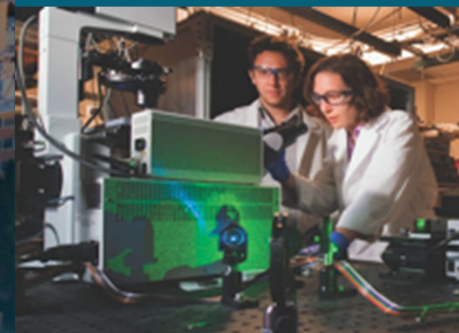
MELCOR Overview

SAND2023-01793PE



PRESENTED BY

Larry Humphries

SAND2023-

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Objective of Presentation

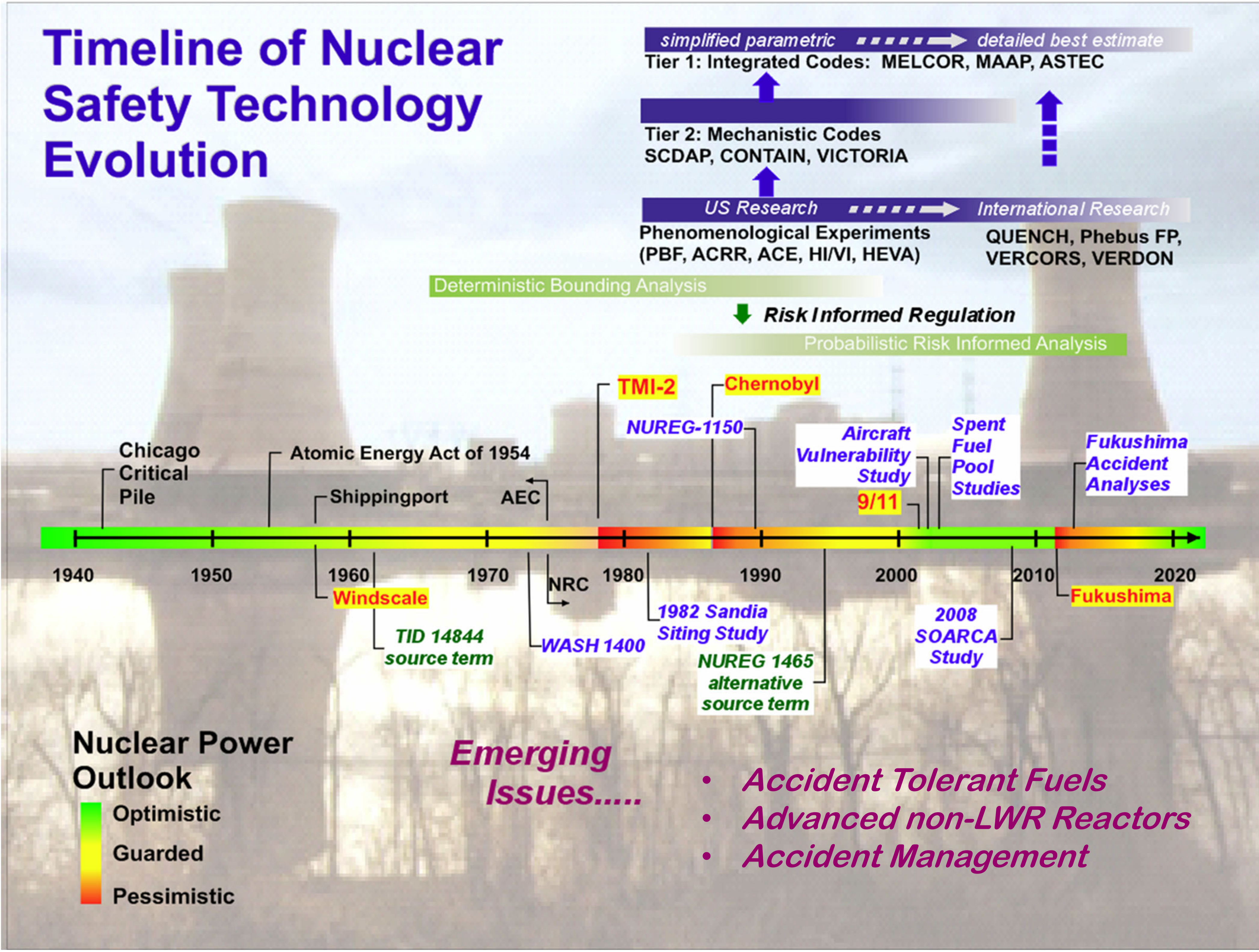
Introduce MELCOR simulation code

- What is it, and what it does
- General view of phenomena modeled
  - Provide specific examples of MELCOR models with illustrative workshop examples.

Code Development Timeline & Modeling Strategy

Show top level organization of MELCOR

- MELGEN and MELCOR executables
- Organization of modeling as "Packages"
  - Phenomena modeled in various packages
  - Interfaces between packages
  - Illustrate the utility of the Control Function Package in interfacing with MELCOR



Timeline of Nuclear Safety Technology Evolution
simplified parametric
detailed best estimate
Tier 1: Integrated Codes: MELCOR, MAAP, ASTEC
Tier 2: Mechanistic Codes
SCDAP, CONTAIN, VICTORIA
US Research
International Research
Phenomenological Experiments
(PBF, ACRR, ACE, HI/VI, HEVA)
QUENCH, Phebus FP,
VERCORS, VERDON
Deterministic Bounding Analysis
Risk Informed Regulation
Probabilistic Risk Informed Analysis
TMI-2
Chernobyl
NUREG-1150
Aircraft Vulnerability Study
Spent Fuel Pool Studies
Fukushima Accident Analyses
Chicago Critical Pile
Atomic Energy Act of 1954
Shippingport
AEC
9/11
1940
1950
1960
1970
1980
1990
2000
2010
2020
Windscale
NRC
Fukushima
TID 14844 source term
WASH 1400
1982 Sandia Siting Study
NUREG 1465 alternative source term
2008 SOARCA Study
Nuclear Power Outlook
Optimistic
Guarded
Pessimistic
Emerging Issues.....
• Accident Tolerant Fuels
• Advanced non-LWR Reactors
• Accident Management

Requirements of an Integrated Severe Accident Code

Fully Integrated, multi-physics engineering-level code
- Thermal-hydraulic response in the reactor coolant system, reactor cavity, containment, and confinement buildings;
- Core heat-up, degradation, and relocation;
- Core-concrete attack;
- Hydrogen production, transport, and combustion;
- Fission product release and transport behavior

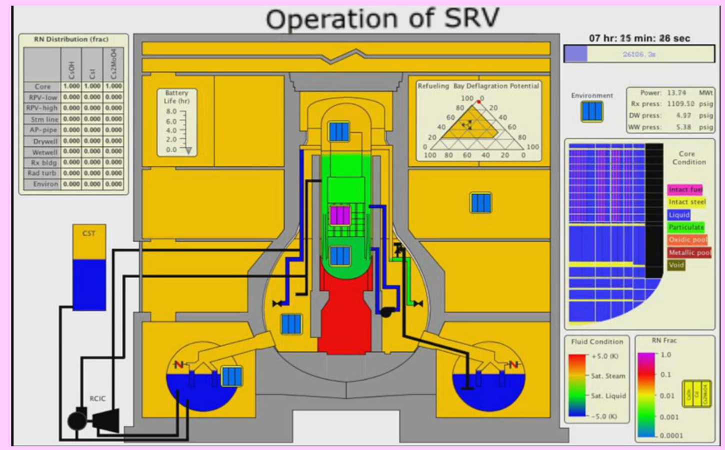
Diverse Application
- Multiple 'CORE' designs
- User constructs models from basic constructs
- Adaptability to new or non-traditional reactor designs
  - ACR700, ATR, VVER, HTGR, …

Validated physical models
- ISPs, benchmarks, experiments, and accidents

Uncertainty Analysis & Dynamic PRA
- Relatively fast-running
- Reliable code
- Access to modeling parameters

User Convenience
- Windows/Linux versions
- Utilities for constructing input decks (GUI)
- Capabilities for post-processing, visualization
- Extensive documentation

Multi- Physics

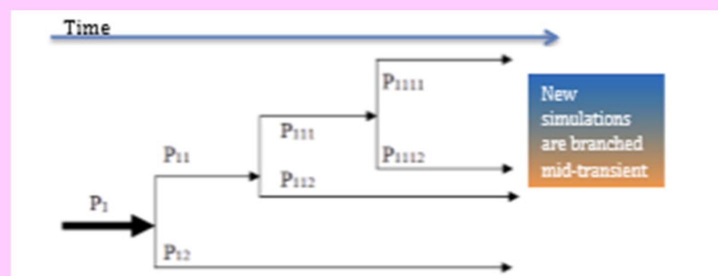


SOARCA LTSBO

Diverse Application

Advanced Test Reactor

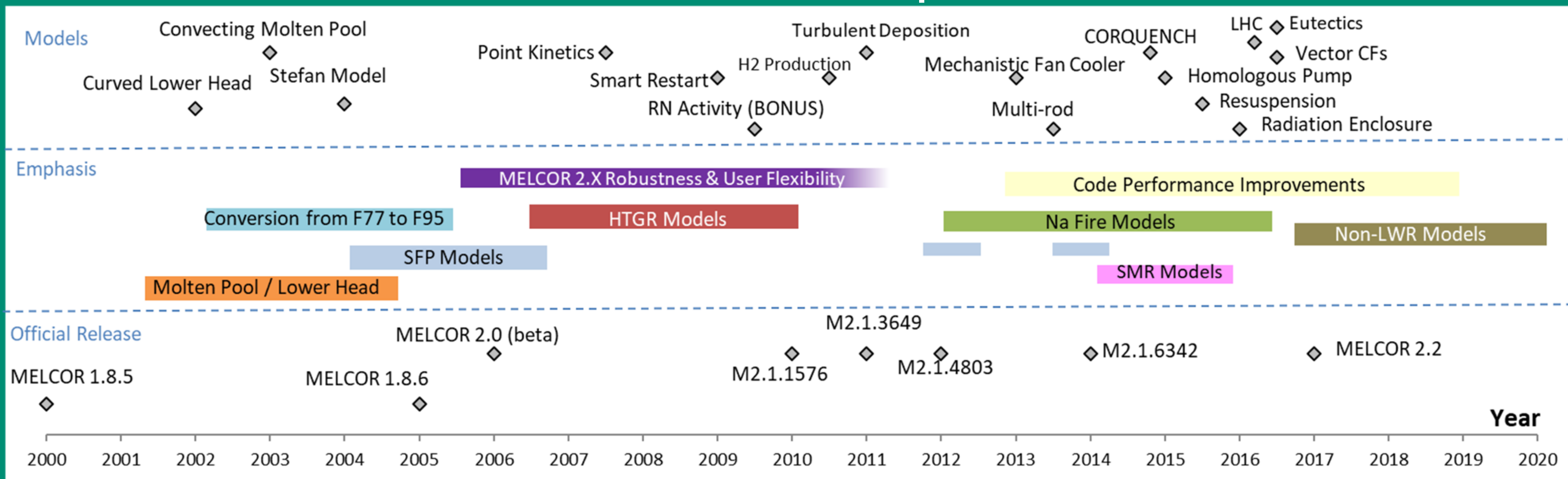
Uncertainty & Dynamic PRA

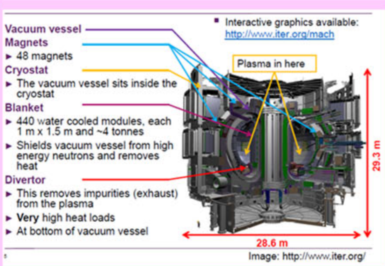


Dynamic Event Tree

MELCOR Model Development

MELCOR Code Development





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 f... l risl... studi...

Multi... iden... area ...n)

Dry S...

HTGR Reactors

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

Sodium Reactors

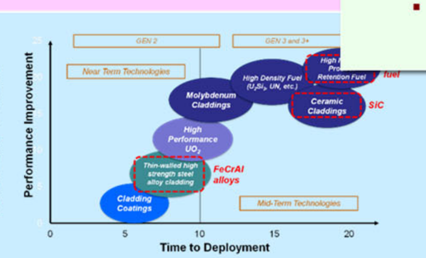
...odium Properties
- Sodium Equation of State
- Sodium Thermo-mechanical properties

...ontainment 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

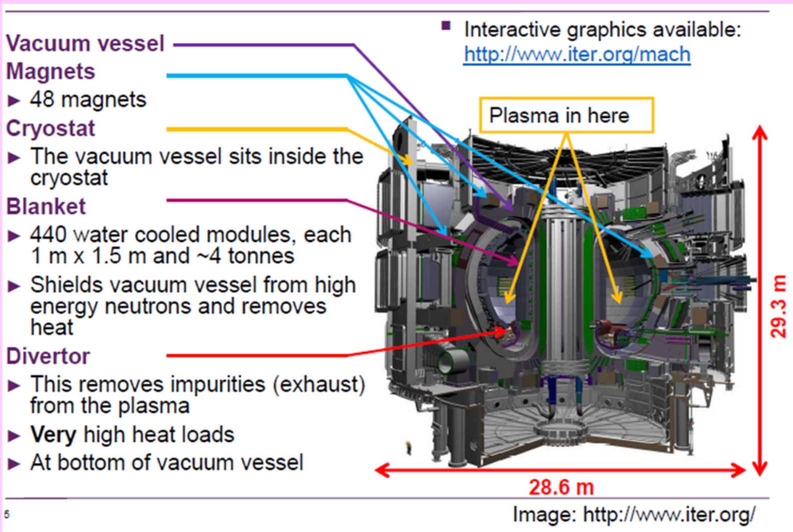
...Tolerant Fuels



Non-Reactor Applications

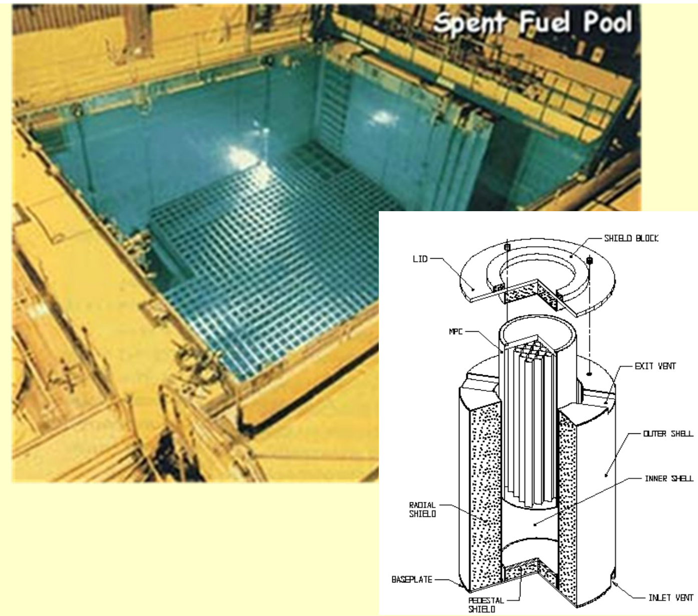
Advanced Reactor Applications

Non-Reactor Applications



Spent Fuel

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



Fusion

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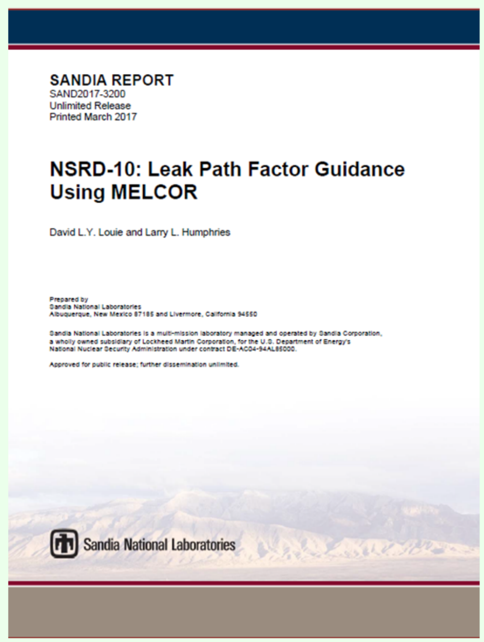

SANDIA REPORT
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NSRD-10: Leak Path Factor Guidance Using MELCOR

David L.Y. Louie and Larry L. Humphries

Prepared by
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Sandia National Laboratories

Non-Nuclear Facilities

- Leak Path Factor Calculations (LPF)
  - Release of hazardous materials from facilities, buildings, confined spaces
- DOE Safety Toolbox code
- DOE nuclear facility users
  - Pantex
  - Hanford
  - Los Alamos
  - Savannah River Site

LWR/Non-LWR/ATF Fuels Development

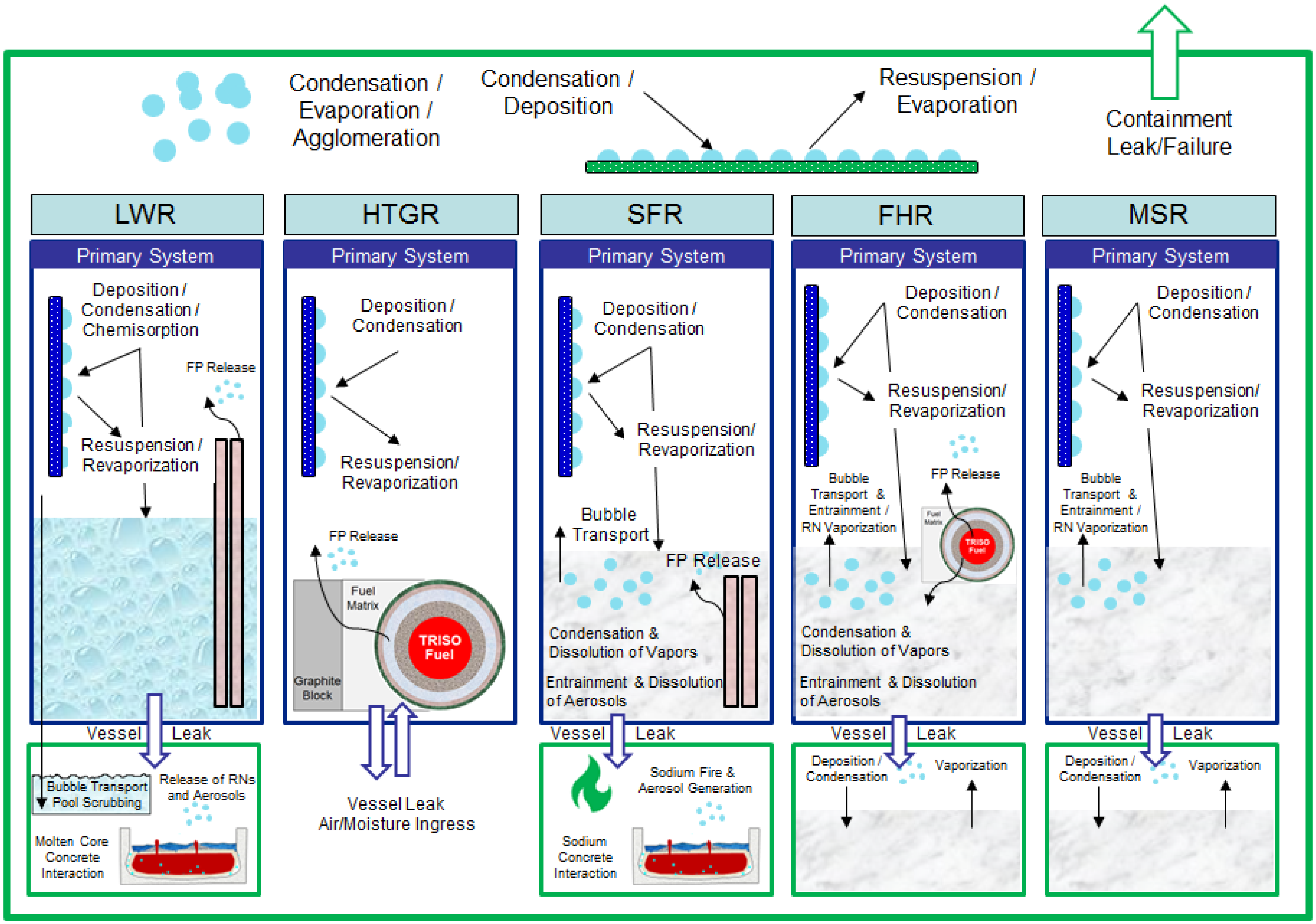
LWR and General MELCOR development

Advanced Technology Fuels (ATF)

Non-LWR Reactors

- HTGR
- Sodium
- Molten Salts

Spent Fuel Pools



Phenomena Modeled by MELCOR

Goal of modeling "all" relevant phenomena is quite ambitious

Main phenomena modeled include

- Two-phase hydrodynamics, from RCS (Reactor Coolant System) to environment
- Heat conduction in solid structures
- Reactor core heatup and degradation
- Ex-vessel behavior of core debris
- Fission product release and transport
- Aerosol and vapor physics

Others will be mentioned in presentation

There is no detailed neutronics model

- Fission power history can be user-specified
- Point kinetics model available

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

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 are 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 are 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

MELGEN and MELCOR

"MELCOR" is actually two executables that perform different parts of the simulation

MELGEN is run first

- Its basic task is to set up the desired calculation
  - Problem definition, input checking, and initial and boundary conditions
- Has no time-advancement capability

MELCOR is run next

- Its basic task is to advance the simulation in time and provide output
- Reads complete problem description from a file
- Has limited ability to modify that description before starting the time advancement

Two codes share many subroutines

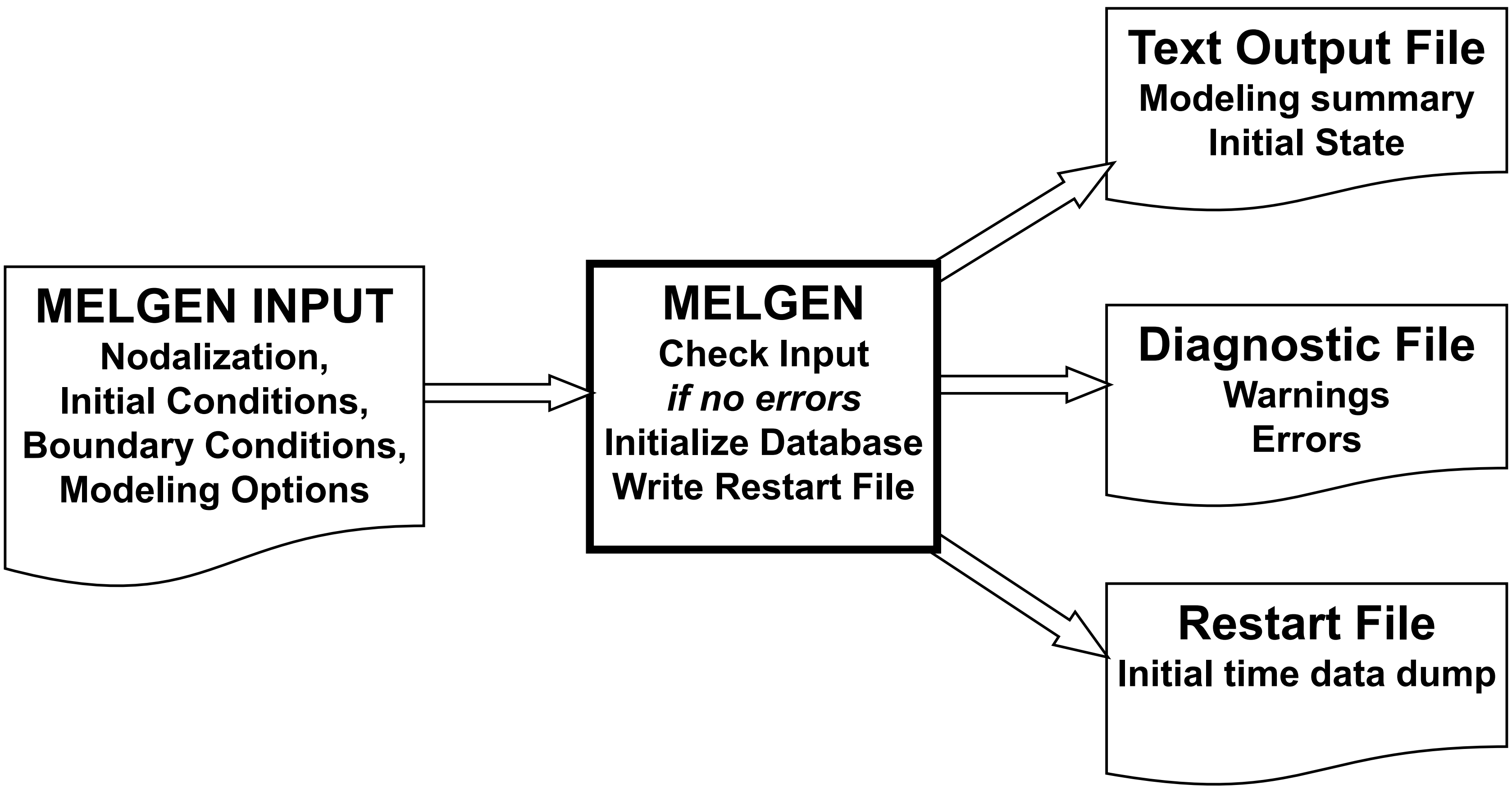
- I/O, properties, etc.

MELGEN

MELGEN execution

- Basic task is to set up the desired calculation
- Input focuses on problem definition
  - Reads description of system to be simulated as provided through user input, including:
    - Nodalization to be used
    - Initial and boundary conditions
    - Modeling options
  - Checks input for completeness and consistency
  - Issues diagnostic warnings and/or error messages when appropriate
- If (and *only* if) input contains no errors
  - Initializes all time-dependent data
  - Writes full text edit with model and state description
  - Writes restart file dump with complete database

MELGEN Files and Information Flow

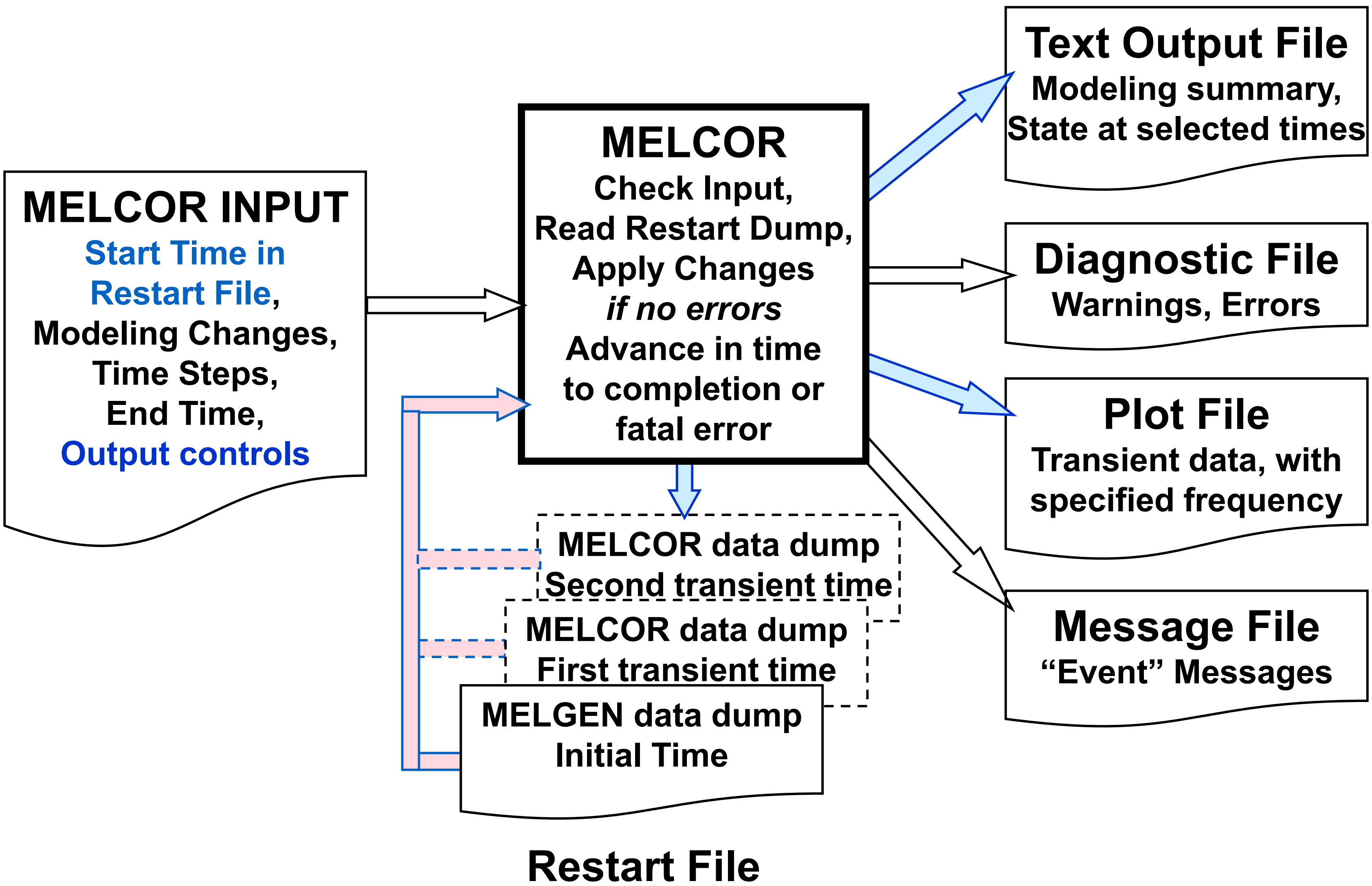


MELCOR

MELCOR execution

- Basic task is to advance simulation in time
- Always run in "restart" mode
  - Reads time-independent and initial time-dependent data from a restart file "dump"
    - May be more than one, corresponding to different simulation times
      - First restart file was written by MELGEN
      - Can have later ones written by previous MELCOR execution(s)
  - Advances time-dependent data through time
- Input focuses on control of advancement
  - Start time, end time, time steps, output frequency
  - Limited capability to modify problem description
    - Useful for sensitivity studies, treatment of branches in event trees
  - Writes text edits, restart, and plot files as requested
    - Any point in the restart file can be used as the initial state for a subsequent MELCOR execution

MELCOR Files and Information Flow



MELCOR Packages

Major pieces of MELCOR called "Packages"

- Each handles a set of closely-related modeling functions
- Do *not* correspond to ancestral codes

Three general types of packages in MELCOR

- Basic physical phenomena
  - Hydrodynamics, heat and mass transfer to structures, gas combustion, aerosol and vapor physics, etc.
- Reactor-specific phenomena
  - Core degradation, ex-vessel phenomena, sprays and other ESFs (Engineered Safety Features)
- Support data and functions for general use
  - Thermodynamic equations of state, other material properties, decay heat generation data
  - Data-handling utilities, equation solvers

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.

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

COR Package
COR Components, Lower Head, Oxidation, Molten Pool, Eutectic Models, TRISO Models, Heat Pipes,...

CAV Package
- Core Concrete Interactions
- Quenching of flooded cavity. Material Interactions

Reactor specific Models

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

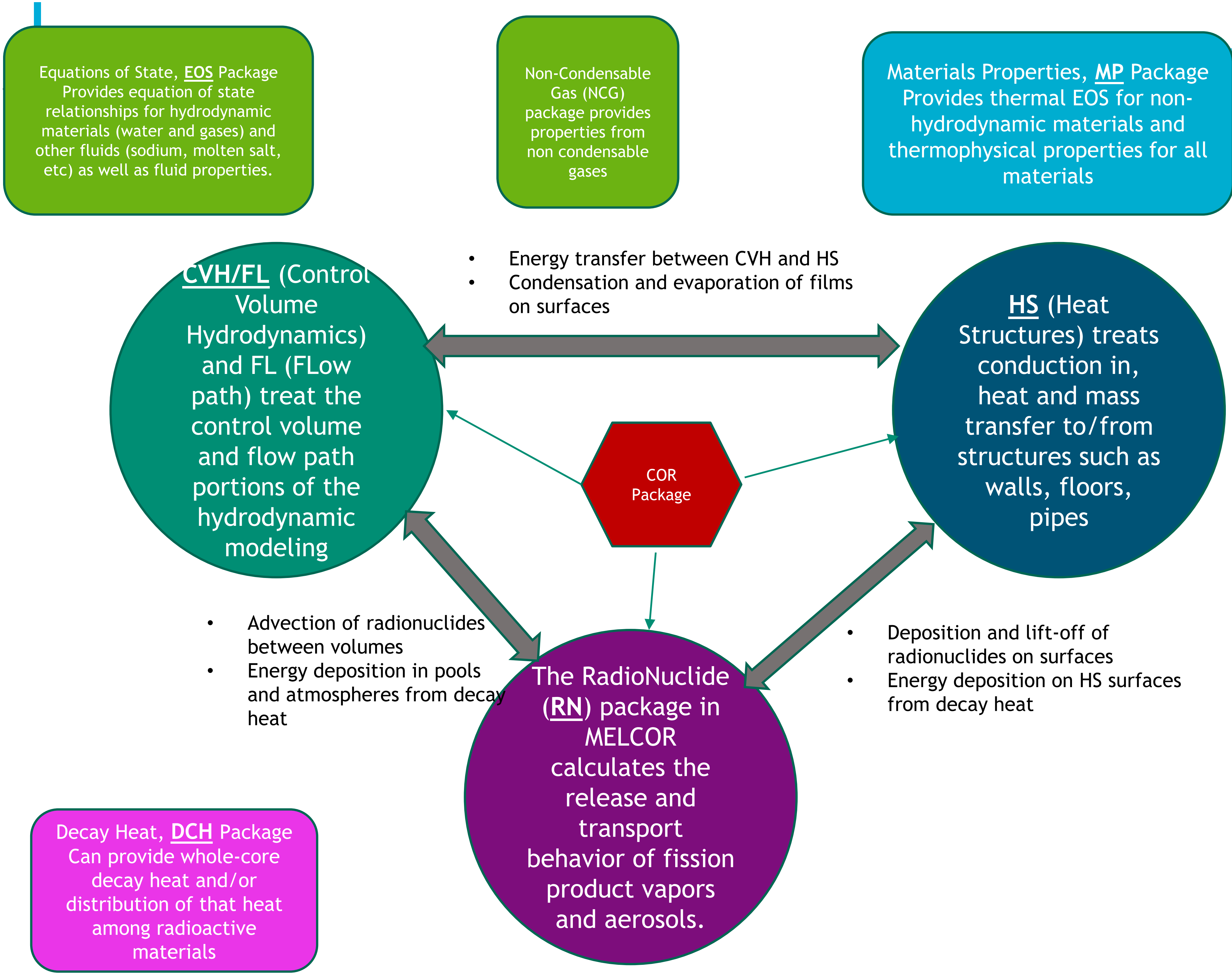
Non-Condensable Gas (NCG) package provides properties from non condensable gases

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

CAV Package
- Core Concrete Interactions
- Quenching of flooded cavity. Material Interactions

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

Misc Engineering Systems/Safety Packages: SPR, PAR, FDI, LHC, CND, NAC,BUR, ACC, etc.



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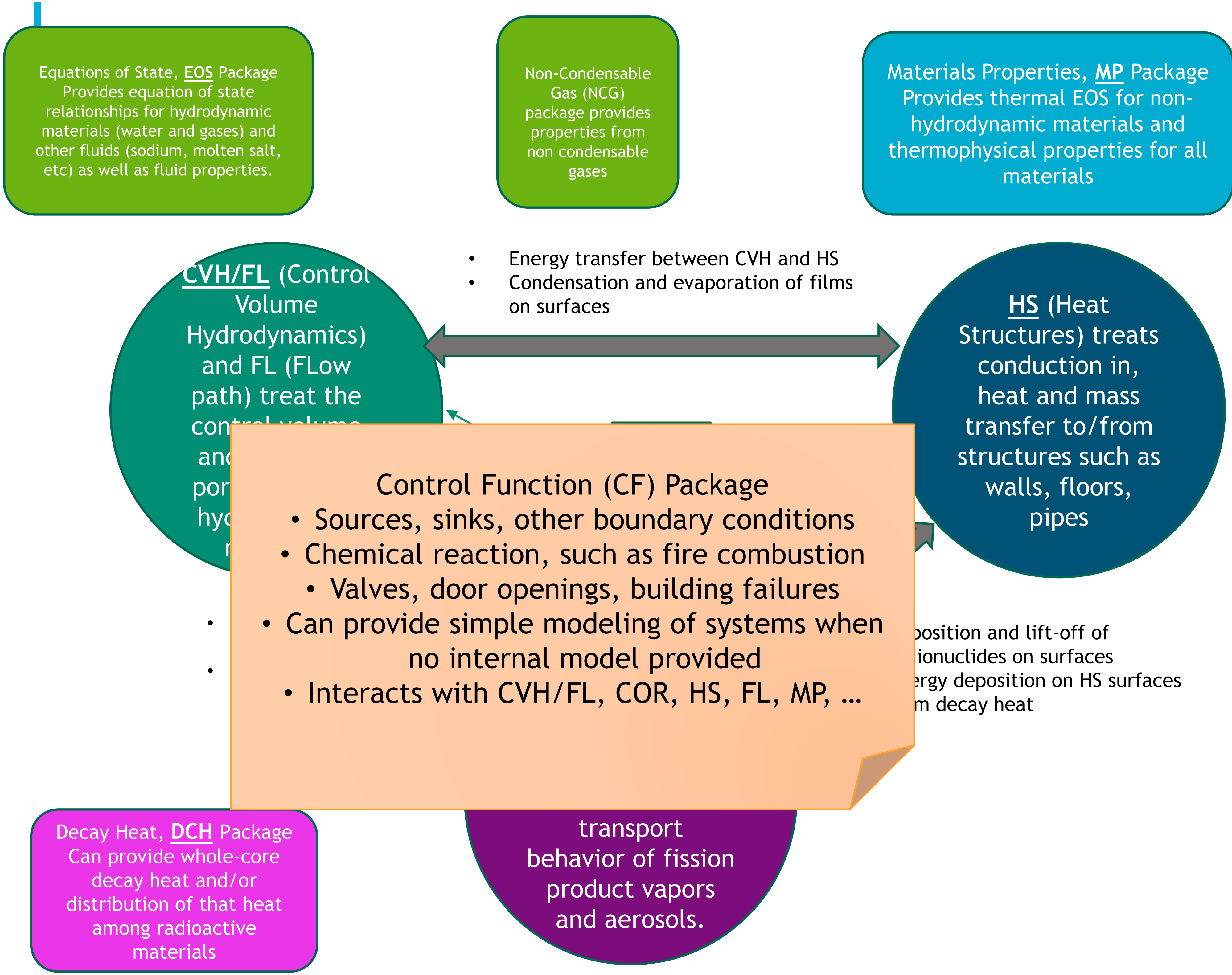
Non-Condensable Gas (NCG) package provides properties from non condensable gases
Materials Properties, MP Package
Provides thermal EOS for non-hydrodynamic materials and thermophysical properties for all materials
CVH/FL (Control Volume Hydrodynamics) and FL (FLow path) treat the control volume and flow 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
COR Package
• 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



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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
• Interacts with CVH/FL, COR, HS, FL, MP, …
position and lift-off of
ionuclides on surfaces
ergy deposition on HS surfaces
m decay heat
Decay Heat, DCH Package
Can provide whole-core decay heat and/or distribution of that heat among radioactive materials
transport behavior of fission product vapors and aerosols.

MELCOR Code Structure

Code structure reflects basic phenomena more than reactor design

- Same general control-volume/flow-path hydrodynamics used in reactor cooling system and containment
- There is NO single package that deals with the vessel and all its contents or with a steam generator
  - This generality makes MELCOR ideally suited for facility safety modeling

Time advancement for each package is local to that package but coordinated within the overall MELCOR system time step.

- Reduces need for simultaneous solutions of many equations
  - Solution strategy for each can be appropriately chosen
- Possible through carefully designed package interfaces
  - Restricted information exchange between packages
  - Use of partially-implicit "predictor/corrector-like" methods to deal with stiffness of equations

MELCOR Top-Level Control (1)

Executive level coordinates other modules

- Manages input, output, time step definition, etc.
  - Each package has its own i/o routines, called in turn
  - Time step chosen subject to various constraints
    - Executive input defines maximum and minimum timesteps
    - Any package can request a limit on timestep for next advancement
    - Executive considers all requests and reconciles with bounds
      - Calculation will be terminated if no acceptable timestep
- Controls time advancement of each package's data, in turn
  - 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

MELCOR Top-Level Control (2)

Executive deals with advancement problems

- Any package can force a "fallback"
  - Problems in advancement of package itself
    - Convergence problem or other failure of solution algorithm
    - Change in properties too large (excessive rate of change)
  - Problems with end-of-step data from *another* package
    - Change too large (e.g. advection far overshoots ignition limit for combustion)
  - Requests repeat of advancement attempt with a reduced timestep
- Executive provides graceful termination with final text edit and restart dump if advancement fails
  - Time step less than minimum
  - Error in any package where reduced step wouldn't help
  - "Logic Error", meaning occurrence of a situation that the code developer considered impossible

More about MELCOR Packages

Packages conventionally referred to by 2- or 3-letter names, mnemonic of functions, e.g.

- CVH (Control Volume Hydrodynamics) and FL (FLow path) treat the control volume and flow path portions of the hydrodynamic modeling
- EOS (Equations of State) provides thermodynamic state equations
- HS (Heat Structures) treats conduction in, heat and mass transfer to/from structures such as walls, floors, pipes
- COR (CORe) treats reactor core response and degradation phenomena
- DCH (DeCay Heat) generates decay power history
- MP (Material Properties) provides various properties
- TF (Tabular Function) is a general table utility

In general, no duplication of function

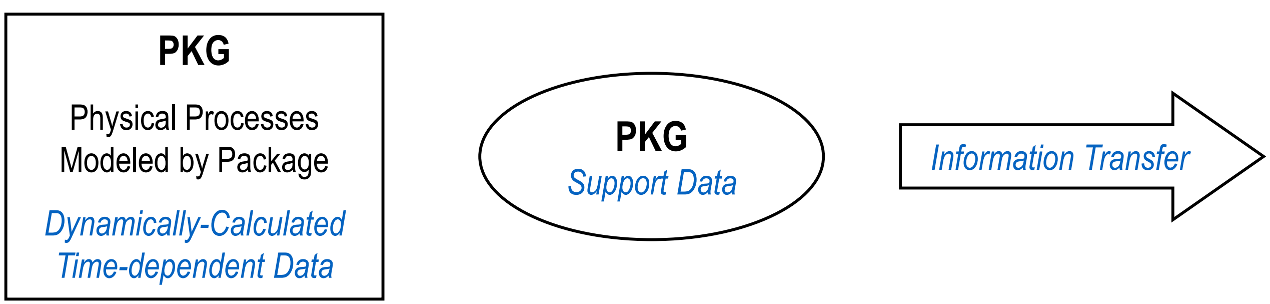
- No in-line materials properties; (should) use MP package
- All input data tables (should be) processed and stored by TF package

Basic Thermal Hydraulic Packages

Next several slides describe modeling in a few of the major packages in MELCOR

Illustrative data flow charts provide the following:

- Dynamic data associated with each package
- Information flow between packages
  - Rectangles for packages that model physical phenomena,
  - Ovals for packages that provide support data
  - Arrows for information transfer between packages



Phenomena Modeled by MELCOR, Packages Involved – Thermal Hydraulics

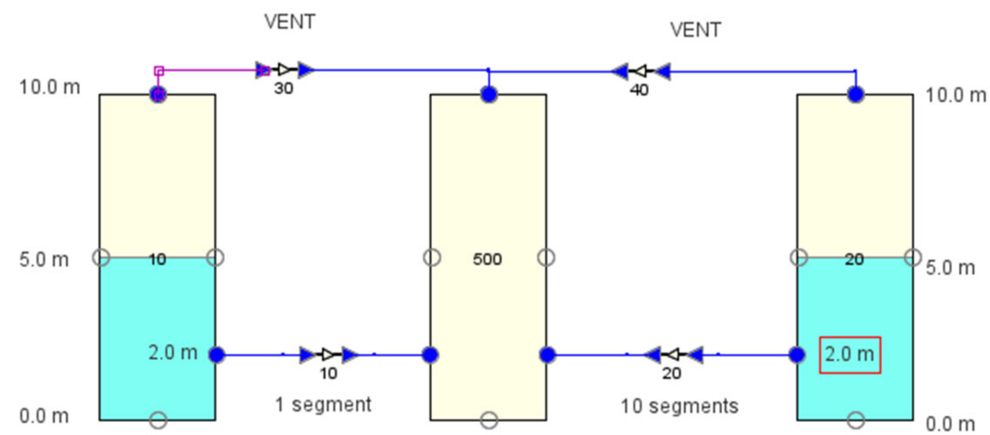
Hydrodynamics involves several packages

- CVH and FL packages treat control volume and flow path aspects (inventories and advective transport, respectively)
- EOS package provides Equations Of State (for closure)
- Interfaces to almost everything else in MELCOR
  - Provides boundary conditions to other packages
  - "Sees" most other packages only as sources and sinks of mass, energy, and volume available to fluids
    - Zircaloy oxidation in core is a sink of H_2O with source of H_2 and/or sink of O_2
    - Movement of core debris changes volume available to fluids in CVH
  - Changes in core geometry can change flow resistance
    - Not default, requires optional user input to relate nodalizations
- Most other packages are advanced first, with sources accumulated for inclusion in Hydro solution
  - Will show order later

Snaplette: Multiple FP Segments for a Simple Uniform Pipe

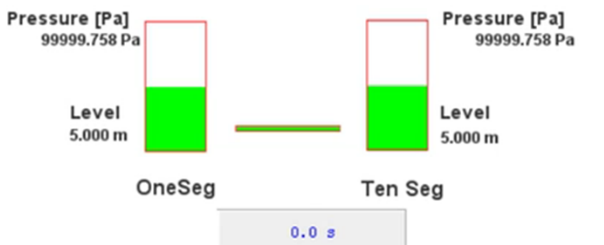
- Input Files
  - Seg_uniform.med
  - Seg_uniform_anim.med
- Job Stream/Data Source
  - Unif_Seg

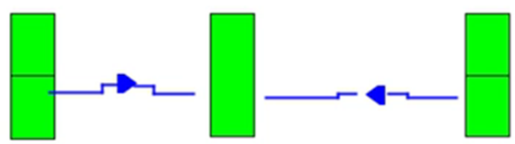
- Two identical control volumes
- Both Vented at top
- Both with uniform flow paths at 2 m, draining to sump
- One flowpath subdivided into 10 equal segments
- No difference in results

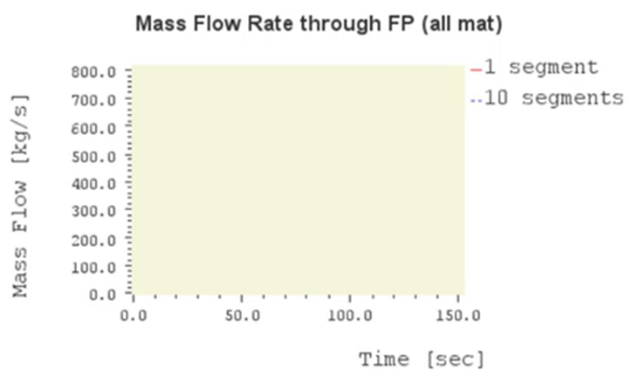


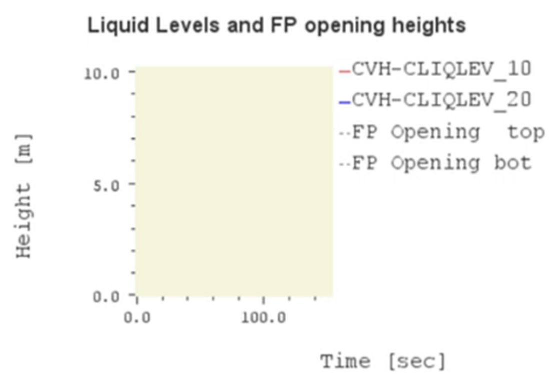

```
FL_SEG   1 !n sarea slen shyd srgh lamflg slam
          1  0.1  1.0  0.1
```

```
FL_SEG  10 ! n sarea slen shyd srgh lamflg slam
  1  0.1  0.1  0.1
  2  0.1  0.1  0.1
  3  0.1  0.1  0.1
  4  0.1  0.1  0.1
  5  0.1  0.1  0.1
  6  0.1  0.1  0.1
  7  0.1  0.1  0.1
  8  0.1  0.1  0.1
  9  0.1  0.1  0.1
  10  0.1  0.1  0.1
```







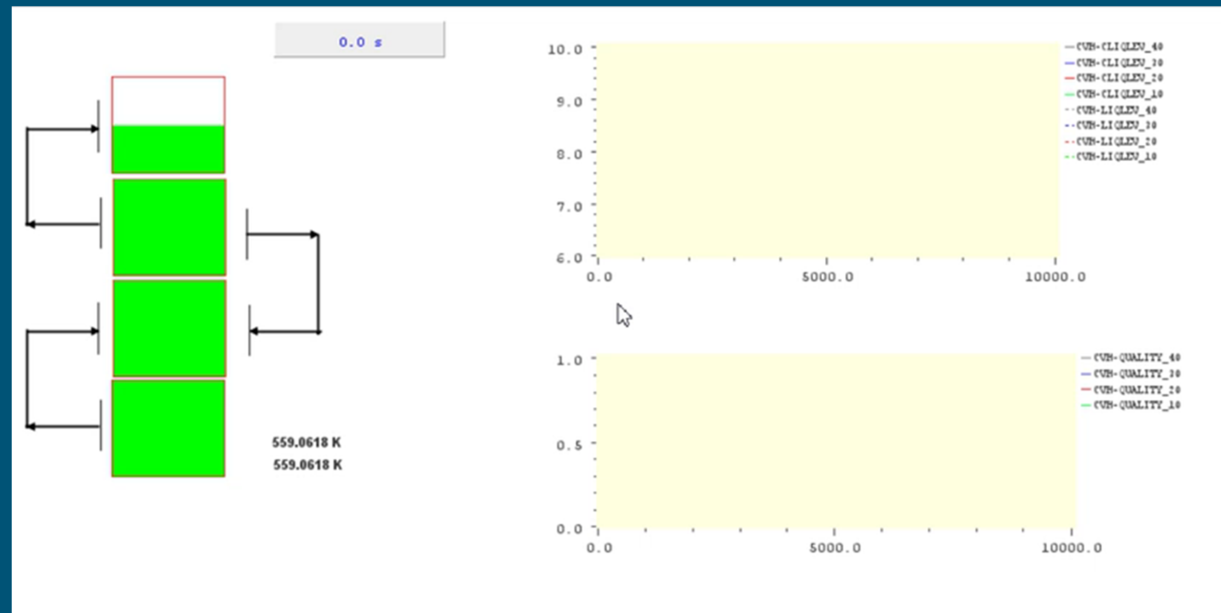


- Liquid levels & flow rates identical
- Inflection in flow rate as water level reaches top of opening
- Flow stops when water level reaches bottom of opening

CVH Modeling – User Choice of Junction Elevations and Opening Heights for Vertically Stacked CVs

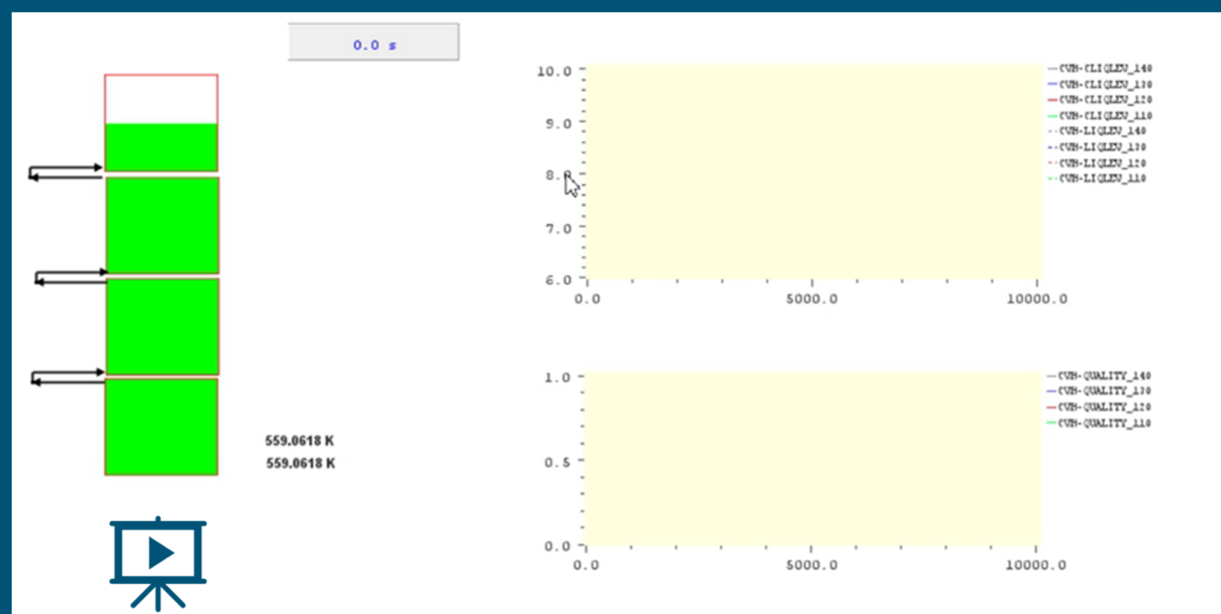
Setting FP junction elevation to midpoint of CV more representative of forced flow boiling

- Leads to layering of pool and atmosphere
- MELCOR lacks a flow regime map



Setting FP Junction Elevation to top/bottom elevation is more representative of quiescent boiling

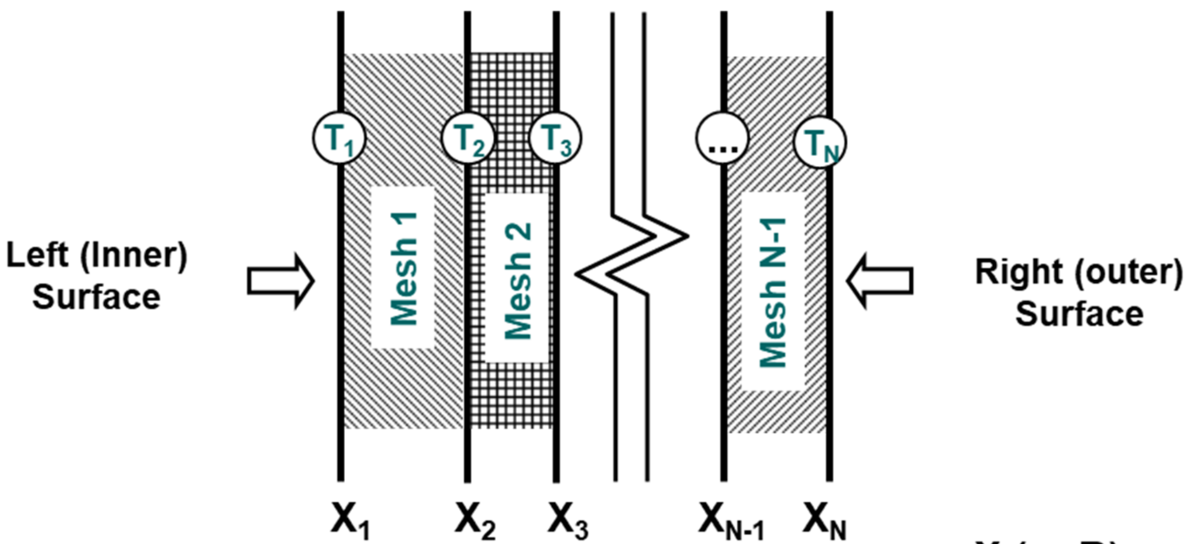
- Eliminates layering of pool/atmosphere



Phenomena Modeled by MELCOR, Packages Involved – Heat/Mass Transfer to Heat Structures

Heat Structures, HS Package

- Treats heat transfer to and within non-core structures
  - Walls, floors, ceilings, pipes, etc.
  - Ice condensers
  - Most of reactor vessel, PWR core support barrel, BWR core shroud, upper internals in PWR and BWR
- Also treats mass transfer and water films on surfaces
  - Condensation and evaporation, drainage to other structure surfaces and/or volume pools
- Some structures can decompose or melt
  - Degassing of concrete walls and floors, melting of ice in ice condensers, steel in some reactor internals
- Gets boundary conditions from, transfers mass and energy to/from CVH
- Receives energy from COR, can transfer mass to COR

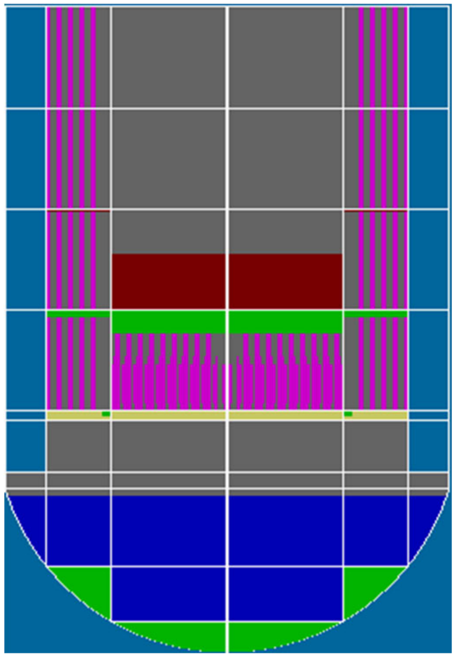


- Currently limited to 1-D structures.
- 2-D Structures in 2022 release

Phenomena Modeled by MELCOR, Packages Involved – COR Package

Core Response, COR Package

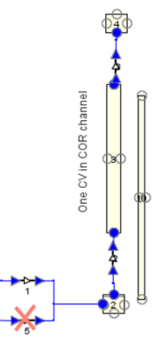
- Calculates heatup, degradation, oxidation, relocation of materials in core structures
  - Fuel, BWR canisters, PWR shroud and formers
  - Control elements
  - Supporting structures like plates and columns
- Handles debris until it leaves the vessel
  - "Passed off" to FDI or CAV (described later)
- Also calculates response of vessel lower head
- Gets boundary conditions from CVH
- Displaces fluid in, transfers mass and energy to/from CVH
- BWR core baffle, PWR core support barrel, all upper internals are modeled as heat structures
  - Radiates to these heat structures
  - Receives mass from them if they melt (optional)



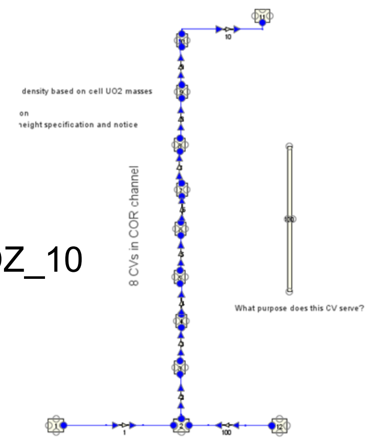
SNAPlette: COR dTdZ Model

- Simple one ring, 10 elevation COR package
  - Uniform power profile
  - Oxidation disabled for illustration
  - FL opening heights reduced to minimize stratification of pool % atmosphere below pool height
  - Same number of HS with same nodalizations. Uses local dtdz temperatures
- Steam injection cuts off at 500 seconds
- DTDZ_1
  - 1 CVH volume in active core, HSs uses local dtdz temperatures
- DTDZ_2
  - Same as DTDZ_1 except HSs uses CVH temperature
- DTDZ_10
  - 8 CVH volume in active core
  - HSs use local dtdz temperatures

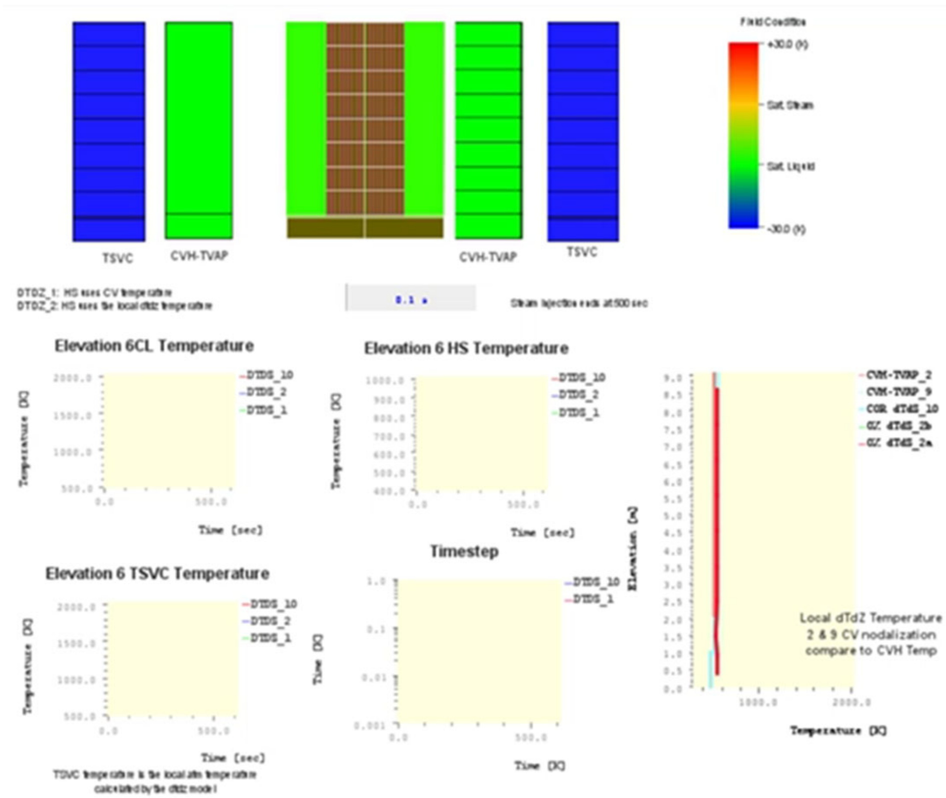
DTDZ_1



DTDZ_10



- Input Files
  - DTDZ_1.med
  - DTDZ_2.med
  - DTDZ_10.med
  - DTDZ_anim.med
- Job Stream/Data Source
  - DTDZ_1
  - DTDZ_2
  - DTDZ_10



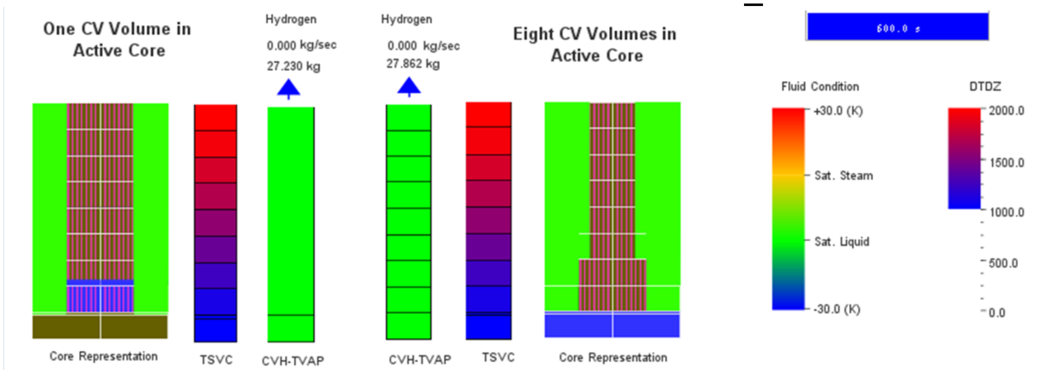
- Things to try
  - Disable FL height specification in DTDZ_10
  - Disable dTdZ model in DTDZ_2

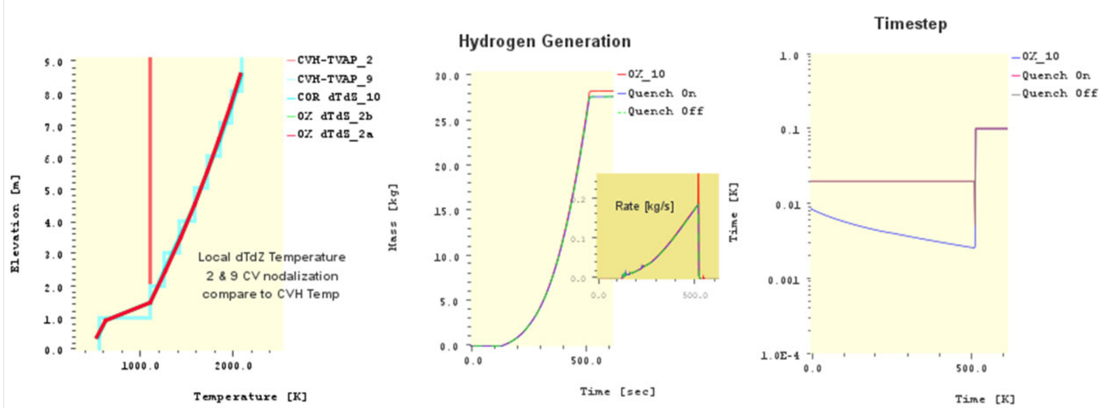
SNAPlette: COR Oxidation Modeling

- Simple one ring, 10 elevation COR package
  - Uniform power profile
  - FL opening heights reduced to minimize stratification of pool % atmosphere below pool height
  - Same number of HS with same nodalizations. Uses local dtdz temperatures
- OX_1a & OX_1b
  - 1 CVH volume in active core
- OX_10
  - 8 CVH volume in active core

- Input Files
  - OX_1a.med
  - OX_1b.med
  - OX_10.med
  - OX_anim.med
- Job Stream/Data Source
  - OX_1a
  - OX_1b
  - OX_10

- Things to vary
  - Increase the steam flow into the bundle
    - Observe the effect of convective cooling of rods
    - Observe the effect on temperature profiles due to steam starvation
  - Enable reflood(quench front)
    - How sensitive are results?
    - Disable oxidation for submerged surfaces
      - How sensitive are results





Ex-Vessel Debris Phenomena (I)

If reactor vessel fails, debris can be ejected

- Ends up on floor
- Can interact with gases and/or water pools on the way

CAV (CAVity) Package models behavior of "core on the floor"

- Essentially CORCON Mod 3
  - Concrete ablation
    - Release of interstitial and hydrated water
    - Decomposition of hydroxides and carbonates
    - Addition of oxides to debris
  - Oxidation of metal in debris by released H_2O and CO_2
- Mass sources, heat transfer to CVH fluids
  - Heat transfer from debris surface
  - Reduced gases, primarily H_2 and CO

Ex-Vessel Debris Phenomena (2)

FDI (Fuel Dispersion Interactions) Package models interactions between vessel and floor

- Use is optional, depends on user input
- Low pressure melt ejection (LPME) option
  - Debris falls under gravity
  - Break up of debris in water pool
  - Heat transfer to water pool in CVH
- High pressure melt ejection (HPME) option
  - More violent expulsion of debris
  - Heat transfer to CVH fluids
  - Oxidation of debris
  - Deposition of some debris on structure surfaces

Ex-Vessel Debris Phenomena (3)

TP (Transfer Process) Package handles bookkeeping for transfers between packages

- Just a clean interface used for flexibility
  - "Insulates" each package from unneeded details
    - Whether transfer is COR → CAV or COR → FDI → CAV
    - Structure of database in the various packages
  - Motivated by code developer concerns
    - Greatly simplifies code structure
    - Need for user input sometimes seen as an annoyance
- Provides temporary storage for information about parcels of debris leaving COR or FDI (or any other) package
  - Stored in standard format
  - Source doesn't need to know where they are going
- Allows these parcels to be picked up by FDI or CAV (…)
  - Recipient doesn't need to know where they came from

Radionuclide Package

Transport of vapor and aerosols
- Fission product vapors & aerosols
- Traces materials hosted by other materials
  - Negligible volume and heat capacity

Aerosol physics
- MAEROS
- Agglomeration of aerosols
  - Several mechanisms cause agglomeration to produce larger particles
    - Brownian diffusion
    - Differential gravitational settling
    - Turbulence by shear and inertial forces

Hygroscopic effects

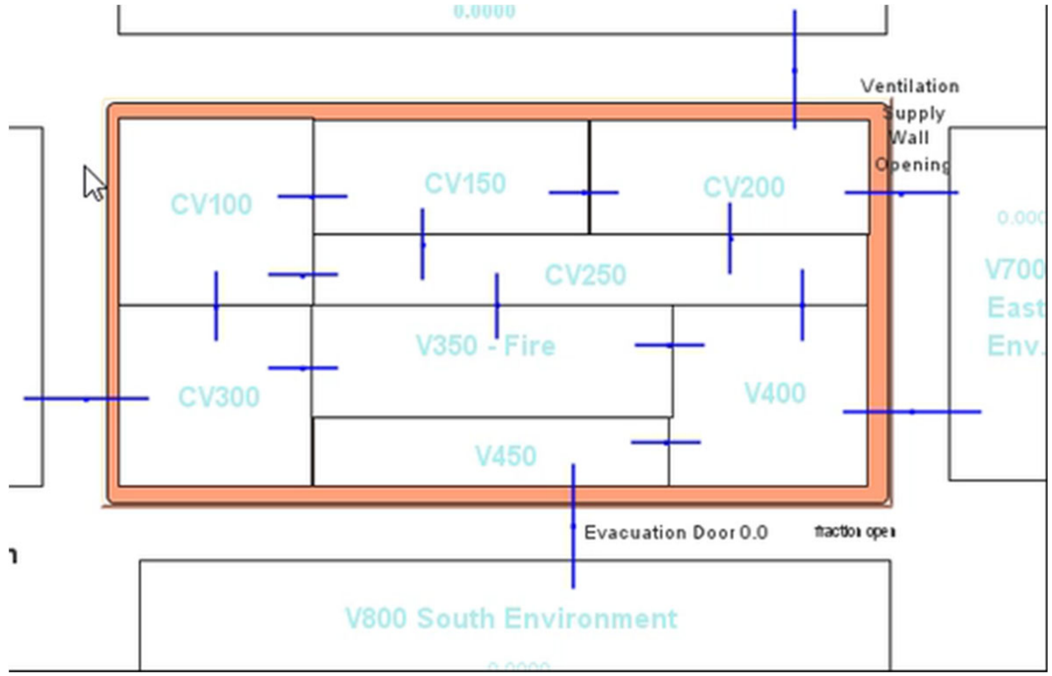
Condensation & evaporation
- TRAP-MELT

Deposition on surfaces
- Modeled as adhering to surfaces contacted unless subsequently resuspended by sufficient flow over surfaces
- Several mechanisms drive aerosols to surfaces
  - Gravity
  - Brownian diffusion
  - Thermophoresis
  - Diffusiophoresis
  - Turbulent deposition

Resuspension

Pool Scrubbing
- SPARC

Iodine Pool Chemistry



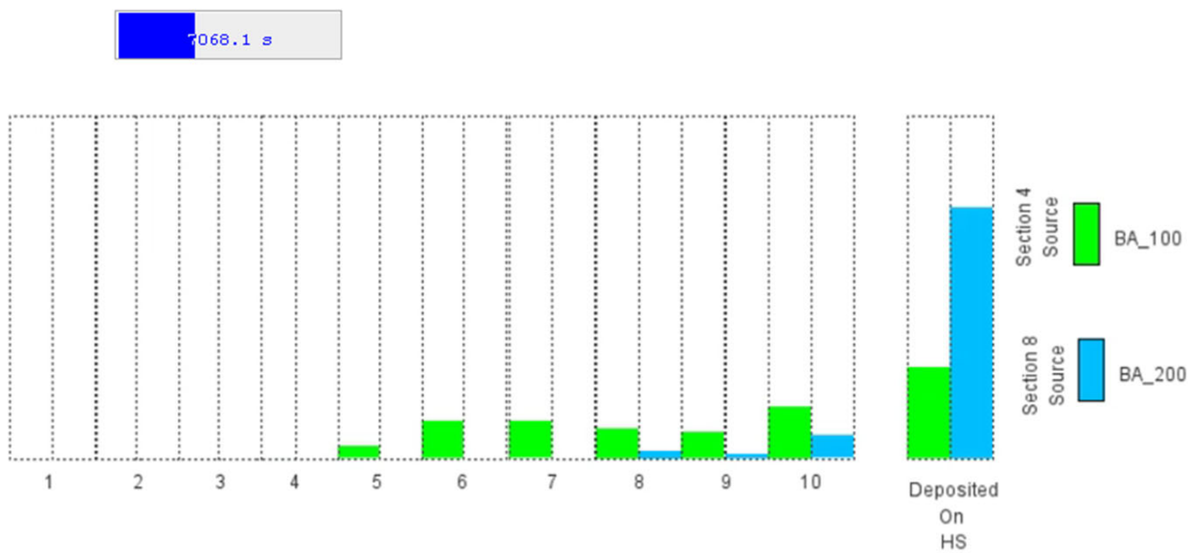
As an example of it's generalized modeling capabilities, RN in MELCOR can be used for tracking "trace" materials in non-reactor situations Transport of radiological releases, toxins, and biohazards in buildings, building complexes

SNAPlette: MAEROS Agglomeration

- Model contains 2 simple CVs
  - 45 m3 CV
  - 3m high
  - Initial temperature = 310K
- 1 Heat structures
  - Floor
    - 1.0D-10 m2
    - Steady State Initialization

- Input File
  - Aerosol.med
  - Aerosol_anim.med
- Job Stream/Data Source
  - Agglomeration

- Things to vary
  - Disable agglomeration by setting sticking factor small 1.0E-10
  - Disable gravitational deposition



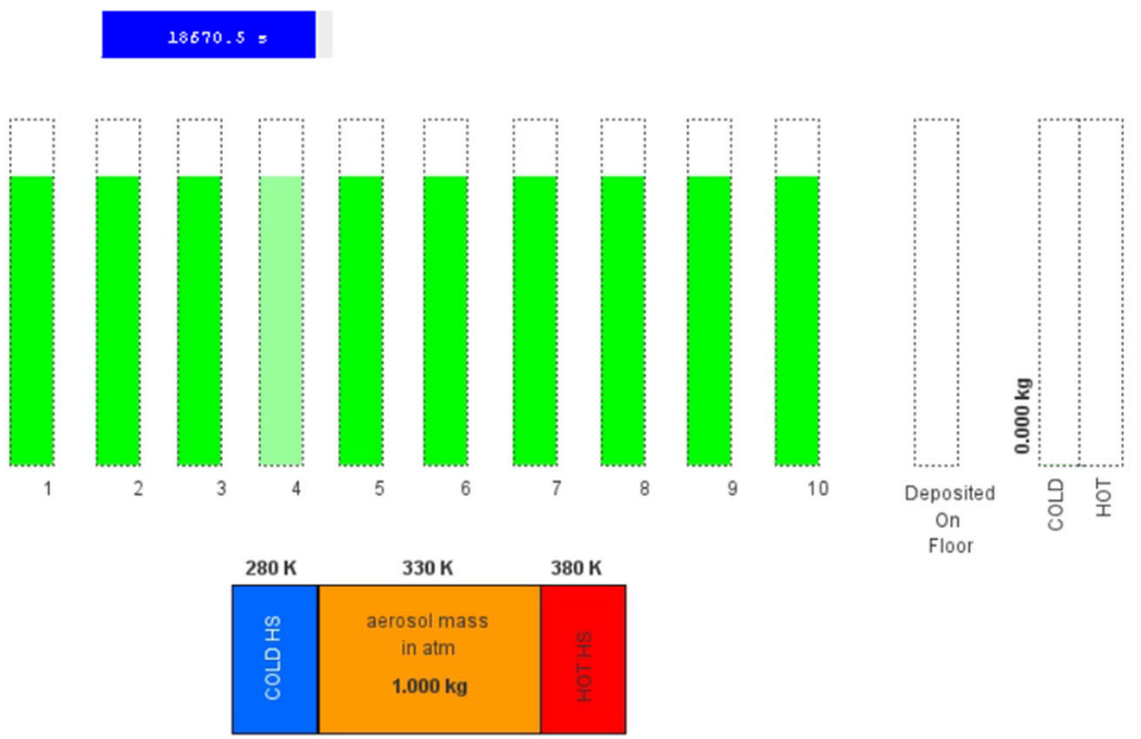
Try setting the sticking factorto something small (1e-14). Note that this essentially disables agglomeration.
Setting the sticking factor to zero leads to numerical issues (divide by zero).

SNAPlette: Deposition from Thermophoresis

- Simple CV
  - 45 m3 CV
  - 3m high
  - Initial temperature = 330K
- 3 Heat structures
  - Floor
    - 1.0D-10 m2
    - Steady State Initialization
  - Cold
    - T.VAP(CV100)-50 K
    - 1.0 m2
  - Hot
    - T.VAP(CV100)+50 K
    - 1.0 m2

Agglomeration disabled
Gravitational and diffusive deposition disabled

- Input File
  - Thermophoresis.med
  - Thermophoresis_anim.med
- Job Stream/Data Source
  - Thermophoresis



- Things to Vary
  - Surface areas of HSs
  - Temperatures of HSs
  - Enable agglomeration
  - Enable Gravitational and diffusive deposition

A Few Important Support Packages

Equations of State, EOS Package

- Implements a mixed-material equation of state for hydrodynamic materials (water and gases)
  - Water properties from H2O package
  - <u>N</u>on<u>C</u>ondensible <u>G</u>as properties from NCG Package
- H2O and NCG properties are also available separately

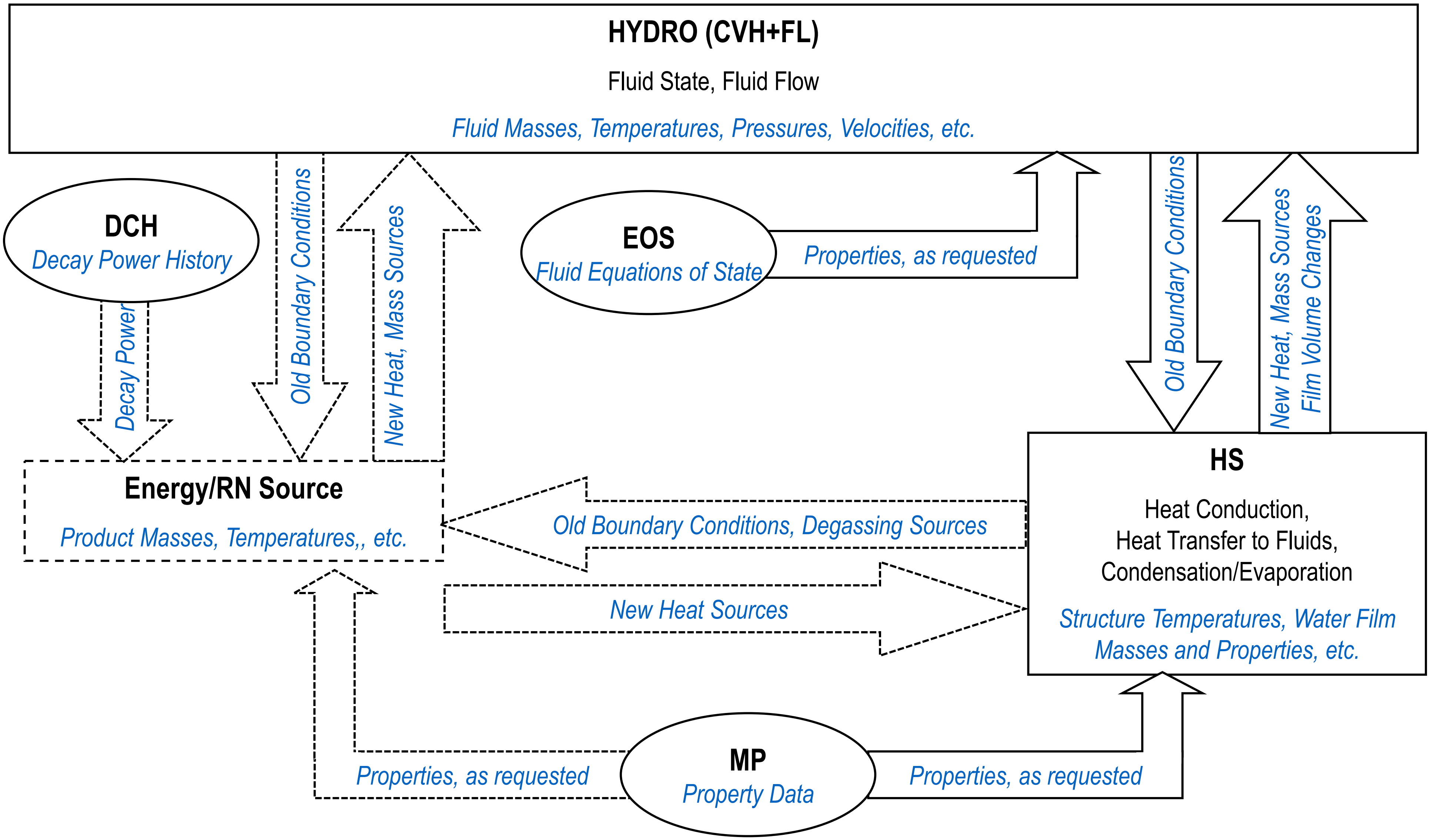
Materials Properties, MP Package

- Provides thermal EOS for non-hydrodynamic materials
- Provides thermophysical properties for all materials
  - Thermal conductivity, viscosity, diffusivity, etc.
  - Mixture rules used where appropriate
- Recent generalization for User Defined Materials and

Decay Heat, DCH Package

- Can provide whole-core decay heat and/or distribution of that heat among fission products (discuss later)

Data and Data Flow for CVH, FL, HS, and RN



Phenomena Closely Tied to Hydro (1)

BUR handles combustion (BURn) of H_2, CO

- Permitted in any volume
- Deflagration only (no detonations)
- Includes modeling of igniters

Various containment models, some grouped as ESFs (Engineered Safety Features)

- SPR models containment SPRays
- PAR models Passive Autocatalytic Recombiners
- FCL models Fan CooLers
- CND models an Isolation CoNDenser System (ICS) and/or Passive Containment Cooling System (PCCS)

Phenomena Closely Tied to Hydro (2)

Modeling in BUR, SPR, PAR, FCL, and CND

- All get boundary conditions from CVH
  - Pressure, temperature, saturation state, concentrations of noncondensible gases, etc.
- All have relatively simple internal modeling, appropriate to phenomena treated
- All transfer mass and/or energy to/from CVH
  - Chemical reactions "look like" sink of reactants, source of products to CVH
    - Equations of state for hydro fluids have thermochemical reference points, like JANNAF tables
      - Heats of reaction implicit in reference points

Order of Advancement

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

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

Control Functions, the “Crown Jewel”

Control Functions, CF Package

- Heart of MELCOR power and flexibility
- Comes close to letting user write code as part of input

Allows user input to define functions of MELCOR-calculated time-dependent variables

- Values can be REAL or LOGICAL, are part of time-dependent database with all other time-dependent data
  - Calculated from definition using *current* conditions
  - Relatively easy, *very* flexible way to model complex systems
- Older versions used own “language”, difficult to read
- MELCOR 2.X adds ability to write function as a FORMULA, that looks much like fortran
- Many (not all) variables are available as arguments
- Recent version permits vector CFs and CF arguments

Control Function Use

Can be used to generate custom output

- Values can be printed, plotted
- Change in value of logical can produce event message

Function values can be used in calculations

- Input to many packages allows reference to the value of a control function rather using than a fixed constant
  - Sources, sinks, other boundary conditions
    - Allow dependence on current state
      - Drain liquid currently present in volume with correct enthalpy
  - Valves, pipe failures, containment failures
    - Complex control logic
    - Larson-Miller cumulative damage strain model
  - Can provide simple modeling of systems (injection, cooling, etc.) when no internal model provided
    - Define mass/energy sources and sinks with appropriate logic
    - PAR could have been done entirely with CFs

Summary

MELCOR has benefited from a long-term, sustained commitment in development from the NRC over more than 40 years

MELCOR models a wide range of physics with models extended, refined, validated, and documented for users.

It has evolved in its capabilities and design to meet the needs of users

- Though originally parametric, models have become more mechanistic where needed
- New capabilities beyond light-water application
- Modernization of code architecture to improve numerics, code capabilities, and extensibility.

Modeling approach allows users to model/expolore new technologies

- Building-block approach to model development
- Extensive use of Control functions
- EOS libraries

MELCOR architecture has always been modular in design which has contributed in its longevity.

- Avoids entanglements of physics