CAV Package
Water Ingression and Melt Eruption Models

SAND2019-6040PE

Presented by:
MELCOR Development Team

Sandia National Laboratories

Outline

- Overview of water ingression and melt eruption models
  - Background
    - Debris pool concept and layer solutions in CAV
    - Theory of pure conduction crust (sublayer) solve
    - Theory of water ingression (WI) and melt eruption (ME)
  - Mathematical implementation of WI and ME in layer solve
  - New debris pool layers ICRST and IDEB for mass/energy accounting
  - Example Problem(s)
  - Summary

Debris Pool Layer Solutions

- Setting the stage…
  - Recall debris in cavity is modeled as a "pool" consisting of one or more stratified layers
  - WI and ME – when selected by the user - are imposed at the layer/sublayer level and:
    - Only for the top-most occupied debris layer (potentially in contact with overlying water pool)
    - Only for the axial layer configuration where crusts (top) and a molten sublayer is present

- Pool solution requires provisional solutions of constituent layers and interfaces
  - Separate axial and radial (essentially two 1-D calculations for every layer)
  - Each layer can have one of several configurations (liquid, liquid with crusts, solid,…)
  - Interface heat fluxes, temperatures, and heat flux derivatives depend on configuration
  - Doubly-iterative scheme to resolve consistent interface temperatures and heat fluxes
  - Layer/interface solutions factor into linearized-implicit part of layer enthalpy equations
    - New-time layer enthalpies use linearized projections of interface heat transfer
    - Interface temperatures and heat flux derivatives construct these projections

Sandia National Laboratories

Background Theory (General Layer Solve 1/2)

- From the general layer energy equation:

$$\rho c_p \frac{dT}{dt} + \nabla \cdot \vec{q}'' = \dot{Q}(\vec{r})$$

- Integrate over volume and employ suitably defined averages:

$$Mc_p \frac{d\bar{T}}{dt} = \frac{dH}{dt} = \langle \dot{Q}(\vec{r}) \rangle V - \int_S \left(\vec{q}'' \cdot d\vec{A} \right) = \langle \dot{Q}(\vec{r}) \rangle V - [-A_B \langle \vec{q}_B'' \rangle + A_T \langle \vec{q}_T'' \rangle + A_R \langle \vec{q}_R'' \rangle]$$

Where: $\langle \dot{Q}(\vec{r}) \rangle = \frac{1}{V} \int_V \dot{Q}(\vec{r}) dV$, a volume average

$\langle \vec{q}'' \rangle = \frac{1}{A} \int_S \left(\vec{q}'' \cdot d\vec{A} \right) = \frac{1}{A} \int_V (\nabla \cdot \vec{q}'')\, dV$, an area average

- Evaluate heat flows $\vec{q}''$ from an equivalent steady-state problem:

$$\nabla \cdot \vec{q}'' = \dot{Q}^*$$

*Layer volumetric generation $\dot{Q}^*$ is chosen such that the same average temperature $\bar{T}$ prevails

- Evaluate heat flows $\vec{q}'' = \hat{q}''$ from a steady, 1-D problem with same $\bar{T}$ and BC's
  - $\hat{q}_T''$ and $\hat{q}_B''$ are determined by T_T, T_B, and $\bar{T}$ and likewise $\hat{q}_R''$ is determined by T_R and $\bar{T}$
  - $\dot{Q}_Z^*$ and $\dot{Q}_R^*$ are implicitly defined by temperatures

Sandia National Laboratories

Background Theory (General Layer Solve 2/2)

- At start of debris layer solve (any configuration), have fixed boundary temperatures, layer average temperature, and layer overall thickness
- Start with solving axial configuration (similar for radial, omit in description here)
  - Discern the configuration: "liquid with crust', 'solid', 'solid with liquid', or 'liquid'
  - Do layer solution using configuration (pure conduction for 'solid', convection for 'liquid')
  - Return with:
    - Interface heat fluxes and derivatives w.r.t temperatures (top, bottom, liquid, layer average)
    - Any sublayer or crust parameters (temperatures, thicknesses)
  - Direct solution for all configurations besides 'liquid with crusts' – requires iteration
    - 2-variable Newton w/ bisection, compute liquid sublayer and solid crusts repeatedly until "targets" hit
    - Targets are average layer temperature and total layer thickness while iteration variables are liquid sublayer thickness and liquid sublayer temperature
  - DO
    - Initialize (or use last-iterate) liquid sublayer thickness and liquid sublayer temperature
    - Calculate liquid sublayer convection for liquid sublayer peripheral heat fluxes
    - Calculate top/bottom crusts (to include WI/ME) for crust temperatures, thicknesses, and peripheral heat fluxes
    - Compute updates to liquid sublayer thickness and temperature according to Newton's method
  - END DO
    - Liquid sublayer temperature/thickness dictates crust temperatures/thicknesses such that all variables satisfy the system of layer equations AND hit the current iteration layer "targets"

Sandia National Laboratories

Background Theory (Top Crust Solve)

- The conventional and only previous CAV approach to solving a top crust (sublayer) in the 'liquid with crust' axial configuration type used a heat equation of the form:

$$\frac{d^2T}{dz^2} = \frac{-\dot{Q}}{k} \qquad \begin{array}{ll} \mathrm{T}(0) = T_S - \mathit{Solidus\ temperature} & ; \quad T(\delta_T) = T_T - \mathit{Layer\ top\ interface\ temperature} \\ -k({}^{dT}/_{dz})_{\delta_T} = q''_T - \mathit{Layer\ top\ heat\ flux} & ; \quad -k({}^{dT}/_{dz})_0 = q''_{TL} - \mathit{Melt\ heat\ flux} \end{array}$$

- Can derive:
  - Temperature profile in crust: $T(z) = \frac{\dot{Q}\delta_T}{2k}\left(z - {}^{z^2}/_{\delta_T}\right) + \frac{z}{\delta_T}(T_T - T_s) + T_s$
  - Derivative profile in crust: $\frac{dT(z)}{dz} = \frac{-\dot{Q}z}{k} + \frac{T_T - T_s}{\delta_T} + \frac{\dot{Q}\delta_T}{2k}$
  - Crust average temperature: $\bar{T}_T = \frac{\dot{Q}\delta_T}{12k} + \frac{T_T}{2} + \frac{T_s}{2}$
  - Crust volumetric energy generation: $\dot{Q} = \frac{q''_T - q''_{TL}}{\delta_T}$
- In the 'liquid with crust' axial configuration solve, must predict δ_T from T_T, T_s, and q''_{TL} from:

$$0 = \dot{Q}\delta_T^2 + 2q''_{TL}\delta_T - 2k(T_s - T_T)$$

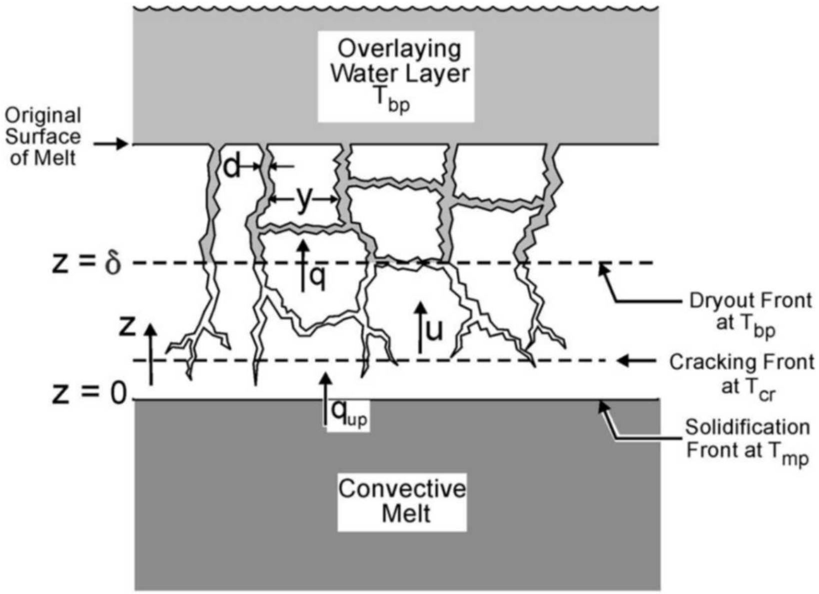
- The top (interface) heat flux follows from the quadratic solve for δ_T: $q''_T = q''_{TL} + \dot{Q}\delta_T$
- This is the top crust dry conduction zone thickness and top crust top heat flux (top layer top interface heat flux) in the absence of any WI or ME modeling

Sandia National Laboratories

Background Theory (Water Ingress Model)

- Based on a dry-out heat flux correlation proposed by Epstein
- Dry-out heat flux from a non-linear algebraic prescription:

$$q = \frac{h_{fg}(\rho_f - \rho_g)g}{\sqrt{2}(12)\nu_g}[\alpha_T(T_{cr} - T_{bp})]^3\left(\frac{32\alpha^2 N\phi\rho^2[h_{fs} + c(T_{mp} - T_{bp})]^2}{(q - q_{up})^2(T_{mp} - T_{cr} + \beta h_{fs}/c)}\right)^{4/5}$$



- Solve for dry-out via bisection algorithm

$$q_0 = \left(\frac{h_{fg}(\rho_f - \rho_g)g}{\sqrt{2}(12)\nu_g}\right)^{5/13}[\alpha_T(T_{cr} - T_{bp})]^{15/13}\left(\frac{32\alpha^2 N\phi\rho^2[h_{fs} + c(T_{mp} - T_{bp})]^2}{T_{mp} - T_{cr} + h_{fs}/c}\right)^{4/13}$$

- Note similarities/differences compared with conventional CAV top crust treatment
  - Presence of a "wet zone" with prevailing temperature T_{sat}
  - Presence of a dry-out front at q''_{dry} and T_{sat}
  - Presence of a dry conduction zone (governed by equations of pure conduction)
  - Presence of a convective melt below, interface at q''_{TL} and T_s

Sandia National Laboratories

Background Theory (Melt Eruption Model)

- The mass transfer rate (volumetric flow per unit area) of molten mass due to sparging gas:

$$j_{melt} = K_{ent} * j_{gas}$$

- The entrainment coefficient is computed with the Ricou-Spalding correlation:

$$K_{ent} = E_{ent}\left(\frac{\rho_{gas}}{\rho_{melt}}\right)^{1/2}$$

- There is a minimum sparging gas rate that can cause melt mass entrainment:

$$j_{min} = \frac{\kappa(\rho_{crust} - \rho_{melt})g}{\mu_g}$$

- Permeability is computed with help from the Epstein dry-out heat flux correlation:

$$\kappa = \frac{2\mu_g q''_{dry}}{\rho_g h_{fg}(\rho_g - \rho_f)g}$$

- Note the melt eruption model depends on the water ingression model via the permeability and dry-out heat flux relationship

- ME cannot be exercised independently of WI

Sandia National Laboratories

Implementation: Water Ingress and Melt Eruption

- Intervene in layer solve ('liquid with crusts') to compute WI/ME if requested and if conditions permit (i.e. wet cavity and a top crust exists)
- Compute WI first, then ME if requested (WI without ME, but no ME without WI)
- Strategy: interject the Epstein model, pre-empt the top crust quadratic equation for δ_T:
  - Proceed with conventional 'liquid with crust' solve, project Epstein prediction inside a given iteration
  - Solve (Newton's method) for q''_{dry} and κ from knowledge of T_s, T_T and liquid sublayer properties
  - Back out a dry conduction zone thickness and a wet "water ingressed" zone thickness

$$\delta_{T,dry} = \left(2*k*(T_S - T_T)\right) \Big/ q''_{dry}$$

  - Compute new crust average temperature (for dry conduction zone only)
  - If melt eruption modeling is requested, j_{melt} is computed if j_{min} is less than j_{gas}
  - The mass inventories of wet crust and of erupted melt can then be computed
- Inventory transfers between layers are performed elsewhere
- Assumptions of IDEB and ICRST layer quench are mathematically imposed

Sandia National Laboratories

Implementation: ICRST and IDEB Layers

- Mass transfers from top-most occupied debris layer to ICRST and/or IDEB
  - "Wet" crust inventory resides in IDEB and is assumed quenched upon formation to water pool T_{sat}
  - "Erupted" debris inventory resides in ICRST and is assumed quenched upon formation to T_{sat}
- Requisite energy transfers to CVH and miscellaneous mass/energy accounting performed
- IDEB and ICRST do not participate in certain calculations of other debris pool physics
- IDEB and ICRST are totally solved upon computation of their masses (T, h are known)

Sandia National Laboratories

Example Problem(s)

- MELCOR (CAV/CORCON-MOD3) to CORQUENCH
- Initialize a debris melt with user-defined concrete and a representative cavity
- Choose similar modeling options for MELCOR and CORQUENCH
  - Water ingress active
  - Melt eruption inactive
  - 2-D erosion calculation in CORQUENCH (as similar as possible to MELCOR axisymmetric model)
  - Same initial debris contents, initial debris temperature, and concrete composition
  - Same wet cavity conditions
  - Similar decay heat generation rate in debris
- Results at end of run – check for general agreement and qualitative similarity
  - Debris pool contents
  - Top crust formation and debris-to-water heat transfer
  - Temperatures and thermophysical properties

Sandia National Laboratories

Example Problem(s)

- Consider extreme concrete decomposition gas migration fractions in CORQUENCH
- Initial debris mass: UO_2 – 300 kg, Fe – 170 kg, Cr – 35 kg
- Neglect species with small mass inventories in summary of TEND compositions below

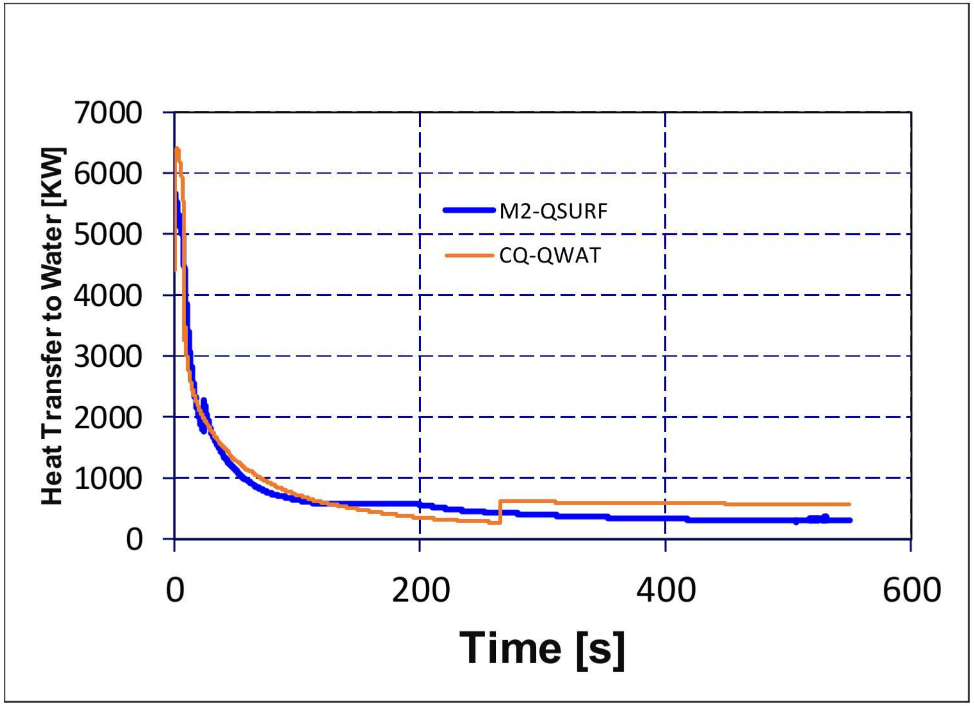
Debris Constituent Masses [kg]

	CQ (no migration)			CQ (full migration)			MELCOR
Species	**Melt**	**Top Crust**	**Overall**	**Melt**	**Top Crust**	**Overall**	**Debris**
UO2	92.368	206.820	299.188	66.570	232.890	299.460	258.540
CR2O3	4.859	5.707	10.566	7.268	13.436	20.704	22.288
FE	52.343	117.200	169.543	37.724	131.970	169.694	146.160
CR	7.464	20.212	27.676	2.819	17.952	20.771	14.920
NA2O	0.016	0.011	0.027	0.022	0.010	0.032	0.050
TIO2	0.035	0.024	0.059	0.047	0.022	0.069	0.109
SIO2	4.636	7.209	11.845	4.251	9.617	13.868	21.630
CAO	4.056	6.300	10.356	3.727	8.398	12.125	18.912
MGO	0.094	0.065	0.159	0.126	0.060	0.186	0.290
AL2O3	0.557	0.634	1.191	0.751	0.643	1.394	2.175
FEO	0.000	0.000	0.000	0.000	0.000	0.000	0.441
FE2O3	0.028	0.019	0.047	0.038	0.018	0.056	0.870
FE3O4	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOTAL	166.456	364.201	530.657	123.343	415.016	538.359	486.385

Sandia National Laboratories

Example Problem(s)

- Top crust formation and water ingress
- Timing:
  - CQ – First formation of top crust – 4.4s and water ingress begins at 396 s
  - M2 – First formation of top crust – 14.7 s and water ingress begins at 506 s
- Final top crust thicknesses are: CQ – 181 mm and M2 – 177 m
- Heat transfer rate to overlying pool:



Sandia National Laboratories

Example Problem(s)

- Compare TEND temperatures:
  - CQ TMELT / M2 TAVE-Z : 1795 [K] / 1741 [K]
  - Oxide/Metal Solidus/Liquidus
    - TSOL_OXIDE (CQ/M2) 1911 [K] / 1732 [K]
    - TLIQ_OXIDE (CQ/M2) 3144 [K] / 2649 [K]
    - TSOL_METAL (CQ/M2) 1791 [K] / 1796 [K]
    - TLIQ_METAL (CQ/M2) 1798 [K] / 1806 [K]

- Compare TEND properties:
  - Specific Heat (CQ/M2) [J/kg/K] 612.5 / 694.7
  - Density (CQ melt / CQ crust / M2) [kg/m^3] 6675 / 8263 / 7043
  - Surface Tension (CQ/M2) [N/m] 0.902 / 0.890
  - Thermal Expansivity (CQ/M2) [1/K] 9.323*10-6 / 3.409*10-5
  - Thermal Conductivity (CQ melt / CQ crust / M2) [W/m/K] 7.16 / 7.11 / 87.93
  - Viscosity (CQ/M2) [kg/m/s] 4.67 / 499.3

Sandia National Laboratories

Example Problem(s)

- MELCOR-to-MELCOR test problem demonstrating action of water ingress

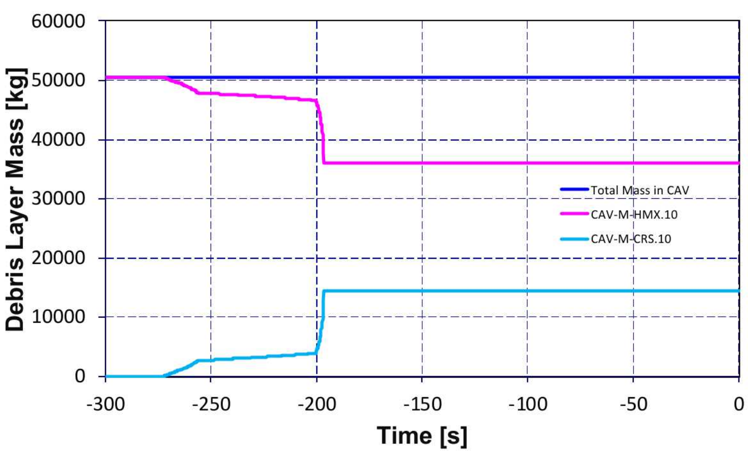
```
!                  cavnam
CAV_ID            'Sump'
!                  volref
CAV_CV            'RSUMP'
!                    type               name
CAV_C0       STANDARD 'CORCON BASALT'
!
!            densct        tsolct        tliqct        tablct         tinct          emisct
CAV_C2       2100.0        1520.0        1570.0        3000.0         300.0             0.7
!      ipdhflg         ipoxflg          ipmflg
CAV_DH   CF  'NZL'  CF  'NZL_FRC_OX'  CF  'NZL_FRC_MET'
!              nrays          zo
CAV_G1          100          -2.0
!              zt          rad          hit        radc
CAV_G2        -4.0        8.0          5.0         0.2
!          flag_rw    rw       hbb      nbot      ncorn
CAV_G3       VALUE     13.0     2.3      53         5
!              novc
CAV_RR       CONTINUE
!              novc
CAV_RA       CONTINUE
!
!     size
CAV_U    6 ! n       keyword       value[1]       value[2]
             1    WATINGR       NONE
             2    BOILING       MOD3
             3    ERUPT         NONE
             4    GFILMBOTT     SLAG
             5    HTRINT      MULTIP 5.0
             6    COND.CRUST 3.0

!
CAV_L1   DEFINE   1800.0   3   ! NUMBER  MATNAM   MASS
                                  1       FE       17000.0
                                  2       CR       3500.0
                                  3       UO2      30000.0
```

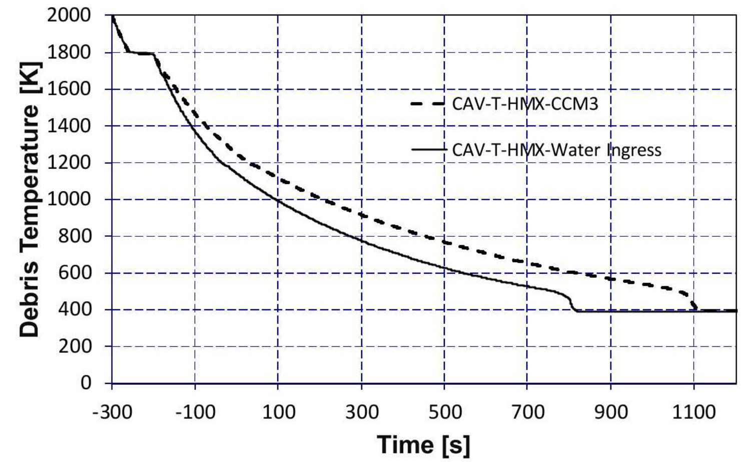
- Two variants
  - — Initialize debris as all molten
  - — Initialize debris as partially solid
- Demonstrate water ingress…
  - — As an initial condition
  - — As an evolved condition
- Description:
  - — Initially wet cavity
  - — Built-in concrete type
  - — Representative cavity geometry
  - — Initialized debris with three components (UO_2, Fe, Cr) and some temperature
- Options: MOD3 boiling, enforced mixing, HTRINT and COND.CRUST

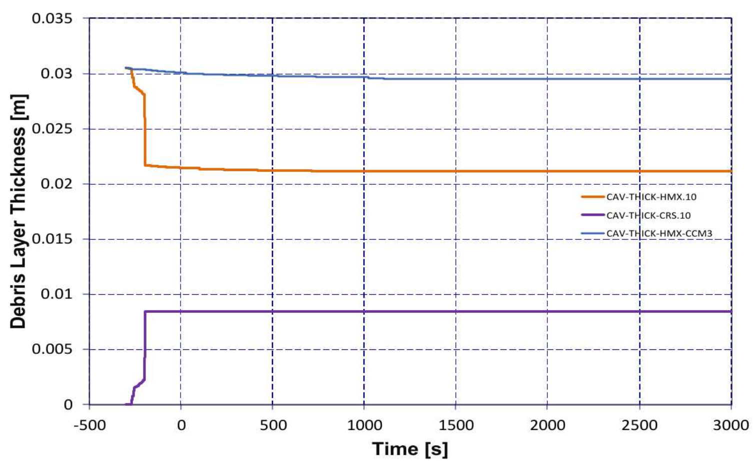
Sandia National Laboratories

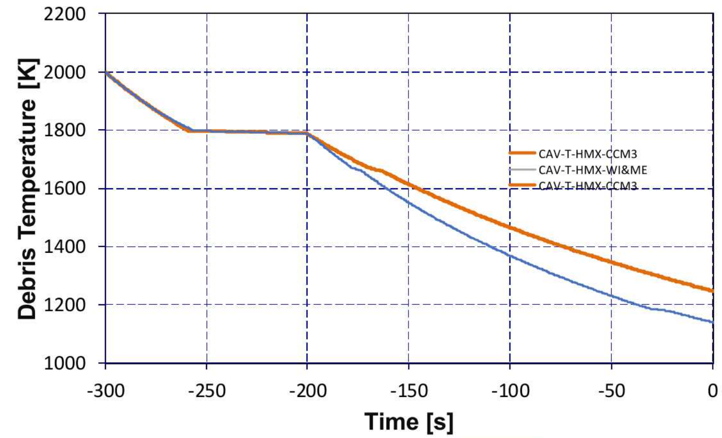
Example Problem(s)

- Initial temperature at 2000 K (initialized molten debris without crusts)





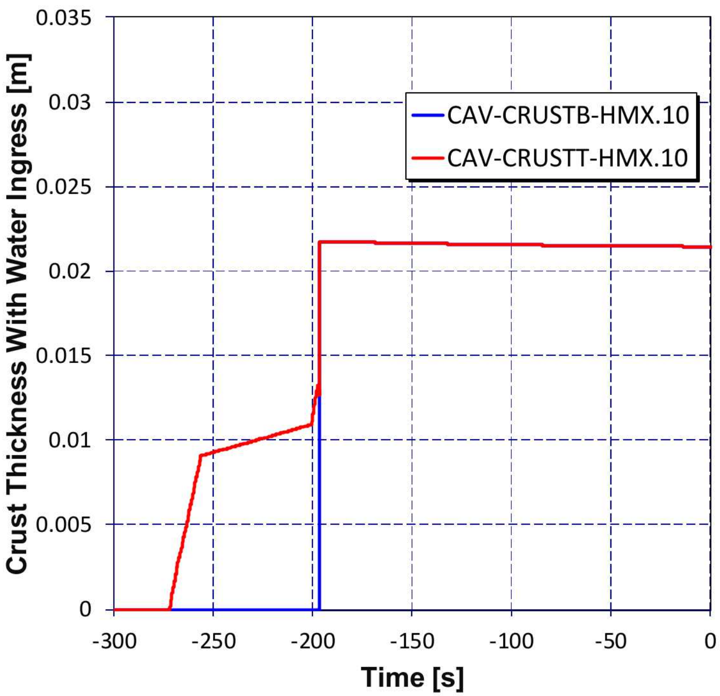


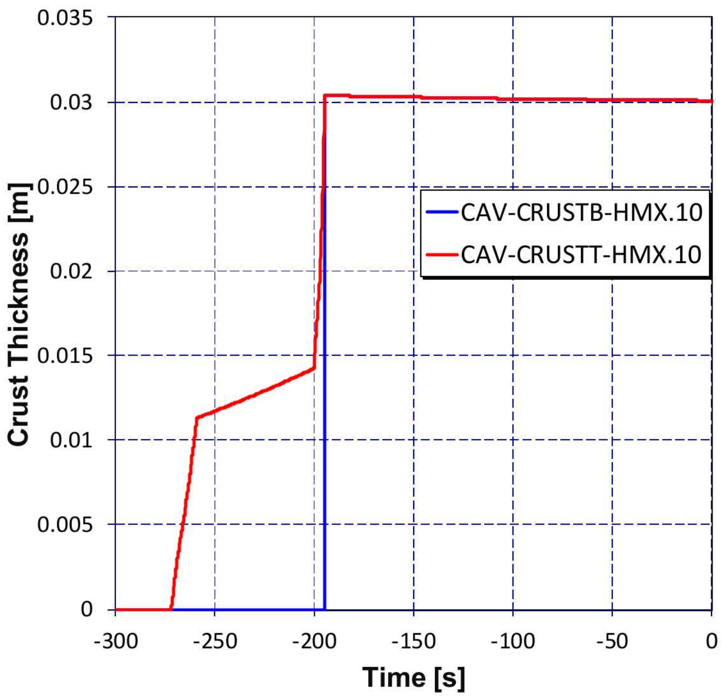


Sandia National Laboratories

Example Problem(s)

- Initial temperature at 2000 K (initialized molten debris without crusts)



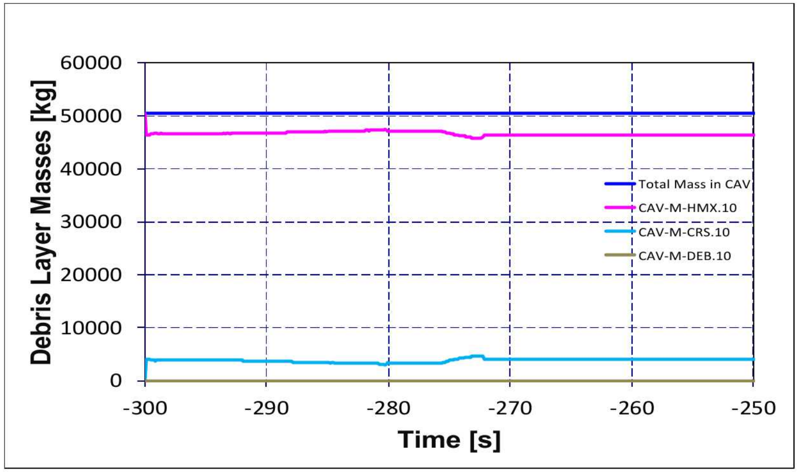


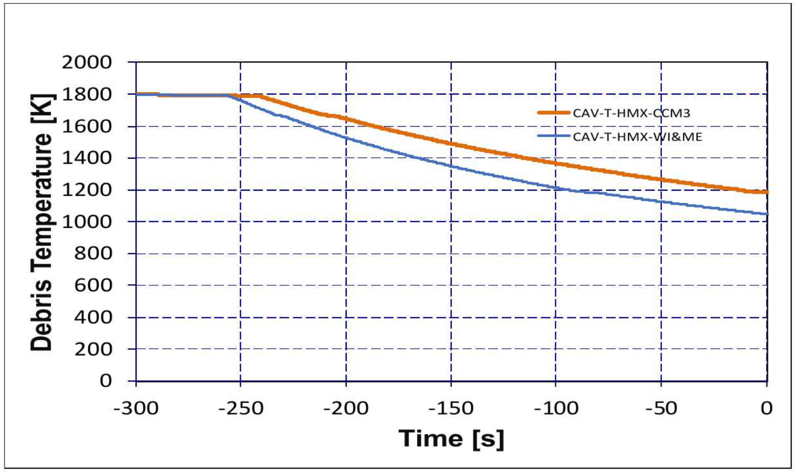
- Cooling through the all-molten configuration is identical
- At onset of crust formation, water ingress cools the debris more quickly
  - Bottom crust formation sooner in problem time
  - No longer a linearly-increasing dry conduction zone growth trend (due to water ingress)

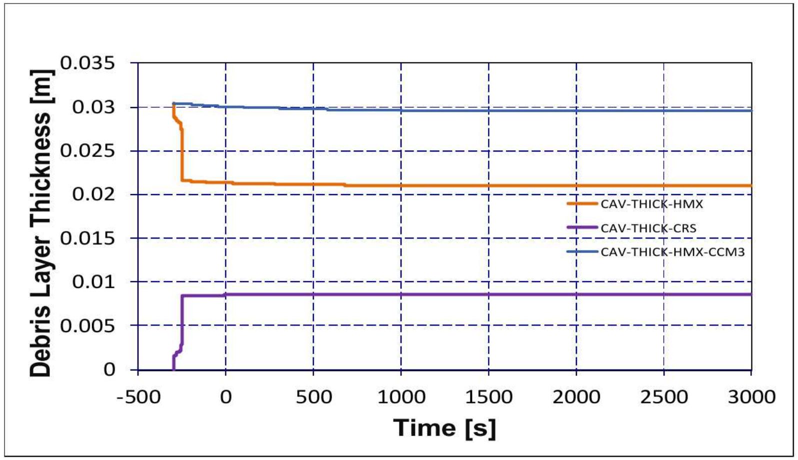
Sandia National Laboratories

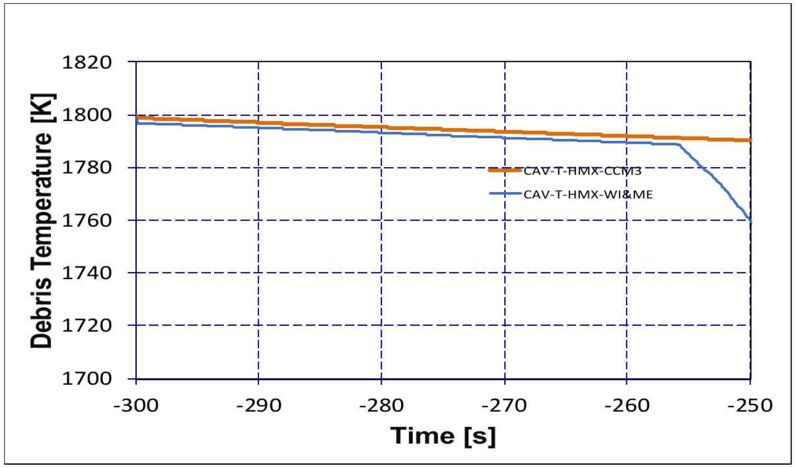
Example Problem(s)

- Initial temperature at 1800 K (initialized molten debris with crusts)





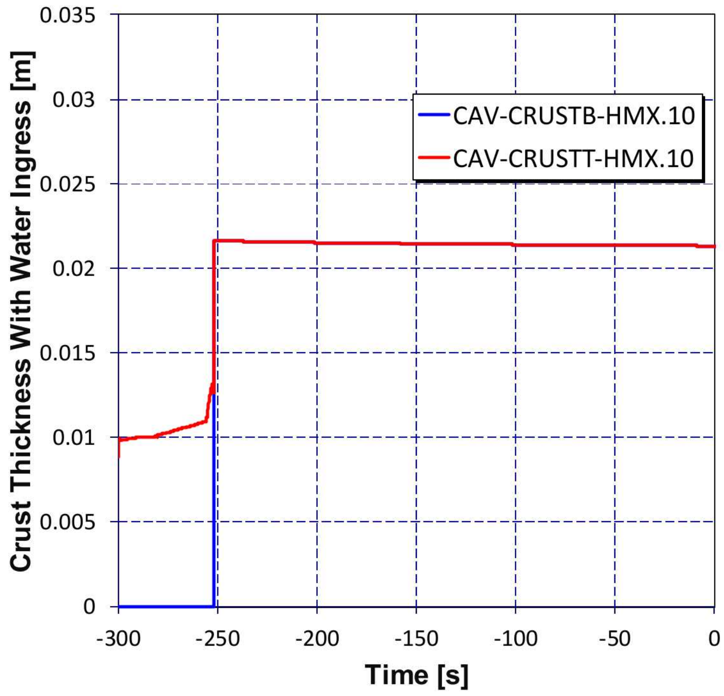


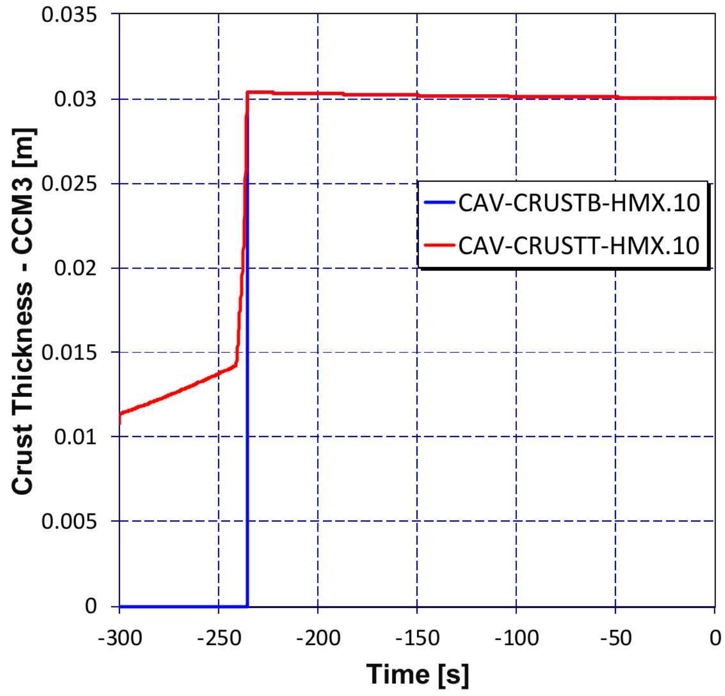


Sandia National Laboratories

Example Problem(s)

- Initial temperature at 1800 K (initialized molten debris with crusts)





- Bottom crust forms sooner in problem time…water ingress cools debris more quickly

Sandia National Laboratories

Summary

- CAV revised to account for water ingress and melt eruption
  - Eliminate previously observed FORTRAN crashes, failures, non-physical behavior, and axial/radial convergence warnings/errors
  - Attempt to capture effects of enhanced molten debris cooling
    - WI permits enhanced cooling of underlying molten pool, quenches cracked crust to saturation temperature
    - ME brings molten material straight to cooling water, subsequent quenching to saturation temperature
- CAV modified to include new layers ICRST and IDEB
- Example problems:
  - Comparison to CORQUENCH seems reasonable (top crust formation and QWAT)
  - M2-to-M2 comparisons behave as expected

Sandia National Laboratories