 17 axial (LOCA depressurization)	4:40:35	-	7:01:57	-	6:22:09	-
PWR – 6 radial 19 radial (SBO)	14:47:02	24015	10:28:33	24015	14:06:32	24015
BWR -6 radial 17 axial (SBO)	23:17:38	24778	16:03:39	24778	16:50:25	25000

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#### **Cooling of a 1-D Heat Structure Comparison with Analytic Results**



Thermal conductivity	50.0 W/m-K
Density	1.0 kg/m3
Specific heat capacity	1500 J/kg-K
Heat transfer coeff	50.0 W/m2-K
HS initial temperature	1000 K
Fluid initial temp	500 K
Cylindrical radius	0.1 m
Cylindrical height	1.0 m





#### Flow Blockage Friction Parameter SC4413(5)

- SC4413(5)
- Minimum porosity to be used in evaluating the correlation, imposed as a bound before the Ergun equation is evaluated.

$$K_{eff} = \left[ C4413(1) + C4413(2) \left( \frac{1-e}{Re} \right) + C4413(3) \left( \frac{1-e}{Re} \right)^{C4413(4)} \right] \frac{(1-e)L}{eD}$$

- 1.0e-6 (Old Default)
- 0.05 (New Default)





#### SC4413(5) Performance Comparison

	New Defaults SC4413(5)=0.05		Old Defaults SC4413(5)=1E-6	
Test Case	Run time seconds	Vessel Failure	Run time seconds	Vessel Failure
BWR	17:20	6693	35:27	6693
PWR	18:33	5297	12:54	5297
Test_lnew	14:37	6888	21:04	6888
LOFT	11:20	-	12:38	-
Falcon1	24:50	-	15:24	-
PWR – 6 radial 17 axial (LOCA depressurization)	4:34:46	-	7:01:57	-
PWR – 6 radial 19 radial (SBO)	13:54:48	24015	11:15:00	24015
BWR -6 radial 17 axial (SBO)	17:34:39	26673	17:31:55	24778

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# Multipliers for Surface Boiling Heat Transfer and Material Conductivity

- CAV\_U (MELCOR 2.1)
  - BOILING
    - CORCON-Mod3 (Old Default)
    - 10.0 (New Default)
- SC4055(2)
  - COND.OX multiplier for oxidic phase thermal conductivity
    - 1.0 (Old Default
    - 5.0 (New Default)
- SC4413(5)
  - COND.MET: multiplier for metallic phase thermal conductivity
    - 1.0 (Old Default)
    - 5.0 (New Default)





#### **Review of MACE Test Results**

• The simplified onedimensional geometric configuration of the debris underestimates heat fluxes observed in the MACE experiments.

•MACE tests showed cracking and multidimensional effects that greatly enhanced the amount of cooling when water was present.

• The debris thermal conductivity (i.e., a method to reflect cracks and multidimensional effects) and surface heat flux were enhanced to replicate the heat fluxes observed in the MACE tests.



Heat Transfer from an Overlying Water Pool to an Ex-vessel Debris Bed.

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## Effect of Increasing Pool Heat Transfer Independent of Crust Thermal Conductivity

• Increasing the pool heat transfer alone cannot increase the cooling rate.

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• Increasing the crust conductivity together with an increase in the pool heat transfer can produce debris cooling by overlying water.





#### **Debris Coolability With Conductivity Multiplier**



Corium cooling resulting from different values of the conductivity multiplier. (The concrete ablation temperature is 1650K.)





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