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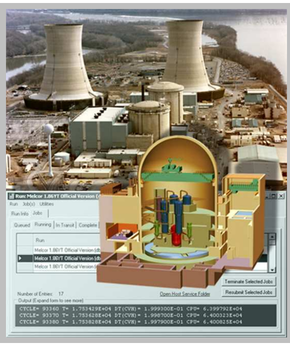
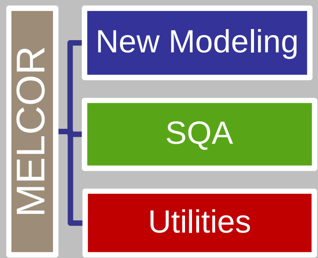


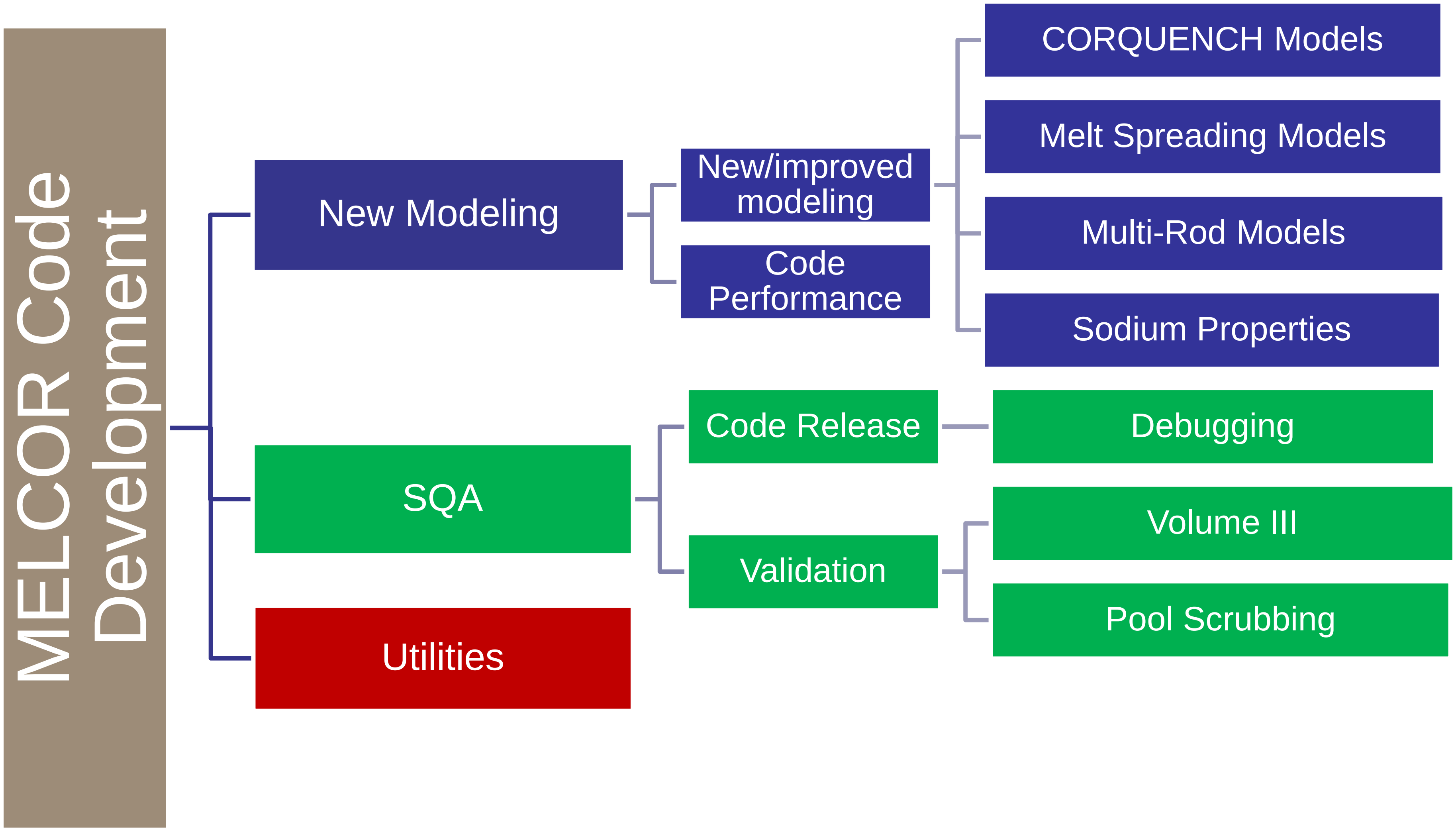


MELCOR Code Development Status

Presented by Larry Humphries

llhumph@sandia.gov

MELCOR Code Development



Current Code Development Tasks

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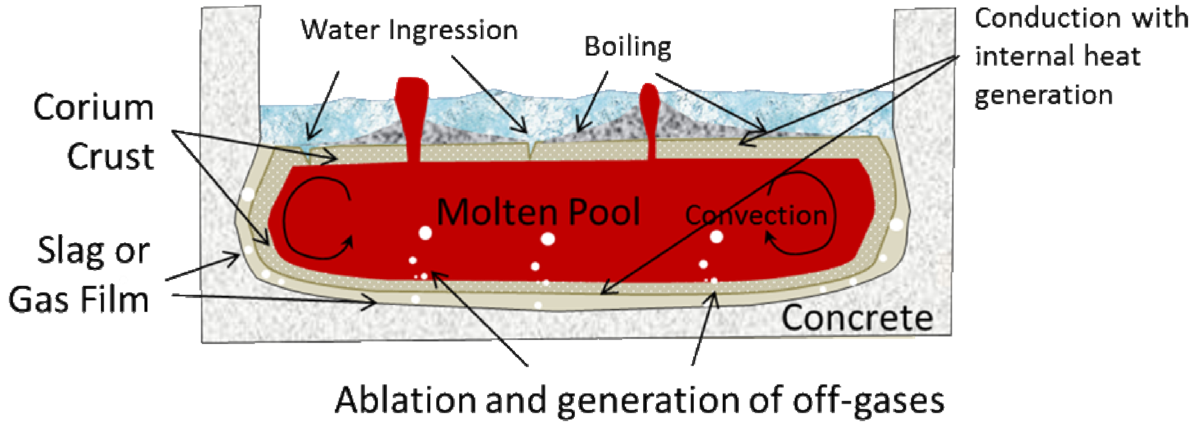
- CORQUENCH modeling to be added to CAV package
- Spreading model implemented into CAV package
  - Balance between gravitational and viscous forces
- Liquid metal reactors
  - Sodium properties to be added to MELCOR
    - Substitute working fluid
  - Other CONTAIN/LMR modeling to be added for modeling sodium fires
- Multiple fuel rod types in a COR cell
- CVH/FL Numerics
- RN groups

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
- 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

Current MELCOR Best Practice

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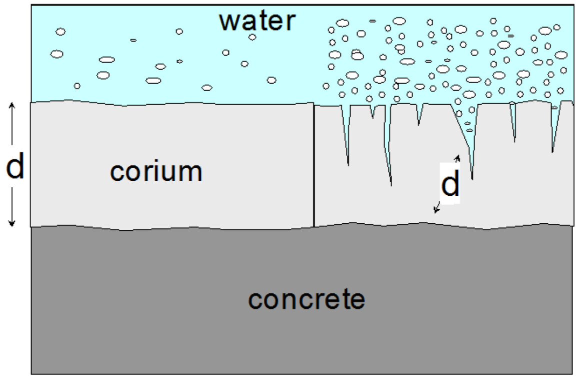
- Water ingression will increase the contact surface area between water and the corium
- Decrease the conduction path length through the corium, both of which will enhance the heat transfer through the crust



$$Q = -A \cdot k\frac{dT}{dz} \sim -\frac{\mathbf{A}}{\mathbf{d}}k\Delta T \sim -\frac{A}{d}\mathbf{k}\Delta T$$

- 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

CORCON/CORQUENCH

- Water ingress model.
  - Added water ingress criterion from Epstein,
  - Coding to allow the top crust to remelt and combine with other layers.
  - Special coding for case when no top crust on melt
  - Added parameters needed for the criterion that were not in CAV, such as mechanical properties used to calculate T_{crack}.
    - Not calculated in CAV but are constants.
- Testing the water ingress model
  - Testing on CCI3 problem now looks reasonable.
- Melt eruption model,
  - Code structure was also added for a coolable debris layer for use with melt eruptions.
  - The melt eruption model is activated with iuseerupt=.true.
  - Eruption criteria for CAV.

CORCON/CORQUENCH

Enhanced Conductivity Old Model

```
CAV_U   10
    1 CTOXYREA   INCLUDE
    2 EMISS.OX   0.8
    3 EMISS.MET  0.8
    4 MIXING     ENFOR
    5 BOILING    value  10.0
    6 COND.OX    mult 1.0
    7 COND.MET   mult 1.0
    8 HTRINT  multip 1.0
    9 HTRSIDE multip 1.0
   10 COND.CRUST  5.
```

Water Ingression New Model

```
CAV_U   9
    1 CTOXYREA   INCLUDE
    2 EMISS.OX   0.8
    3 EMISS.MET  0.8
    4 MIXING     ENFOR
    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
```

MELCOR Debris Spreading Model

- By default, corium relocated to the cavity will spread instantaneously
- Users are able to specify a spreading radius through a CF or TF
- Current model development will add an internally calculated spreading radius.

CAV_SP – Definition of Parametric Debris Spreading
Optional

This record may be used to model the spreading of debris in the cavity. Users can define a maximum debris radius as a function of time through a tabular function, control function, channel of an external data file, or an internal model.

(1) SOURCE

Source of data for maximum debris radius as a function of time

1 or 'TF'
: Use data from tabular function.

-1 or 'CF'
: Use data from control function.

2 or 'CHANNELEDF',
: Use data from channel of external data file NameCF_TF_EDF.

0 or 'MODEL',
: This option allows the code to internally calculate the debris radius as a function of time. However, this option requires the initial debris radius (RADTINI).

If SOURCE = 0, the following record is required:

(2) RADTINI - Initial time-dependent debris radius for the internal model

MELCOR Debris Spreading Model Development

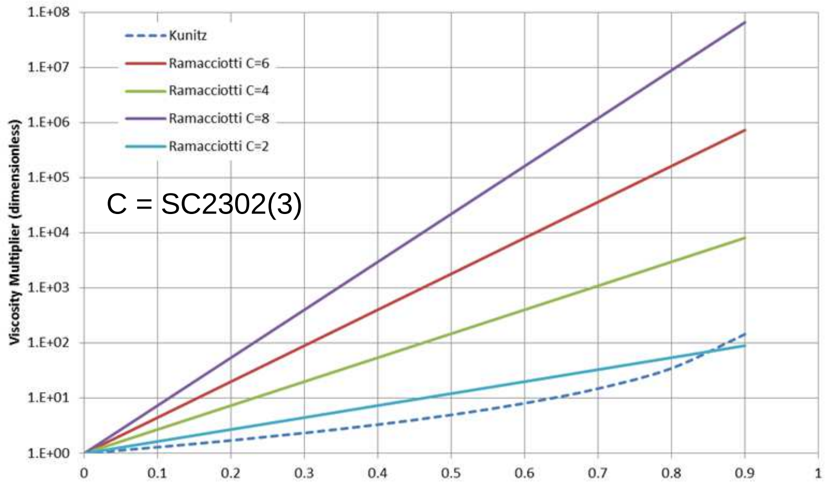
- An analytical melt spreading model based on the difference between the gravitational and viscous forces has been developed and implemented

$$\frac{dR}{dt} = C_1 \frac{\rho\, g}{\mu} \left(\frac{V}{\pi R^2} \right)^3 \frac{1}{R}$$

$$R(t) = \sqrt[8]{R(t_0)^8 + C_1 \cdot \frac{\rho\, g}{\mu\, \pi^3} V^3 (t - t_0)}$$

- Melt viscosity enhancement using Ramacciotti correlation has been added to MELCOR. This correlation is being used in other spreading codes, such as MELTSPREAD. The current MELCOR viscosity enhancement is done through the use of Kunitz two-phase viscosity multiplier

$$\eta = \eta_0 \cdot \exp(2.5 \cdot C \cdot \phi)$$



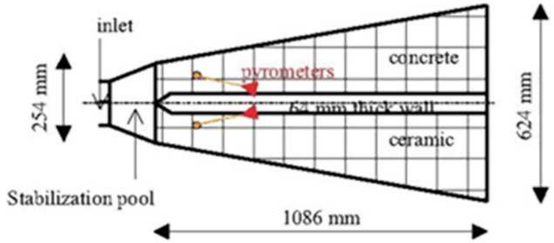
ϕ is the melt solid fraction

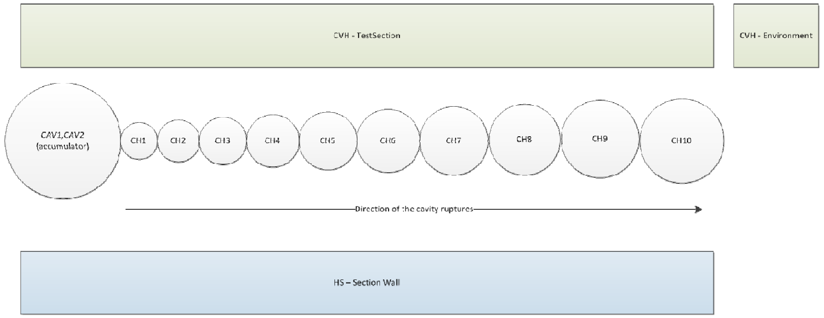
MELCOR Debris Spreading Model Development

- Melt spread stopping models based on MELTSPREAD code and crust fraction have been implemented.
  - MELTSPREAD assumes a fixed volume fraction of oxide in the melt to stop spreading when melt temp < oxide solidus temp or a fixed volume fraction of metal in the melt to stop spreading when melt temp < metal solidus temp.
    - If the oxide phase has a volume fraction > 64.1 vol%, then the debris is considered to be immobile when the debris temperature falls below the oxide solidus temperature
    - If the metal fraction of the debris is greater than 39.9 vol%, then the debris is immobilized when the debris temperature falls below the metal solidus temperature
  - Crust fraction model assumes a fixed length fraction of crust in the melt – radially or axially – crust height over total melt height and crust radial thickness over melt radius are greater than the fixed length fractions (radially or axially) to stop spreading.

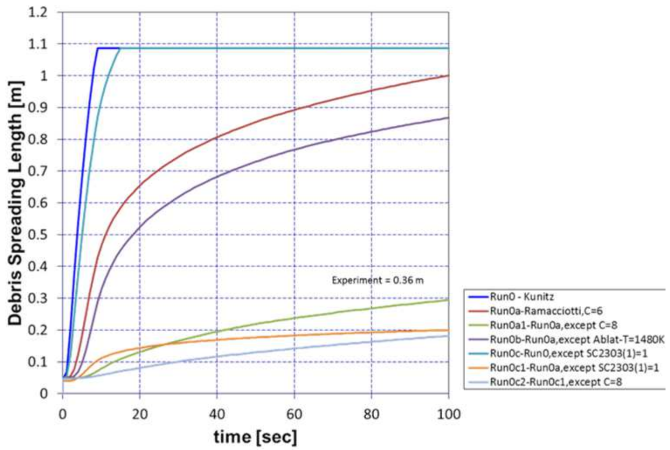
MELCOR Debris Spreading Model Testing

- VULCANO-7 experiment
  - Modeling in MELCOR is challenging because of the geometry
  - Modeled as several connected cavities
  - Figures at right for the VULCANO assessments





- MELTSPREAD simulation for Peach Bottom cavity melt spreading
  - Direct code-to-code comparison
  - MELCOR pancake geometry
  - not yet completed



DOE Project for Integration of CONTAIN-LMR Models Into MELCOR

- Project Motivation and Objective
  - Address the regulatory infrastructures requirements regarding accident analyses for reactor systems,
    - A sodium coolant accident analysis code is necessary to provide regulators with a means to perform confirmatory analyses for future sodium reactor submissions.
- Solution Strategy
  - Implementation of models for sodium phenomenology simulation into an integrated, full-featured, actively maintained, severe accident code
    - CONTAIN/LMR models implemented into the MELCOR code

Liquid Metal Working Fluid

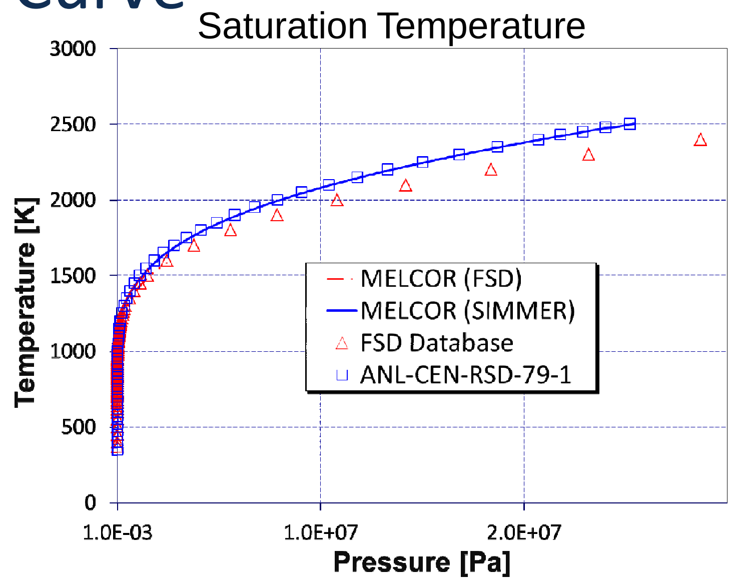
DOE Project Strategy

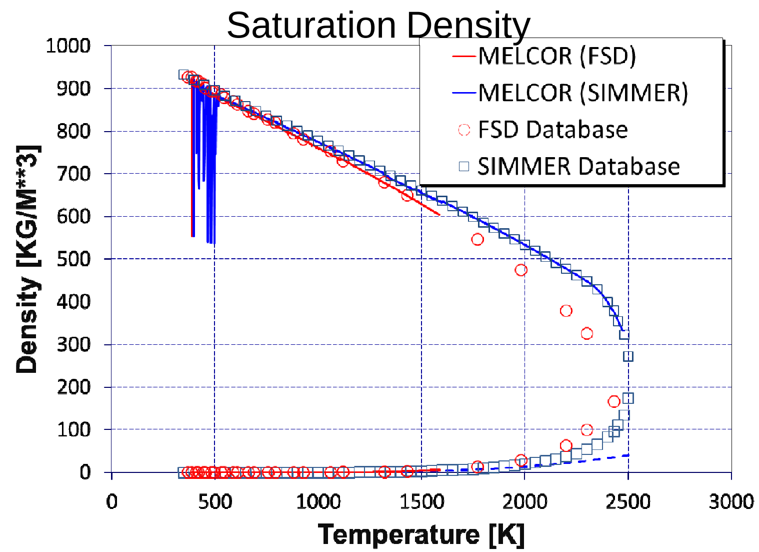
- Phase 1 – Implement sodium as replacement to the working fluid for a MELCOR calculation
  - Implement properties & Equations Of State (EOS) from the fusion safety database
  - Implement properties & EOS based on SIMMER-III
- Phase 2 – Review of CONTAIN/LMR and preparation of design documents
  - Detailed examination of LMR models with regards to implementation into MELCOR architecture
  - Condensation of sodium
- Phase 3 – Implementation and Validation of:
  - Sodium spray fires
  - Upper cell chemistry
  - Sodium pool chemistry
- Phase 4 – Implementation and Validation of:
  - Sodium pool modeling,
  - Sodium pool fire models
  - Debris bed/concrete cavity interactions.

Liquid Metal Working Fluid

Testing Results - Saturation Curve

- FSD – Fusion Safety Database
  - More stable at very low temperatures
  - Calculations reproduce the saturation pressure and density curves for the database.
  - MELCOR reads binary EOS library file
- SIMMER Database
  - More stable over a wider range of temperatures.
  - Calculations reproduce the saturation pressure and density curves for the database except for atmosphere densities at temperatures approaching the critical point.





Liquid Metal Working Fluid

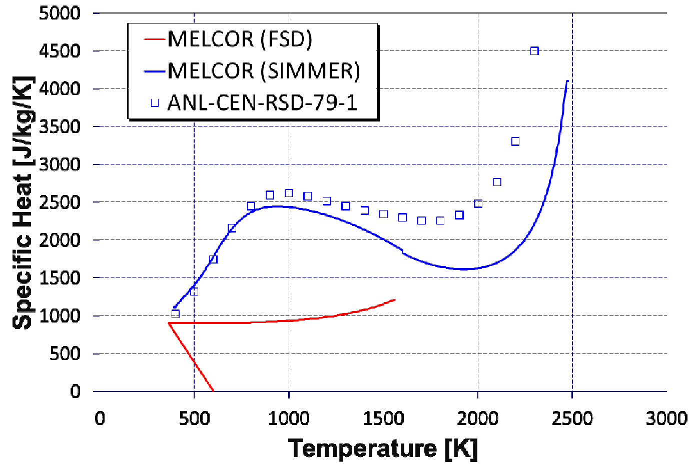
Testing Results -Specific Heat at Constant Pressure

- Where the specific heat at constant pressure is needed, it is evaluated from the standard relationship

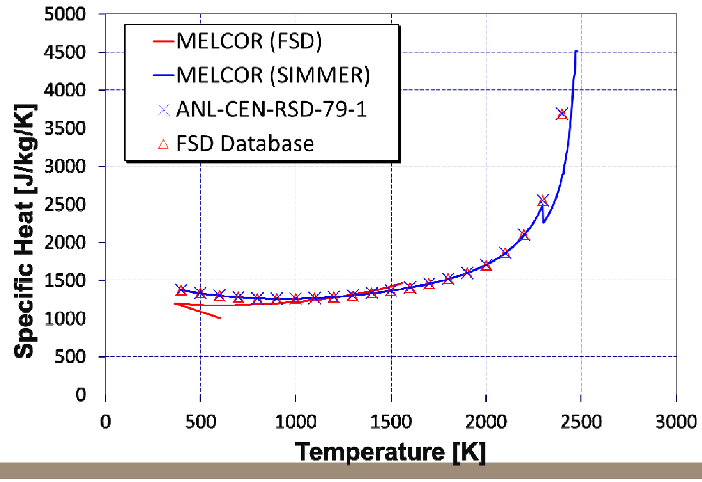
$$c_p = c_v + \frac{T\left(\frac{\partial P}{\partial T}\right)_\rho^2}{\rho^2\left(\frac{\partial P}{\partial \rho}\right)_T} \quad .$$

- Comparison of this variable with the database provides a good test on the derivatives used by MELCOR
  - Indicator of code stability

Atmosphere



Pool



Modeling Improvements for PWR SFP

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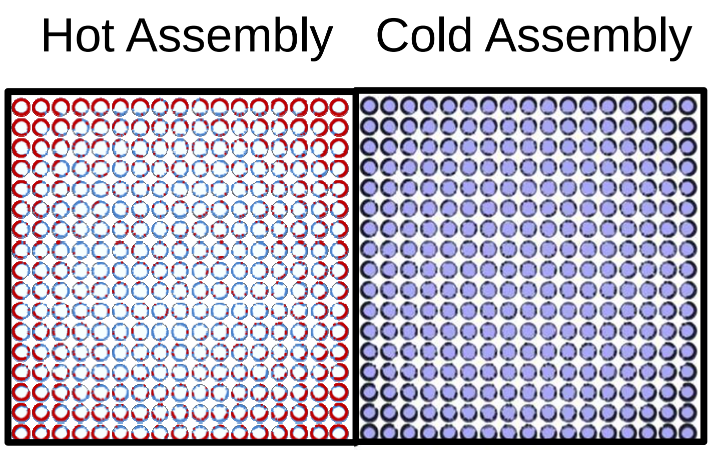
- Motivation
  - It is desirable to model an entire assembly within a single MELCOR ring
    - Reduction in CPU time for SFP models
    - Simplified input requirements
- Challenge
  - When hot assembly reaches ignition, heat transfer to cold assembly is problematic
    - – All fuel assemblies in assembly have same average temperature
    - – Large temperature gradients across cell
    - – Ignition in cold assembly can only be reached when entire assembly reaches ignition
    - For a BWR, the outer canister captures the temperature in the edge regions so this is not as much of an issue



Multi-Rod Model

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- Proposed Solution
  - Implement additional fuel rod components to capture temperature gradient
    - Temperature in edge region simulated
    - Oxidation and ignition captured
  - Implement sub-grid radiation model
    - User provides view factors between rows of rods
      - Geometric viewfactor now meaningful
- Benefits
  - Input greatly simplified compared to multi-cell
    - No input for surface area, temperatures, mass equivalent diameter for each COR cell
  - Code performance greatly improved.

Fraction of mass for each rod type

COR_ROD2 2
1 rfrac1, rfrac2, rfrac3, rfrac4
2 rfrac1, rfrac2, rfrac3, rfrac4

View Factor Matrix

COR_ROD_VF 5
1 VF11 VF12 VF13 VF14 VF15 VF1RK
2 VF21 VF22 VF23 VF24 VF25 VF2RK
3 VF31 VF32 VF33 VF34 VF35 VF3RK
4 VF41 VF42 VF43 VF44 VF45 VF4RK
5 VF51 VF52 VF53 VF54 VF55 VF5RK

Fraction of mass for each control rod type

COR_CR2 2
1 CRfrac1 CRfrac2 CRfrac3 CRfrac4
2 CRfrac1 CRfrac2 CRfrac3 CRfrac4

Validation of Multi-Rod Model

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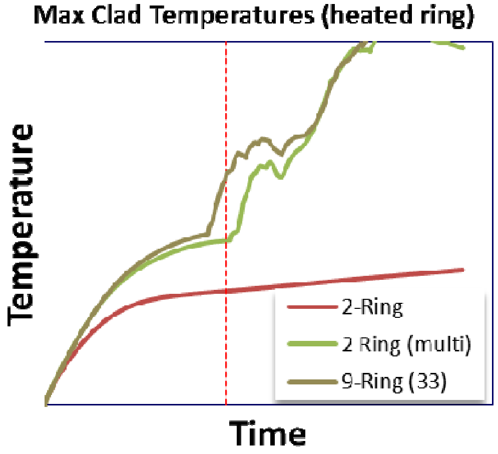
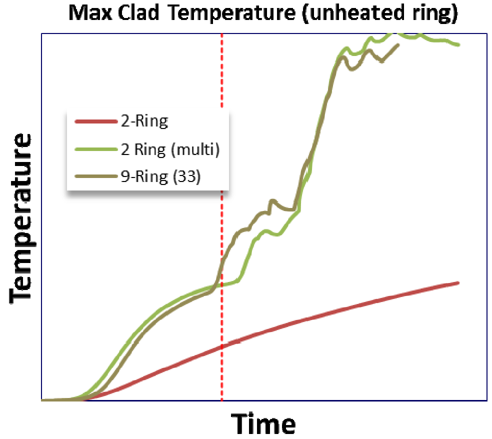
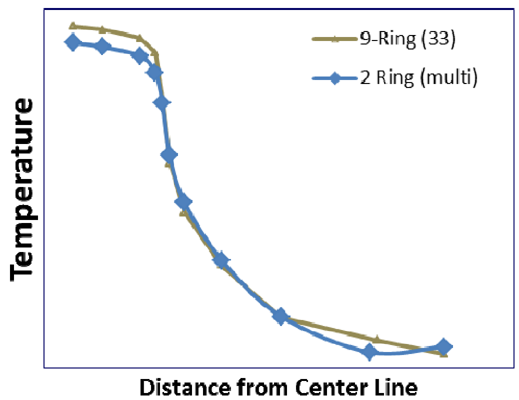
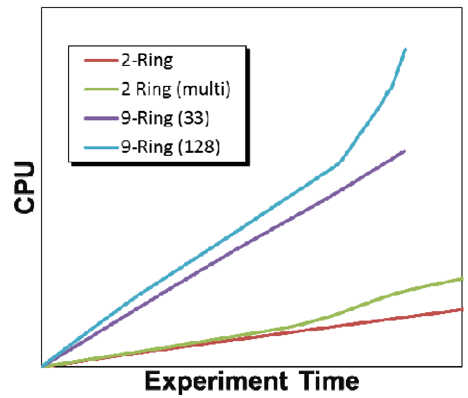
- Validation
  - Validation was performed against the Sandia PWR Spent Fuel Pool Experiments
  - Comparisons between 2-ring model; 2-ring, 9-rod model; and 9-ring model.
    - 9-ring and 2-ring 9-rod give very similar results for both heated and unheated ring
    - 2-ring (2-rod) model is incapable of capturing the temperature gradient and oxidation.
  - Data not shown because it is proprietary
- CPU time is greatly reduced for multi-rod model
- Model development is not complete
  - Core degradation and melting not currently handled
  - To be completed for September code release









CVH/FL Numerics
The Implicit Continuous-fluid Eulerian (ICE) Method

MELCOR version

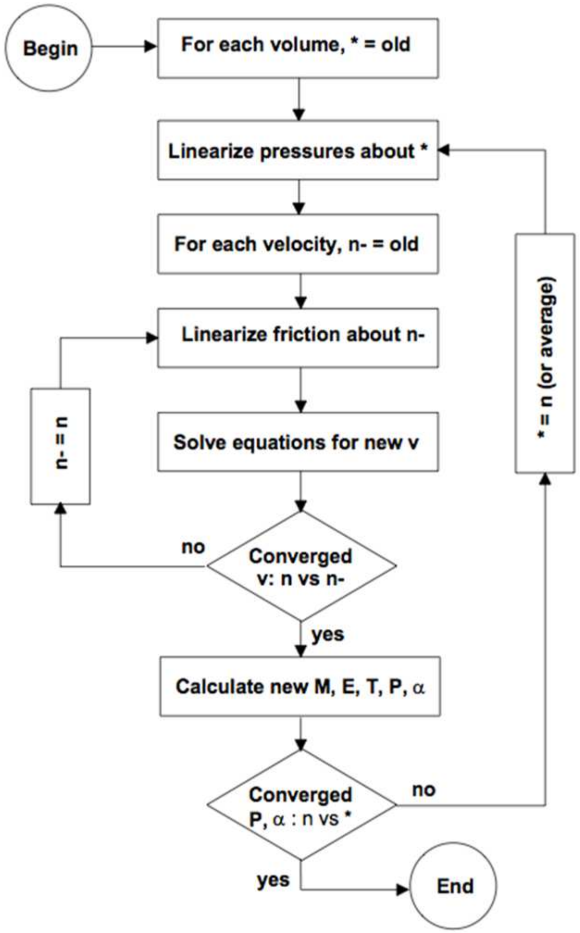
- Substitute mass equation into momentum equation
- Solve a matrix for velocity
- Back solve for density
- Pressure from linearized EOS
- Iterate to get pressure correct

TRACE version

- Substitute momentum equation into mass equation
- Solve a matrix for pressure
- Density comes from linearized EOS
- Back solve for velocity
- Iterate to conserve mass.

CVH/FL Numerics
MELCOR vs. TRACE

- TRACE – fewer iterations (speed at the cost of accuracy), designed for boiling, few models, many closures caused by many flow regimes.
- MELCOR – multiple nested iterations (accuracy at the cost of speed), designed for flow, many models, few closures since only one flow regime.



New Plot Variables & CF Arguments

Parameter	Plot Variable	CF Argument	Details
Emissivity	COR-EM-sss.ia,ir	COR-EM(IA,IR,sss)	Enabled by input; Local emissivity for each component surface
Oxide Thickness	COR-OXTH-sss.ia,ir	COR-OXTH(IA,IR,sss)	Enabled by input; Local oxide thickness for each component surface
Linear Power Density	COR-POW-Z.ia,ir	COR-POW-Z(IA,IR)	Enabled by input: Local total linear power density (includes decay, fission, and oxidation)
Component HTC to Atm	COR-HTCA-sss.ia,ir	COR-HTC(IA,IR,sss,A)	Enabled by iinput: Local heat transfer coefficient to atmosphere used for each surface
Component HTC to Pool	COR-HTCP-sss.ia,ir	COR-HTC(IA,IR,sss,A)	Enabled by iinput: Local heat transfer coefficient to poolused for each surface
Component HTC to Pool Surface	COR-HTCS-sss.ia,ir	COR-HTC(IA,IR,sss,S)	Enabled by iinput: Local heat transfer coefficient to pool/atm interface used for each surface
Hydrogen generated by component	In Progress	In Progress	

Customizable Plot File

- User can remove individual plot variables from a binary plot file
  - Users often request additional plot variables in the plot file
  - However, plot files can become extremely large with gigabytes of data
  - Customizable plot files puts the burden of choosing important parameters on the user
    - Beware, when you remove a plot variable , that's just when you find you need it.
- Currently only implemented for COR package
  - COR_PLOT 2

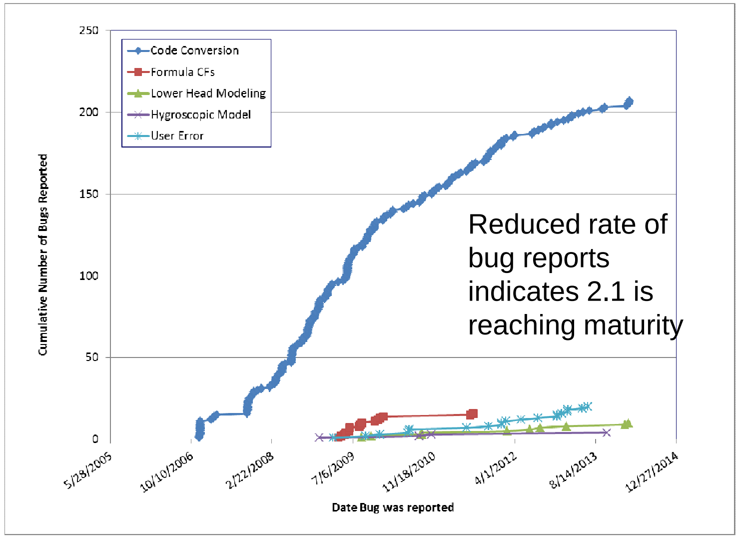
    1 COR-SS-STRESS OFF

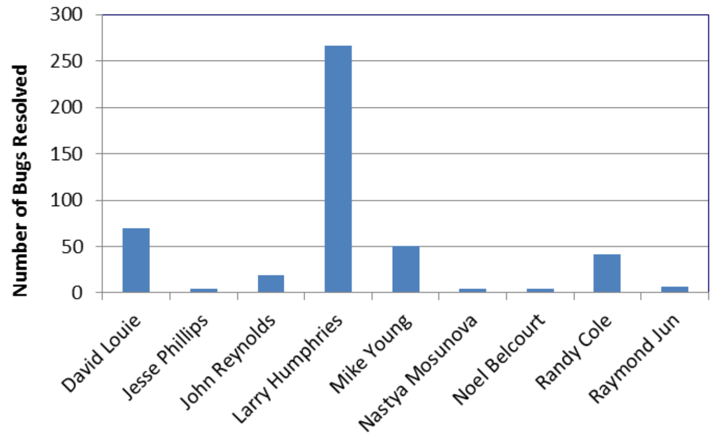
    2 COR-EM ON
- Certain energy error, mass error, CPU, NCYCLE variables necessary for diagnostics are not permitted to be removed

MELCOR
New Modeling
SQA
Utilities

Preparing for Code Release

- Last Official Code Release
  - Rev4803 – Sep 2012
  - Significant code improvements have been made.
    - Improved stability
    - Addressed bug issues
- Code release is high priority
  - Plan to release code in May
  - Tasks necessary for code release
    - Address outstanding Bugzilla issues
      - Over 100 bugs resolved in the past two months
      - 90 bugs remain unresolved
    - Test code
    - Documentation of tests
  - Follow-on release in September





Recently Corrected Code Issues

- No warning/error when RPV heat structures were not using local dtdz temperatures (1.8.6 & 2.1 issue)
- Diagnostic messages missing for time-dependent volumes(2.1 issue)
- CORCON termination due to numerical issues with CCSAXC matrix inversion routine – terminates with error message (1.8.6 & 2.1 issue)
- Error in partitioning radiation between PD & PB (or MP1 & MB1) components when channel box is gone and one of the 2 components is missing – excessive heating in component leading to COREU3 error (1.8.6 & 2.1 issue)
- Corrections to hygroscopic model to ensure that convergence is bounded by available mass –terminates with error message (1.8.6 & 2.1 issue)
- In some cases COR cuts the time step to tmin rather than cutting the time step in half - performance issue only (1.8.6 & 2.1 issue)
- ESF_CND model did not work in M2.1 – terminates with error message (2.1 issue)

Duplicate Errors SC1502(2)

- **1502** – Minimum Component Masses
  - These coefficients specify the minimum component mass below which the masses and energies will be discarded and the minimum component mass below which the component will not be subject to the maximum temperature change criterion. <u>The default value of C1502(2) must be reduced to successfully simulate small-scale experiments.</u>
  - Minimum total mass of component subject to the maximum temperature change criterion for timestep control.
    - (default = 10.0, units = kg, equiv = XMCMN2)
- Problem
  - The default may be too large for experiments or when lower head is finely nodalized or low density insulation on outer surface
- Resolution
  - User Impact:An error check is added to pass 2 to detect lower head node masses that are less than XMCMN2. A strong warning is issued with the minimum node mass provided and a recommendation to reduce SC1502(2).
  - Bug#: 1253
  - Revision: 5492
  - Date: 3/5/2014 3:54:11 PM

Hygroscopic Model

- Mass conservation of water for the hygroscopic model has been a subject of uncertainty (Phillips, EMUG 2013)
- MELCOR does an internal check on mass and energy when it is moved, but does not provide an explicit accounting of all 'varieties' of water
- Challenging to perform water mass balance. Water mass is tracked by HS and RN package and can be generated or removed from a number of MELCOR models
  - Some of these variables are not available as plot variables

Hygroscopic Model Inactive	Hygroscopic Model Active
CV volume mass (active volumes) CVH water sources Water generated from burns Water removed from oxidation Water generated from PARS Water generated from melting heat structures Water accounted for in HS package as films on structures CVH Water flow to inactive or time-independent CV volumes Water generated from MCCI.	CV volume mass (active volumes) CVH water sources Water generated from burns Water removed from oxidation Water generated from PARS Water generated from melting heat structures Water accounted for in HS package as films on structures CVH Water flow to inactive or time-independent CV volumes Water accounted for in RN masses in active cells RN water advected to inactive or time-independent CV volumes RN water settling into inactive or time-independent CV volumes Water generated from MCCI.

Hygroscopic Model

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- A plot variable has been added to provide a global water mass error
- Water mass is tracked in all its forms
- Mass sources are accounted for
- Mass sinks are accounted for

$$Total\ Error = \sum_{All\ \ active\ \ CVs} Error_{icv}$$

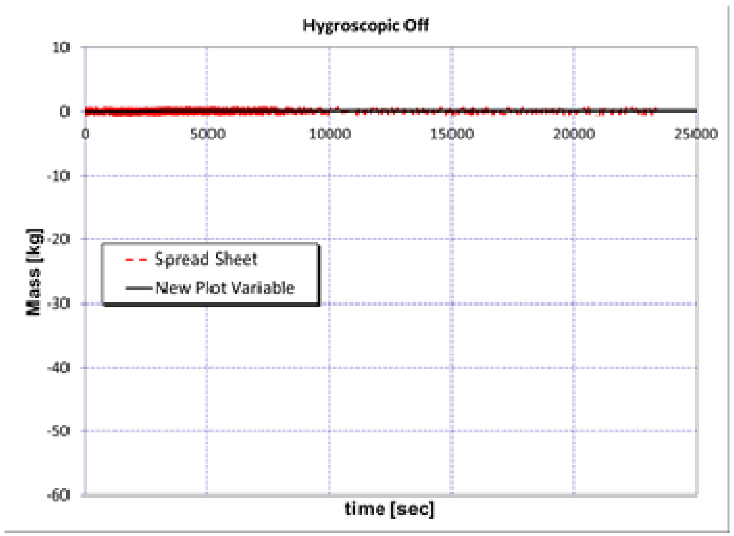
$$\begin{aligned} Error_{icv} = \ & CVmass_{icv} + RN_{H20\ icv} + HS_{H20\ icv} + NetFlowOut_{icv} + RNadvected_{icv} + RNsettled_{icv} + CVsources_{icv} \\ & + MH2O_{Oxidation\ \ ,icv} - dMH2O_{PARS,icv} - dMH2O_{degas\ ,icv} - dMH2O_{MCCI,icv} - dMH2O_{H2\ Burns\ ,icv} \\ & -(CVmass_{icv} + RN\_H2O_{icv} + HS\_H2O_{icv})_{at\ time\ =0} \end{aligned}$$

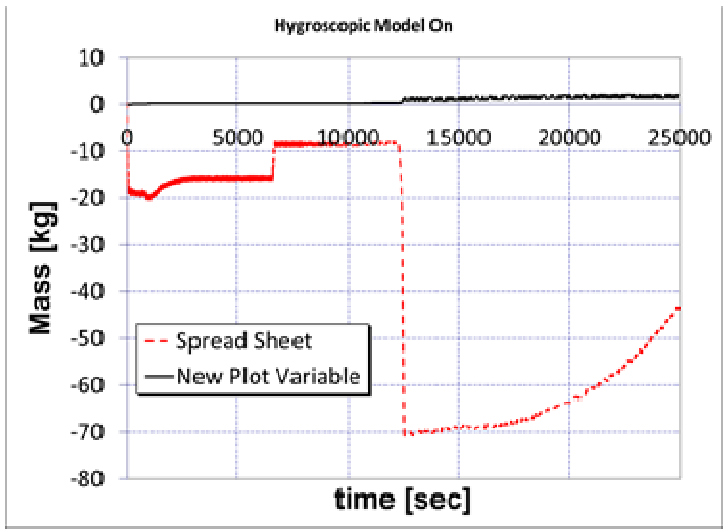
Where

$CVmass_{icv} =$	$Total\ CV\ mass\ (pool, atm, and\ fog)$
$RN_{H20\ icv}$	$Total\ water\ RN\ aerosol\ mass$
$HS_{H20\ icv}$	$Total\ HS\ film\ masses\ on\ all\ HS\ surfaces\ in\ contact\ with\ CV$
$NetFlowOut_{icv}$	$Net\ flow\ of\ all\ water\ flowing\ out\ of\ CV$
$RNadvected_{icv}$	$Net\ water\ RN\ mass\ advected\ with\ flow$
$RNsettled_{icv}$	$Net\ water\ RN\ mass\ settling\ out\ of\ CF$
$CVsources_{icv}$	$Sum\ of\ all\ CV\ sources\ associated\ with\ CV$
$MH2O_{Oxidation\ \ ,icv}$	$Mass\ of\ all\ H2O\ removed\ from\ this\ CV\ from\ oxidation$
$dMH2O_{PARS,icv}$	$Mass\ of\ all\ H2O\ generated\ in\ this\ CV\ from\ PARS$
$dMH2O_{degas\ ,icv}$	$Mass\ of\ all\ H2O\ generated\ in\ this\ CV\ from\ associated\ degassing\ sources$
$dMH2O_{MCCI,icv}$	$Mass\ of\ all\ H2O\ generated\ in\ this\ CV\ from\ MCCI$
$dMH2O_{H2\ Burns\ ,icv}$	$Mass\ of\ all\ H2O\ generated\ in\ this\ CV\ from\ hydrogen\ burns$

Hygroscopic Model- No Mass Conservation Error

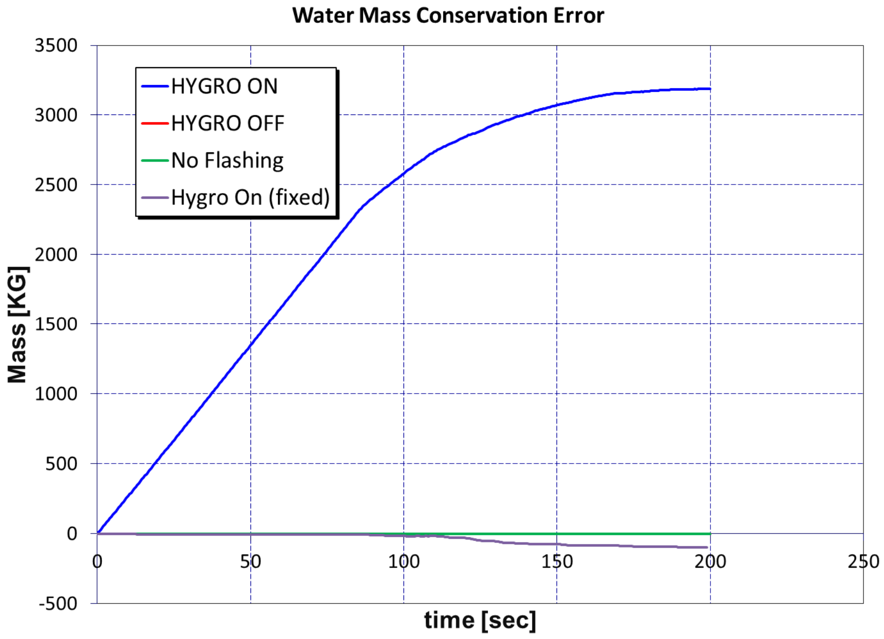
- Tested on a number of simple decks as well as several plant decks
- No mass conservation error found in hygroscopic model. Mass error is within reasonable tolerance.
- Hygroscopic model currently used by NRC for filtered vent analysis and Surry UA
- Only place where mass conservation was an issue was when flashing model was invoked (next slide)





Flashing Model and Mass Conservation

- An error <u>was</u> identified for the flashing model (superheated pool flow) <u>with</u> the hygroscopic model active
  - Flow partitioning can place some mass in fog (managed by RN)
- CVH mass was added to RN package without removing mass from CVH
- Correction shows improvement
  - Still reviewing to possibly reduce error further



Simple 4 Volume Flashing Test Deck

MELCOR Volume III: Code Assessment Report

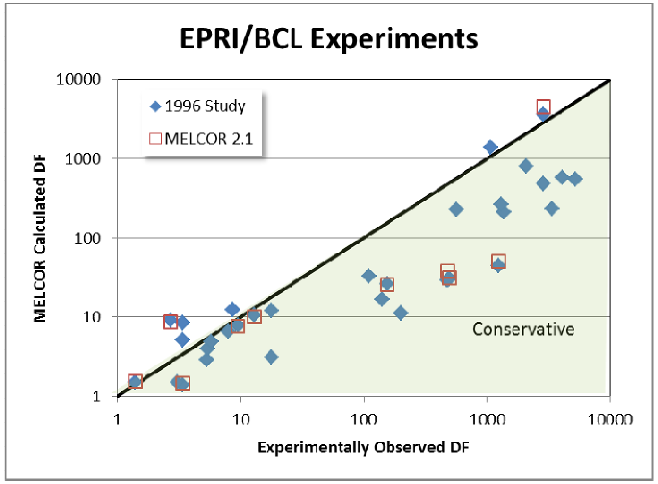
- MELCOR Documentation
  - Volume I: User Guide
  - Volume II: Reference Manual
  - Volume III: Code Assessment Report
  - Volume IV: Modeling Guide
- Currently completing the Volume III Assessment report
  - Reviewing and re-running historic assessments
  - Adding new assessments for un-assessed physics
    - POSEIDEN (Pool scrubbing – SPARC-90)
    - ACE (Pool scrubbing – (SPARC-90)
    - MARVIKEN CFT-21 & JIT-11 (Critical Flow)
    - LACE LA1 & LA3 (Turbulent Deposition)
    - LHF, OLHF (Lower Head Failure)

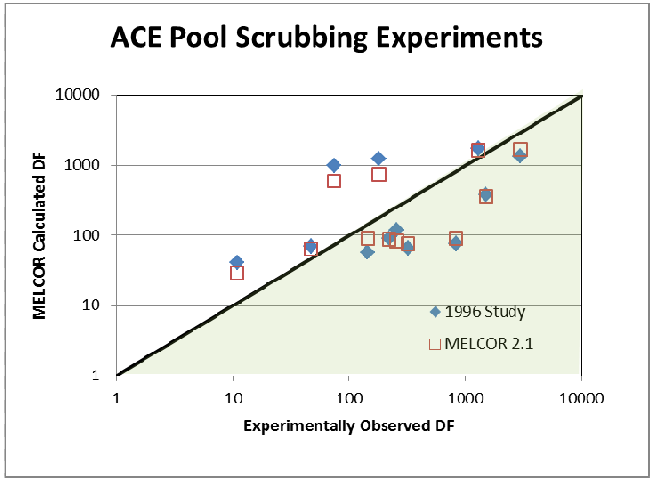
Fission Product Retention in Pools - Pool Scrubbing

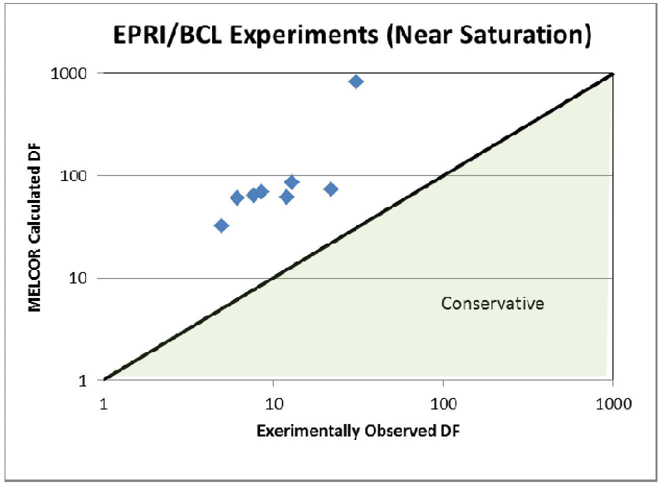
- SPARC 90 Model
  - Thermodynamics of bubble interactions with a pool
  - Scrubbing and retention radionuclides by pool
    - Original SPARC 90 model only accounted for scrubbing of aerosols and Iodine vapor
      - Species such as CsOH and CsI sometimes are released at high temp in vapor form
      - Such vapors would not have been condensed and scrubbed
  - Code Versions
    - Implemented in MELCOR 1.8.4
    - MELCOR 1.8.6 - extended to include scrubbing of vapors
- Observations
  - Calculation trends consistent with experiment
    - A deeper pool resulted in more aerosol capture and a larger DF
      - However, MELCOR overestimated DFs for deep pools (169.0 compared to 21.4 for 4 m deep pool). Edge effects may be important.
    - MELCOR overestimates DFs for near-saturated pool conditions
- Validation Cases
  - ACE Pool Scrubbing Tests
  - PSI Poseidon Experiments (PA06, PA07, PA08, PA12 and PA17)

Assessment with EPRI/BCL and ACE experiments

- MELCOR 2.1 calculations show slight improvement
- MELCOR DF is overestimated near saturation
  - We haven't run these calculations with MELCOR 2.1







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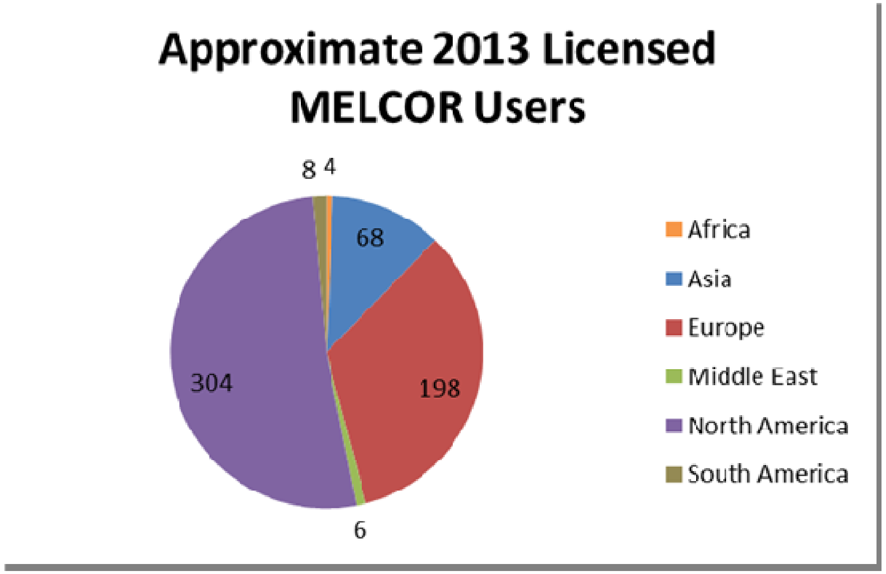
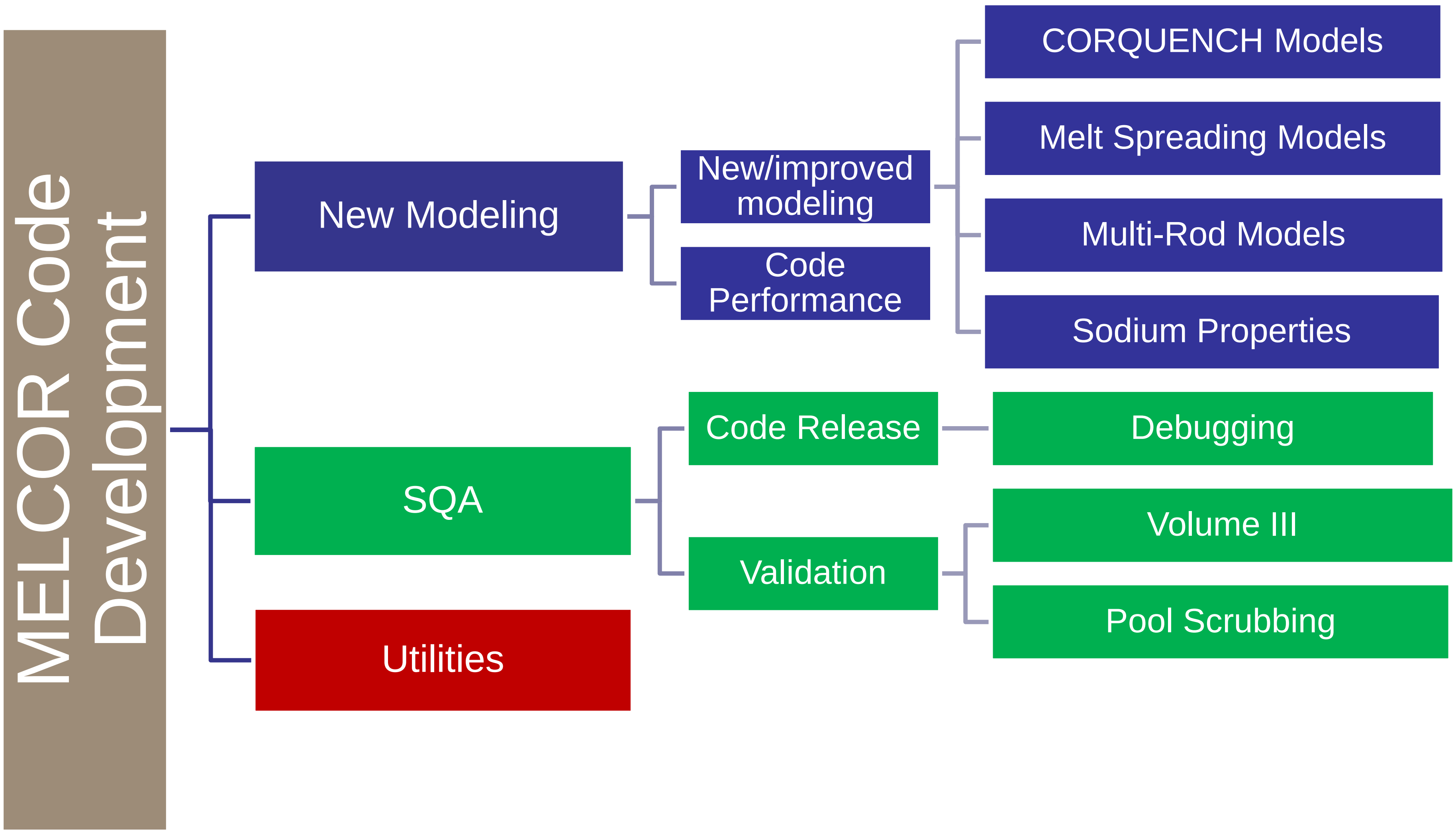
Meetings & Workshops

- CSARP/MCAP (Sept 16-19)
  - Watch MELCOR website for details
- MELCOR Workshop (Sept 8 -12)
  - Week long beginner workshop
  - Possible use of SNAP again
- EMUG (April 15-16, 2014)
  - hosted by VUJE Slovak Nuclear Regulatory Authority and VTS at VUJE,
  - Bratislava, Slovakia.
- Asian MELCOR User Group
  - Discussing a regional workshop in October



Questions?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