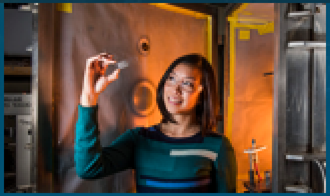
SAND2022-2825C

Sandia National Laboratories

MELCOR INTEGRATED SEVERE ACCIDENT CODE FOR NON-LWR APPLICATIONS

SAND2022-1819 PE



PRESENTED BY

Larry Humphries

MELCOR “Systems-level” Modeling Approach

Modeling is as mechanistic as possible, consistent with a reasonable run time.

- Examples: Zonal diffusion release in TRISO particles, Lagrangian droplet combustion models for sodium spray fires, multi-component/multi-particle size aerosol physics models, etc.
- Advances in computer run-time over the past few decades has led to increased mechanistic modeling in MELCOR.

Simplified models where appropriate consistent with available supporting experimental data

- Example: Simple force balance model vs kinetic “rock’n’ roll” model for resuspension
  - Kinetic model based on data that is unavailable, difficult/impossible to characterize under accident conditions
  - Simple model performs as well on fundamental validation experiments

Some parametric models, where appropriate

- Example: Data for large scale core degradation is sparse or non-existent.
  - Validation limited to small-scale bundle experiments or post-accident conditions for Fukushima and TMI-2 and indirect temperature/pressure measurements
  - Use of Cross-walk comparisons to other codes.
- Parametric models are general enough that they do not force a particular outcome (i.e., TMI-2)
- Core degradation not a concern of facility SB and therefore such uncertainties do not exist

Modeling is consistent with current state of practice in modeling phenomena

Uses general, flexible models rather than models for specific system components

- Relatively easy to model unique safety systems
- Puts greater burden on analyst to develop input deck that well-represents problem

Significance of a fully-integrated source term tool

MELCOR is a fully-integrated, system-level computer code

- Prior to the development of MELCOR, separate effects codes within the Source Term Code Package (STCP) were run independently
  - Results were manually transferred between codes leading to a number of challenges
    - transferring data
    - ensuring consistency in data and properties
    - capturing the coupling of physics

Advantages of using a fully-integrated tool for source term analysis

- Integrated accident analysis is necessary to capture the complex coupling between a myriad of interactive phenomenon involving movement of fission products, core materials, and safety systems.
- A calculation performed with a single, integrated code as opposed to a distributed system of codes reduces errors associated with transferring data downstream from one calculational tool to the next.
- Ensures consistency in material properties and thermal hydraulic properties.
- Performing an analysis with a single integrated code assures that the results are repeatable.
- Methods for performing uncertainty analysis with an integrated tool such as MELCOR are well established.
- Time step issues are internally resolved within the integral code

Equations of State, EOS Package
Provides equation of state relationships for hydrodynamic materials (water and gases) and other fluids (sodium, molten salt, etc) as well as fluid properties.

Non-Condensable Gas (NCG) package provides properties from non condensable gases

Materials Properties, MP Package
Provides thermal EOS for non-hydrodynamic materials and thermophysical properties for all materials

CVH (Control Volume Hydrodynamics) and FL (FLow path) treat the control volume and flow path portions of the hydrodynamic modeling

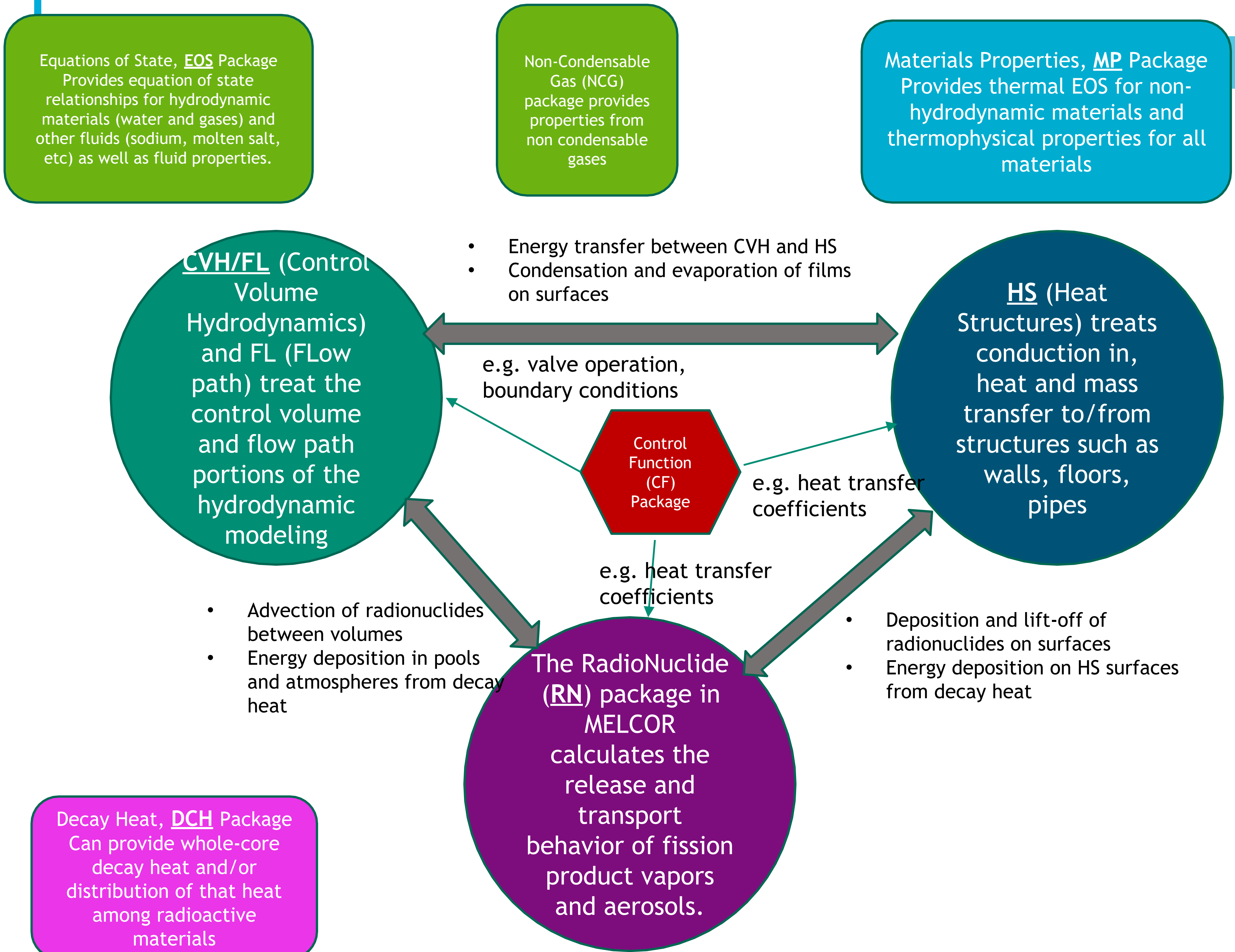
Control Function (CF) Package

- Sources, sinks, other boundary conditions
- Chemical reaction, such as fire combustion
- Valves, door openings, building failures
- Can provide simple modeling of systems when no internal model provided

HS (Heat Structures) treats conduction in, heat and mass transfer to/from structures such as walls, floors, pipes

The RadioNuclide (RN) package in MELCOR calculates the release and transport behavior of fission product vapors and aerosols.

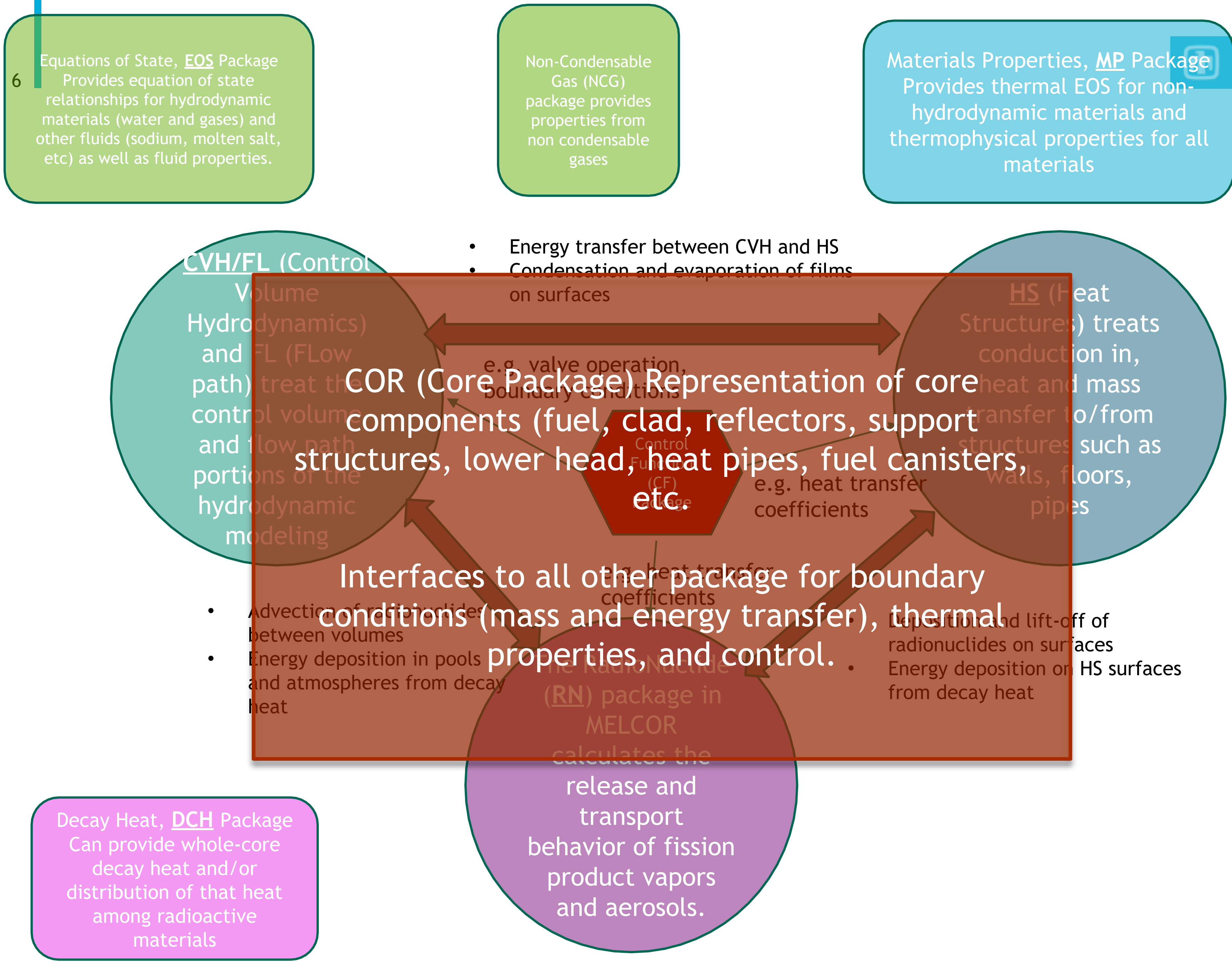
Decay Heat, DCH Package
Can provide whole-core decay heat and/or distribution of that heat among radioactive materials



Equations of State, EOS Package
Provides equation of state relationships for hydrodynamic materials (water and gases) and other fluids (sodium, molten salt, etc) as well as fluid properties.
Non-Condensable Gas (NCG) package provides properties from non condensable gases
Materials Properties, MP Package
Provides thermal EOS for non-hydrodynamic materials and thermophysical properties for all materials
CVH/FL (Control Volume Hydrodynamics) and FL (FLow path) treat the control volume and flow path portions of the hydrodynamic modeling
• Energy transfer between CVH and HS
• Condensation and evaporation of films on surfaces
HS (Heat Structures) treats conduction in, heat and mass transfer to/from structures such as walls, floors, pipes
e.g. valve operation, boundary conditions
Control Function (CF) Package
e.g. heat transfer coefficients
e.g. heat transfer coefficients
• Advection of radionuclides between volumes
• Energy deposition in pools and atmospheres from decay heat
• Deposition and lift-off of radionuclides on surfaces
• Energy deposition on HS surfaces from decay heat
The RadioNuclide (RN) package in MELCOR calculates the release and transport behavior of fission product vapors and aerosols.
Decay Heat, DCH Package
Can provide whole-core decay heat and/or distribution of that heat among radioactive materials

COR (Core Package) Representation of core components (fuel, clad, reflectors, support structures, lower head, heat pipes, fuel canisters, etc.

Interfaces to all other package for boundary conditions (mass and energy transfer), thermal properties, and control.



Explicit Coupling of Packages

Package coupling numerically explicit
Each package uses start-of-step data from other packages (with a very few exceptions, where end-of-step data are used)
Pass changes (e.g. heat and mass transfers) to other packages
Order of advancement chosen to facilitate this

- Some packages can call for a subcycle
  - Reduce package timestep and run subcycles to complete system time step
- Any package can force a "fallback"
  - Rewinds calculation to beginning of time step and runs with reduced system time step.
  - Calculation terminates if system timestep too small.

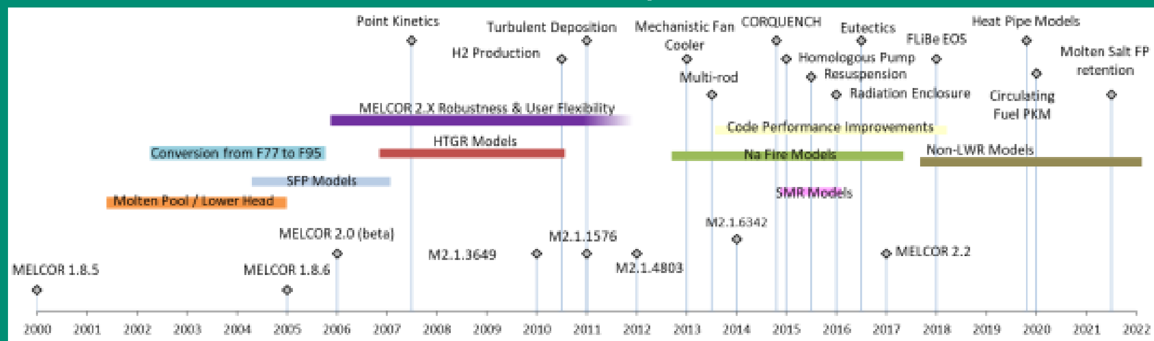
Advance packages that evaluate sources or relocations before those that use them

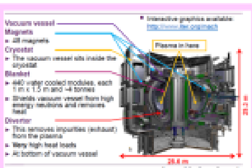
- DCH: First to update time-dependent decay heat data
- COR: Before CVH and HS that will receive heat/mass
- LHC: After COR which may receive debris, before CVH
- SPR: Before CVH that will receive heat/mass
- BUR: Before CVH that will receive mass changes
- FDI: After COR to receive debris, before CAV and CVH
- CAV: After COR and FDI to receive debris, before CVH
- ESF: Before CVH
- RN1: After COR and CAV to receive releases
- HS: After COR to receive sources, before CVH
- CVH: After COR, CAV, and HS to receive sources
- RN2: After CVH to use fluid relocations
- CF: After all physics packages

MELCOR Model Development

8

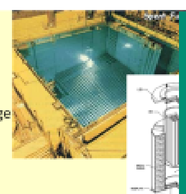
MELCOR Code Development Timeline





Fusion
- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

Spent Fuel
- Spent fuel pool risk studies
- Multi-unit accidents (large area destruction)
- Dry Storage

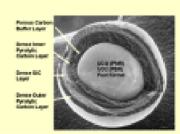


Non-Nuclear Faciliti
- Leak Path Factor Calcu (LPF)
  - Release of hazardo materials from fac buildings, confined
- DOE Safety Toolbox co
- DOE nuclear facility us
  - Pantex
  - Hanford
  - Los Alamos
  - Savannah River Sit

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

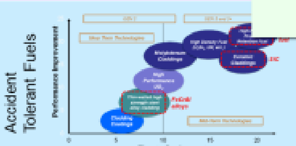
HTGR Reactors
- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- Modified Fuel components (PMR/PBR)
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure



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

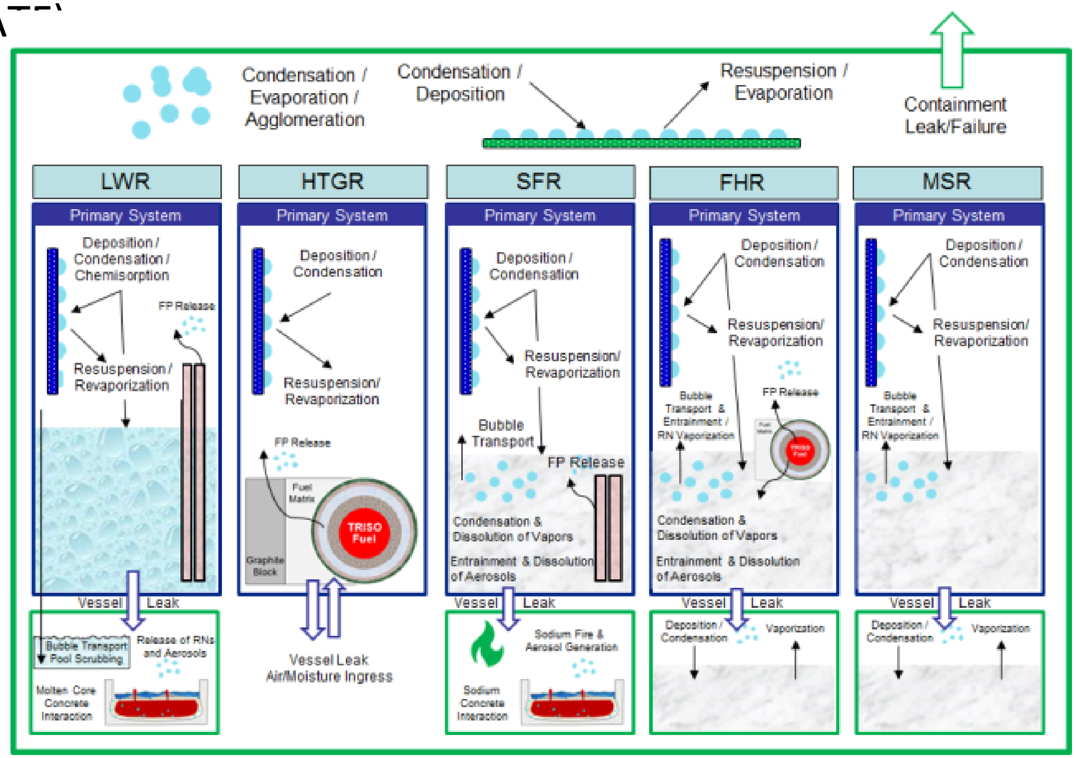
LWR and General MELCOR development

Advanced Technology Fuels (A

Non-LWR Reactors

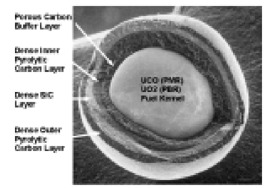
- HTGR
- Sodium
- Molten Salts

Spent Fuel Pools



High Temp Gas-Cooled Reactors

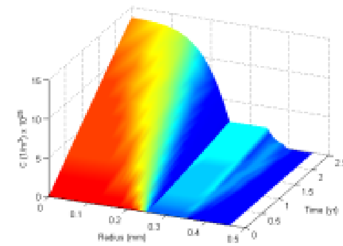
- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- New COR components for PBR and PMR designs
- Core conduction
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure
- Graphite dust transport
  - Turbulent deposition,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

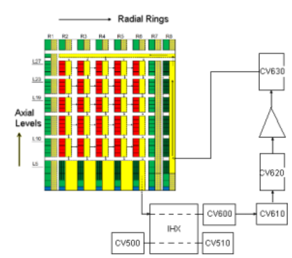


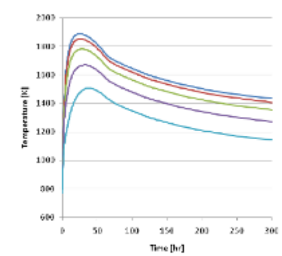
$$\frac{\partial C}{\partial t} = \frac{1}{r^m}\frac{\partial}{\partial r}\left(r^m D \frac{\partial C}{\partial r}\right) - \lambda C + S$$

$m = 1$ (*cylindrical*)

$m = 2$ (*spherical*)







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.

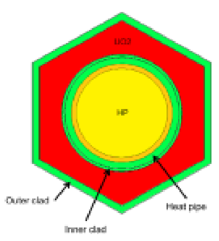
MELCOR accommodates HP models of different fidelity through a common interface.

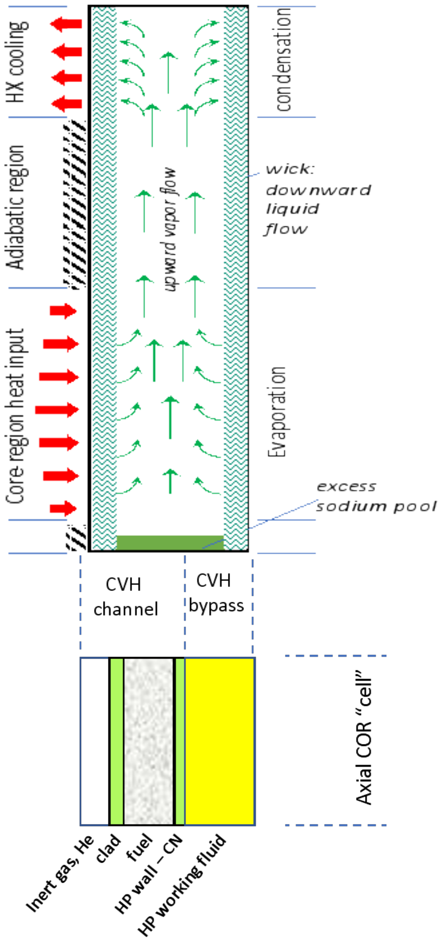
- Model 1: working fluid region modeled as high thermal conductivity material
- Model 2 (new in 2020 release): thermodynamic equilibrium approximation of working fluid (sodium or potassium EOS). P, T and liq/vap fraction evolve in time. Sonic, capillary and boiling limits enforced.
- If needed, higher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

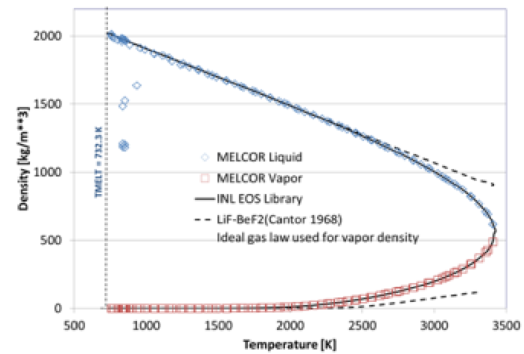
At failure, HP materials and regions transition to COR and CVH modeling.

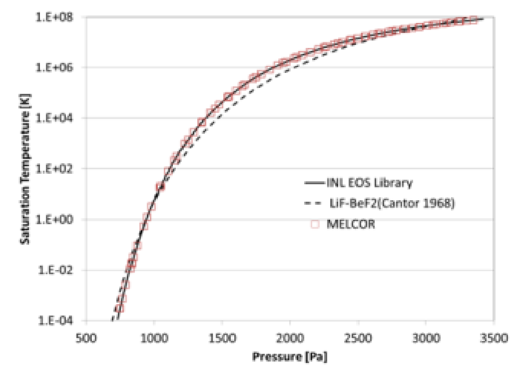




Molten Salt Reactors

- Properties for LiF-BeF2 have been added
  - Equation of State
  - Thermal-mechanical properties
  - EOS for other molten salt fluids would need to be developed
- Two reactor types envisioned
  - Fixed fuel geometry
    - TRISO fuel models
  - Liquid fuel geometry
    - MELCOR CVH/RN package can model flow of coolant and advection of internal heat source with minimal changes
  - Framework for fission thermal power generation without COR package
    - 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
    - Calculation of neutronics kinetics for flowing fuel
- Radionuclide Transport
  - Molten salt fission product release models
  - Thermochemistry modeling using Thermochemica





Circulating Fuel Point Kinetics Model

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

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

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

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

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 Chemistry and Radionuclide Release

Model Scope

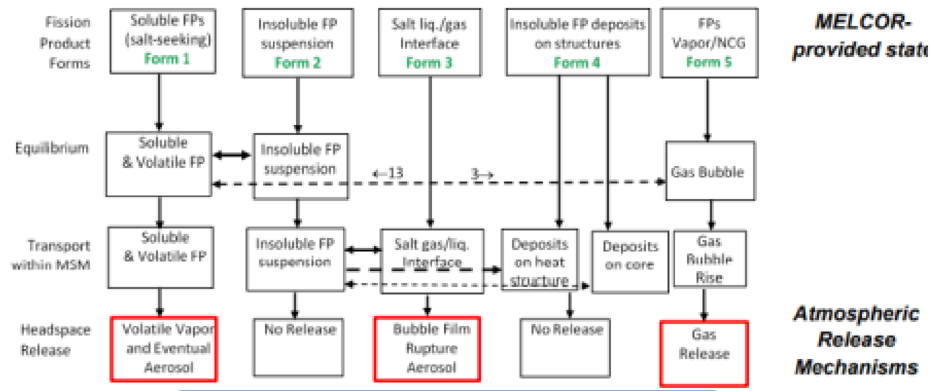
Evaluation of thermochemical state

- Gibbs Energy Minimization with Thermochimica
- Provides solubilities and vapor pressures

Thermodynamic database

- Generalized approach to utilize any thermodynamic database
- An example is the Molten Salt Thermal Database
  - FLiBe-based systems
  - Chloride-based systems

Radionuclides grouped into forms found in the Molten Salt Reactor Experiment



Initial Model Form

Solubility determined from empirical evidence (P. Britt ORNL 2017)

Solubilities mapped to 17 MELCOR fission product classes

Insoluble MELCOR classes are assigned to be colloidal

MELCOR Software Quality Assurance Best Practices

MELCOR SQA Standards

SNL Corporate procedure IM100.3.5
CMMI-4+
NRC NUREG/BR-0167

Emphasis is on Automation

Affordable solutions
Consistent solutions

MELCOR Wiki
- Archiving information
- Sharing resources (policies, conventions, information, progress) among the development team.

Code Configuration Management (CM)
- 'Subversion' (Transitioning to Git)
- TortoiseSVN (Transitioning to TortoiseGit
- VisualSVN integrates with Visual Studio (IDE)
- Transitioning to GitLab

Code Review
- Code Collaborator (Transitioning to GitLab)

Continuous builds & testing (Transitioning to CMAKE)
- DEF application used to launch multiple jobs and collect results
- Regression test report
- More thorough testing for code release

Bug tracking and reporting
- Bugzilla online (Transitioning to GitLab)

Code Validation
- Assessment calculations
- Code cross walks for complex phenomena where data does not exist.

Documentation
- Available on repository with links from wiki
- Latest PDF with bookmarks automatically generated from word documents under Subversion control
  - Links on MELCOR wiki

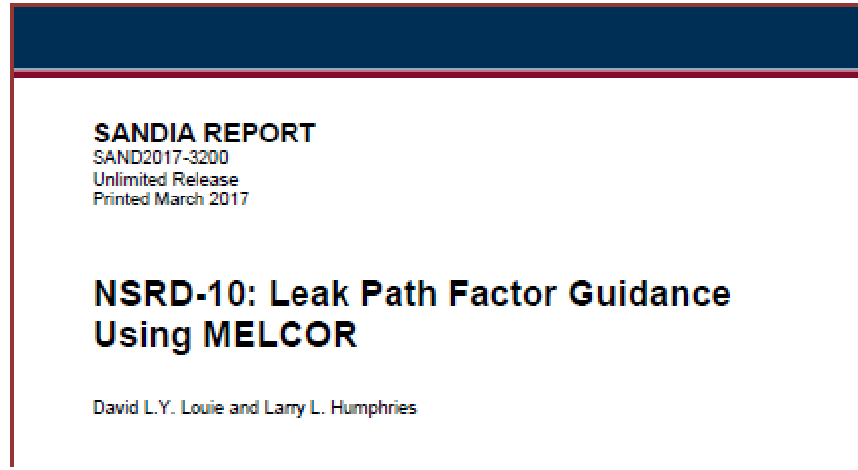
Project Management
- Jira for tracking progress/issues
  - Can be viewable externally by stakeholders

Sharing of information with users
- External web page
- MELCOR workshops
- MELCOR User Groups (EMUG & AMUG)

Annual NRC audits

Verification & Validation of Models for Nuclear Facility Safety

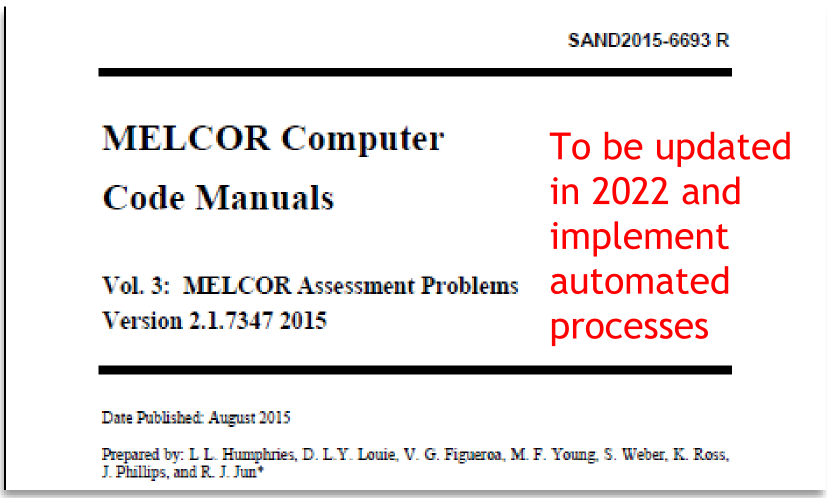
- MELCOR 2.1 guidance was developed, including V&V
  - V&V from
    - Selected DOE-HDBK-3010 experiments
    - Applicable validations from SAND2015-6693 R
    - CFAST validation benchmark experiment
    - Verifications from MELCOR 1.8.5 guidance report



SANDIA REPORT
SAND2017-3200
Unlimited Release
Printed March 2017

NSRD-10: Leak Path Factor Guidance Using MELCOR

David L.Y. Louie and Larry L. Humphries



SAND2015-6693 R

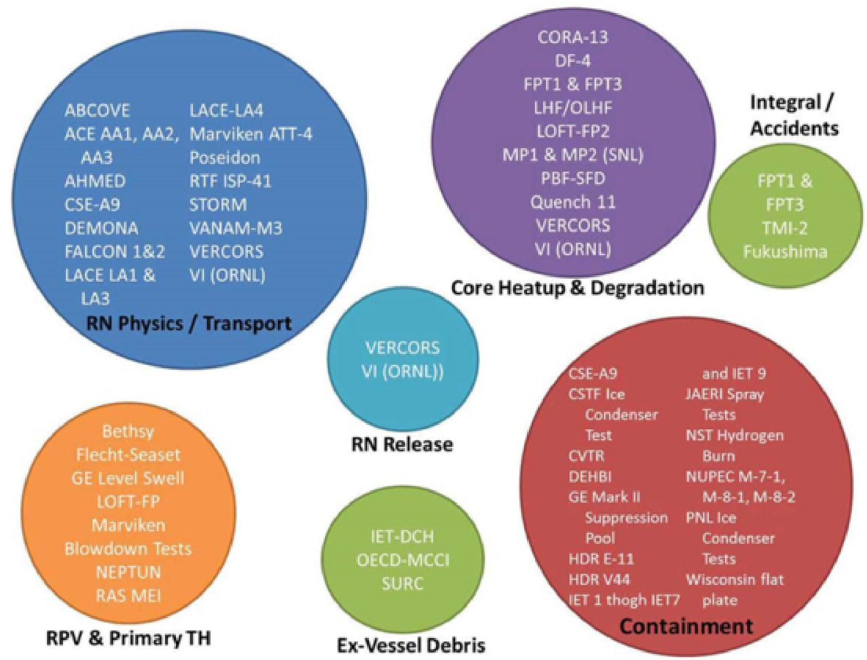
MELCOR Computer Code Manuals

Vol. 3: MELCOR Assessment Problems
Version 2.1.7347 2015

Date Published: August 2015

Prepared by: L. L. Humphries, D. L.Y. Louie, V. G. Figueroa, M. F. Young, S. Weber, K. Ross, J. Phillips, and R. J. Jun*

To be updated in 2022 and implement automated processes



- Only separate effect tests of reactor experiments are applicable to SB
  - RN physics/transport
  - Containment

Code Validation

Importance of Code Validation

- Code Developers
  - provide the necessary guidance in developing and improving models
  - Desirable to have validation test at time of model implementation
- Code Users
  - Increased confidence in applying code to real-world application
  - Improved understanding of modeling uncertainties

Sources of Validation

- Analytical Methods
  - Limited in terms of problem types that can be assessed
  - Isolates physics and removes complications from multiple physics
  - Removes uncertainty from experimental operations and measurements
- Separate Effects Tests
  - Isolates physics and removes complications from multiple physics
  - Often it is difficult or impossible to isolate physics in an experiment
- Integral Tests (No SB integral tests in validation database)
  - Examines relationships between coupled processes
  - Tests should be selected that are applicable to the calculation domain of the code.
- Actual Incidents (Currently no such events for SB analysis have been added to MELCOR validation)
  - Captures all relevant physics
  - Poorly ‘instrumented’

Validations should focus on what can be learned from the exercise

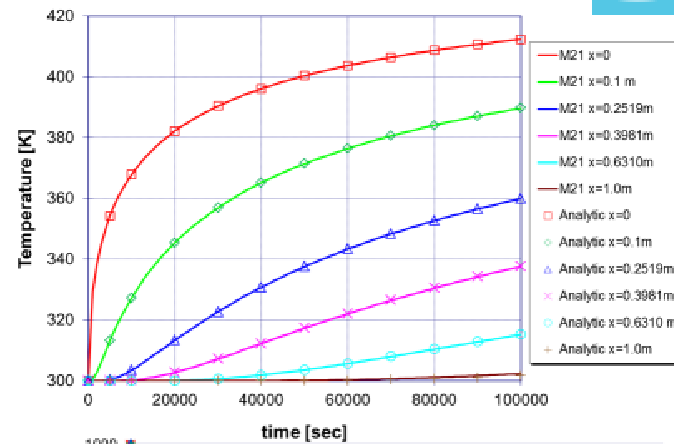
Validation must avoid trying to ‘tune’ results

Use default values for all models or justify the use of any non-default parameters

Analytic Solutions for Heat Structures

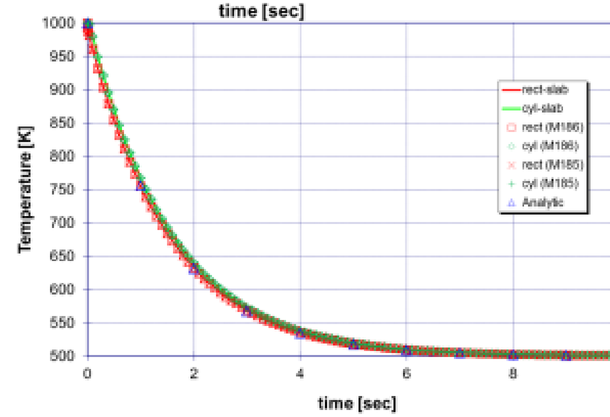
Transient Heat Flow in a Semi-Infinite Heat Slab

$$\frac{T-T_i}{T_o-T_i}=1-erf\left[\frac{x}{2\sqrt{\alpha t}}\right]-\exp\left[\frac{hx}{k}+\frac{h^2\alpha t}{k^2}\right]\left[1-erf\left(\frac{x}{2\sqrt{\alpha t}}+\frac{h\sqrt{\alpha t}}{k}\right)\right]$$



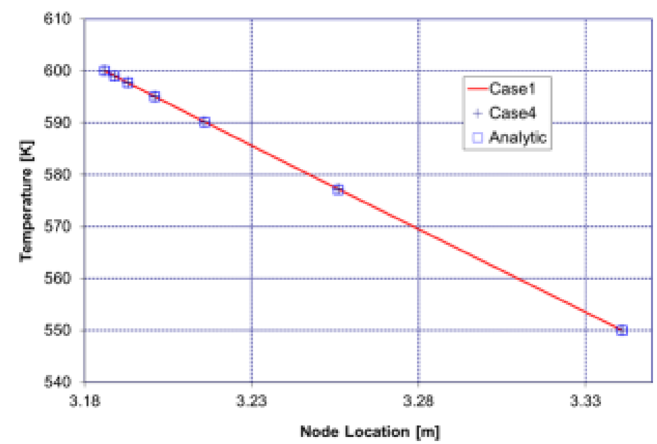
Cooling of Heat Structures in a Fluid

$$T=T_f+\left(T_i-T_f\right)\left[\exp\left(\frac{-hAt}{\alpha V}\right)\right]$$

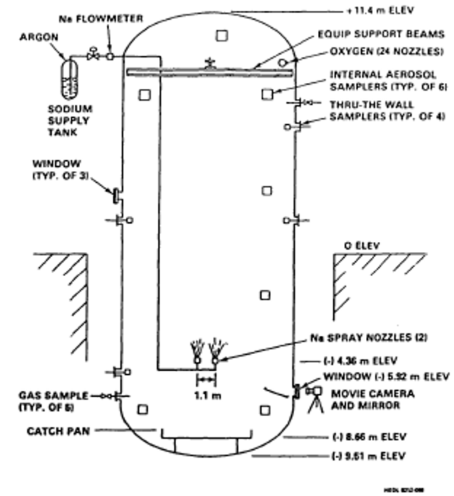


Radial Heat Conduction in Annular Structures

$$T=T_{em,i}-\left(\frac{\ln\left(r_i/r_o\right)}{k}+\frac{1}{h_i r_i}\right)\left(\frac{\left(T_{em,i}-T_{em,o}\right)}{\frac{\ln\left(r_o/r_i\right)}{k}+\frac{1}{h_i r_i}+\frac{1}{h_o r_o}}\right)$$

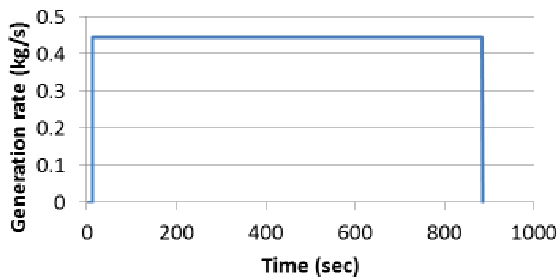


ABCOVE: Background



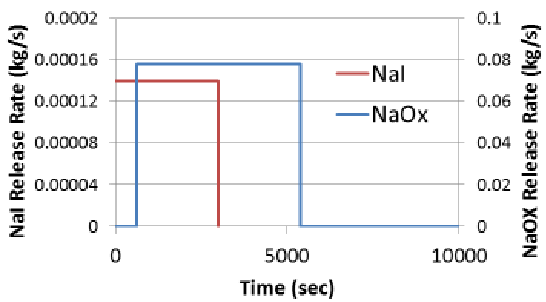
General Description:

- Simulation of the dry atmosphere conditions of an LMFBR containment with a sodium fire, i.e., sodium combustion product aerosols.
- AB6 modeled fission product aerosols, sodium iodide (NaI), in the presence of sodium combustion product aerosol (NaOx).



Important Physics:

- Agglomeration behavior of two aerosol species (hygroscopic and non-hygroscopic), condensation of water vapor.

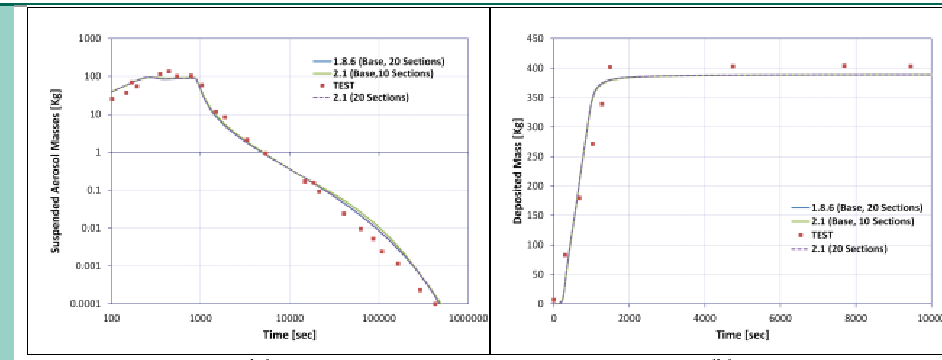


References

- Souto, F.J., Haskin, F.E., Kmetyk, L.N., “MELCOR 1.8.2 Assessment: Aerosol Experiments ABCOVE AB5, AB6, AB7, and LACE LA2,” SAND94-2166 (1994),

ABCOVE: Status

- AB5
  - Predicted airborne mass is in very good agreement with the experimental results

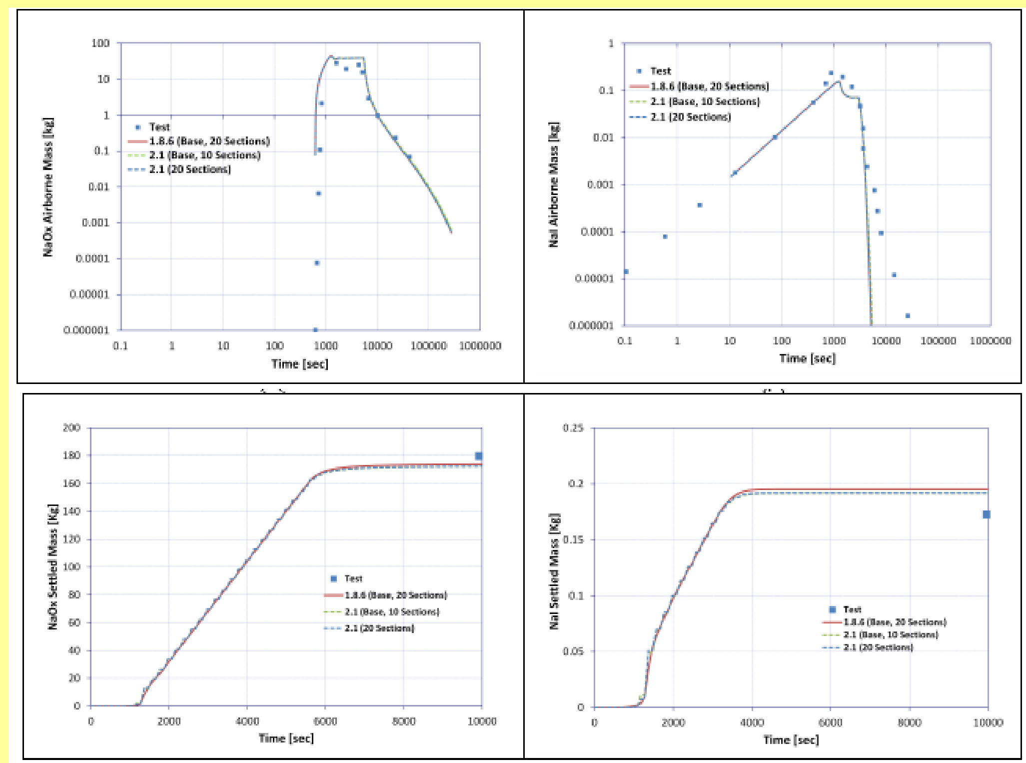


Airborne Mass | Deposited Mass

- AB6
  - MELCOR adequately predicts deposition of the sodium combustion, NaOX, aerosols
  - MELCOR overpredicts aerosol depletion of NaI, possibly due to lack of resuspension modeling

Airborne Mass

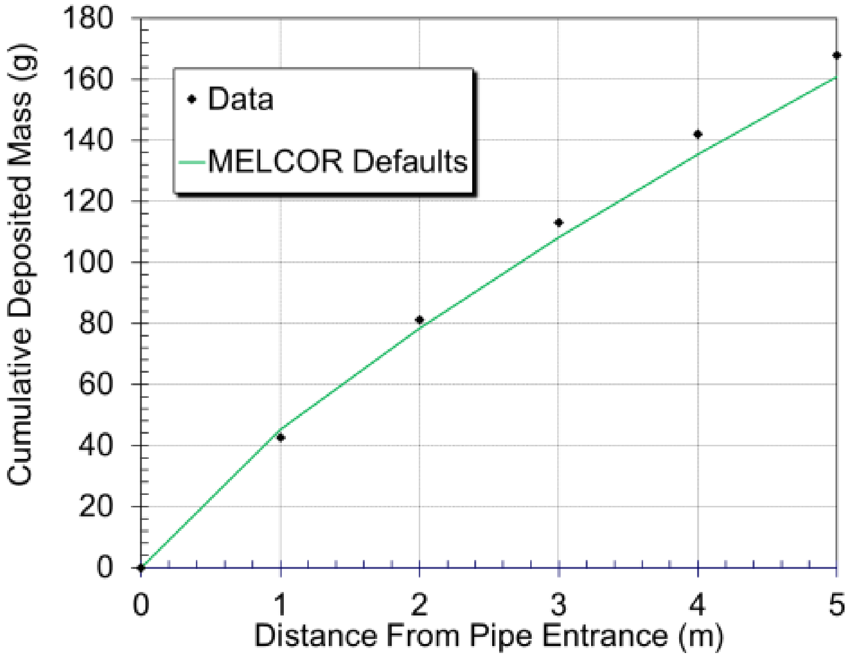
Settled Mass



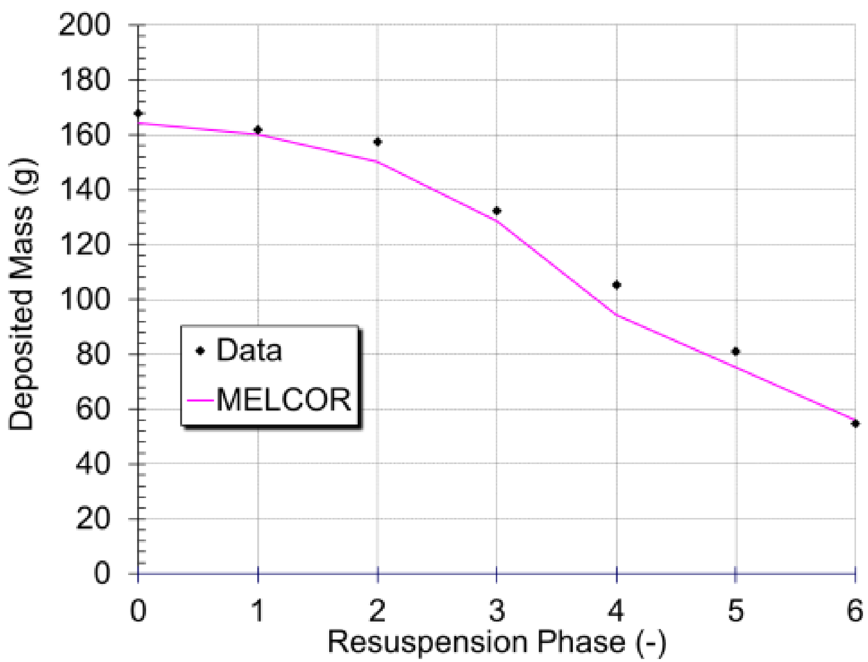
NaOx | NaI

STORM Tests Thermophoresis and Resuspension Validation

Deposition Phase



Resuspension Phase



General Description:

- A series of hygroscopic aerosol experiments were conducted at the AHMED Test Facility by injecting NaOH in aerosol form into an atmosphere with controlled humidity.

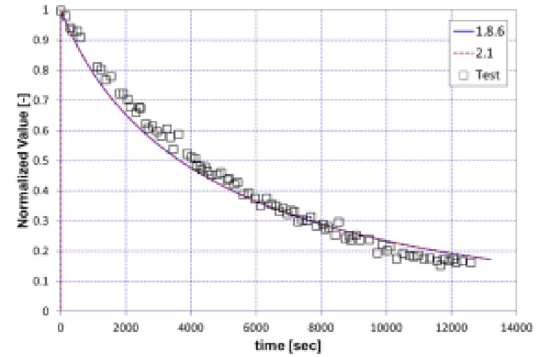
Important Physics:

- Hygroscopic effects under differing humidity conditions and the impact on aerosol masses available for release.

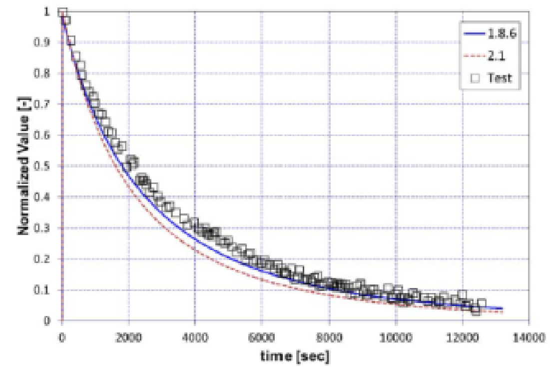
AHMED Test Results

Both MELCOR 2.x and 1.86 simulations were performed at various RH and their results were compared with experiment data. At these RHs, the MELCOR simulations always yielded results that were close to the test data.

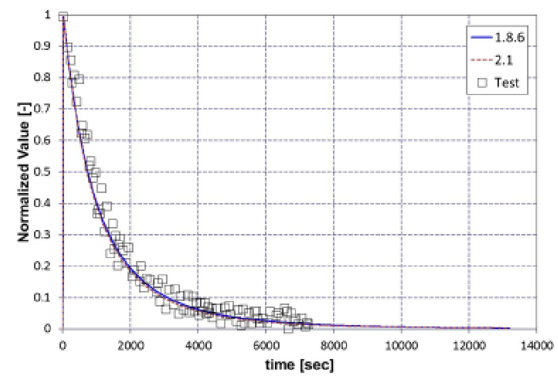
RH=22%



RH=82%



RH=96%



NUPEC M-7-1, M-8-1, and M-8-2

Validation objectives

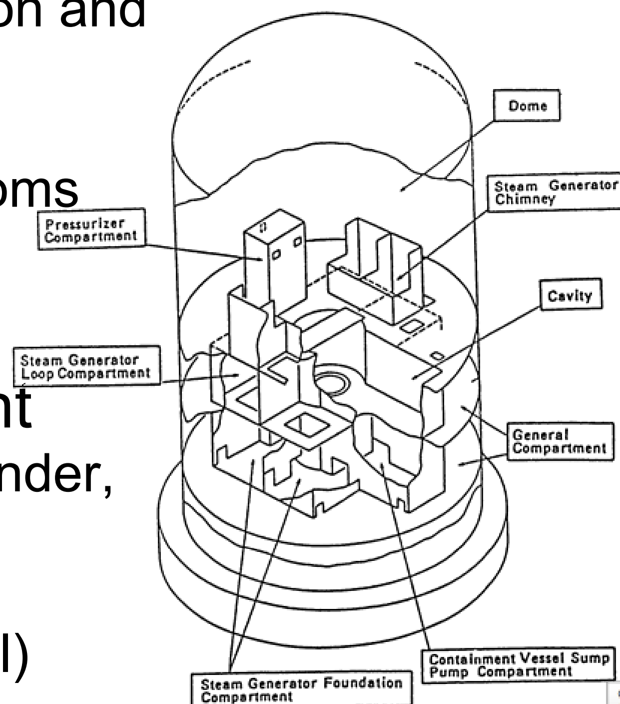
- Pressure response;
- Temperature distribution and stratification
- Hydrogen mixing
- Advection between rooms
- Spray modeling
- Film Tracking Model

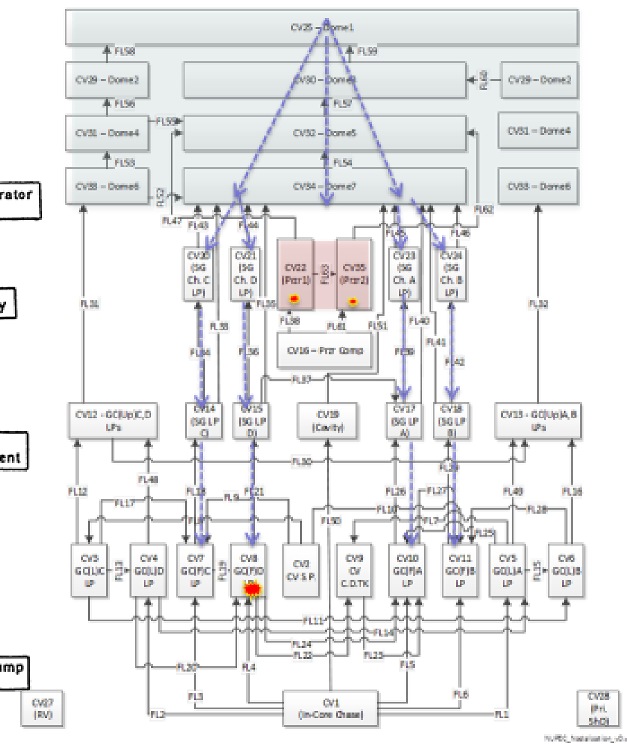
¼ Scale Containment

- 10.8 m OD domed cylinder,
- 17.4 m high
- 25 interconnected compartments (28 total)

Sprays

- M-8-1 No Sprays
- M-7-1 and M-8-2 Sprays modeled





He Concentration Distributions

Without sprays

- Slightly overprediction of He concentration in lower general compartments

With sprays

- He concentration well-predicted for all compartments