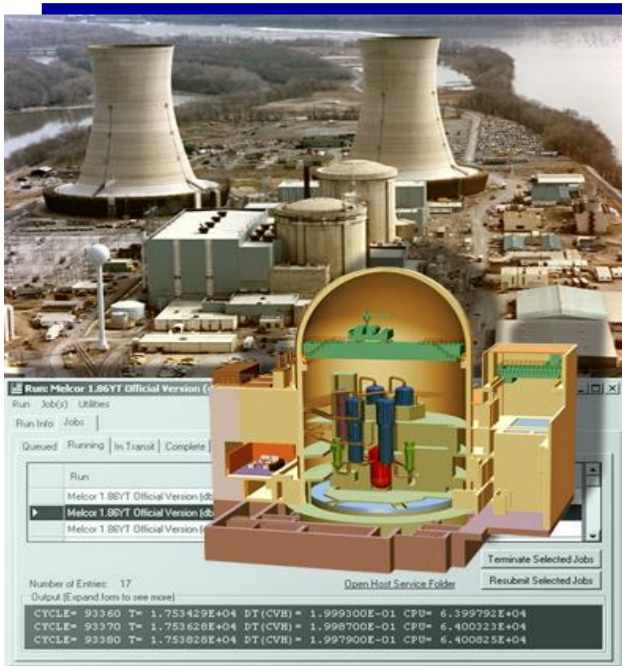

Introduction to MELCOR and the RN Package

Session 1

Presented by

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MELCOR Physics

- Thermal/hydraulic response
- Combustible gas generation, transport, and deflagration
- Aerosol/vapor release, behavior, transport, deposition
- Core heatup and degradation
  - PWRs, BWRs, and other designs (e.g., SFP)
- Ex-vessel molten core/concrete interactions
- Relocation of decay heat sources
- High pressure melt ejection, direct containment heating
- Performance and impact of Sprays and Engineered Safety Systems
  - Sprays, filters, fans, coolers, ice condensers, hydrogen recombiners

MELCOR Code Structure

- Major pieces of MELCOR referred to as “Packages”
  - Larger than usually implied by “module”
  - 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
  - Reactor-specific phenomena
    - Decay heat generation, core degradation, ex-vessel phenomena, sprays and ESFs
  - Support functions used by both
    - Thermodynamics, equations of state, other material properties, data-handling utilities, equation solvers

MELCOR Building Block Approach

- Generic models
  - No "built-in" nodalization
- Building block approach
  - More flexibility means greater user responsibility
  - Now developing engineering interface to simplify input
    - Anticipate that it will contain "templates" for some common subsystems
- Maintainable code structure
  - Modular architecture, portable to new systems

MELCOR Control Functions

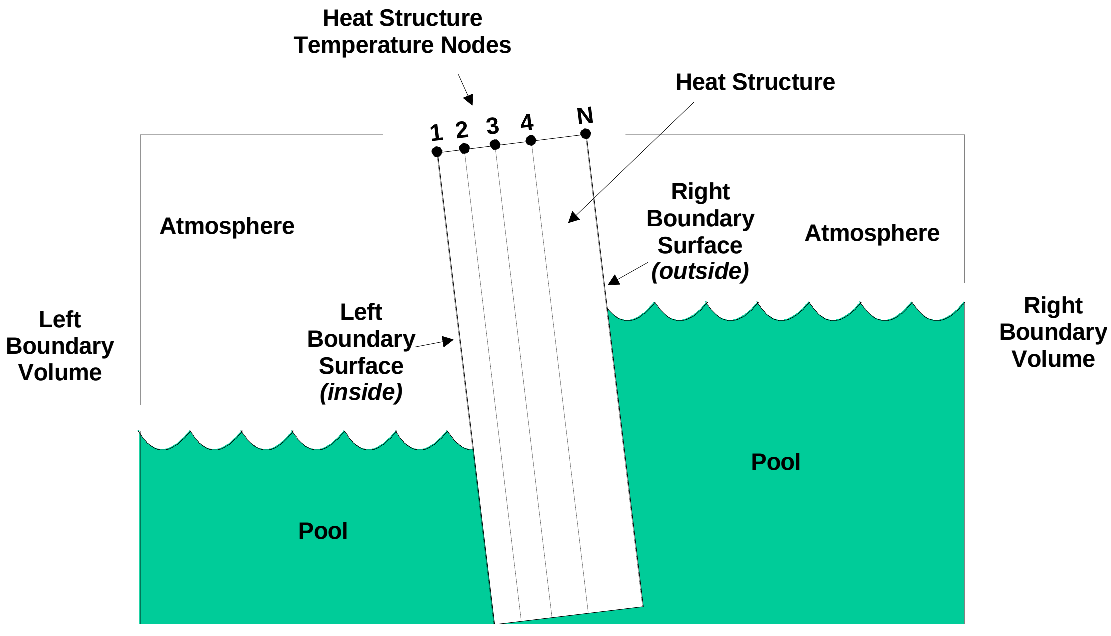
- "Control Functions" are simply user-defined functions
  - May be LOGICAL- or REAL-valued
  - All functions are evaluated at the start of every time step
    - All control-function-based models numerically explicit
- They have many uses, not just control
  - Define valve behavior, failure conditions, SCRAM criteria
    - Little predefined logic, but great flexibility
  - Define internally-calculated sources, boundary conditions
- Many variables in the MELCOR database are available as arguments for control functions
  - Any such variables can be written to an external data file
  - Any such variable can be added to the plot file

```
! Stress in a thick-walled pipe as function of pressures
CF_ID  'Stress'  FORMULA
CF_SAI  1.0
CF_FORMULA 4 ((C1^2+C2^2)*A-2*C2^2*B)/(C2^2-C1^2)
              1  A  CVH-P(CV500) ! Inner pressure (hot leg)
              2  B  CVH-P(CV8)   ! Outer pressure (containment)
              3  C1 0.37         ! Inner radius
              4  C2 0.45         ! Outer radius
```

Control Volume

- A region of space that contains hydrodynamic materials
- Properties correspond roughly to “cell centered” variables in finite-difference CFD formulations
- Need to define:
  - –Geometry
  - –Contents (liquid water, water vapor, N_2, O_2, etc.)
  - –Thermodynamic states (equil, nonequil)
  - –Pressure and temperature
  - –Boundary of pool

Heat Structures (HS)

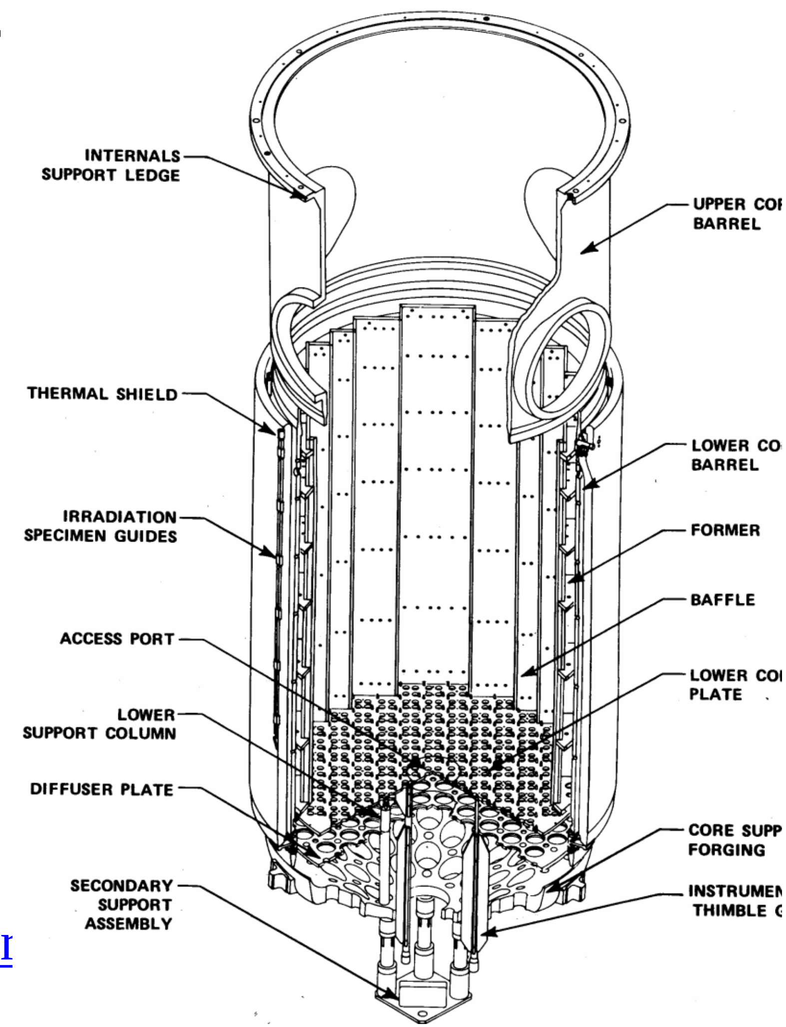


- Heat structure may be inclined
- Partially immersed
- May have rectangular, cylindrical, spherical or hemispherical 1-D geometry

- HS nodalized with N temperature nodes
- Node 1 is at the left boundary surface (or inside), must define it
- Node N is at the right (outside)
- Region between two nodes is called mesh interval (N-1 meshes)

COR Package Modeling

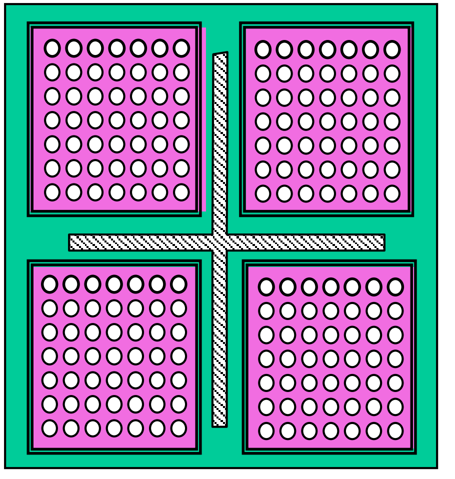
- MELCOR COR package models core-specific structures in the core and lower plenum
  - Fuel assemblies
    - Fuel rods (and grid spacers), BWR canisters (channel box)
  - Control elements
    - PWR rods, BWR blades
  - Structural elements
    - Core plate
    - BWR control-rod guide tubes
    - Core shroud/baffle
    - Formers
    - Vessel lower head
      - Including penetrations
      - Includes some of the lower vessel
- It *does not* model boundary structures
  - Core barrel, upper vessel, upper inter
  - Modeled as Heat Structures



COR Package Modeling (2)

- Same representation used for PWR and BWR
  - In a BWR, MELCOR calls the region outside the canisters (channel boxes) in the core region the "bypass"
  - In a PWR, MELCOR calls the region outside the core shroud the "bypass"
  - Everything else is called the "channel"
    - In a BWR, "channel" includes the interior of canisters and the lower plenum
- Input specifies the CVH volume representing channel and bypass for each core cell
  - Distinction only in core region of a BWR or outer peripheral core ring of PWR
  - Common to interface several cells to a single CVH volume

BWR

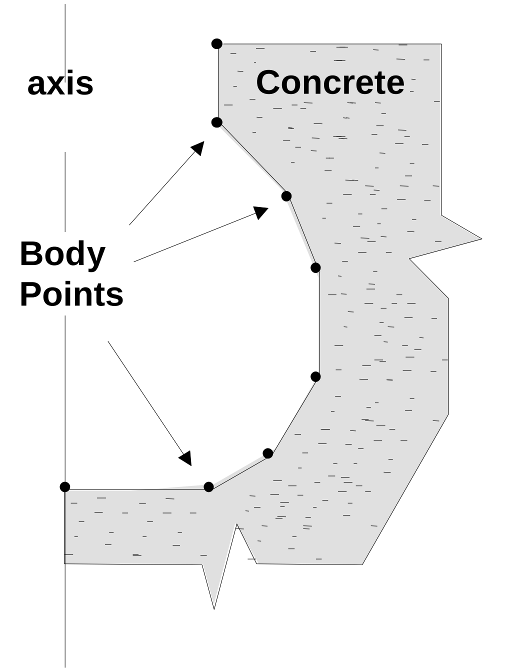


Channel Region

Bypass Region

Cavity (CAV) Package

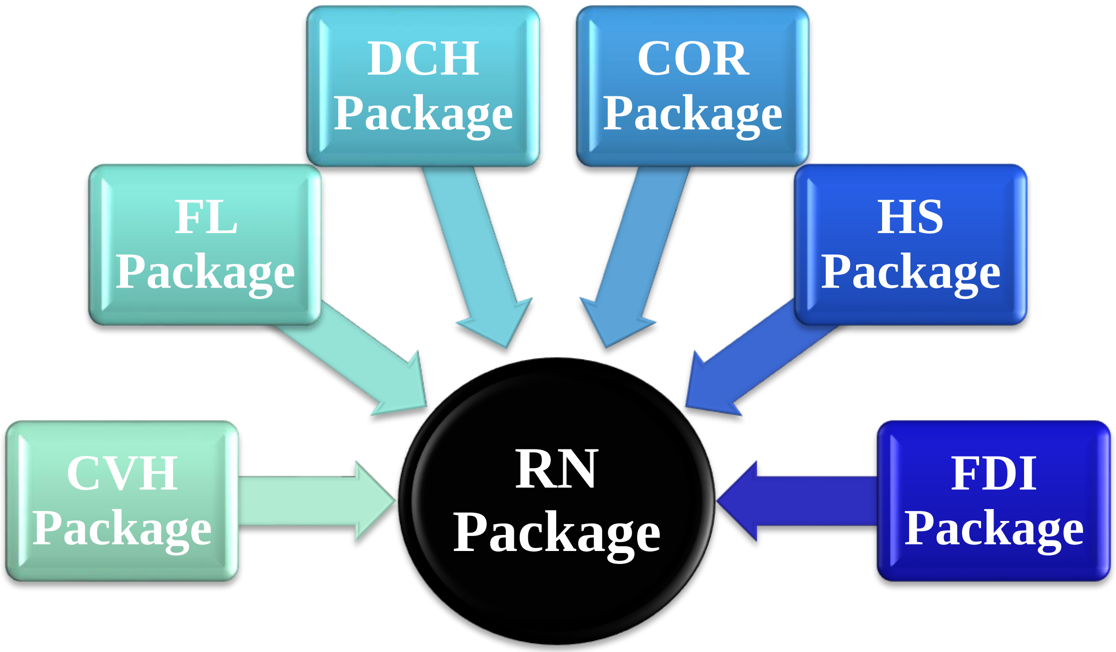
- Debris geometry
- Mass and energy transport and conservation
  - Concrete ablation
  - Chemistry
- Debris ejected from vessel attacks concrete
  - Attack is primarily thermal: surface ablates
    - Concrete decomposes
    - Gases (H_2O and CO_2) interact with debris
    - Oxides (CaO, SiO_2, Al_2O_3, etc.) add to debris
- Top surface communicates with surroundings
  - Heat is lost by radiation, convection, or boiling
  - Gaseous reaction products pass to atmosphere
- Sustained by decay and chemical heat
  - Heat balance determines progression



MCCI*: Framework

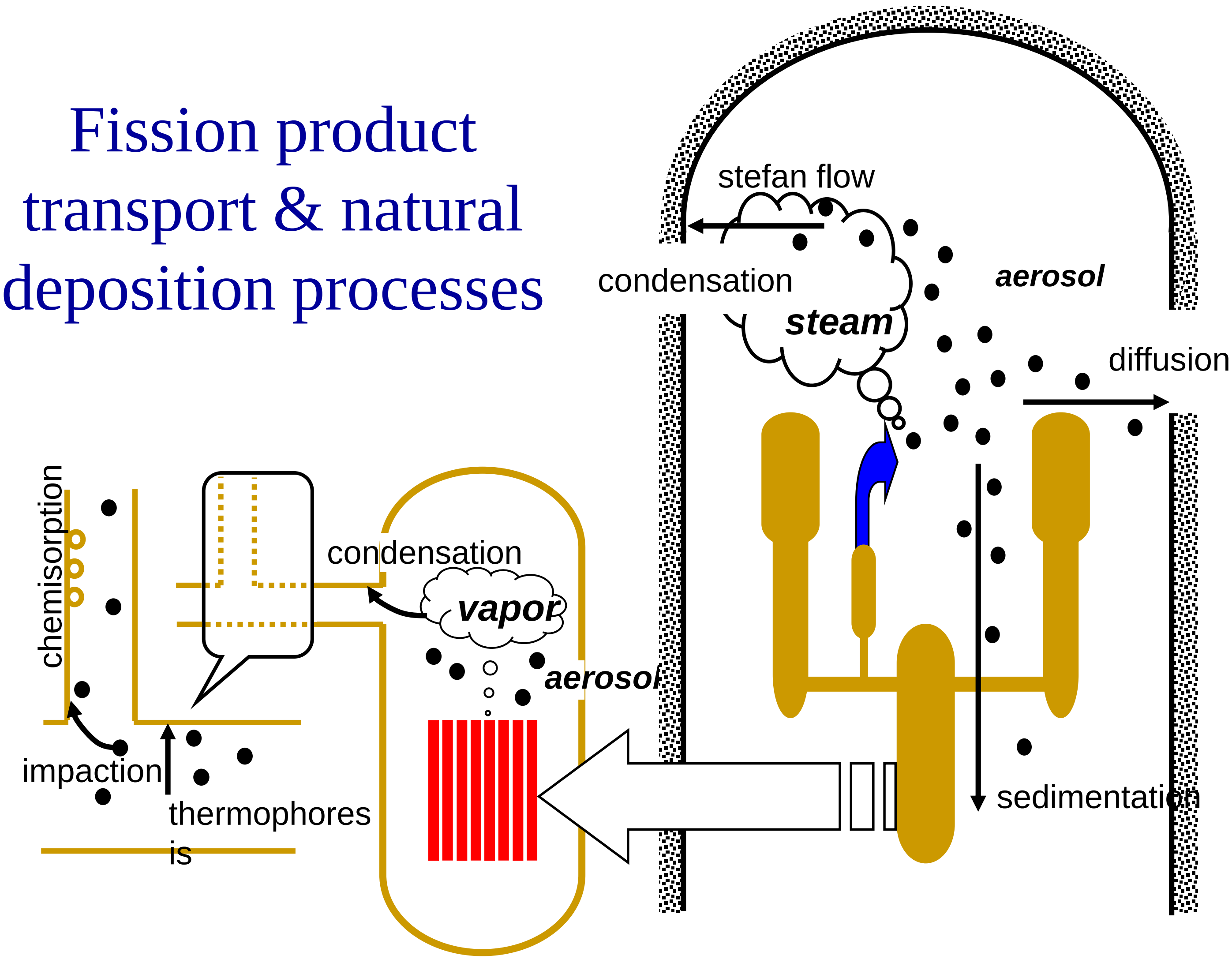
- MELCOR models based on CORCON-Mod3
  - Uses CCM3 routines for phenomenological models
    - Geometry, heat transfer, chemistry, concrete ablation
  - Obtains boundary condition and source data from other MELCOR packages rather than user input
    - Stand-alone options available (in MELCOR format)
  - Interface to VANESA preserved
    - VANESA is fission product release model
      - Implemented as part of the RN package
      - Separate scrubbing model replaced by general SPARC model
- MELCOR executive replaces top coding levels
  - Controls input, advancement, output
  - Input format consistent with other MELCOR packages
  - Allows integrated restart, plot, and fallback capabilities

Packages Interactions w/ RN Package



RadioNuclide Overview

Fission product transport & natural deposition processes



RN Package Physics

- Initial RadioNuclide inventories (ORIGEN)
- Release of radionuclides (CORSOR, VANESA)
- Aerosol dynamics (MAEROS)
- Condensation/evaporation (TRAP-MELT2, thermodynamics routines)
- Decay heat distribution
- ESF models (pool scrubbing, filters, sprays)
- Fission product chemistry
- Chemisorption on surfaces
- Hygroscopic aerosols
- Flashing jet impaction model
- Iodine pool model

RN: Boundary Conditions

- Obtained from other MELCOR packages
  - CVH
    - Fluid conditions
    - Radionuclide advection between control volumes done using CVH flows
  - COR & CAV
    - Fuel and debris temperatures
    - Provides information regarding bulk debris relocation
    - {allows RN to perform relocation of unreleased fission products}
  - HS
    - Structure surface temperatures
    - Wash-off of radionuclides deposited on heat structures is determined from drainage of water films calculated by this package
- RN package determines decay heat power for current radionuclide inventories from the Decay heat (DCH) package
  - Requires request from both packages

Initial Radionuclide Inventories

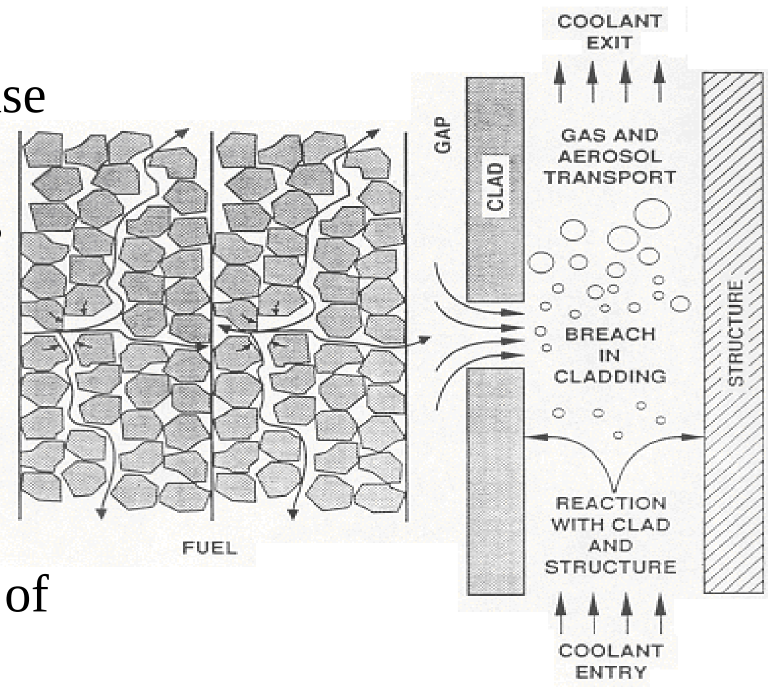
- RN Classes
  - species with similar chemical properties.
- Elemental inventories from tables of ORIGEN calculations
  - Can be user specified
- Spatial distributions
  - Fuel in the core
    - Radial & axial profiles
  - Fuel-cladding gap
  - Any initial cavity debris, and
  - Atmosphere and pool (of any control volume)
- Fuel FPs are transported with the fuel until released

Class	Name	Element	All Member Elements
1	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	Alkaline Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	Halogens	I	F, Cl, Br, I, At
5	Chalcogens	Te	O, S, Se, Te, Po
6	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	Early Transition	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, TC, Ta, V
8	Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Gd, Sm, Eu, Tb, Dy, Ho, Er, Tm, Yb, Cm, Lu, Am, Bk, Cf
10	Uranium	U	U
11	More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl,
12	Less Volatile Main Group	Sn	Ga, Ge, In, Sg, Ag
13	Boron	B	B, Si, P
14	Water	H2O	H2O
15	Concrete	–	-
16	Cesium	iodide	CsI-

Fission product release/transport is governed primarily by thermo-chemical characteristics of species, not their radioactive properties. Therefore, species with similar chemical properties are combined.

RN Release

- Can occur from
  - Fuel-cladding gap exceeding a failure temperature criterion (or losing intact geometry)
  - Material in the core using the various CORSOR empirical release correlations [based on T_{fuel}]
  - During core-concrete interactions in the reactor cavity using the VANESA release model
- After release to a control volume, masses may exist as aerosols and/or vapors
  - Depending on the vapor pressure of the radionuclide class and the volume temperature



RN Release: Test Environment

- Oxidizing (steam) environment
  - –Cladding oxidizes (exothermic reaction) and holds bundle together
  - –Release favors diffusive RN’s & volatile oxides
  - –Nobles, I, Cs, & Te
- Reducing (hydrogen) environment
  - –Cladding melts and runs off
  - –Release favors diffusive RN’s & volatile hydrides
  - –Nobles, I, Cs, Te, Ba, Ru, and Eu

RN Release Tests

- Out of Pile

– Parker	ORNL	1955-1980	Oxidizing fuel chips	800-1500 K
– SASCHA	KfK	1975-1979	Oxidizing fuel pellets	800-1500 K
– Albrecht	Chalk R	1975-1979	Oxidizing fuel chips	1700-3000 K
– HBU	ORNL	1978	Oxidizing	800-1500 K
– HT	ORNL	1980	Oxidizing	1600-1900 K
– HI	ORNL	1981-1985	6 Oxidizing	1675-2250 K
– MCE-1-8	AECL	1984-1991	5 Air, 3 Air&H2	1973-1350 K
– VI 1-4	ORNL	1989	3 Oxidizing, 1 Reducing	2000-2700 K
– Vercors 1-6	IRSN	1989-1994	1 Oxidizing, 1 Reducing, 4 Both	2130-2620 K
– VI 5-7	ORNL	1991-1992	1 Oxidizing, 1 Reducing, 1 Both	2000-2700 K
– HT 1,3	IRSN	1996-2001	2 Reducing	2900 K-melting
– RT 1,3-5	IRSN	1998-1999	2 Oxidizing, 1 Reducing, 1 both	2600 K-melting

- In Pile

– PBF ST,1	INEL	1986-1992	2Oxidizing	2000-2400 K
– PBF 2,4	INEL	1986-1992	2Reducing	2000-2400 K
– ST 1& 2	SNLA	1988	2Reducing	2400 K
– PHEBUS	FPT0,1	1999-2001	2Oxidizing	fuel melting

MELCOR RN Release Models

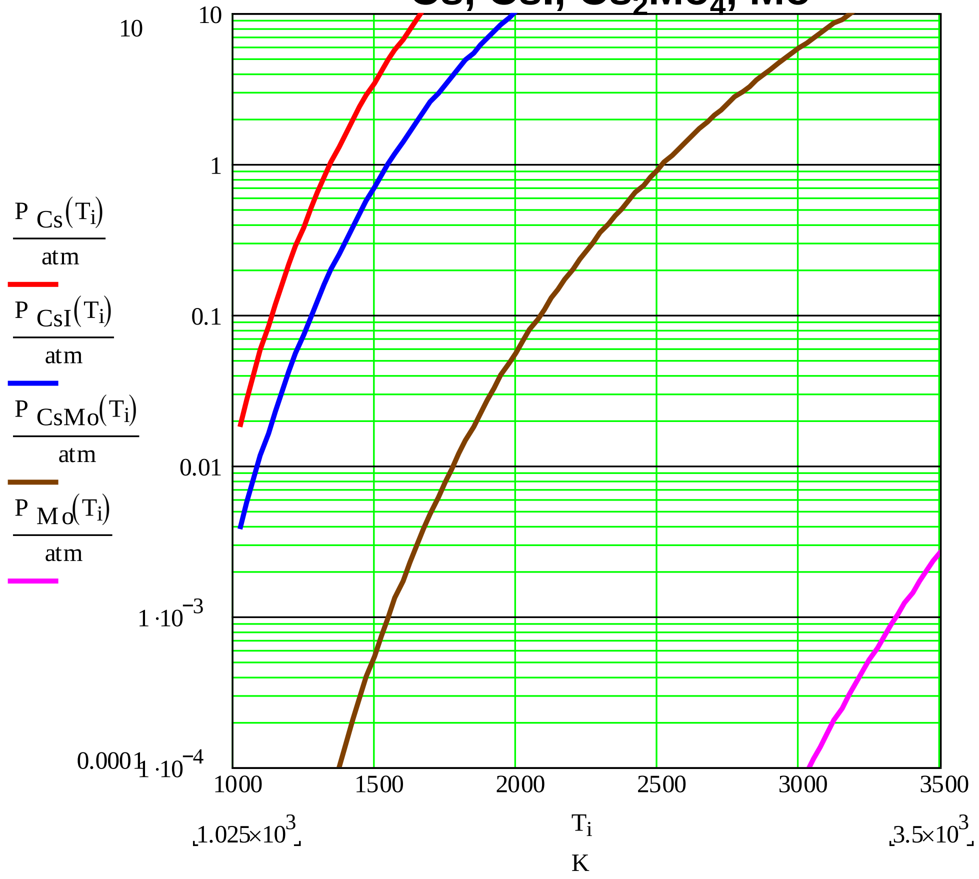
- Four basic release models, with options
  - CORSOR
  - $k = A \exp(BT) \quad for\, T \geq T_i$ where k is the release rate
  - CORSOR-M,
  - $k = k_o \exp(-Q/RT)$
  - CORSOR-Booth*,
    - Limited by mass transport in fuel
    - $D_0 \exp(-Q'/RT)$
    - Also limited by mass transfer through gas phase
    - Options for high- or low-burn-up fuel

MELCOR RN Release Models

- Modified ORNL Booth
  - Same equation set
    - Known Limitations
  - Cs_2MoO_4 vapor pressure
  - Modified scaling factors
- Improved results
  - FPT-1
    - Cs, I, Mo
  - ORNL VI Tests
    - VI 2 (oxidizing)
    - VI 3 (oxidizing)
    - VI 5 (reducing)
  - Vercors 4 (oxidizing)
    - Cs, I, Mo

Vapor Pressure

Cs, CsI, Cs_2Mo_4, Mo

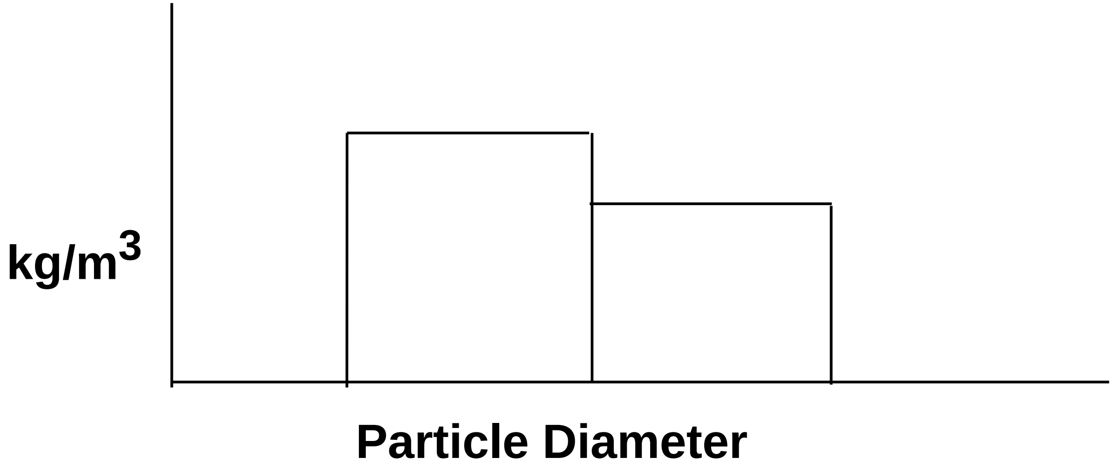


Aerosol Component/Class Mapping

- MELCOR uses CLASS grouping to represent FP species
  - Common physical/chemical characteristics (e.g., volatility)
- MAEROS recognizes and operates on the aerosol portions of these FP (radioactive and non-radioactive) classes
  - Component ≡ a particular type of aerosol material
- MELCOR allows the user to define aerosol ***Components*** which are groupings of one or more fission product ***Classes*** (the mapping between RN classes and MAEROS aerosol components)
  - These components are allowed to have distinct size distributions
    - The size distributions are characterized by the amount of aerosol mass within a range of aerosol particle sizes
    - Size ranges are called ***Sections***

Aerosols (Mass Distributions)

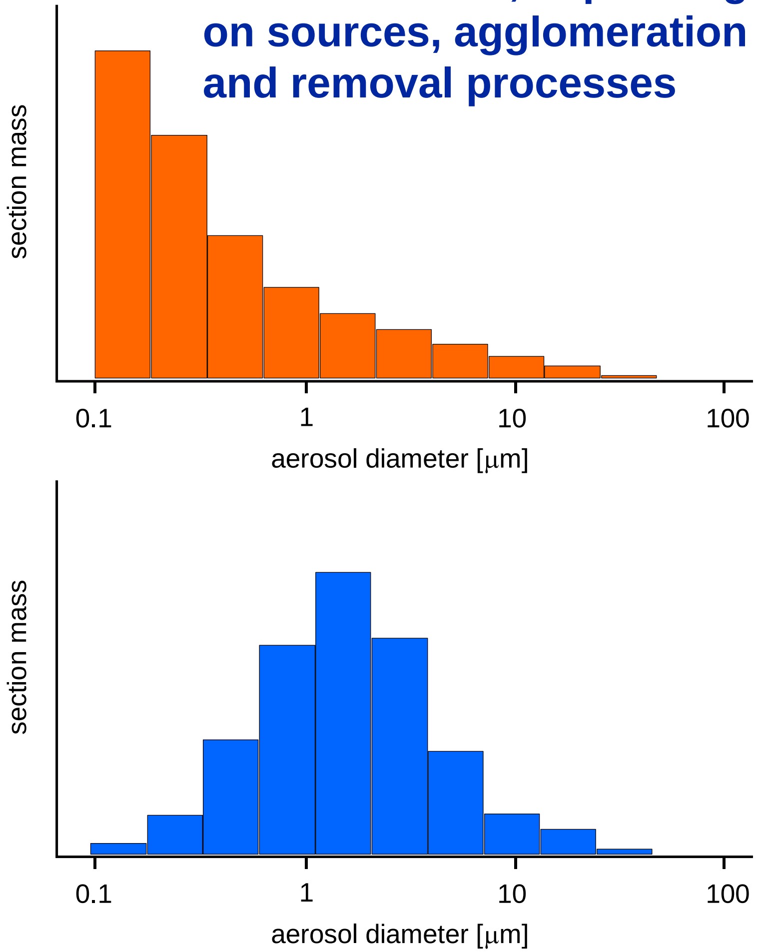
- Sections (size bins)
  - Discretized representation of (mass) concentration
  - Typically 10 sections, uniformly spaced in log of particle (volume-equivalent) diameter
  - Limited to section boundary diameters varying geometrically (i.e. $d_i >= 2^{(1/3)} d_{i-1}$) (use up to 9 sections per decade in particle diameter.)



Aerosols: MAEROS

- MAEROS sectional model of Fred Gelbard
  - 10 sections [.1 - 50 μm]
  - Condensed FP vapor sourced into smallest section
- Particles grow in size
  - Agglomeration
  - Water condensation
- Particle fallout by gravitational settling
- Particle deposition processes
  - Thermophoresis
  - Diffusiophoresis
  - Brownian motion
- PWR Ag aerosol release from control rods modeled
  - Significant aerosol mass
  - Affects agglomeration, growth and fallout
- Cs chemisorption in RCS modeled
  - Iodine from CsI revolatilizes when reheated

Aerosol size distribution evolves in time, depending on sources, agglomeration and removal processes



Aerosols: Resuspension and Sources

- New resuspension incorporated into MELCOR
  - Particle deposits maintain original bin size
  - Characteristic diameter of each bin is compared to a critical diameter lofted by local velocity
- Inter-volume phenomena
  - Flow through by gravitational settling/fall-out from cell above.
  - Flow through by advection.
- Source models
  - Release of radionuclides from fuel and debris
  - Aerosol creation from molten debris/concrete interactions
  - User defined sources

Condensation/evaporation

- FPs & water can condense/evaporate onto/from
  - Aerosols; heat structure surfaces; and/or water pools
- Aerosol water ≡ fog (CVH pkg)
  - Change in fog mass
    - Determined by thermodynamics
    - Distributed over aerosol sections
- Water condensation/evaporation for heat structure and water pool surfaces
  - Mason equation
- Calculation of FP vapor condensation/evaporation
  - TRAP-MELT2 rate equations based on
    - Surface areas, mass transfer coefficients, atmosphere concentration, and the saturation concentrations corresponding to the temperatures of the surfaces

Decay Heat Distribution (CV)

- All decay heat released by radionuclides in a control volume pool is assumed to be absorbed by that pool
- Decay heat released by radionuclides in the control volume atmosphere and from those deposited on the various heat structure surfaces can be apportioned according to user specifications among the
  - Volume atmosphere
  - Surfaces of heat structures in that volume
  - Pool surface (if a pool is present)

Decay Heat Distribution (FP)

- Simulation of decay radiation transmitted through flow paths
  - Specify the fraction going to the atmosphere and surfaces of other volumes
- Decay heat generated as
  - γ-radiation (~½) & β-radiation (~½)
- Deposition of decay heat in a volume atmosphere results primarily from absorption of β-radiation

Pool Scrubbing

- Adapted from SPARC-90 code
  - Steam condensation at the pool entrance
  - Aerosol deposition by Brownian diffusion, gravitational setting, and inertial impaction
  - Subject also to evaporative forces, for the rising bubble
- Aerosols and iodine vapor are removed
  - Removal of other vapor species can be treated identically to iodine vapor
- Model treats
  - Regular flow paths that vent through pools,
  - Gases generated by core-concrete interactions flowing through overlying pools
- Decontamination factor calculated

Filter Trapping (1)

- Some fraction of the transported RN materials may be removed by the action of filters in the flow paths
  - Calculated by CVH: aerosols & vapors transported through flow paths with the bulk fluid flow of pool and/or atmosphere
- Flow path can contain more than one filter
  - Single filter can remove either, but not both, aerosol or fission product vapor
- Filter efficiency, user-specified DFs per bin size or vapor
  - By default, a DF (= 1) is applied to all RN classes except water
- User-specified maximum loading
  - Loading reached, no further RN materials are removed (i.e., DF = 1)

Filter Trapping (2)

- Effect of filter loading on flow resistance of the associated flow path modeled through user input
  - Requires construction of a CF to link the laminar loss coefficient for the flow path to the filter loading (see FL User's Guide)
  - Filter loading may be obtained from one or more of the CF arguments (see RN User's Guide)
- Decay heat energy from radionuclides deposited on filters is given to the downstream control volume according to the vapor flow direction

Sandia National Laboratories

Spray Scrubbing (1)

- Model, same as in HECTR code
- Calculates the T-H behavior associated with spray systems
  - Coupled to the RN pkg for the calculation of aerosol washout and atmosphere decontamination by the sprays
  - SPR-RN interface may produce nonphysical results if the SPR pkg is required to make multiple passes through the same CV on a given timestep
    - Avoid by limiting the spray activity to a single drop size in each spray train
    - Restriction: only 1 spray train should pass through each CV

Spray Scrubbing (2)

- Particulate removal by sprays is a mechanistic treatment of removal processes
  - Modeled as a first-order rate process
  - Different rate constants are used for vapors and aerosols because the removal processes are different
    - Vapor removal by adsorption is calculated using a stagnant film model for the adsorption efficiency
      - The vapor removal is calculated as an injection spray removal rate; no recirculation of spray liquid is considered
- Limit on iodine adsorption by spray droplets (user specified) using a partition coefficient (equilibrium ratio of the iodine density in the liquid to its density in the gas)
  - LWR accident conditions, iodine may exist as a vapor over relatively long time periods in containment pressure/ temperature conditions. Other materials have low vapor pressures at accident conditions that preclude their extended existence as vapors; that is, they condense to aerosol forms.

Spray Scrubbing (3)

- Aerosol removal also included
  - Inertial impaction and interception
    - Primary removal mechanisms as long as droplet radii are in the 10 – 100 micron size range
  - Diffusiophoresis and diffusion effects
    - 1–10 μm diffusiophoresis becomes an important contributor
    - Diffusion only becomes important for droplets with radii , 0.1 μm
  - Rate constant are a function of collection efficiency
    - Viscous and well as potential flow around a sphere are considered for both impaction and interception
    - Collection efficiencies for different processes are combined
- No droplet interactions are considered

T-H Modeling: Spray

- Spray droplets are assumed spherical, isothermal, and falling through containment at their terminal velocity (w/o horizontal velocity component)
- Droplet heatup & cooldown in a steam environment
  - Modeled using a correlation for forced convection heat transfer coefficients
- Evaporation/condensation are modeled
  - using a correlation for mass transfer coefficients
- Final droplet mass ($m_{droplet}$) & temp (T_{drop}) obtained
  - By use of a std integrator to integrate transfer rates over the fall height of the spray droplet
- Heat and mass transfer to a droplet computed via
  - Comparison of $m_{droplet}$ & T_{drop} at bottom of compartment to the inlet conditions
- Total heat & mass transfer rates calculated by multiplying rates for single droplet by the number of droplets of that size and summing over droplet sizes

Fission Product Chemistry

- Chemistry effects can be simulated in MELCOR through the use of class reaction and class transfer processes
  - class reaction process uses a first-order reaction equation with forward and reverse paths
  - class transfer process
    - can change material class or location of a radionuclide mass (caution: use feature carefully)
    - can be used to simulate fast chemical reactions
- With these two processes (reversible & irreversible reactions) phenomena including adsorption, chemisorption, & chemical reactions can be simulated
- Only FP vapors are considered in the chemistry models
  - Only fission product vapors can react with surfaces and only vapors and ions produced from them can undergo chemical transformations in the pool

FP Chemistry: Example

Consider the adsorption of CsI on a surface with a known deposition velocity which is then transformed immediately to CsOH plus HI when adsorbed water is present. After the transformation, the revaporization of CsOH is delayed until the surface temperature reaches T_1 while the HI revaporization is simply mass transfer limited. In this case, CsI, CsOH, and HI are separate material classes.

$$CsI(\text{gaseous}) \rightarrow CsI(\text{adsorbed})$$

$$\downarrow H_2O$$

$$CsOH(\text{gaseous}) \leftrightarrow CsOH(\text{adsorbed})$$

$$+(\text{depends on } \mathrm{T}_1)$$

$$HI(\text{gaseous}) \leftrightarrow HI(\text{solid})$$

Chemisorption

- Forms chemical bond with surface
- Currently can only be done on materials in the MELCOR database & does not function for user-defined materials

Chemisorption Transport	
CsOH	Stainless steel
CsOH	Inconel*
CsI	Stainless steel
CsI	Inconel*
I_2	Stainless steel
HI	Stainless steel
Te	Stainless steel
Te	Inconel*

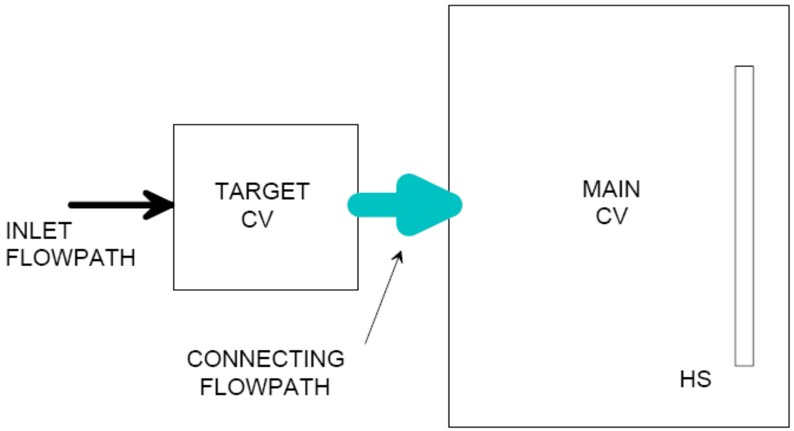
*not in database

Hygroscopic Models

- Mason Equation
- Model describes diffusion of water vapor molecules to the surface of an aerosol particle, and the conduction of the latent heat of vaporization away from the particle and to the bulk atmosphere
  - Solubility effect: hygroscopic
  - Kelvin effect: surface tension
  - Free molecule effects: noncontinuum
- Aerosol particles that are soluble in water exhibit hygroscopic properties such that they can absorb moisture from an atmosphere with relative humidity less than 100%
  - Effect leads to particle size growth as water vapor condenses onto the soluble particle
  - Consequence:
    - Increase in gravitational settling rate
    - Subsequent depletion of airborne FP aerosols

Jet Impaction

- Impingement of a flashing water jet on a plate
  - Water jet enters volume at lower pressure than the inlet pressure, flashes, and then expands according to regular jet expansion formulation until deflected by a plate
  - Droplets larger than a cutoff diameter hit the plate and are removed from the jet (becoming part of water film on HS & drain according to film model)
  - Droplet size distribution
    - Determined by flashing model (FL pkg) and is sourced into RN pkg
- No flash, no aerosol

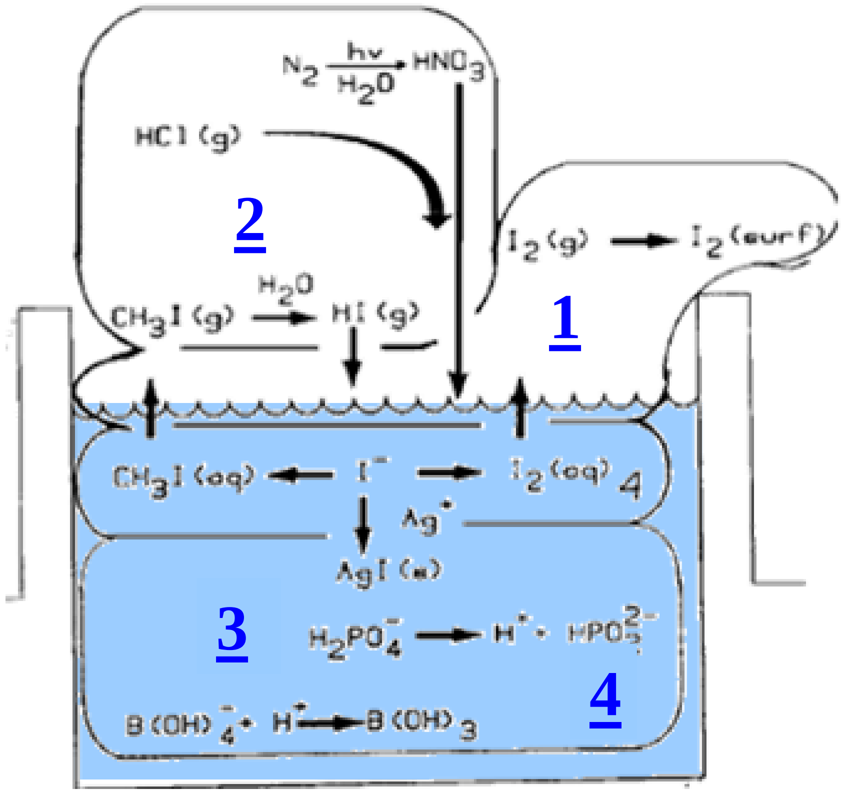


Iodine Control

- Amount of iodine released is reduced by controlling atmospheric iodine concentration
  - Iodine can be confined in aqueous forms in pools and sumps, but
    - radioactive iodine may not remain trapped in water because of its relatively dynamic chemical behavior
      - There are important processes that can regenerate gaseous forms of iodine that release into the containment atmosphere from the water, thus becoming available for release to the environment for long times after the accident initiation
      - Chemical and radiolytic oxidation of iodine in the pool can lead to the formation of a variety of chemical forms of iodine, such as elemental iodine and volatile organic iodides
    - Formation of volatile forms of iodine in solution depends on
      - Dose rate to aqueous phase; temperature; pH; and total iodine concentration

Iodine Transformations Considered

- Seven sub-models



- Acid generation and transport models (walls & pools)
- Pool pH calculation
- Silver iodine model
- Iodine aqueous pool chemistry (276 equation set)
- Pool atmosphere mass transfer
- Iodine atmospheric radiolysis and recombination
- Iodine atmosphere wall deposition