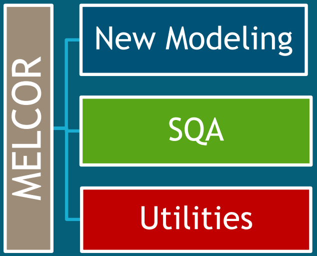
Sandia National Laboratories



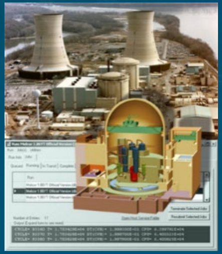
MELCOR

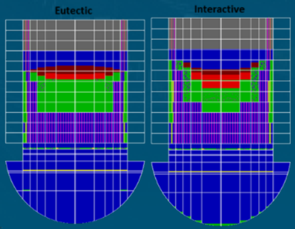
New Modeling

SQA

Utilities

MELCOR Code Development Status
EMUG 2021





MELCOR Team, Sandia National Laboratories

SAND2021-4647 PE

PRESENTED BY

Larry Humphries, Sandia National Laboratories

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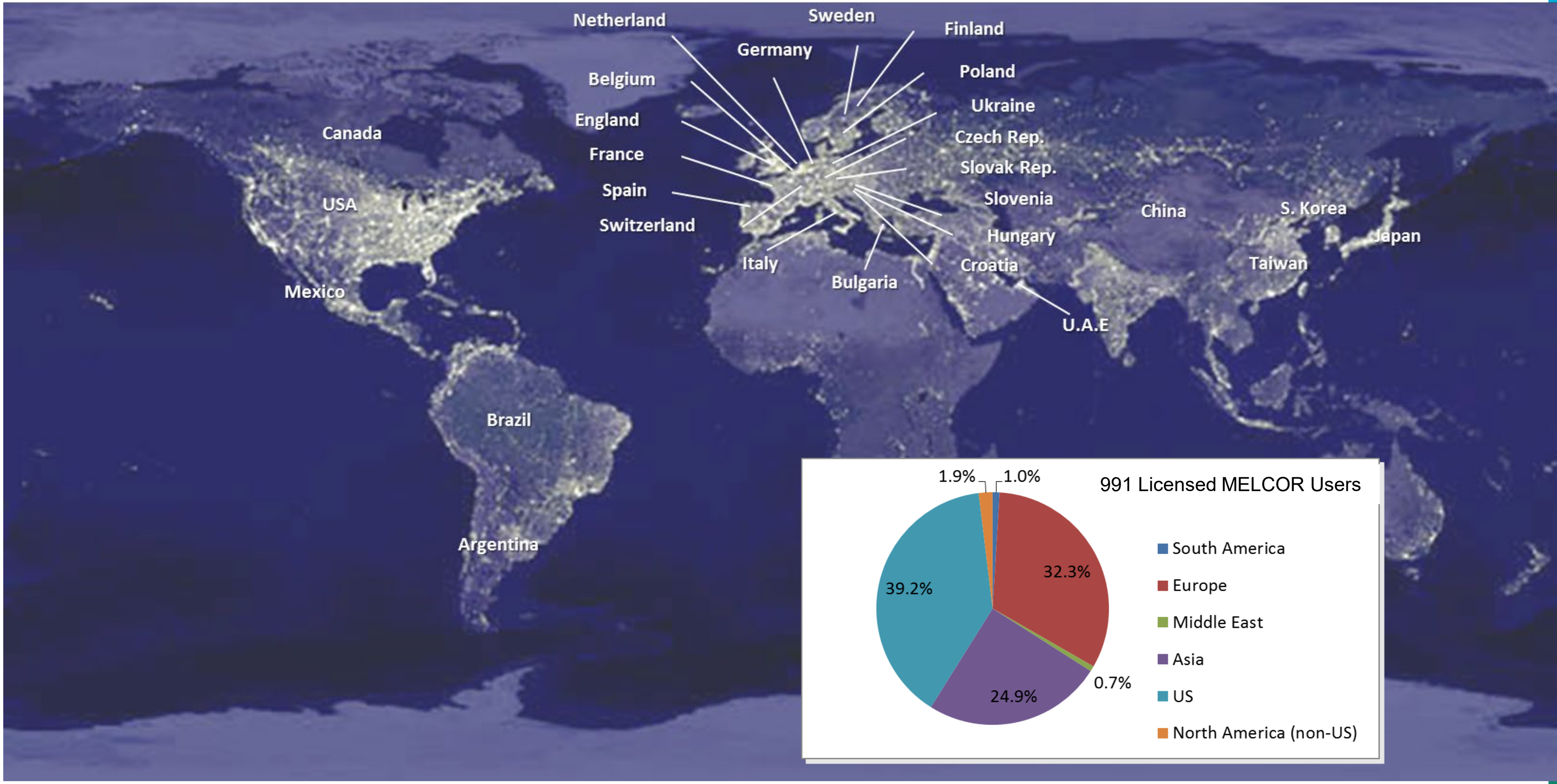
International Use of MELCOR



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

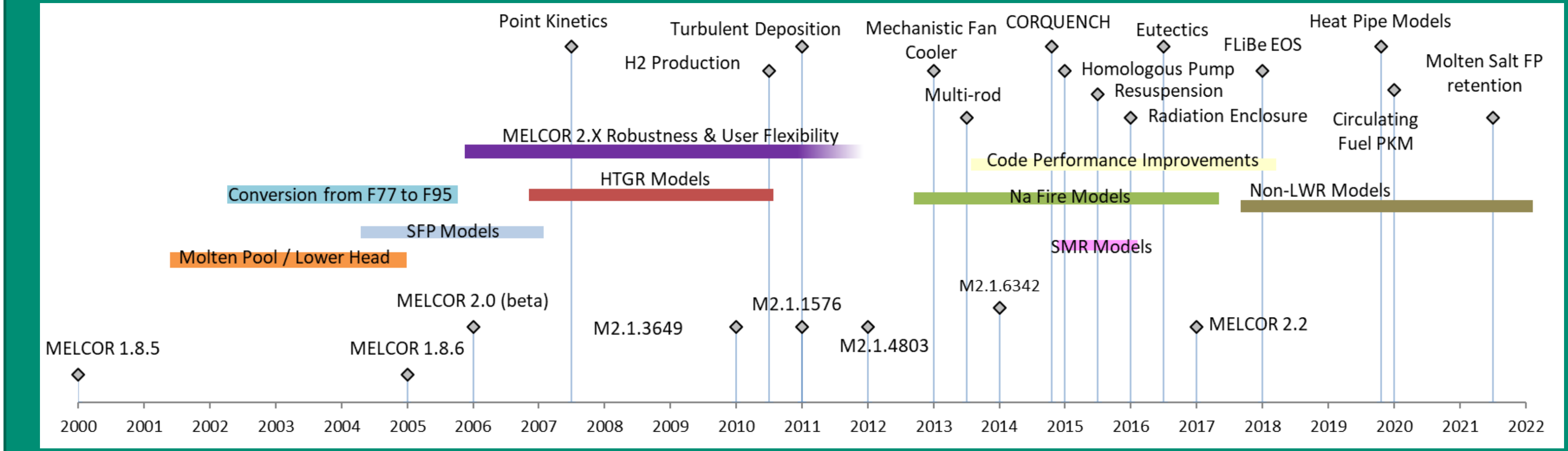
- CSARP (June 3-5), MCAP (June 5-6), Workshop (June 6 afternoon)
- Albuquerque, NM
- ½ day workshop with focused topics on ex-vessel corium modeling

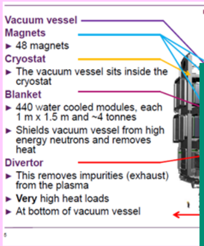
2019 Asian MELCOR User Group (AMUG)

- Hosted by KAERI
- November 2019

MELCOR Model Development

MELCOR Code Development Timeline





Vacuum vessel

Magnets
- 48 magnets

Cryostat
- The vacuum vessel sits inside the cryostat

Blanket
- 440 water cooled modules, each 1 m x 1.5 m and ~4 tonnes
- Shields vacuum vessel from high energy neutrons and removes heat

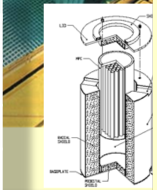
Divertor
- This removes impurities (exhaust) from the plasma
- **Very** high heat loads
- At bottom of vacuum vessel

- Interactive graphics available: http://www.iter.org/mach

Fusion

- Neutron Beam (LOVA)
- Li Loop LOFA t analysis
- ITER Cryostat
- Helium Lithium
- Helium Cooled Bed Test Blank (Tritium Breed

Spent Fuel



M2x Official Code Releases

Version	Date
2.2.18019	December 2020
2.2.14959	October 2019
2.2.11932	November 2018
2.2.9541	February 2017
2.1.6342	October 2014
2.1.4803	September 2012
2.1.3649	November 2011
2.1.3096	August 2011
2.1.YT	August 2008
2.0 (beta)	Sept 2006

ear Facilities

th Factor Calculatio

Release of hazardous materials from facilities, buildings, confined spac

fety Toolbox code

clear facility users

Pantex

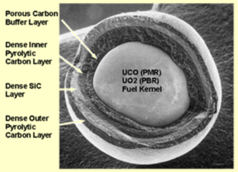
Hanford

Los Alamos

Savannah River Site

HTGR Reactors

- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- Modified Fuel components (PMR/PBR)
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure


Porous Carbon Buffer Layer
Dense Inner Pyrolytic Carbon Layer
Dense SiC Layer
Dense Outer Pyrolytic Carbon Layer
UCO (PMR)
UO2 (PBR)
Fuel Kernel

Sodium Reactors

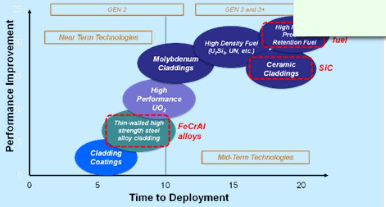
Sodium Properties
- Sodium Equation of State
- Sodium Thermo-mechanical properties

Containment Modeling
- Sodium pool fire model
- Sodium spray fire model
- Atmospheric chemistry model
- Sodium-concrete interaction

Molten Salt Reactors

- Properties for LiF-BeF2 have been added
  - Equation of State
  - Thermal-mechanical properties

Accident Tolerant Fuels



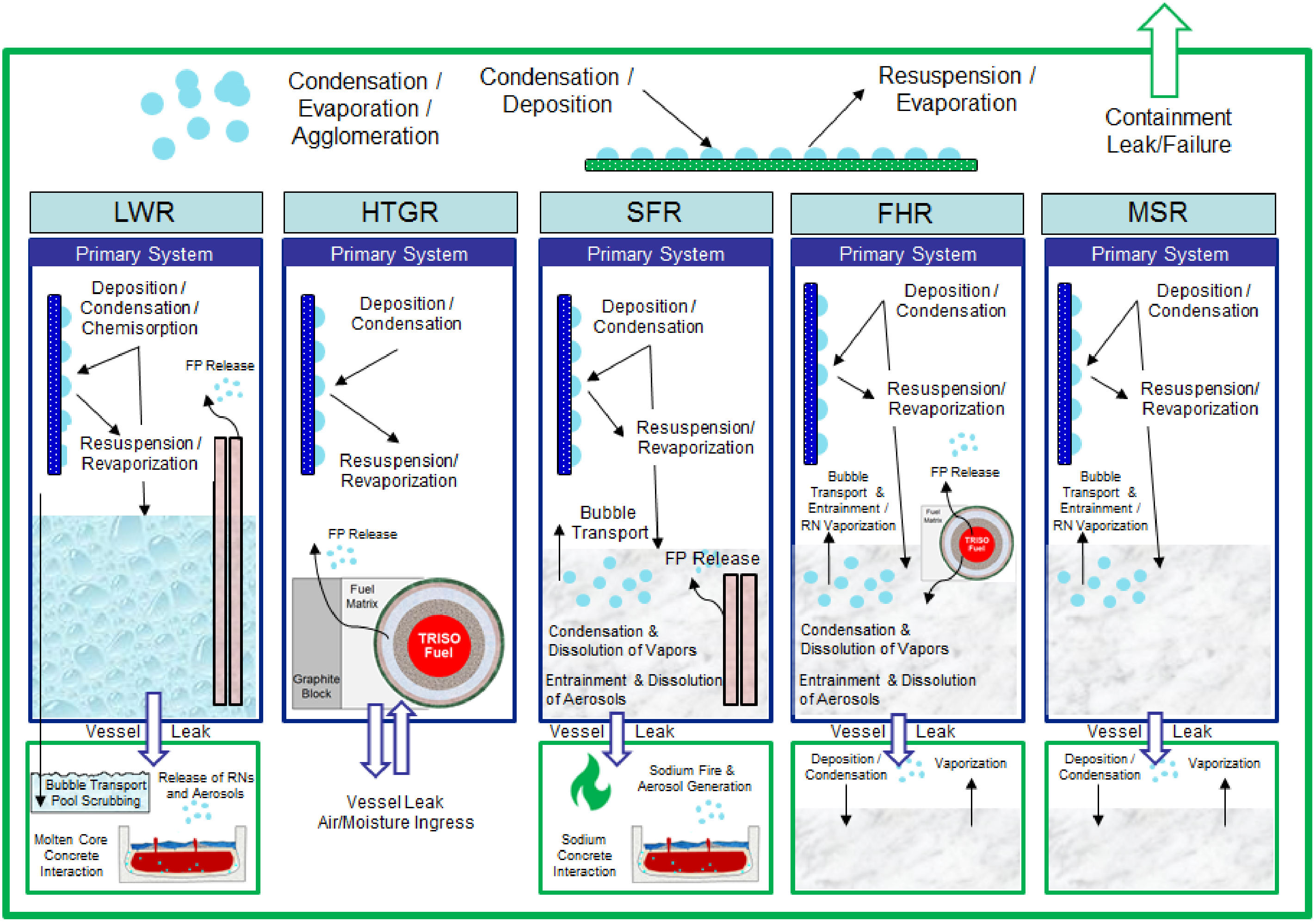
LWR/Non-LWR/ATF Fuels Development

LWR and General MELCOR development

Advanced Technology Fuels (ATF)

Non-LWR Reactors
- HTGR
- Sodium
- Molten Salts

Spent Fuel Pools


Condensation / Evaporation / Agglomeration
Condensation / Deposition
Resuspension / Evaporation
Containment Leak/Failure
LWR
HTGR
SFR
FHR
MSR
Primary System
Deposition / Condensation / Chemisorption
FP Release
Resuspension / Revaporization
Vessel Leak
Bubble Transport Pool Scrubbing
Release of RNs and Aerosols
Molten Core Concrete Interaction
Deposition / Condensation
Resuspension/ Revaporization
FP Release
Fuel Matrix
Graphite Block
TRISO Fuel
Vessel Leak
Air/Moisture Ingress
Deposition / Condensation
Resuspension/ Revaporization
Bubble Transport
FP Release
Condensation & Dissolution of Vapors
Entrainment & Dissolution of Aerosols
Vessel Leak
Sodium Fire & Aerosol Generation
Sodium Concrete Interaction
Deposition / Condensation
Resuspension/ Revaporization
Bubble Transport & Entrainment / RN Vaporization
FP Release
Fuel Matrix
TRISO Fuel
Condensation & Dissolution of Vapors
Entrainment & Dissolution of Aerosols
Vessel Leak
Deposition / Condensation
Vaporization
Deposition / Condensation
Resuspension/ Revaporization
Bubble Transport & Entrainment / RN Vaporization
Vessel Leak
Deposition / Condensation
Vaporization

New Defaults (2019 Code Release)

Sub-cooled Heat Transfer New Default

- New COR default enables lower head segment-to-pool heat transfer when segment surface temperature is sub-cooled with respect to the pool
  - Default in 2019 release

- Previously, outer surfaces of LH segments submerged in a CAV/LHC pool do not transfer heat unless surfaces are superheated with respect to the pool

- No new physics, apply existing convection correlations (HS subroutine)

- 5th field **ILHHT** on **COR_MS** - “1”/“ACTIVE” to deactivate

```
!         IEUMOD      IHSDT      IDTDZ      ICORCV      ILHT
COR_MS       0          0          0          0           1    ! Activate sub-cooled LH HT to pool
```

Heat Transfer Coefficients for Lower Head New Default

Parameters for modeling heat transfer to the lower head are provided on the COR_LHF record.

User specifies heat transfer for the following:

- Debris to penetrations
- Debris to lower head
- Heat transfer from oxidic molten pool to lower head
- Heat transfer for 'stray' metallic molten pool to lower head

User can optionally specify a control function for each HTC

	Conduction Path Length (m)		
	0.5	0.25	0.1
UO2	4.4	8.8	22
ZR	83.6	167.2	418
ZRO2	4.88	9.76	24.4
SS	69	138	345
SSOX	40	80	200.

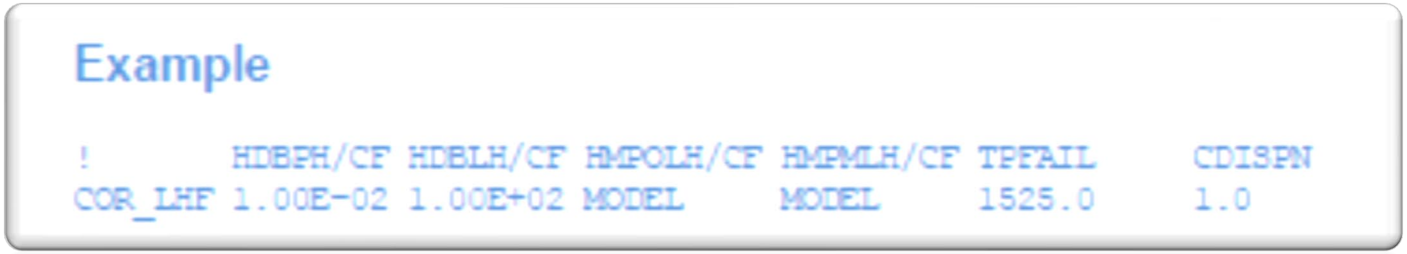
Using Thermal Conductivity of Material at 1700 K

Previous default: All heat transfer coefficients were assumed to be 1000.0 W/m2-k

- Completely arbitrary and not always representative
- Does not reflect thermal conductivities of materials and composition
- Does not reflect conduction path which is dependent on nodalization

MELCOR 2019 release default: an internal model for calculating heat transfer.

- Available for PD to LH and MP1 to LH and MP2 to LH
- Model uses locally calculated thermal conductivity and a conduction path using half the current calculated component height
- These internal models will become default in next code release



Example

```
!        HDBPH/CF HDBLH/CF HMPOLH/CF HMPMLH/CF TPFAIL     CDISPN
COR_LHF 1.00E-02 1.00E+02 MODEL     MODEL     1525.0     1.0
```

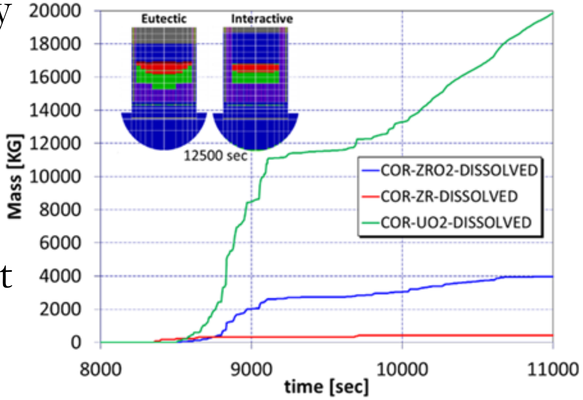
Eutectic Model Enabled by Default

Interactive Materials Model

- Historically, for users to simulate intermetallic formations and their effect on core degradation, users were required to specify surrogate material with effective melt temperatures, UO2-INT and ZRO2-INT.
- However, use of these materials was often overlooked, even by experienced users.

Eutectics Model

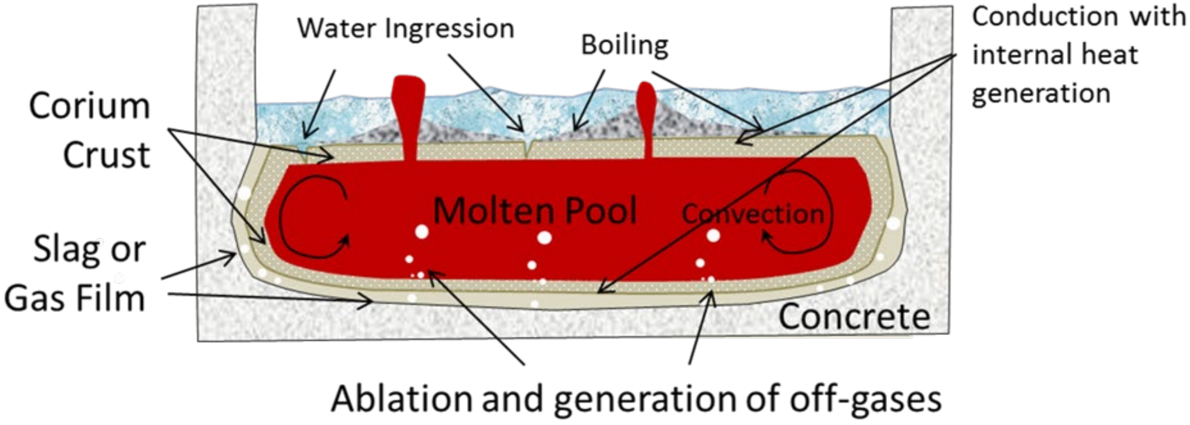
- Improvements to the COR eutectics model were introduced in revision 11932 but were not activated by default until the 2019 release.
- With the new eutectic model, materials in their intact form melt at the molecular liquidus, i.e., UO2 melts at 3113 K and ZRO2 melts at 2990 K.
- However, when UO2 and ZRO2 are in a mixture, the melt temperature is dependent on the fractional content of UO2 and ZRO2 with a minimum melt temperature of 2450 K at 0.5 mole fraction (default).
- In addition, models for liquefaction of intact materials assumed in contact with a eutectic mixture are calculated using a parabolic rate limitation and dependent on the updated melt temperature of the conglomerate.



The new model is activated using the COR_EUT record and specifying ON for the first field. Similarly, OFF will deactivate the eutectic model.

- Should a user incorporate material UO2-INT or ZRO2-INT, the eutectic models will be deactivated.

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

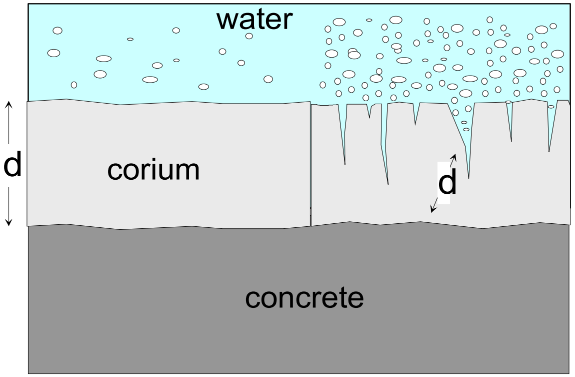
- Water ingression reduces conduction path to molten pool and increases surface area of contact

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

New Defaults (2019 Code Release)

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
```

2018: 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
```

2019 Release: Current default

New in MELCOR 2019 Release

Explicitly set all multipliers for 2018 Bes Practice	New keyword to automatically set all multipliers to 2018 best practice
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	CAV_U 5 … 5 WATINGR MULTIPLIER

Only used as a convenience in comparing to previous best practice using multipliers. New water ingression model is recommended

New Defaults (2019 Code Release)

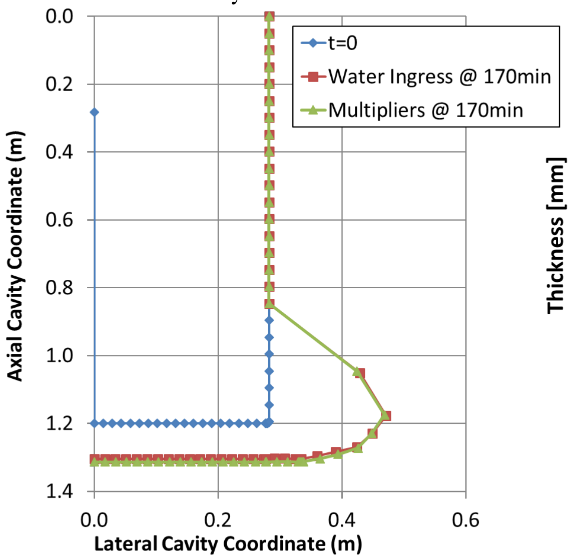
Modifications to CAV Energy Error Accounting (New in 2020 Release)

Previously, wet cavity calculations invoking revised water ingress model demonstrated relatively high CAV and relative global energy errors due to poor accounting

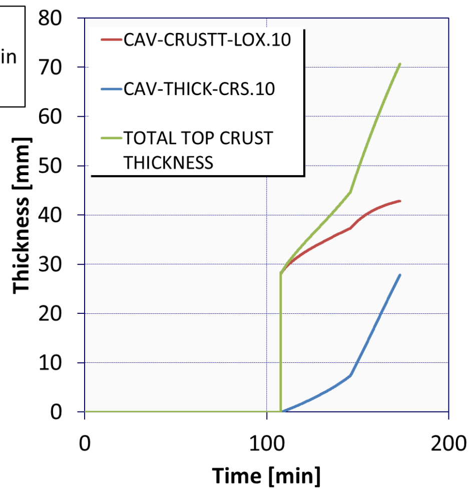
Solution: 1) Revise energy accounting given debris pool layer dyr
2) Test on validation cases (e.g. CCI experiments)

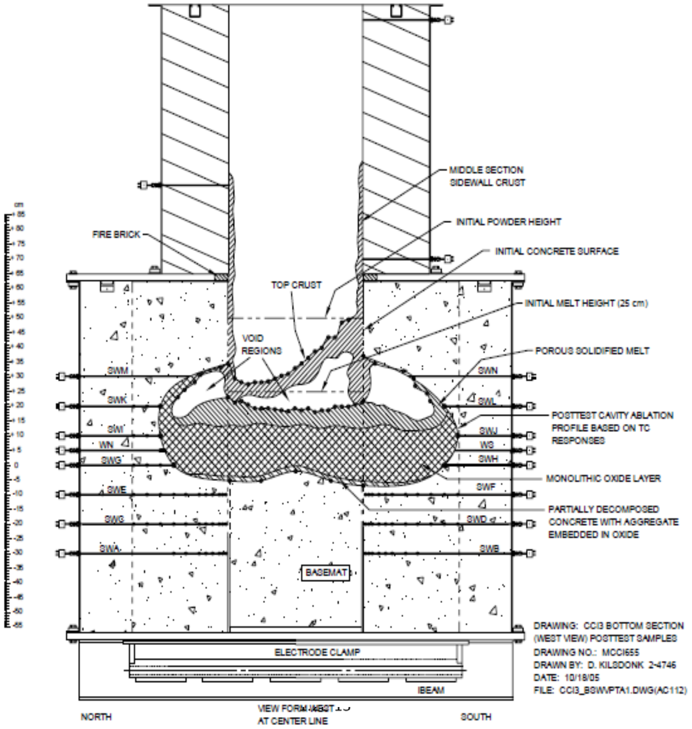
CCI-3 Results and Improved Energy Balance

Concrete Cavity Ablation

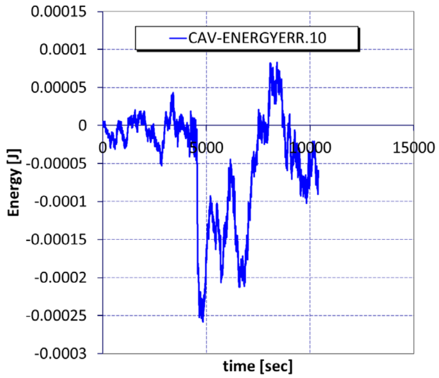


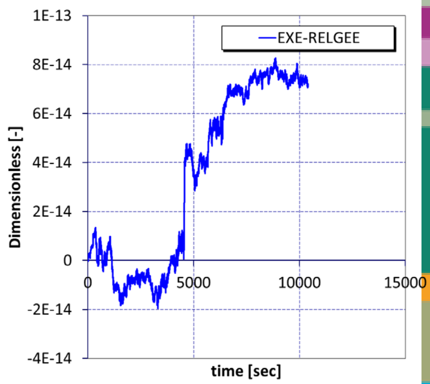
Top Crust Formation




MIDDLE SECTION SIDEWALL CRUST
INITIAL POWDER HEIGHT
FIRE BRICK
INITIAL CONCRETE SURFACE
TOP CRUST
INITIAL MELT HEIGHT (25 cm)
VOID REGIONS
POROUS SOLIDIFIED MELT
SWM
SWN
SWK
SWL
SWI
SWJ
WN
WS
SWG
SWH
POSTTEST CAVITY ABLATION PROFILE BASED ON TC RESPONSES
MONOLITHIC OXIDE LAYER
SWE
SWF
PARTIALLY DECOMPOSED CONCRETE WITH AGGREGATE EMBEDDED IN OXIDE
SWC
SWD
SWA
SWB
BASEMAT
ELECTRODE CLAMP
IBEAM
NORTH
VIEW FORM WEST
AT CENTER LINE
SOUTH
DRAWING: CCI3 BOTTOM SECTION (WEST VIEW) POSTTEST SAMPLES
DRAWING NO.: MCCI655
DRAWN BY: D. KILSDONK 2-4746
DATE: 10/18/05
FILE: CCI3_BSWVPTA1.DWG(AC112)
cm

Measurement	Top Dry Crust [cm]	Top Wet Crust [cm]
CCI-3 Experiment	5 +/- 2	-
MELCOR w/ new WI	4.3	2.75
MELCOR w/ multipliers	13.0	-
CORQUENCH	5 “porous”	-





User plot variables
(New in 2020 Release)

COR-HP-T.n.j Temperature of heat pipe wall at each axial level “j” for heat pipe “n”.
(units = K, default =ON)
(units = K, default =)

COR-HP-T_EWF.n Temperature of equilibrium working fluid region for heat pipe “n”. (Heat Pipe Model 2 only) .
(units = K, default = ON)

COR-HP-P_EWF.n Pressure of equilibrium working fluid region for heat pipe “n”. (Heat Pipe Model 2 only) .
(units = Pa default = ON)

COR-HP-QHP_IN.n Energy transfer rate into heat pipe “n” from surrounding fuel in evaporator region.
(units = W, default =ON)

COR-HP-QHP_OUT.n Energy transfer rate out of heat pipe “n” to surrounding CVH coolant in condenser region
(units = W, default =ON)

COR-VOLF-HP.n Volume fraction of heat pipe in cell n
(units = - , default = ON)

COR-MOLTEN.n Mass of all molten material in cell n . This includes MP1, MP2, MB1, MB2, and any molten conglomerate material associated with particulate debris (PD and PB).
(units = kg, default = ON, Keyword=COR-MOLTEN)

COR-M-LHMELT The total mass that has melted from the LH structure and moved to boundary COR cells
(units = kg, default =ON)

COR-E-LHMELT The total ethalpy of the melted from the LH structure and added to boundary COR cells
(units = kg, default =ON)

COR-V-LHMELT The total volume of the melted from the LH structure and added to boundary COR cells
(units = m3, default =ON)

COR-MPOOL-HGT Height of lower head molten pool
(Units = m default =OFF, keyword=COR-MPOOL-HGT)

COR-MP-HEIGHT.n Molten pool height (thickness) within each cell n
(Units = m default =OFF, keyword=) COR-MPOOL-HEIGHT

COR-MPOOL-Area Surface area of lower head molten pool
(Units = m**2 default =OFF, keyword=COR-MPOOL-AREA)

User plot variables (New in 2020 Release)

COR-TQ-k.n Temperature of the quenched portion of the surface of the clad component
(Units = W, default =ON, Keyword=COR-TQ)

COR-QRAD.k.n Heat radiated to component k in cell n.
(Units = W, default = OFF, COR_EDV(5) required, Keyword = COR-DCZ-M)

COR-EEJEC-TOT Total enthalpy of mass ejected through vessel breach.(units = J)
(Units = W, default =ON, Keyword=COR-MEJEC)

COR-EMIX-TOT Total mixing energy associated with oxidation.(units = J)
(Units = W, default =ON)

COR-EMIX-RAT Total rate of mixing energy associated with oxidation.(units = W)
(Units = W, default =ON)

COR-VOLT.n Total Volume of a COR cell
(Units = W, default =ON)

COR-MASSERR Total mass error for COR package.(units = kg)
(Units = W, default =ON)

COR-CPUDIF2 Total CPU usage by HTGR FP release model COR_DIF2 routine call.(units = s
(Units = W, default =ON)

COR-COR DAMAGE Fraction of the core fuel that is no longer intact due to loss of support, liquefaction, or melting.
(Units = -, default =ON)

COR-WLEVEL Waterlevel in COR package (channel volumes)
(Units = m default =ON)

COR-CWLEVEL Collapsed Waterlevel in COR package(channel volumes)
(Units = m default =ON)

Extensions to the CF Package

Ranges

- User defined construct that generates an ordered list of objects to be used by vectorized CFs

Vectorized CF arguments

- Control Function arguments can now be specified as a vector of values by specifying and index with a range

Vector Control Functions

- Certain control functions now permit vector operations such as add, multiply, divide, equals, L-GT, L-GE, etc.

Package input support of vector CFs

- Some input records have been modified to allow vector fields in place of scalar fields

Analytic Control Functions

- Ultimate flexibility allowing users to pass vectors to a user specified FORTRAN function.

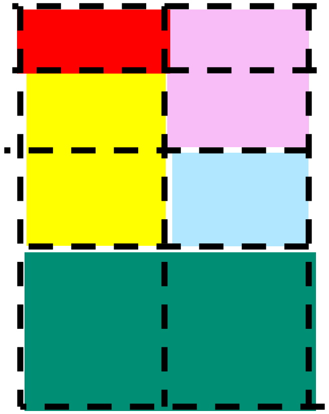
Vectorized Formula type CF (NEW in 2019 release)

- Integrates ranges into the 'Formula' type CF

Dependent Ranges for Vector CFs (New in 2020 Release)

A new keyword for constructing a range was added to facilitate the use of vectors in analytic functions. This new keyword references another range (i.e., #Range1) since it is entirely dependent on the other range for definition. As an example,

- A range was constructed for all COR cells of interest in the calculation
- it is required that the CV volume that is associated with a COR cell also be provided for each COR cell associated with that COR cell range and in the appropriate order.
- This new construction keyword generates that range automatically and guarantees a one-to-one correspondence.



- COR cells indicated by dashed lines
- CV volumes indicated by colors

```
CF_RANGE  CORCELLS2  CELLS  10
CONSTRUCT  1
   1 ALL
CF_RANGE  CVCELLS  CVOLUMES  20
CONSTRUCT  1
   1 #CORCELLS2
```

CORCELLS2	CVCELLS
Cell101	CV_GREEN
Cell102	CV_Yellow
Cell 103	CV_Yellow
Cell 104	CV_Red
Cell 201	CV_GREEN
Cell 202	CV_Blue
Cell 203	CV_Pink
Cell 204	CV_Pink

Improvements to Lower Head Model (New in 2020 Release)

Spheroidal Lower Head

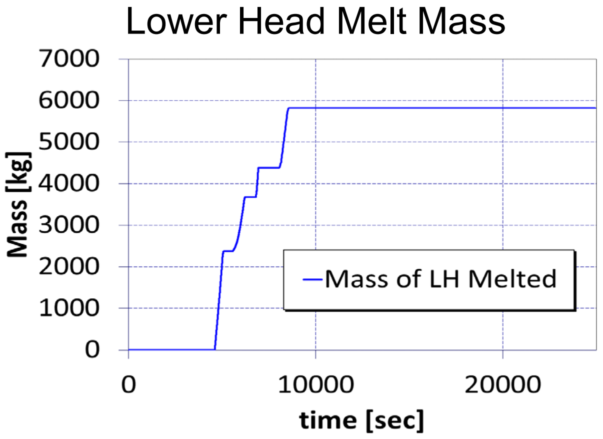
- Generalization of hemisphere model to allow for an oblated lower cap
- Two distance to specify: a horizontal radius and a vertical radius

Spheroidal Lower Head

```
!       RCOR  RVESS  ILHTRN  DZRV  DZLH  ILHTYP     ELLIPA  ELLIPC
COR_VP  1.8   2.2    RVESS   0.24  0.24  SPHEROIDAL 2.5     1.25
```

Melting Lower Head

- Debris relocating to the lower head contains sufficient decay heat to lead to melting of the interior surface of the lower head.
- Though MELCOR already accounts for the reduction in load-bearing material as the lower head melts, it does not allow the melted material to become part of the COR package where it
  - can affect heat transfer (focusing effect) of molten materials,
  - can be oxidized (contributing to hydrogen production),
  - can be transferred to the CAV package for MCCI.
- This code modification will source steel into the calculation along with the associated thermal energy where the COR package then takes control for further relocation



Limitations:

Currently only accounts for melting carbon steel

Mass, energy, and available volume sourced into the COR package

Currently only SS can receive the melting carbon steel

Mechanical Properties of Lower Head

SC 1602 – Vessel Steel Elastic Modulus Parameters

The elastic modulus of vessel steel is given as a function of temperature, T, by

$$E(T) = C1602(1)\cdot\left(\left\{1+[T/C1602(3)]^{C1602(4)}\right\}^{-1} - \left\{1+[C1602(2)/C1602(3)]^{C1602(4)}\right\}^{-1}\right)$$

(1) Leading multiplicative constant.
(default = 2.E11, units = Pa, equiv = none)
(2) Temperature at which elastic modulus vanishes.
(default = 1800.0, units = K, equiv = none)
(3) Temperature at which elastic modulus is approx halved.
(default = 900.0, units = K, equiv = none)
(4) Exponent of scaled temperatures.
(default = 6.0, units = none, equiv = none)

SC1603 – Vessel Steel Yield Stress Parameters

The yield stress of vessel steel is given as a function of temperature, T, by

$$\sigma_Y(T) = C1603(1)\cdot\left(\left\{1+[T/C1603(3)]^{C1603(4)}\right\}^{-1} - \left\{1+[C1603(2)/C1603(3)]^{C1603(4)}\right\}^{-1}\right)$$

(1) Leading multiplicative constant.
(default = 4.E8, units = Pa, equiv = none)
(2) Temperature at which yield stress vanishes.
(default = 1700.0, units = K, equiv = none)
(3) Temperature at which yield stress is approx halved.
(default = 900.0, units = K, equiv = none)
(4) Exponent of scaled temperatures.
(default = 6.0, units = none, equiv = none)

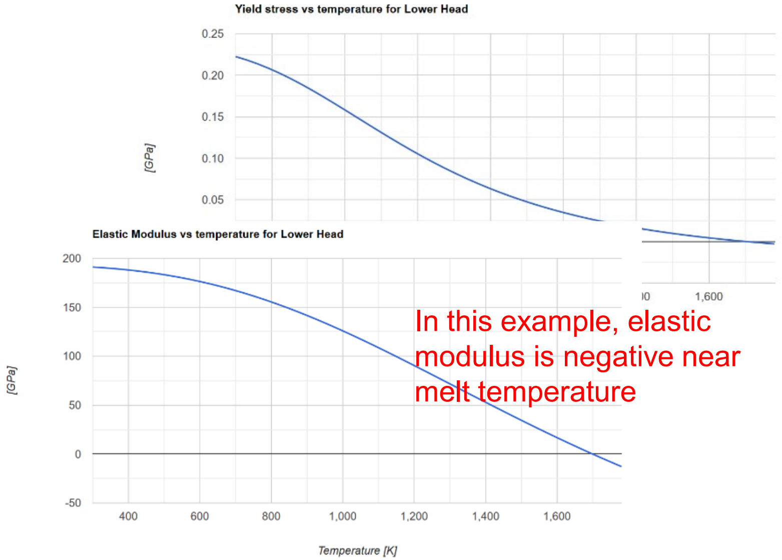
New in 2020 Release

- Lower Head Yield Stress & Elastic Modulus can now also be specified by a Tabular Function with optional fields on COR_LH

```
COR_LH    8   0  ElasticModulus YieldStress

 TF_ID 'ElasticModulus'    1.0 !(
 TF_TAB   2
                 1       273.15     0.15E9
                 2       1.0E+5     0.15E9
```

- Lower Head Yield Stress & Elastic Modulus plotted in HTML during MELGEN



In this example, elastic modulus is negative near melt temperature

Generalized Fission Product Release Model

A cumulative burst fission product release fraction is described by the following equation:

$$FB_{j,i} = a\_burst_j\left(c_0 + c_1 * T_i + c_2 * T_i^2 + c_3 * T_i^3\right)$$

Where

T_i is the fuel temperature that existed during the time interval Dt_i
c_0, c_1, c_2, c_3 are constant coefficients provided in user input
a_j is a constant class dependent coefficient provided in user input.

A cumulative diffusive fission product release fraction is described by the following equation:

$$FD_{j,i} = b\_diff_j\left(FD_{j,i-1} + \left(1 - FB_{j,i-1} - FD_{j,i-1}\right) \cdot \left[1 - e^{-kd_{j,i} \cdot \Delta t_i}\right]\right)$$

Where

$FD_{j,i}$ is the cumulative fraction of diffusive fission product released up to time t_i
B_diff_j is a constant class dependent coefficient provided in user input
$FD_{j,i-1}$ is the cumulative fraction of diffusive fission product released up to time t_{i-1}
FB_i is the cumulative fraction of burst fission product released up to time t_i
$\left[1 - e^{-kd_{j,i} \cdot \Delta t_i}\right]$ is the fractional release due to diffusion during the time interval Dt_i
$kd_{j,i}$ is the release rate coefficient for fission product class j calculated using the temperature, Ti, that existed during the time interval Dt_i

$$kd_{j,i} = A_j e^{-B_j/(RT_i)}$$

Where A_j and B_j are class dependent coefficients provided in user input.

The total cumulative fission product release fraction at time t_i for fission product j is determined by:

$$F_{j,i} = d\_total_j \cdot \left(FB_{j,i} + FD_{j,i}\right)$$

The cumulative release fraction cannot exceed the amount of fission product available

$$FB_{j,i} = FB_{j,i-1} \; and \; FD_{j,i} = FD_{j,i-1} when \; FD_{j,i} \geq 1.0$$

The derivative of the cumulative burst release with respect to time cannot be less than zero; if the temperature decreases, the cumulative burst release remains constant.

$$FB_{j,i} = FB_{j,i-1} \; when \; T_{i-} \geq T_{B-max} \; or \; T_{melting}$$

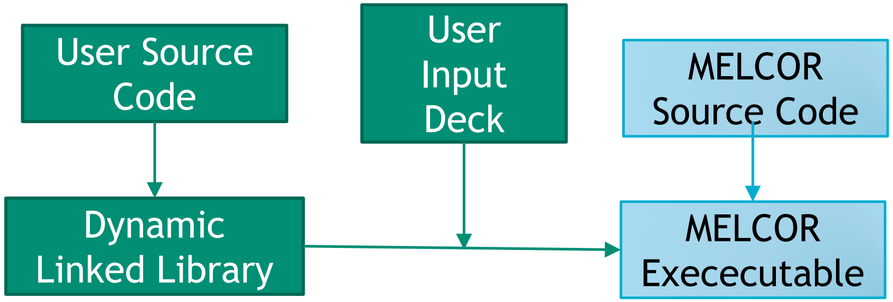
The cumulative burst release reaches its maximum when the fuel temperature reaches $T_{B\text{-max}}$ or $T_{melting}$ whichever is lower

$$FB_{j,i} = FB_{j,i} \; when \; T_i \geq T_{B-max} \; or T_{melting}$$

LWR and General Development

Generalized Fission Product Release Multiplier (New in 2020 release)

$$FD_{new}(k) = b_{diffusive}(FD_{old}(k) + (1 - FB_{new}(k) - FD_{old}(k)) * RF) \cdot \boldsymbol{GFPR_{mult}}$$



Objective:

Allow a user to define a multiplier on the diffusion release factor that can be coded in a very general way as an analytical control function contained within a dynamically linked library (DLL).

The development of a physical fission product release model was not performed, only the development of the infrastructure for passing and processing the new input, utilizing the results of the analytical control function, and passing the necessary data into the analytic control function.

MELCOR's previously existing analytic control function feature makes this possible, though modifications were needed to the code to use a control function as a multiplier as well as adjustments to the interface and exchange of data between MELCOR and the DLL.

Input for Fission product release

```
RN1_GREL 3
   1 CE 0.0 1.0  -
   2 I2  1.0 0.0  1.0       USER_I2
   3 CS -    -   D_TOTAL  USER_CS
```

Input for analytic control function:

```
CF_ID 'USER_CS' 885 ACF
CF_SAI 1.0 0.0 1.0
CF_VCF #CORCELLS2
CF_MSC 'CS MULTIPLIER' OLD
CF_ARG 10
      1 CVH-P(#CVCELLS) 1.0 0.0
      2 CVH-PPART(#CVCELLS,H2O-VAP) 1.0 0.0
      3 CVH-PPART(#CVCELLS,H2) 1.0 0.0
      4 COR-M(#CORCELLS2,ZRO2)  1.0 0.0  !ZRO2 and
      ZR passed as arguments but add as many
      materials as needed
      5 COR-M(#CORCELLS2,ZR)  1.0 0.0
      6 COR-CELLTEMP(#CORCELLS2) 1.0 0.0
      7 EXEC-TIME 1.0  0.0
      8 EXEC-DT  1.0  0.0
      9 EXEC-CYCLE  1.0  0.0
      10 COR-RELD(#CORCELLS2,CS)  1.0  0.0
```

Input to define Ranges

```
CF_RANGE  CORCELLS2  CELLS  10
CONSTRUCT  1
  1 ALL
CF_RANGE  CVCELLS  CVOLUMES  20
CONSTRUCT  1
  1 #CORCELLS2
```

LWR and General Development

Material Property Development
(New in 2020 Release)

User-defined Materials

- Default material properties can be templated onto new materials
- Can be defined for COR with extra input
  - Emissivity, Viscosity, Thermal expansion coefficient, Oxidation behavior

- COR User-Defined Material

```
MP_ID      NewZirc  COR-USER-METAL  NUZR
MP_BHVR    Zircaloy  METAL   OXIDATION-MODEL
EXEMPT
MP_BETMU   1.65E-5   3313.0  1.076E-3
MP_COREMIS CF  ‘NewEmissivity’  0.0001  0.9999
```

- Initialize Mass in component

```
COR_NMAT 1 ! IA    IR   IC   USRM1   USRM2   USRM3
USRM4
         1   ALL   ALL CL   0.0     0.0     64.2    0.0
```

- Associate with metal pool

```
COR_LAY 1 ! LAYMAT  MPLAY
        1   NUZR    UPPER   ! Associate with MP2
```

LWR and General Development

Generalized Oxidation Model
(New in 2020 Release)

Historically, MELCOR had a specific set of oxidizable material:

- Zirconium, Stainless-steel, Graphite, B_4C, Aluminum
- Now extended to use the user-defined materials (UDMs)

General Oxidation Model makes use of the new UDMs to create a new oxidizable material.

- Define a reactant core material, COR-USER-METAL, and its oxide product, COR-USER-OXIDE.User permitted to fully specify material properties
- May use templating or be wholly user-defined

```
MP_ID FeCrAl COR-USER-METAL UFCA
MP_BHVR    Itself  METAL   OXIDATION-MODEL
EXEMPT
MP_BETMU   3.1e-5 7.7 3313. 1.076e-3
MP_COREMIS linear - 0.0001 0.9999
0.042003702 0.0003474
MP_PRTF 4 ! NPAR PROPERTY DEFAULT/TF/CF(may
be only for THC)
        1 ENH FCA-IntEn
        2 CPS FCA-SpHeat
        3 THC FCA-Conduct TF
        4 RHO FCA-Density

MP_ID FeCrAl-Oxide COR-USER-OXIDE UFCAO
MP_BHVR ITSELF
MP_PRC 5180.0 1901.0 687463.0 193.4102395
MP_COREMIS linear - 0.0 1.0 0.7 0.0
MP_BETMU 3.1e-5 7.7 3313. 1.076e-3
MP_PRTF 4 ! NPAR PROPERTY DEFAULT/TF/CF(may
be only for THC)
        1 ENH FCAO-IntEn
        2 CPS FCAO-SpHeat
        3 THC FCAO-Conduct TF
        4 RHO FCAO-Density
```

ATF – Oxidation Simple Reaction Assumptions

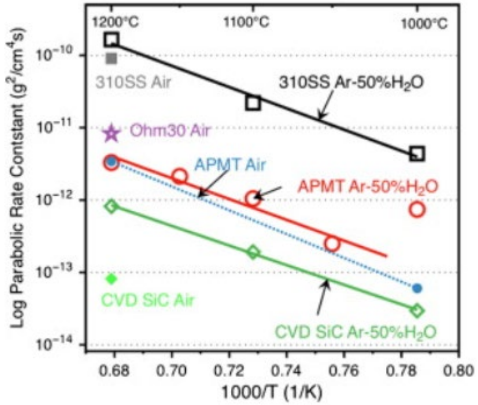
While it is recognized that an alumina layer initially forms, MELCOR materials do not presently track oxidation of constituents individually.

Stoichiometric reactions of the following equations are simply applied producing an assumed FeCrAl-Oxide, similar to the default stainless-steel treatment:

$$\mathrm{Fe} + \frac{4}{3}\mathrm{H_2O} \rightarrow \frac{1}{3}\mathrm{Fe_3O_4} + \frac{4}{3}\mathrm{H_2} + \mathrm{Q_{ox}}$$

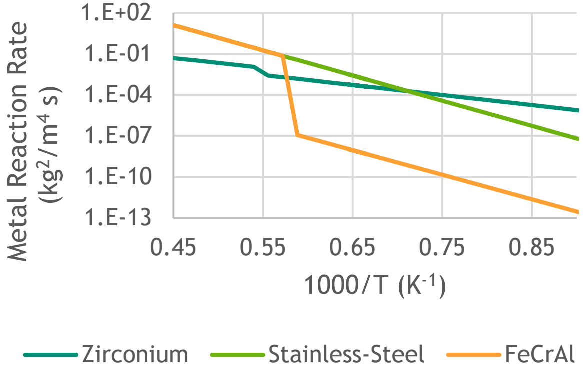
$$\mathrm{Cr} + \frac{3}{2}\mathrm{H_2O} \rightarrow \frac{1}{2}\mathrm{Cr_2O_3} + \frac{3}{2}\mathrm{H_2} + \mathrm{Q_{ox}}$$

$$\mathrm{Al} + \frac{3}{2}\mathrm{H_2O} \rightarrow \frac{1}{2}\mathrm{Al_2O_3} + \frac{3}{2}\mathrm{H_2} + \mathrm{Q_{ox}}$$



Reaction Rates (based on prior work by INL/ORNL)

- Pre-Breakaway
  - Reaction rates apply data from Pint, et.al
- Post-breakaway
  - Rates are taken from Stainless-steel as a surrogate until additional data are available
- Breakaway
  - Based on ORNL experiments, the breakaway transition was set to 1425-1450C by default
    - available as sensitivity coefficients



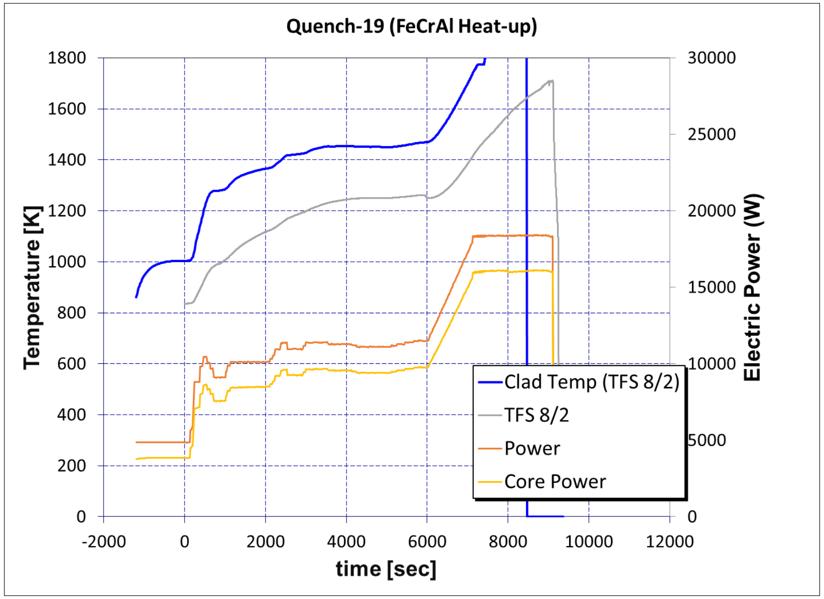
Merrill, B.J., Bragg-Sitton, S.M., Humrickhouse, P.W., Modification of MELCOR for Severe Accident Analysis of Candidate Accident Tolerant Cladding Materials, Nuclear Engineering and Design 315 170-178, 2017

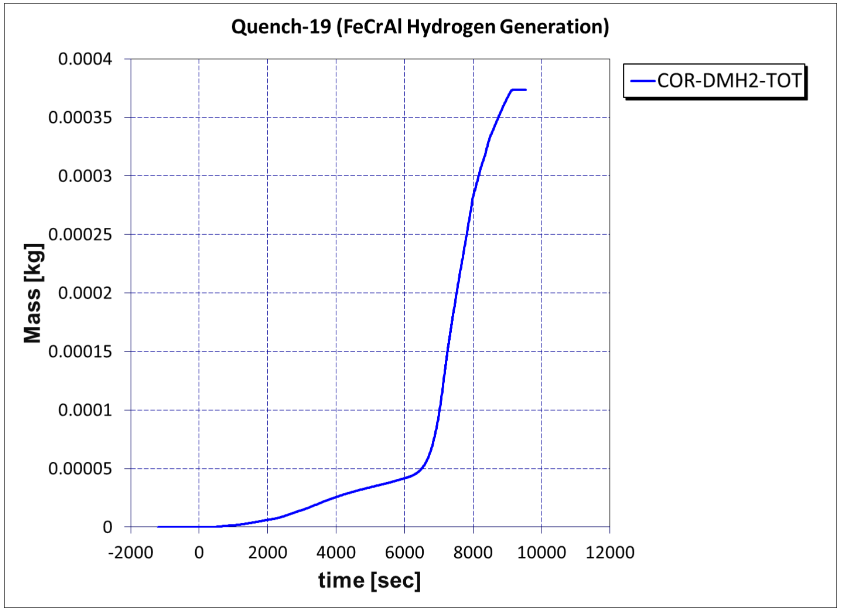
K.R. Robb, H. Howell, and L.J. Ott, “Design and Analysis of Oxidation Tests to Inform FeCrAl ATF Severe Accident Models”, Oak Ridge National Laboratory, ORNL/SPR-2018/893 (July 2018).

B.A. Pint, et al., “High Temperature Oxidation of Fuel Cladding Candidate Materials in Steam-Hydrogen Environments,” Journal of Nuclear Materials 440, pp. 420-427, 2013.

ATF Development (New in 2020 Release)

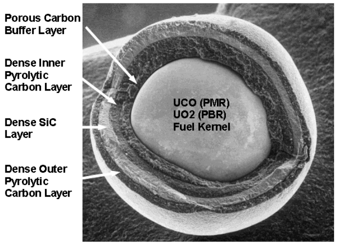
- Adaption of Generalized Oxidation Model for FeCrAl cladding
- Validation against Quench 15/19





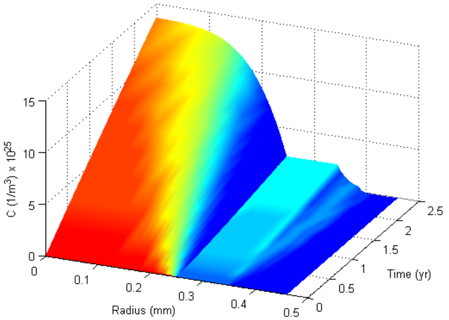
High Temp Gas-Cooled Reactors

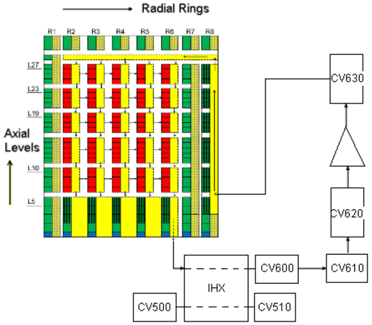
- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- New COR components for PBR and PMR designs
- Core conduction
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure
- Graphite dust transport
  - Turbulent deposition,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

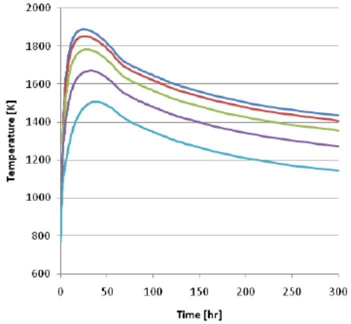

Porous Carbon Buffer Layer
Dense Inner Pyrolytic Carbon Layer
Dense SiC Layer
Dense Outer Pyrolytic Carbon Layer
UCO (PMR)
UO2 (PBR)
Fuel Kernel

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

$$m = 1 \ (cylindrical)$$
$$m = 2 \ (spherical)$$



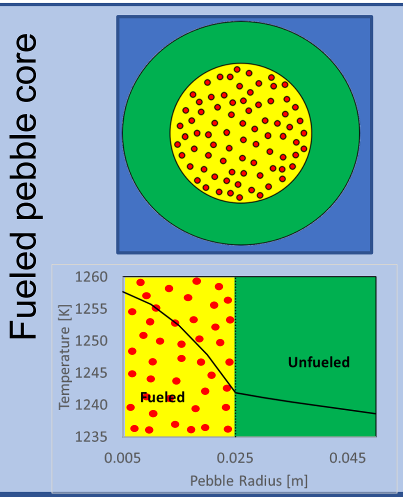


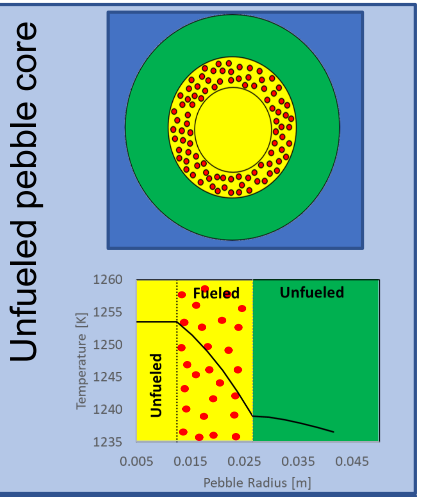


HTGR Components

Pebble Bed Reactor (PBR) Fuel/Matrix Components

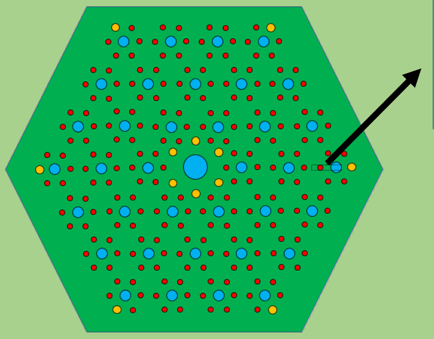
- Fueled part of pebble
- Unfueled shell is modeled as separate component (Matrix)
- Fuel radial temperature profile for sphere
  - Provides peak and surface pebble temperature
  - Modified for unfueled central core

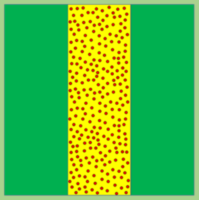


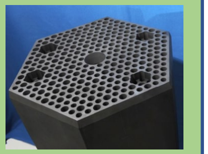


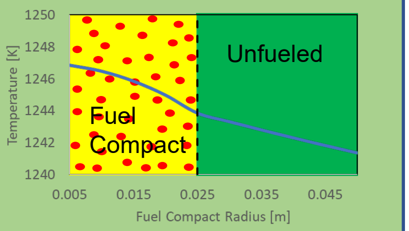
Prismatic Modular Reactor (PMR) Fuel/Matrix Components

- More "rod-like" geometry
- Fuel compacts represented as fuel component
- Part of hex block associated with a fuel channel is matrix component
- Fuel radial temperature profile for cylinder







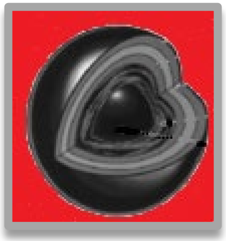


Legend

- 🟥 TRISO
- 🟨 GRAPHITE

Fuel (FU)

- 🟩 GRAPHITE — Matrix (MX)
- 🟦 Fluid B/C



TRISO (FU)

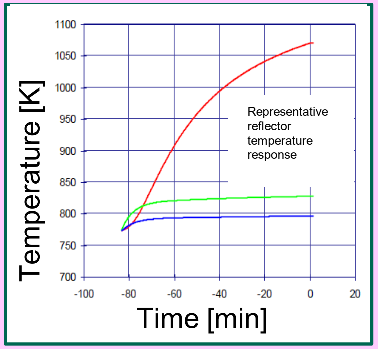
Sub-component model for zonal diffusion of radionuclides through TRISO particle

High Temperature Gas Reactors

Transient/Accident Solution Methodology

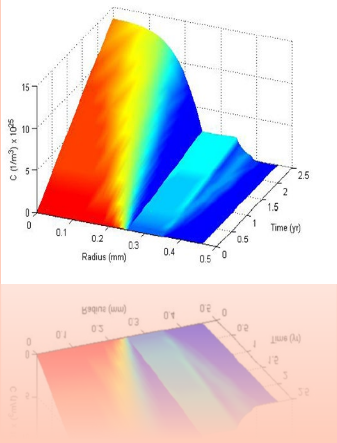
Stage 0:
Normal Operation
Establish thermal state

- *Time constant in HTGR graphite structures is very large*
  - *>24 hours for reflector to reach steady state*
- *Reduce heat capacities for structures to reach steady state thermal conditions.*
- *Reset heat capacities after steady state is achieved.*



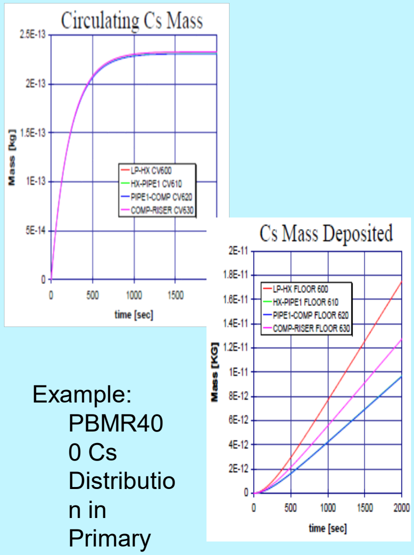
Stage 1:
Normal Operation
Diffusion Calculation

Establish steady state distribution of radionuclides <u>in TRISO particles (and matrix)</u> for normal operation



Stage 2:
Normal Operation
Transport
Calculation

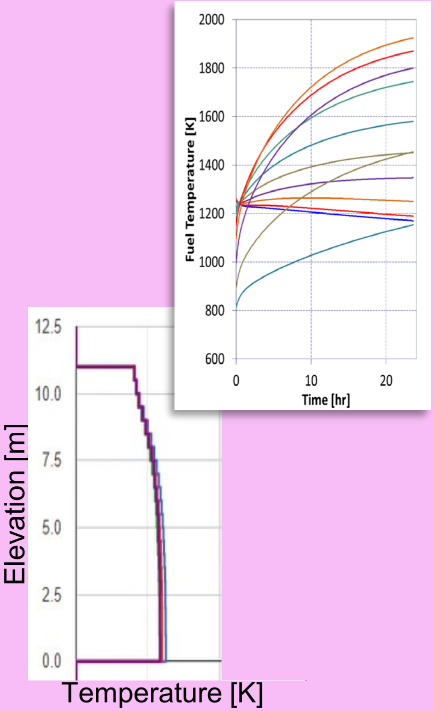
Calculate steady state distribution of radionuclides <u>throughout system</u> during normal operation (deposition on surfaces, convection through flow paths, etc.)



Example:
PBMR400 Cs Distribution in Primary System

Stage 3:
Accident
Diffusion & Transport
calculation

Calculate accident progression and radionuclide release



All steps performed in one run with data passed transparently between stages

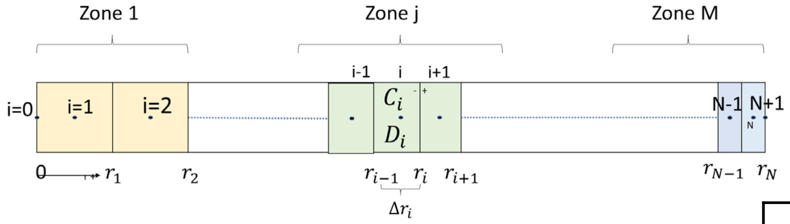
High Temperature Gas Reactors

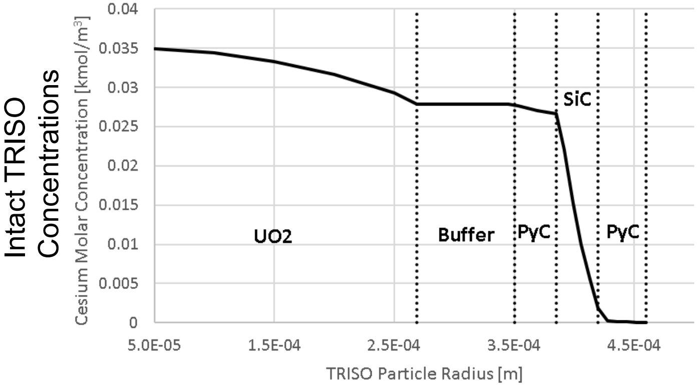
HTGR Radionuclide Diffusion Release Model

Intact TRISO Particles

- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

$$\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \boldsymbol{D}\frac{\partial C}{\partial r}\right) - \lambda C + \beta \quad D(T) = D_0 e^{-\frac{Q}{RT}}$$





Diffusivity Data

Radio-nuclide	UO_2	UCO	PyC	Porous Carbon	SiC	Matrix Graphite	TRISO Overall
Ag	Some	unknown	Some	unknown	Extensive	Some	Extensive
Cs	Some	unknown	Some	unknown	Extensive	Some	Some
I	Some	unknown	Some	unknown	Some	unknown	unknown
Kr	Some	unknown	Some	unknown	unknown	Some	Some
Sr	Some	unknown	Some	unknown	Extensive	Some	Some
Xe	Some	unknown	Some	unknown	Some	Some	unknown

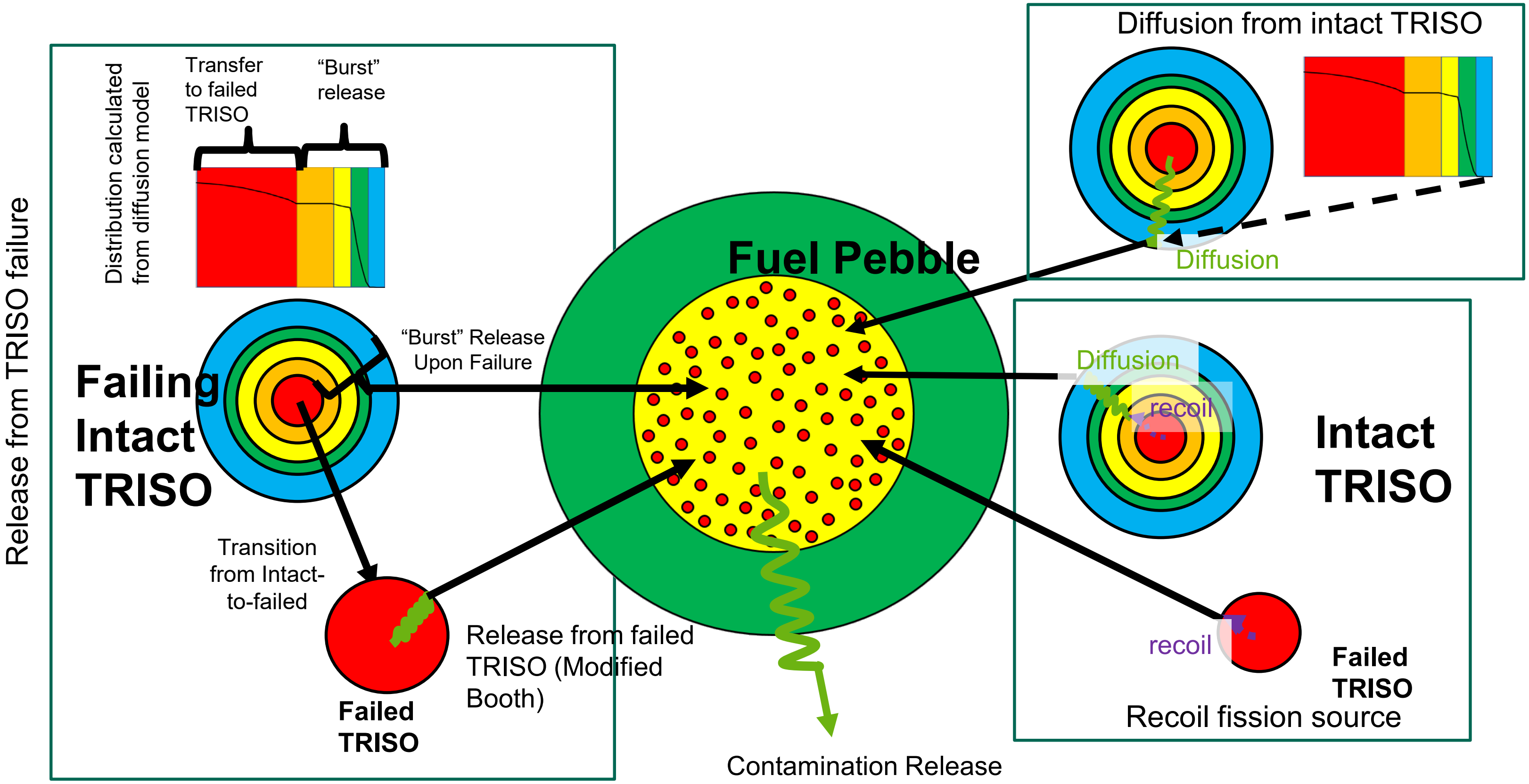
Availability

	FP Species							
	Kr		Cs		Sr		Ag	
Layer	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m2/s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6-8	209000.0	2.2E-3	488000.0	6.75E-9	165000.0
Buffer	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0
PyC	2.9E-8	291000.0	6.3E-8	222000.0	2.3E-6	197000.0	5.3E-9	154000.0
SiC	3.7E+1	657000.0	7.2E-14	125000.0	1.25E-9	205000.0	3.6E-9	215000.0
Matrix Carbon	6.0E-6	0.0	3.6E-4	189000.0	1.0E-2	303000.0	1.6E00	258000.0
Structural Carbon	6.0E-6	0.0	1.7E-6	149000.0	1.7E-2	268000.0	1.6E00	258000.0

Data used [IAEA TECDOC-0978]

HTGR Radionuclide Release Models

- Recent failures – particles failing within latest time-step (burst release, diffusion release in time-step)
- Previous failures – particles failing on a previous time-step (time history of diffusion release)


Release from TRISO failure
Distribution calculated from diffusion model
Transfer to failed TRISO
"Burst" release
Failing Intact TRISO
"Burst" Release Upon Failure
Transition from Intact-to-failed
Failed TRISO
Release from failed TRISO (Modified Booth)
Fuel Pebble
Contamination Release
Diffusion from intact TRISO
Diffusion
Diffusion
recoil
Intact TRISO
recoil
Failed TRISO
Recoil fission source

MELCOR HTGR DEMONSTRATION CALCULATION (PBMR-400 DLOFC)

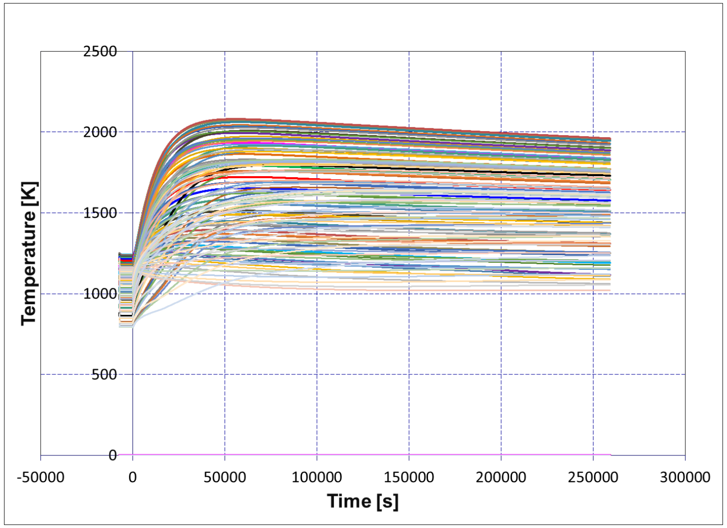
Similar to previous HTGR demonstrations, but now includes more detail

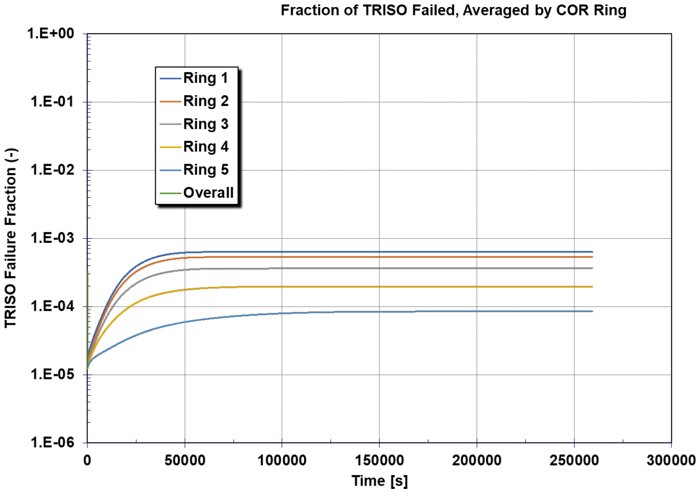
- RN1 elements (in their default class grouping) have mass and specific decay heat tables (SCALE/ORIGEN)
- Reactor building and expanded secondary-side modeling
- Example usage of new CF arguments (including vectorized CFs and with range objects)

Run sequence:

- Pre-performed thermal steady-state (COR component and HS temperatures establish steady values)
- Steady-state diffusion calculation at -7200 s problem time (executed within a time-step)
- Steady-state transport calculation until 0 s problem time (pseudo-time)
- Transient diffusion/transport and DLOFC commences from 0 s problem time
- Foreshortened TEND of ? is long enough for TFU to rise, turn over, and decline

Demonstrates diffusional release model performance and illustrates fuel failure modeling capability





MELCOR/CONTAIN-LMR Implementation

Implement sodium as replacement to the working fluid for a MELCOR calculation

- Implement properties & Equations Of State (EOS) from the fusion safety database
  - Na (tpfna), FLiBe (tpffi), Pb-Li (tpflipb), He (tpfhe), N2(tpfn2)
- Implement properties & EOS based on SIMMER-III

Implementation and Validation of:

- Sodium spray fires
  - Based on NACOM spray model from BNL
  - Input requirement: fall height, mean diameter and source
    - Droplet acceleration model
  - Internal droplet size distribution (11 bins) from Nukiyama-Tanasama correlation
  - Reactions considered:
    - (S1) $2\,Na + {}^{1}/_{2}\,O_2 \rightarrow Na_2O$,
    - (S2) $2\,Na + O_2 \rightarrow Na_2O_2$
- Sodium pool fires
  - 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

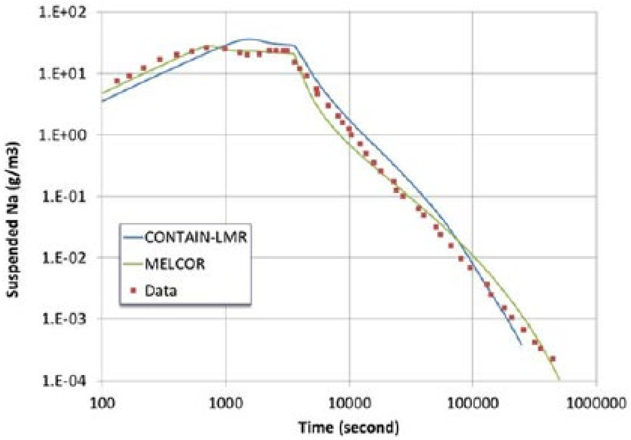


Figure 33. Suspended Na Aerosol Mass - AB1

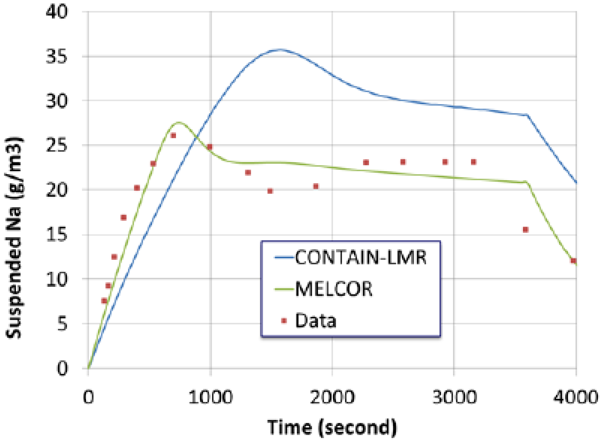


Figure 34. Suspended Na Aerosol Mass-AB1

Atmospheric Chemistry New in 2019 Code Release

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:

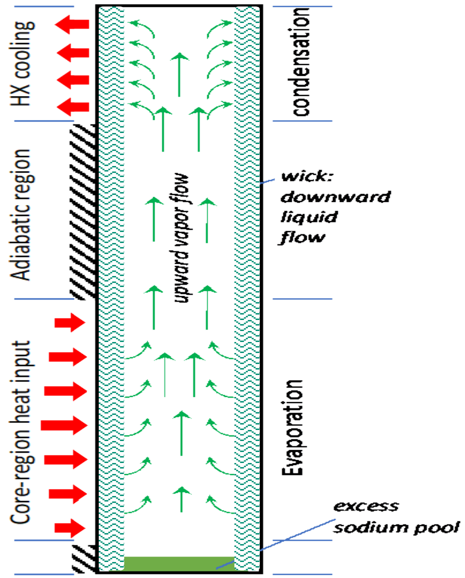
- In the order listed above
- By location of reactions
  - Atmosphere(g), aerosol, surfaces (i.e., HS)

Outputs

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

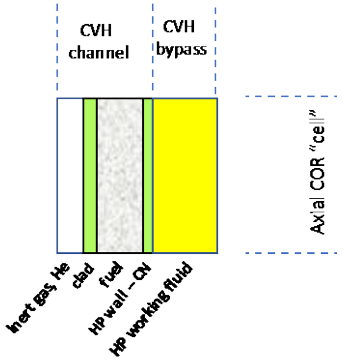
MELCOR Heat Pipe Reactor Modeling

HPs replace conventional convective heat transfer between the fuel and coolant channel with the energy transfer from the fuel to the evaporative region of the HP. Heat rejection from the HP model at the condensation interface is transferred to the CVH package.

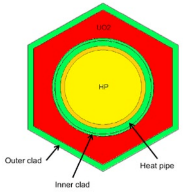


Distinct wall and working fluid region nodalization. MELCOR accommodates HP models of different fidelity through a common interface.

- Model 1: working fluid region modeled as high thermal conductivity material
- Model 2 (new in 2020 release): thermodynamic equilibrium approximation of working fluid (sodium or potassium EOS). P, T and liq/vap fraction evolve in time. Sonic, capillary and boiling limits enforced.
- If needed, higher fidelity models straight-forward to implement to interface.



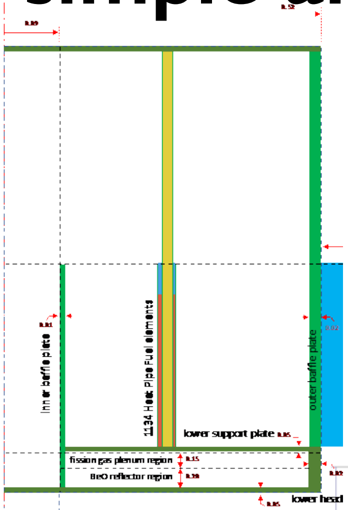
MELCOR heat transfer paths enable radial (lateral) heat transfer in the core among multiple HP regions and to other MELCOR structures.



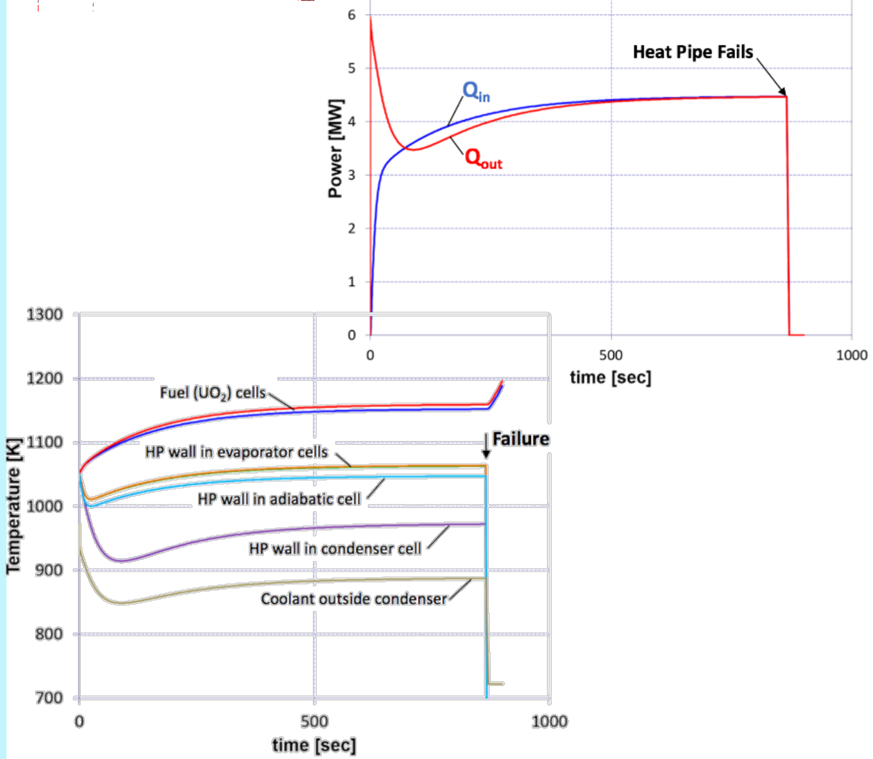
- Thermal resistance network approximation across heterogeneous domain

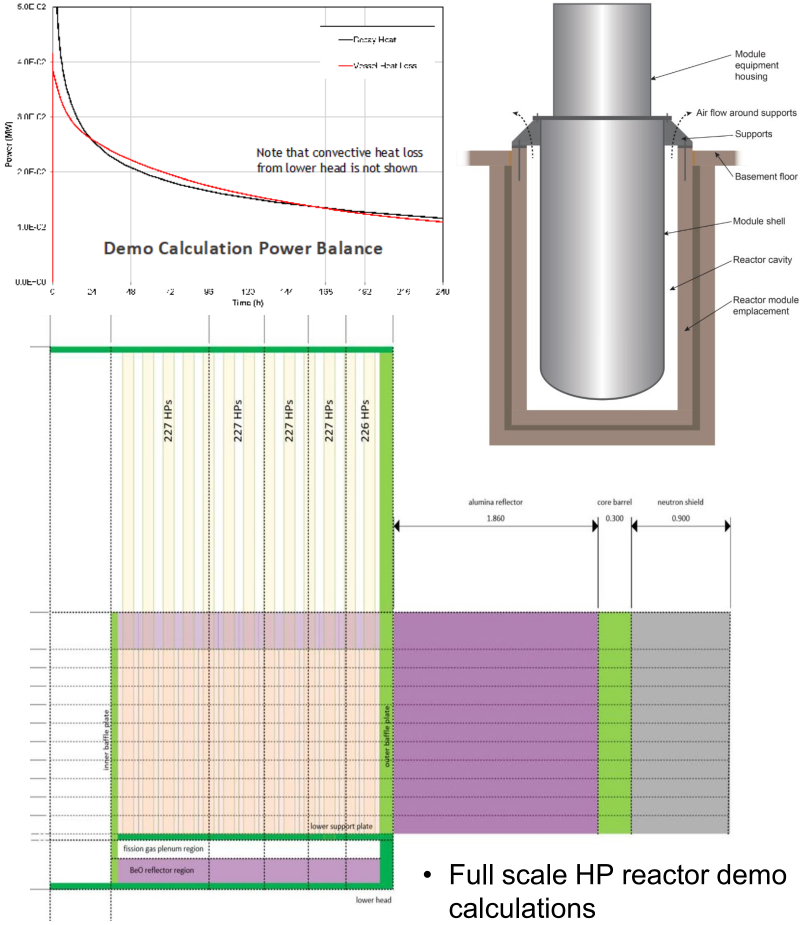
At failure, HP materials and regions transition to COR and CVH modeling.

HP Models being exercised/tested on simple and full plant decks



- 1 representative HP
- 5 axial levels, 2 radial rings
- Contrived simple transient with control function triggered HP failure





- Full scale HP reactor demo calculations

Aerosol Radiation Model New in 2019 Code Release

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.

Molten Salt Reactor

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

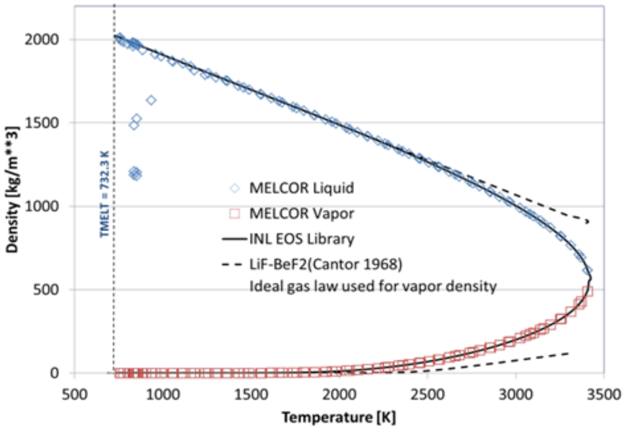
Two reactor types envisioned

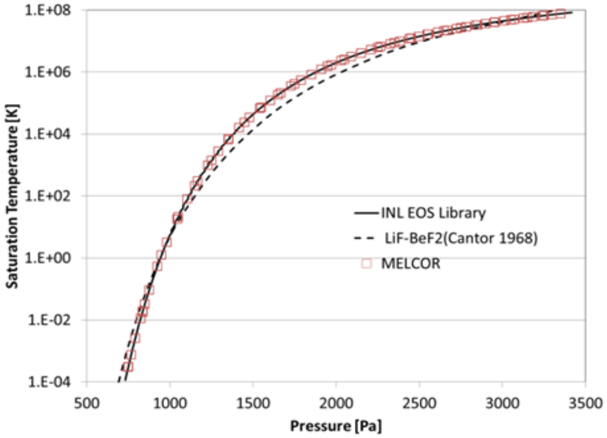
- Fixed fuel geometry
  - TRISO fuel models (current capability)
- Liquid fuel geometry
  - MELCOR CVH/RN package can model flow of coolant and advection of internal heat source with minimal changes (current capability)
  - Framework for fission thermal power generation without COR package (current capability)
    - Control volumes defined as “vessel” type or “loop” type
    - Specify axial/radial power profile shape and magnitude (over “vessel” type CV’s)
    - Specify flow paths constituting transitions between vessel and loop
    - Preserve decay heat deposition capabilities (CVH/RN1 tracks decay heat from aerosol/vapor already)
  - COR package representation no longer applicable but structures can be represented by HS package (current capability)
  - Calculation of neutronics kinetics for flowing fuel (under development)

Radionuclide Transport

Molten salt fission product release models (under development)

Thermochemistry modeling using Thermochemica (under development)



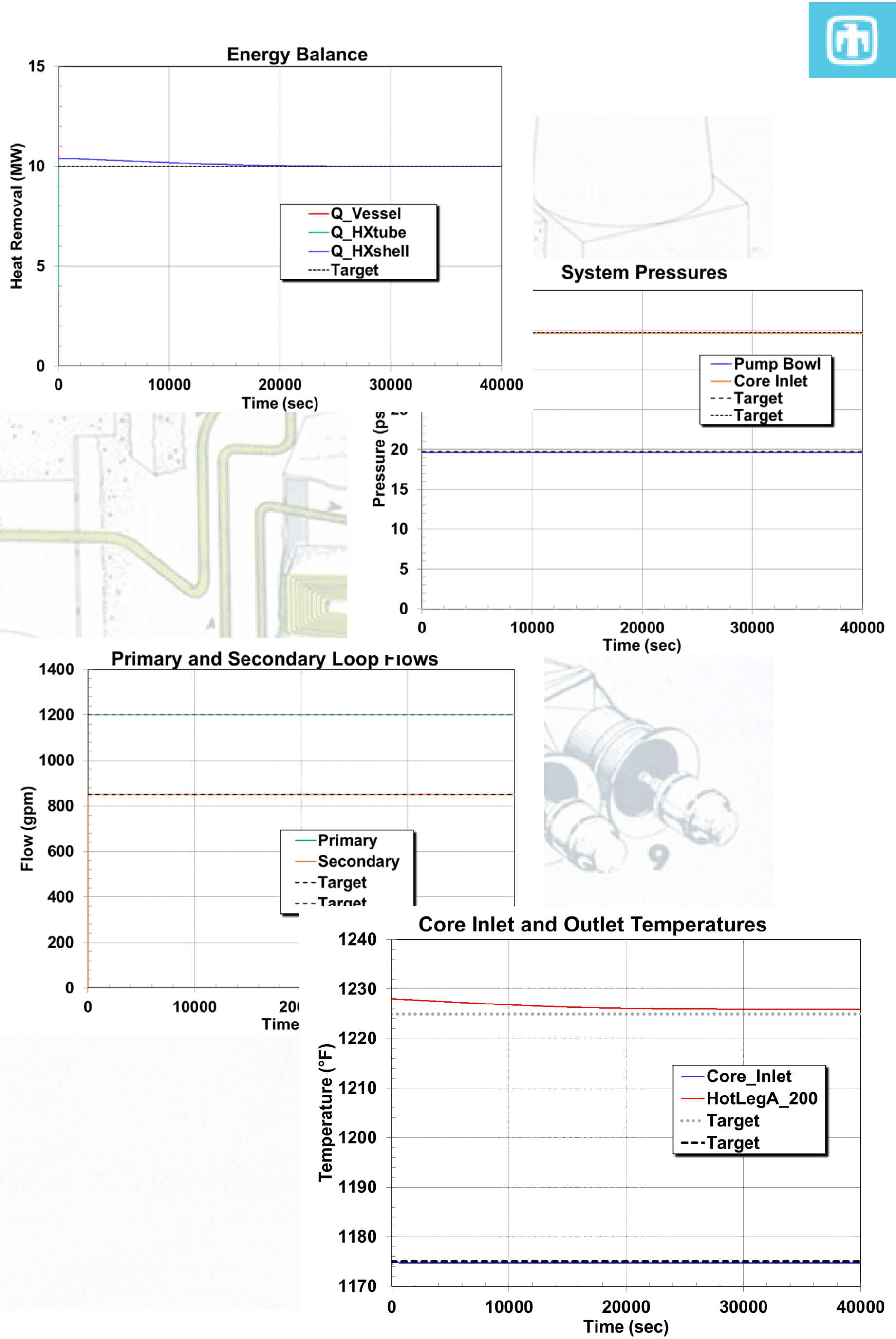


MSRE MELCOR V2.2 Model 2019 Benchmark

Steady state operating conditions

The MELCOR MSRE model includes the following features

- **One-dimensional core**
  - 8 control volumes (2-dimensional enhancement straight-forward)
  - Graphite blocks
  - Connected diversion & drain tank
  - Core-bypass leakage flow
- **Primary system recirculation loop**
  - Schedule 40 INOR-8 piping – a high Nickel alloy (16% Ni, 7% Mo, 5% Cr, 0.05% Fe, 0.05% C)
- **Fuel pump and pump bowl** (aka pressurizer)
  - Connected overflow tank
  - Pump spray with He gas offtake (Xe & Kr removal)
- **Mechanistic horizontal U-tube heat exchanger**
  - 2-dimensional primary system shell-side
  - Secondary coolant flow in U-tube



Circulating Fuel Point Kinetics Model (Under Development)

Code circulating fuel point kinetics models including any requisite reactivity feedback models

$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \bar{\beta}}{\Lambda}\right) P(t) + \sum_{i=1}^{6} \lambda_i C_i^C + S_0$$

$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P(t) - \left(\lambda_i + {}^{1}\!/_{\tau_C}\right) C_i^C(t) + \left(\frac{V_L}{\tau_L V_C}\right) C_i^L(t - \tau_L), \qquad for\ i = 1 \ldots 6$$

$$\frac{dC_i^L(t)}{dt} = \left(\frac{V_C}{\tau_C V_L}\right) C_i^C(t) - \left(\lambda_i + {}^{1}\!/_{\tau_L}\right) C_i^L(t), \qquad for\ i = 1 \ldots 6$$

$$\bar{\beta} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum_{i=1}^{6} \lambda_i C_i^L(t)$$

Where:

$P(t)$= Thermal power due to fission

C_i^C= delayed neutron precursor group i inventory/concentration in-core

C_i^L= delayed neutron precursor group i inventory/concentration ex-core (in loop)

S_0= Thermal power generation rate due to neutron source

$\rho(t) = \frac{k-1}{k}$= Reactivity for k the effective multiplication factor

$\bar{\beta}$= Effective delayed neutron fraction

β= Delayed neutron fraction (static, in absence of drift effects)

$\Lambda = {}^{1}\!/_{\nu V \Sigma_f}$= Neutron generation time

$\tau_{C/L} = {}^{M_{C/L}}\!/_{\dot{m}}$ = Residence time of precursors (core, loop, respectively)

$V_{C/L}$= Fluid volume (core, loop, respectively)

λ_i= Decay constant of delayed neutron precursor group i

Molten Salt Reactor Accident Fission Product Transport (Under Development)

Attractive safety features

1. Molten Salt is an unpressurized coolant.
2. Fluoride salts have broad liquid range (e.g. FLiBe, 459 C – 1430 C).
3. Actinides and most fission products are soluble in molten salt.

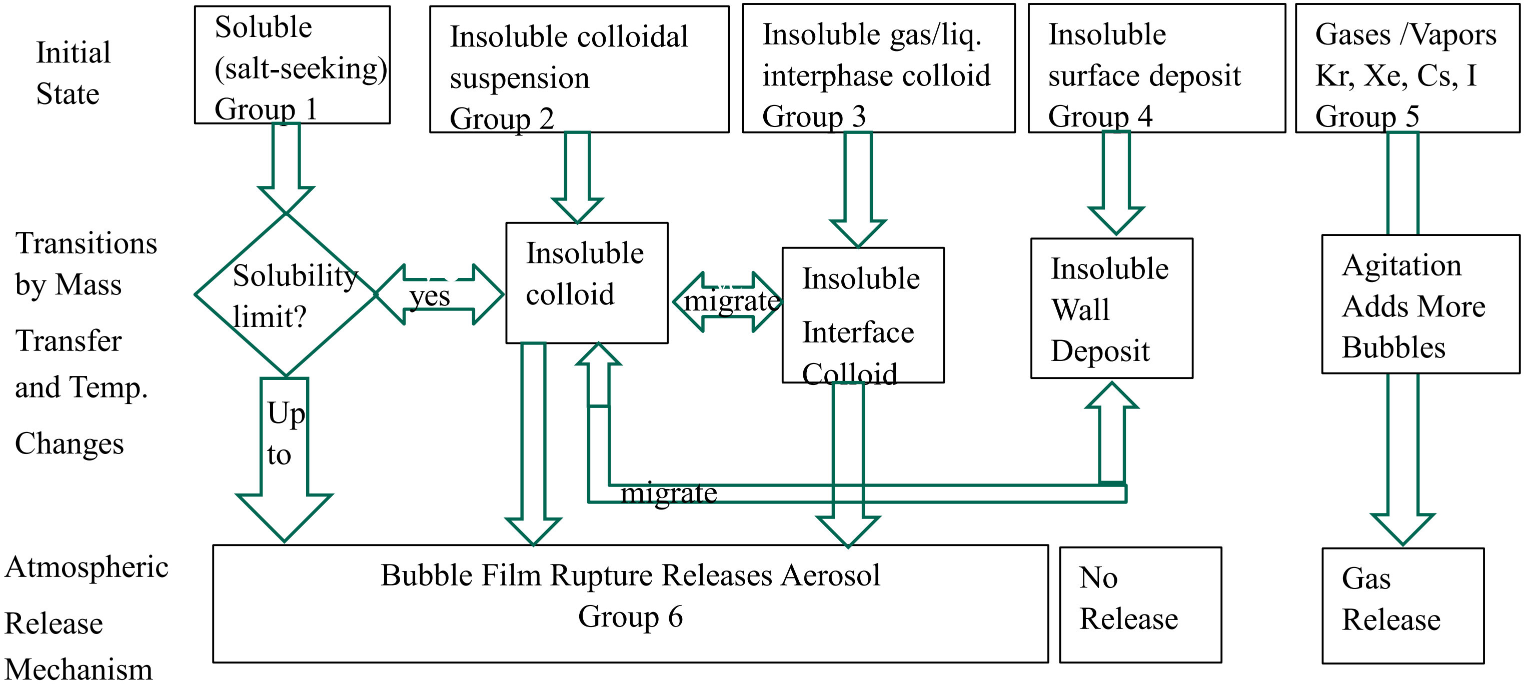
Solubility ≠ Immobility

Release processes

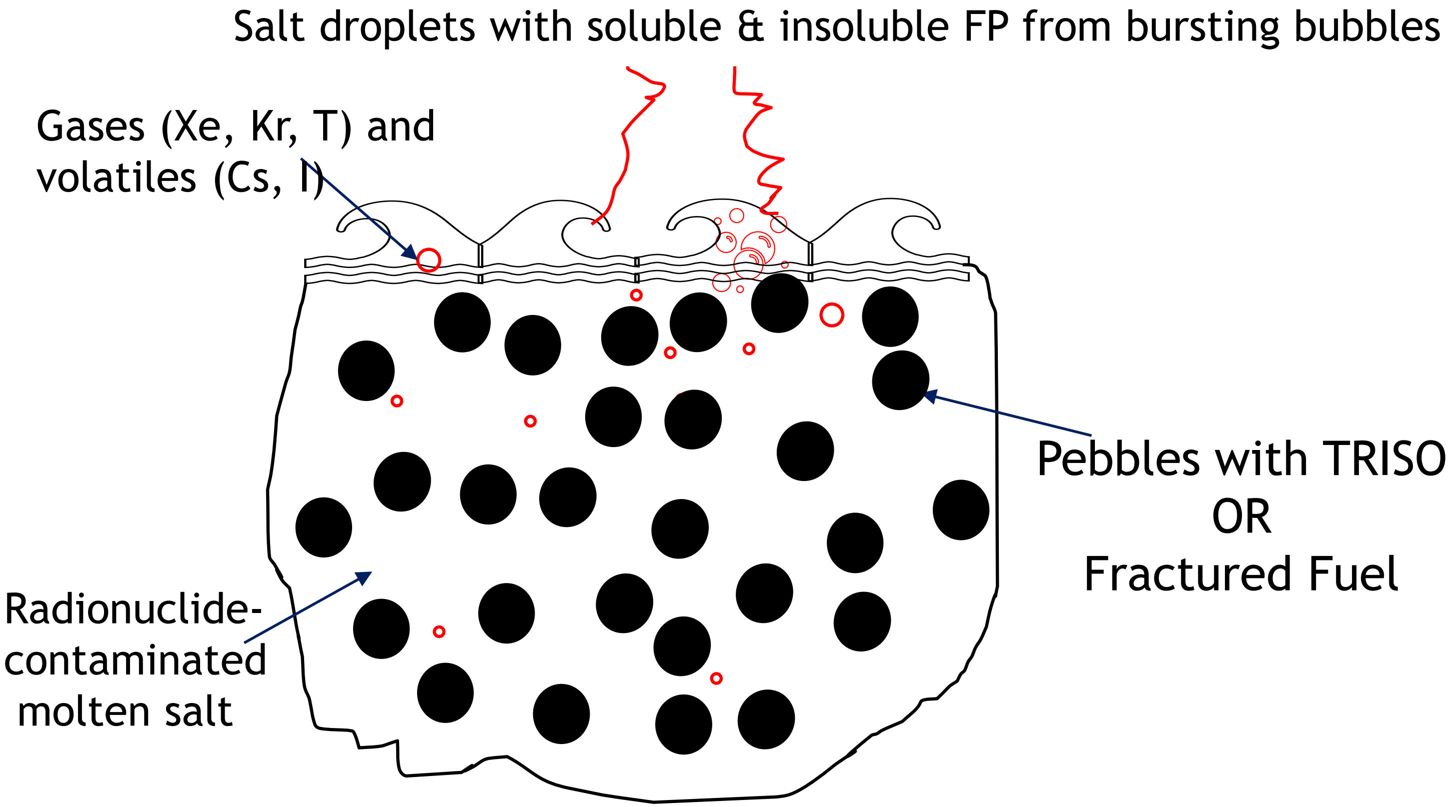
1. MELCOR provides the conditions and species released into salt, and MSM determines how much of that is released to the atmosphere as gas and aerosol particles.
2. Fission products tracked in six areas as observed in MSRE at ORNL.
3. Gases (e.g. Kr, Xe) bubble up through molten salt.
4. Volatile species (e.g. Cs, I) vaporize into bubbles and released at salt top surface, and later condense into particles.
5. Bursting bubbles create aerosol particles of salt droplets containing soluble and insoluble radionuclides.

Schematic of MSM (Molten Salt Model)

Radionuclides grouped into 6 areas as found in the Molten Salt Reactor Experiments at ORNL


Initial State
Soluble (salt-seeking) Group 1
Insoluble colloidal suspension Group 2
Insoluble gas/liq. interphase colloid Group 3
Insoluble surface deposit Group 4
Gases /Vapors Kr, Xe, Cs, I Group 5
Transitions by Mass Transfer and Temp. Changes
Solubility limit?
yes
Insoluble colloid
migrate
Insoluble Interface Colloid
Insoluble Wall Deposit
Agitation Adds More Bubbles
Up to
migrate
Atmospheric Release Mechanism
Bubble Film Rupture Releases Aerosol Group 6
No Release
Gas Release

Schematic of Phenomena (accident not expected to be quiescent)

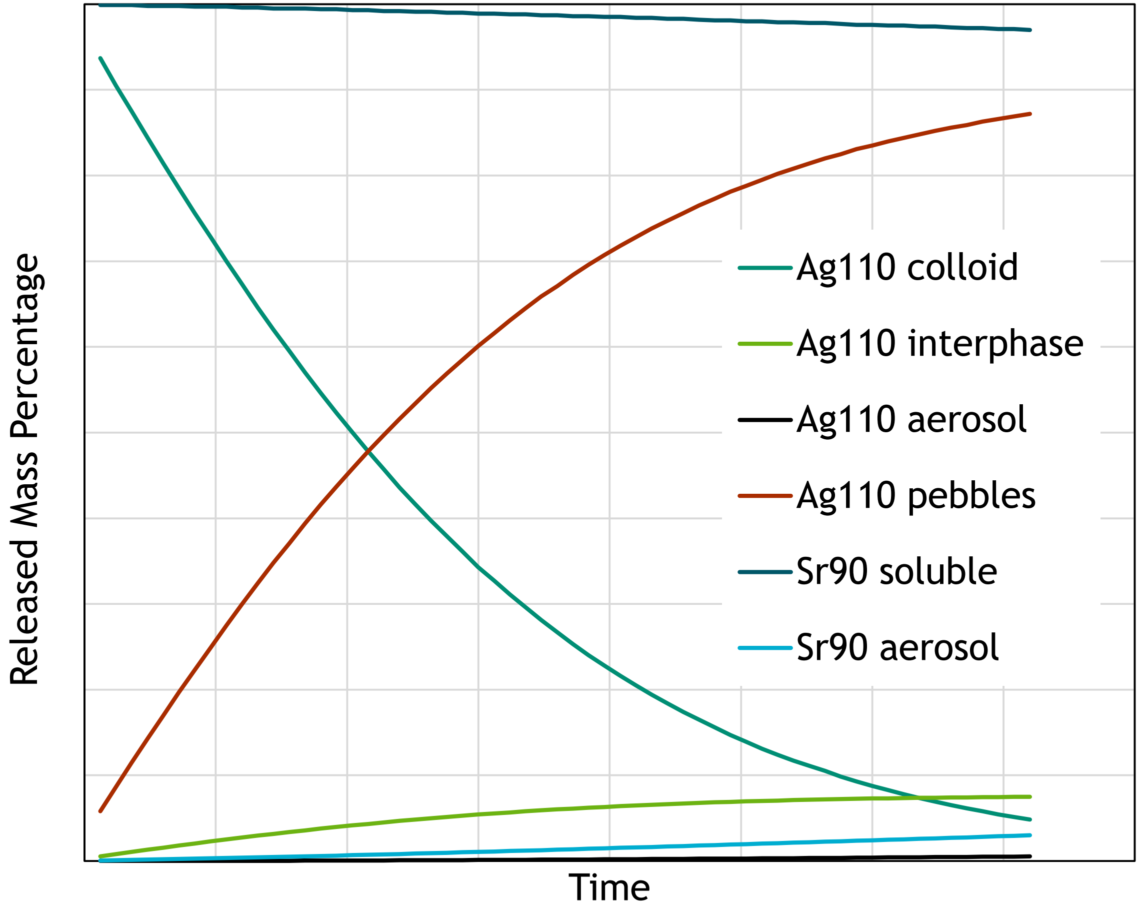

Salt droplets with soluble & insoluble FP from bursting bubbles

Gases (Xe, Kr, T) and volatiles (Cs, I)

Pebbles with TRISO
OR
Fractured Fuel

Radionuclide-contaminated molten salt

Example of soluble and insoluble FP transport calculation



Soluble Sr90 mostly retained in salt, but some aerosolized

Insoluble Ag110 mostly deposits on pebbles with some aerosolized

Radionuclide Transfer between Pool & Atmosphere New in 2019 Code Release

By default, 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.

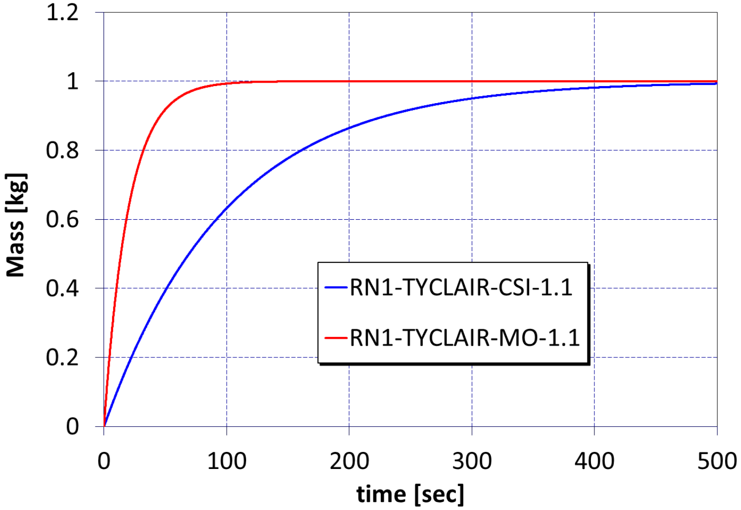
- User specifies table (for each CV) of radionuclides and CFs for calculating RN transfer

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

- 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.

Non-LWR Demonstrations Calculations

Objectives

Develop an understanding of non-LWR beyond-design-basis-accident behavior

- Provide insights for enhancing source-term regulatory guidance
- Provide NRC staff with an understanding of non-LWR beyond-design-basis-accident behavior
  - Identify key accident characteristics influencing source terms
  - Highlight important uncertainties influencing accident progression and source terms

Demonstrate MELCOR for non-LWR beyond-design-basis accidents

- Distribution of non-LWR input models with MELCOR executable
- Shake down the MELCOR modeling and identify missing models or data needs

Non-LWR Demonstrations Calculations

Demo Case Selection

- Demonstrate/exercise breadth of non-LWR physics modeled by MELCOR
- Consider NRC priority relative to timing of licensing submittal
- Utilize non-proprietary designs
- Build on existing decks where possible

Demo Cases

PBMR-400

- Pebble bed HTGR
  - Maturity of plant input deck
  - Modeling of pebble bed supports subsequent modeling of FHR accident progression and source term

Megapower Heat Pipe Reactor

- Heat pipe reactor
  - 1st priority due to imminent submittal of Oklo application
  - Insights into accident progression and source term will support NRC review of Oklo

Flouride Salt Cooled High Temperature Reactor

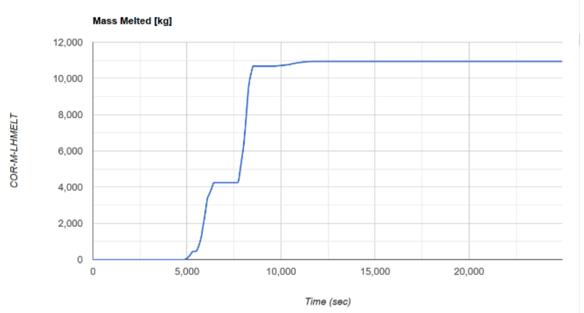
- Pebble bed FHR
  - Builds on work to evaluate pebble bed HTGR
  - Additional modeling capability evaluated related to molten salt working fluid

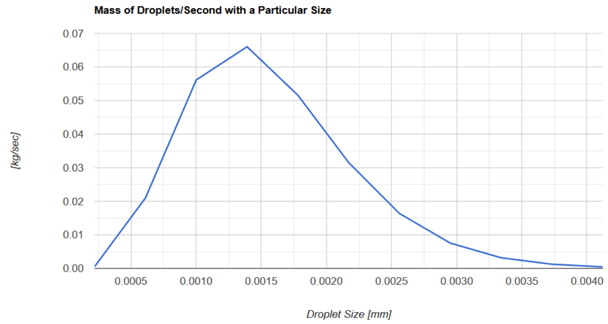
Additions to HTML in MELCOR 2020 Release

New plots generated at each write to text output

- Mass of melt from lower head
- Lower head energy balance
- Polar plot of temperature profile in lower head
- Heat of mixture (eutectics) added to energy balance
- Added plots for sodium spray fire
  - Number (or mass) of droplet of a particular size
  - Droplet velocity with time (by size)
  - Mass fraction burned with time(by droplet size)
  - Droplet temperature with time (by size)
  - Droplet diameter with time (by size)

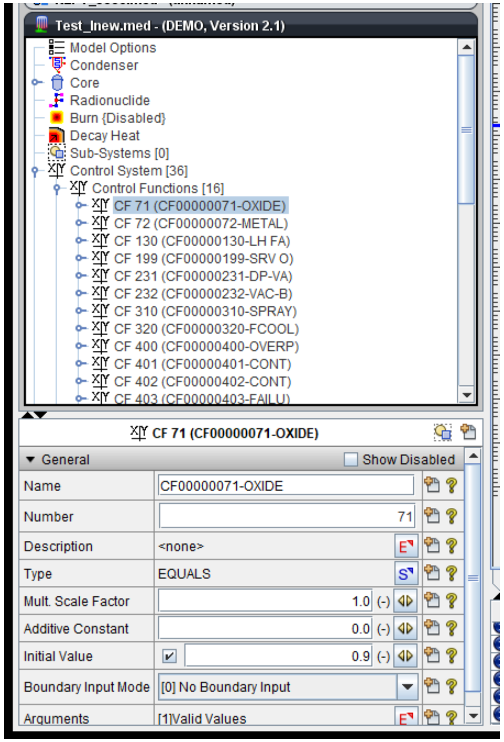
Animation of lower head temperatures





SNAP Upgrade

- MELCOR 2.2 plugin update
  - Support input for new models
    - Vector Control Functions
    - LHC Package
    - Radiation enclosure model
    - New MCCI Models
    - Support for named comment blocks
    - Support for Variable input.
  - Most features have been implemented
  - Post-processing Improvements?



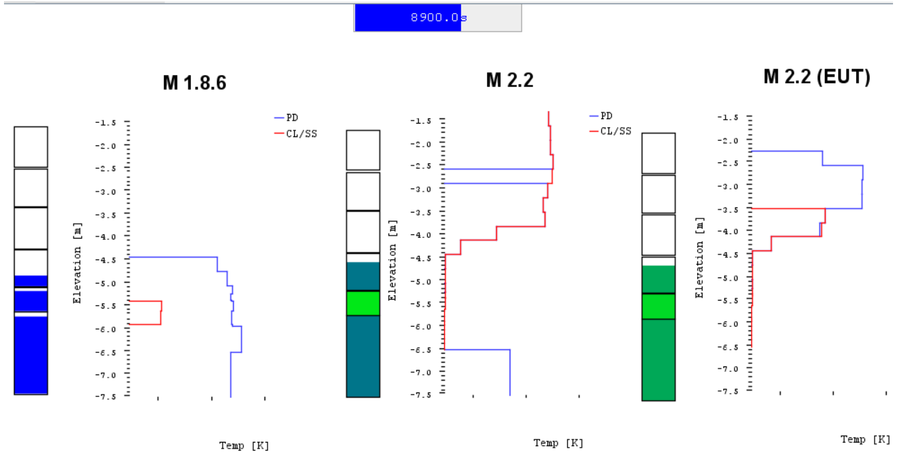
Test_Inew.med - (DEMO, Version 2.1)

- Model Options
- Condenser
- Core
- Radionuclide
- Burn {Disabled}
- Decay Heat
- Sub-Systems [0]
- Control System [36]
  - Control Functions [16]
    - CF 71 (CF00000071-OXIDE)
    - CF 72 (CF00000072-METAL)
    - CF 130 (CF00000130-LH FA)
    - CF 199 (CF00000199-SRV O)
    - CF 231 (CF00000231-DP-VA)
    - CF 232 (CF00000232-VAC-B)
    - CF 310 (CF00000310-SPRAY)
    - CF 320 (CF00000320-FCOOL)
    - CF 400 (CF00000400-OVERP)
    - CF 401 (CF00000401-CONT)
    - CF 402 (CF00000402-CONT)
    - CF 403 (CF00000403-FAILU)

CF 71 (CF00000071-OXIDE)

General ☐ Show Disabled

Name	CF00000071-OXIDE
Number	71
Description	<none>
Type	EQUALS
Mult. Scale Factor	1.0 (-)
Additive Constant	0.0 (-)
Initial Value	☑ 0.9 (-)
Boundary Input Mode	[0] No Boundary Input
Arguments	[1]Valid Values



Proprietary and Markings Records
New in MELCOR 2019 Release

A new capability was added permitting the use of a pre-generated marking message for all text output, diagnostic, and html files as well as the binary plot file. The record is a global data record and will be documented in subsequent releases within the Users' Guide Exec Package as follows:

PROPRIETARY – Prepends a Proprietary Statement Marking to the Output Files

Optional

If this record is present, the following statement will appear in all diagnostic files, text output files and html files:

```
/////////////////////////////PROPRIETARY/////////////////////////////
  The input deck used in this calculation is marked as proprietary. Consequently,
  output files are also assumed to contain information that should be regarded
  as proprietary.
/////////////////////////////PROPRIETARY/////////////////////////////
```

Example

PROPRIETARY

MARKINGS – Prepends a Generic Statement Marking to the Output Files

Optional

If this record is present, a general statement will appear in all diagnostic files, text output files and html files. The user will specify the identification of the marking with a keyword on the first input field.

MARKING

A user specifies a character string to be used to create a general marking statement. The statement is provided below, and "Marking" indicates the fields of the statement which will be replaced by the user specified string.

(type = character*256, default = Proprietary)

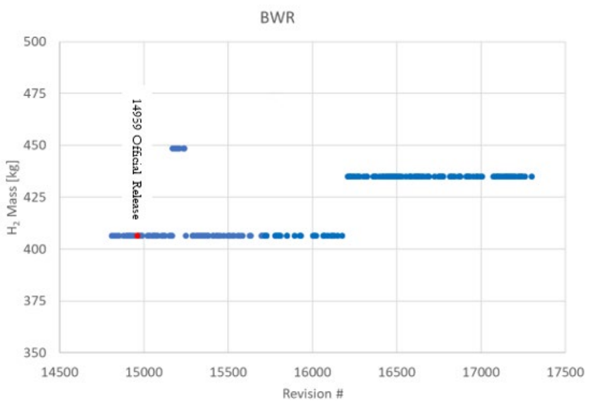
```
///////////////////////////////////MARKING///////////////////////////////
  The input deck used in this calculation is marked as General Access.  Consequently,
  output files are also assumed to contain information that should be regarded
  as General Access.
///////////////////////////////////MARKING///////////////////////////////
```

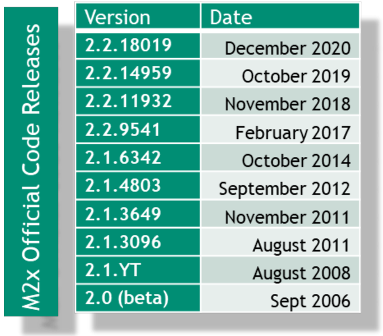
Example

MARKINGS "General Access"

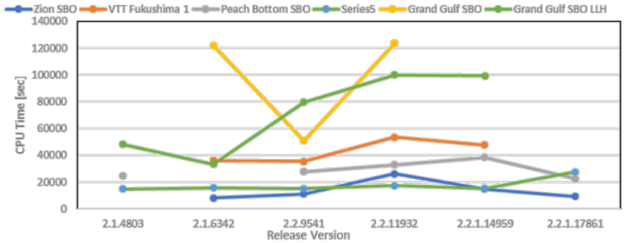
Code Releases

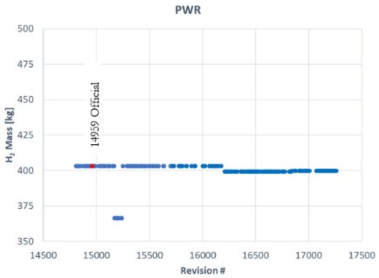
- V 2.2.18019
  - Released December 23, 2020
  - QL, UG, and RM released January 11, 2021
  - Some improvements in performance and small changes in hydrogen and other metrics.
- V 2.3.xxxxx
  - To be released July/August timeframe
  - To include updated assessments report




M2x Official Code Releases

Version	Date
2.2.18019	December 2020
2.2.14959	October 2019
2.2.11932	November 2018
2.2.9541	February 2017
2.1.6342	October 2014
2.1.4803	September 2012
2.1.3649	November 2011
2.1.3096	August 2011
2.1.YT	August 2008
2.0 (beta)	Sept 2006





MELCOR Modernization Plan (5 years)

Modernization

- Improvements in code structure designed to strengthen
  - Performance – shorter run times and more robust calculation
  - Numerics – reduced numerical variance, improved accuracy, and improved characterization of uncertainty
  - Capability – Removal of limitations that hinder modeling of some effects
  - Maintainability – more extensible framework to allow code to adapt to new reactor designs., flexibility in future code/model development
- Maintain currently validated physics
  - Objective is not to add new physics models
  - This is not a re-write of the code (still FORTRAN though incorporating new FORTRAN features and possible other languages in new modules/routines)
- Incremental benefits in the existing code base

Five Year Plan

- Generalized Numerical Solution Engine Module
- MELCOR hydrodynamic modeling
- MELCOR In-Vessel Core Damage Progression
- Ex-Vessel Damage Progression
- Fission Product Release and Transport Modeling
- Rationalization of Current MELCOR Code Base with Modernized MELCOR Code Base / Finalization of the Modernized Code

Generalized Numerical Solution Methods

Implementation of a generalized numerical solution framework that can integrate a range of numerical algorithms required by MELCOR to advance the state of the plant to the next point in simulation time.

- Stateless, Testable, Defined interface

This does not apply to a specific area of phenomenological modeling.

The functionality implemented during this phase enables the modernization of the MELCOR code architecture, separating numerical solution functionality from functionality that implements the representation of physical models in software.

MELCOR hydrodynamic modeling

Reformulation of the hydrodynamic equation set and numerical solution scheme to utilize an enhanced solver. This will enhance overall robustness of the numerical solution, adopting state-of-the-art numerical solution methods developed under Task 1.

This effort is necessary to enhance the capabilities of the hydrodynamics numerical solution strategy to reflect new strategies developed to handle known issues where the hydrodynamic equations are particularly difficult to solve. This task involves modifications to the control volume hydrodynamics and flow path packages (containment vent header/FL) within MELCOR (other packages interfacing with these two packages will also be modified as needed).

MELCOR In-Vessel Core Damage Progression

Generalization of the code architecture to simplify the addition of new components, improve numerics, and restructure the lower head model to improve treatment of melting and interactions with the lower head.

COR component objects

The COR database will be restructured to allow creation of component objects with properties such as oxidation, hold-up, number of surfaces in contact with CVH, etc. to allow templating for new components. This should allow more flexibility for users in defining COR component attributes for specific design needs.

Candling Model

Currently MELCOR will move melting material down a component surface (candle) in a single time step. Such modeling overlooks the oxidation that may occur during the transition and would affects the heat transfer.

Material interactions

Enhancements will enable the code to more adequately reflect new types of material interactions likely to occur in advanced reactors and for ATF, and more generally treat fission product speciation.

Lower Head Structure

- The lower head model will be rewritten to improve the numerical solution of the equations to better account for melting at the interior boundary.

Ex-Vessel Damage Progression

Code Numerics

- The numerical solution and physical modeling functionality will be separated. Introduction of a state-of-the-art numerical solution methodology will be performed.

Generalized Geometry

- A key component of this effort also involves generalization of how ex-vessel geometries (i.e., the cavity beneath reactor vessels) are represented. This will facilitate significantly enhanced functionality in support of greater severe accident modeling realism, critical to evaluating efforts to credit insights from Fukushima Daiichi accident.

Replace Vanessa with a generalized Gibbs free energy minimizer

Fission Product Release and Transport Modeling

Improvements to numerics

- The numerical solution and physical modeling functionality will be separated. Introduction of a state-of-the-art numerical solution methodology will be performed. A result of this effort will be a modernization of the underlying radionuclide transport equations (in the MAEROS model).

Improvements to RN class representations

- Generalized to facilitate more flexible addition of new classes.
- The ability to clone radionuclide classes from an existing class.
- Generalization of chemical interactions to enable modeling radionuclides undergoing chemical reactions and transformations between classes.

MELCOR Modernization Work: Current Progress

Refactorization of CVH package interfaces to pass all CVH package Control Volume and Flow Path state variable data through calling list.

- Eliminate all access through Fortran “include” statements.
- Subroutines become “stateless”.
- Enables any development code that meets interface requirements to be “swapped in” for testing purposes. Required for software “unit testing”.
- *Consistent with modern software development “best practices”.*
- *Affected nearly every CVH package subroutine as well as many other package subs.*

Revised and additional metrics optionally available for developers to better determine solution convergence and “goodness”.

- Calculation of scaled residual vector enables check of solution goodness after the convergence criteria based on relative change is satisfied.
- Scaled convergence metrics. For example, check on $\alpha_{j,\varphi}^{n} v_{j,\varphi}^{n}$ (the scaled quantity of interest) instead of $v_{j,\varphi}^{n}$ (unscaled velocity).
- Eliminates false positives (solution actually bad) and false negatives (solution actually good) that lead to code failures and/or code thrashing.
- *Consistent with modern scientific computing “best practices”.*

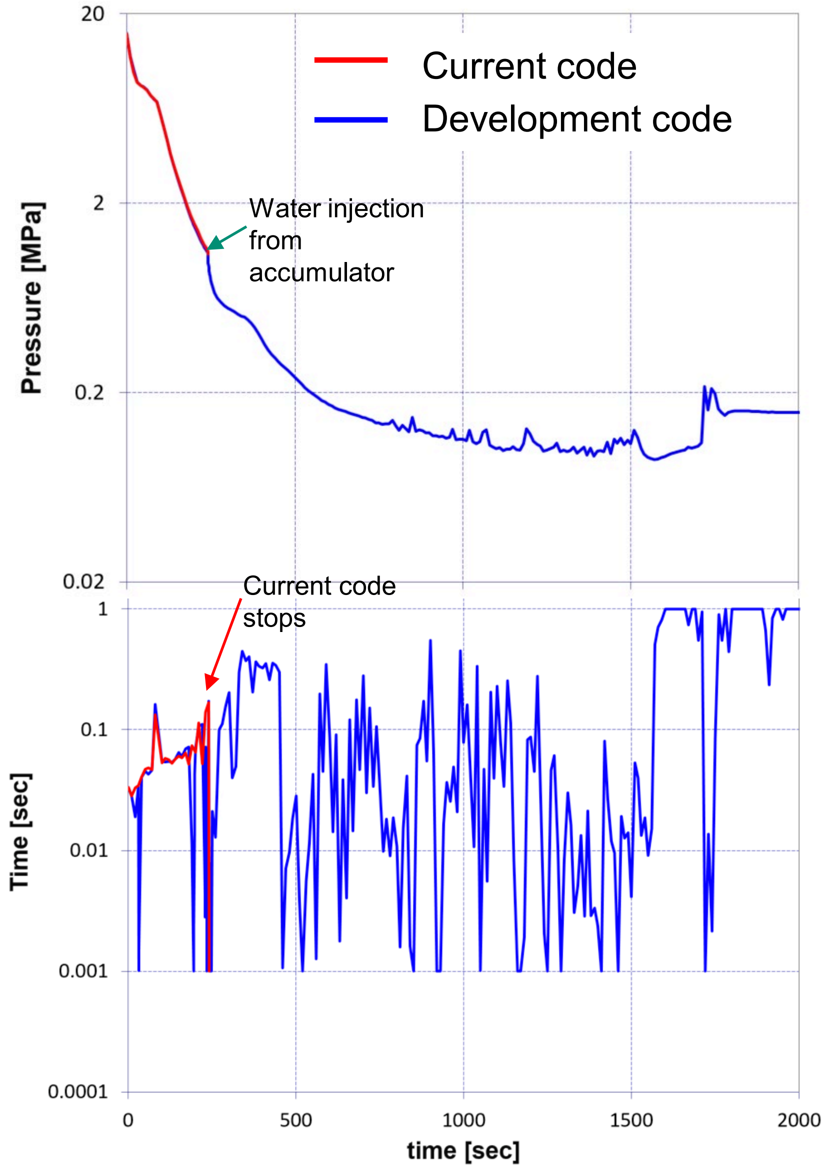
These are largely “under the hood” changes not directly seen by users but should greatly benefit ongoing and future code development and code maintenance.

- Has helped facilitate exploration of revised/modified CVH equations for low pressure flow conditions (e.g. cold water injection after blow down, spent fuel pool analysis)

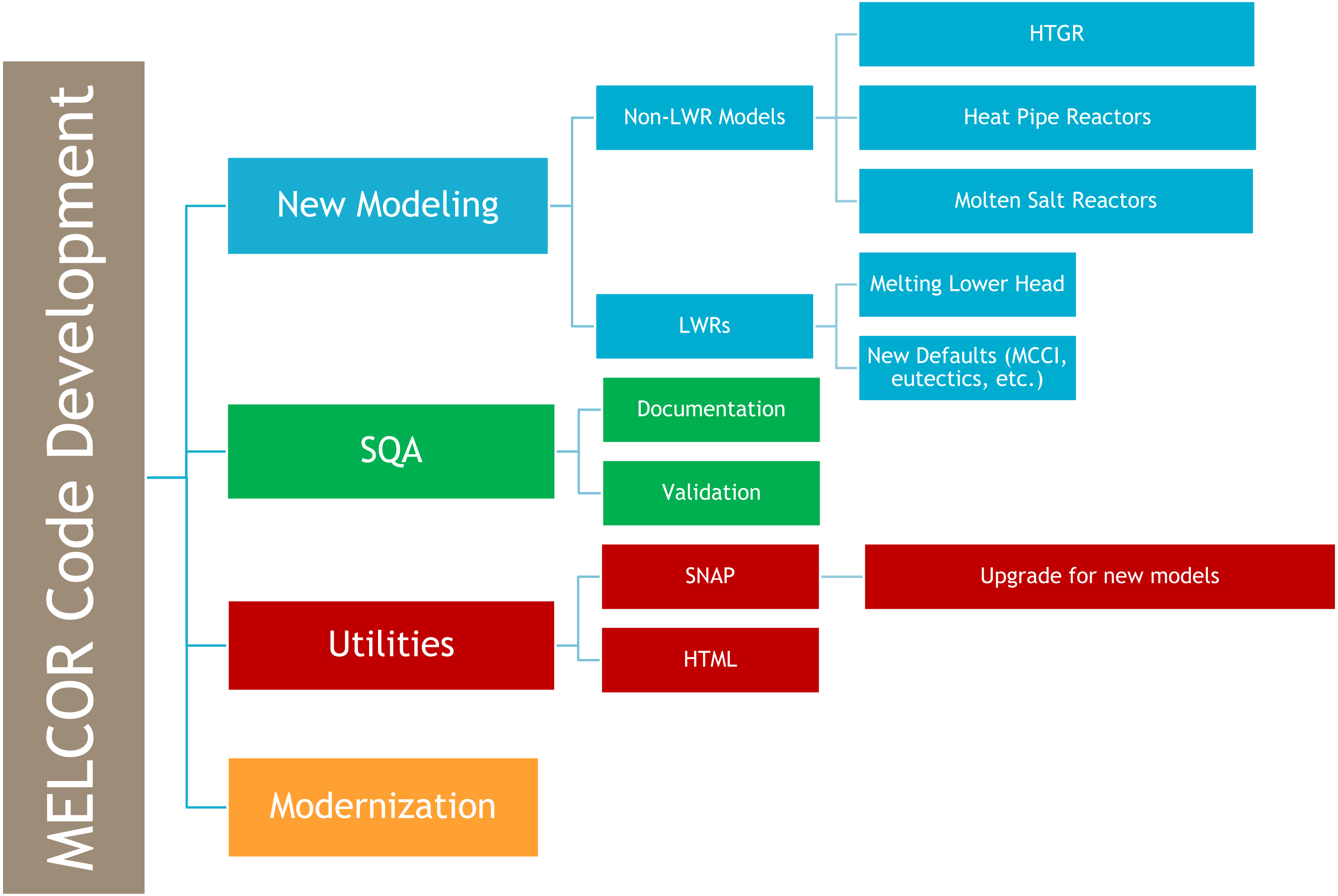
CVH Package Modernization Work Facilitates Code Improvements

Test Problem: Large full-scale plant deck subject to rapid depressurization with subsequent cold water injection.

- Very challenging for current pressure-based formulation and solution algorithm.
- Current code drops dt to dt_{min} and then fails to converge. Run stops after less than 250 sec into transient.
- Development code drops dt to dt_{min} but continues to run robustly and time step recovers (test run out to > 9000 sec).



Questions


MELCOR Code Development
New Modeling
Non-LWR Models
HTGR
Heat Pipe Reactors
Molten Salt Reactors
LWRs
Melting Lower Head
New Defaults (MCCI, eutectics, etc.)
SQA
Documentation
Validation
Utilities
SNAP
Upgrade for new models
HTML
Modernization