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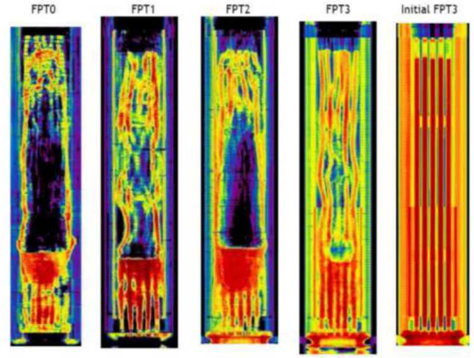

Building a Source Term within the MELCOR/NRC Framework

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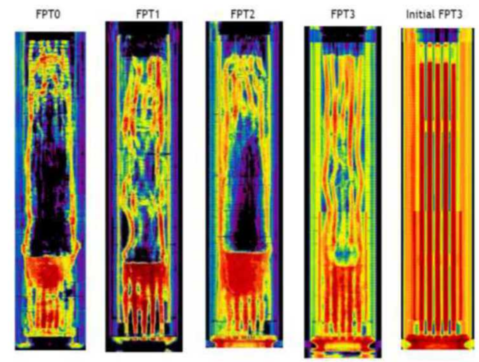
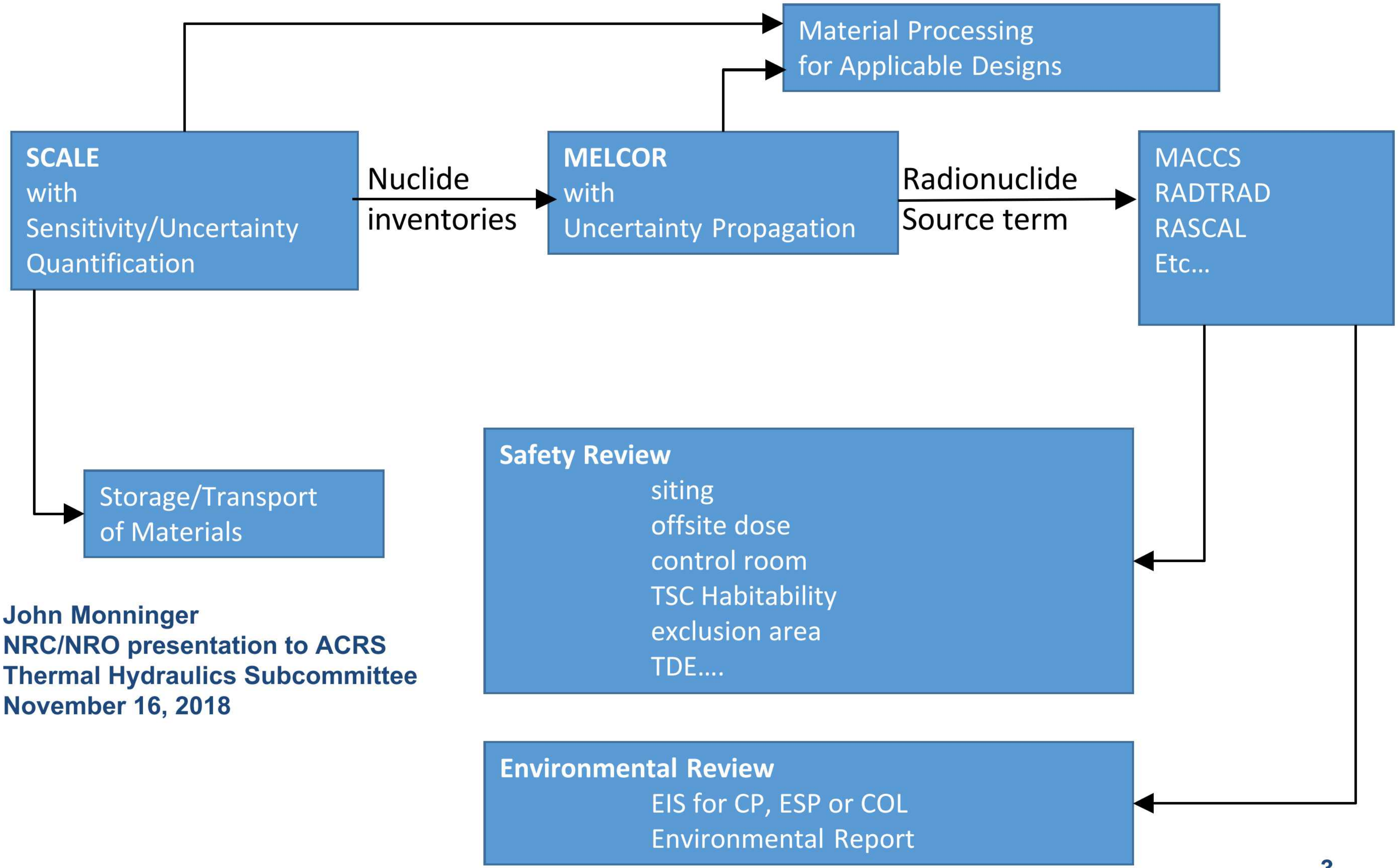


MODELING APPROACH

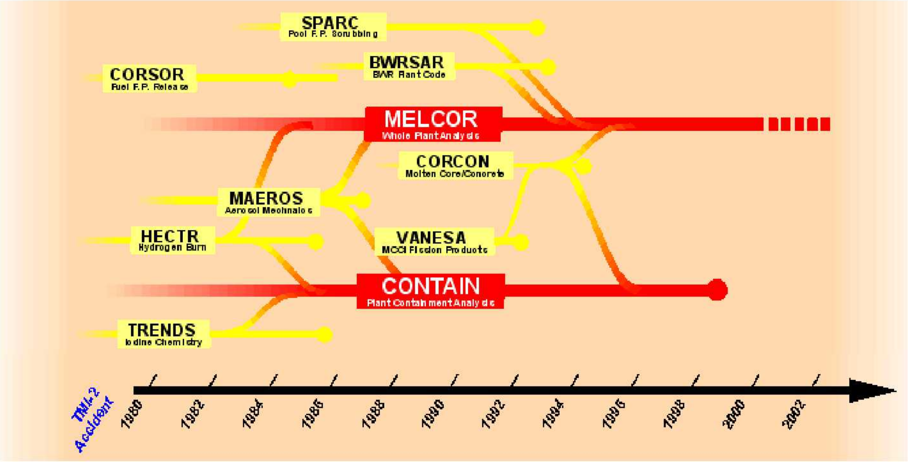
Source Term Use Process

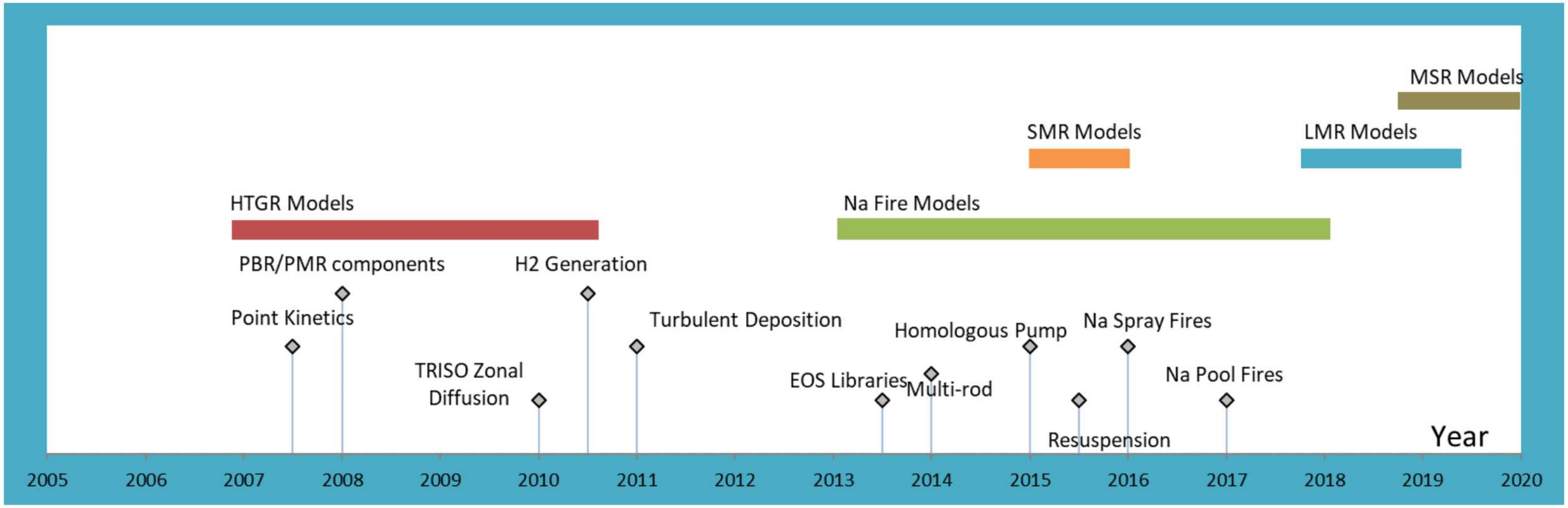


John Monninger
NRC/NRO presentation to ACRS
Thermal Hydraulics Subcommittee
November 16, 2018

MELCOR Activities

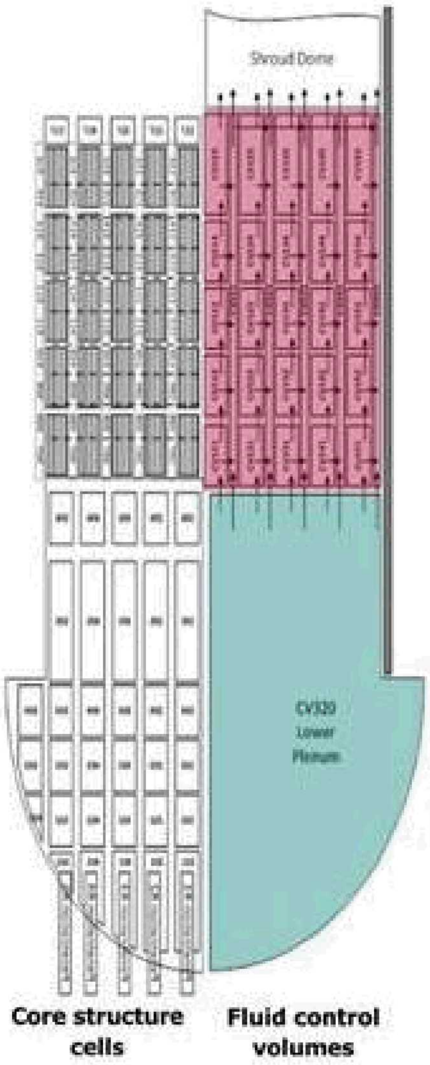
- State-of-the-art tool for severe accident progression and source term analysis.
- Ongoing development of new capabilities
- Replaces collection of simple, special purpose codes, i.e., Source Term Code Package (STCP)
- Eliminate tedious hand-coupling between modules
- Capture feedback effects (i.e., coupling of temperatures, release rates, and decay heating

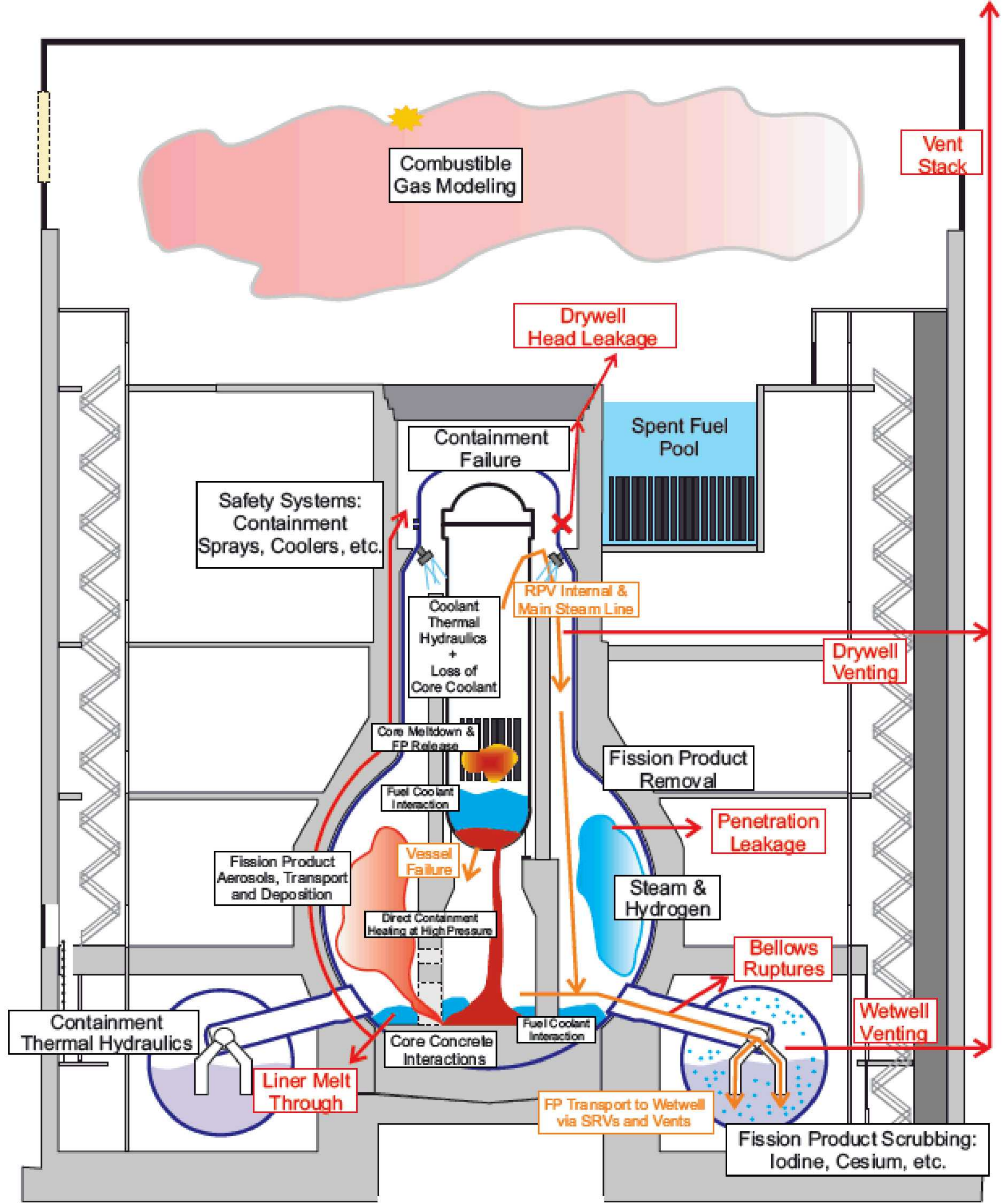




MELCOR Overview

- Fully integrated, engineering-level computer code with the purpose of modeling the progression of accidents in LWRs
  - Evaluate accident progressions
  - Determination of fission product source terms
  - Identify sensitivities and uncertainties of these calculations
- Executive driver and packages, that together model the major systems of a reactor plant and coupled interactions
  - Thermal-hydraulic response of the system
  - Core uncovering, fuel heatup, cladding oxidation & fuel degradation Lower plenum behavior an relocation ex-vessel
  - Core-concrete attack and ensuing aerosol generation
  - In/ex-vessel hydrogen production, transport, combustion
  - Fission product release, transport, and deposition
  - Behavior of radioactive aerosols in the system, including scrubbing in pools, and aerosol mechanics such as particle agglomeration & gravitational settling
  - Impact of engineered safety features on fluids & RN behavior





Physics Captured in MELCOR Framework

- Accurate system description
  - Geometries
  - Leakage parameters for components
  - Safety system modeling
- Transit through the system
  - Vapor, aerosol, gas, pool
  - Into the primary
  - Circulated
  - Interactions w/components and piping

Key Literature

- Develop Source Term → Apply Source Term → Releases → Consequences
- NUREG 1465: Develop a source term, based on reactor type and characteristic scenarios
- RG 1.183: Apply a source term for specified accident scenarios
- SOARCA Program: Application of uncertainty to scenarios and consequence
- NUREG 2161: Spent fuel pool study
- NUREG 2206: Filtered venting study

Radionuclide Group	Title	Elements in Group
1	Noble Gases	Xe, Kr
2	Halogens	I, Br
3	Alkali Metals	Cs, Rb
4	Tellurium Group	Te, Sb, Se
5	Barium, Strontium Group	Ba, Sr
6	Noble Metals	Ru, Rh, Pd, Mo, Tc, Co
7	Lanthanides	La, Zr, Nd, Eu, Nb, Pm, Pr, Sm, Y, Cm, Am
8	Cerium Group	Ce, Pu, Np

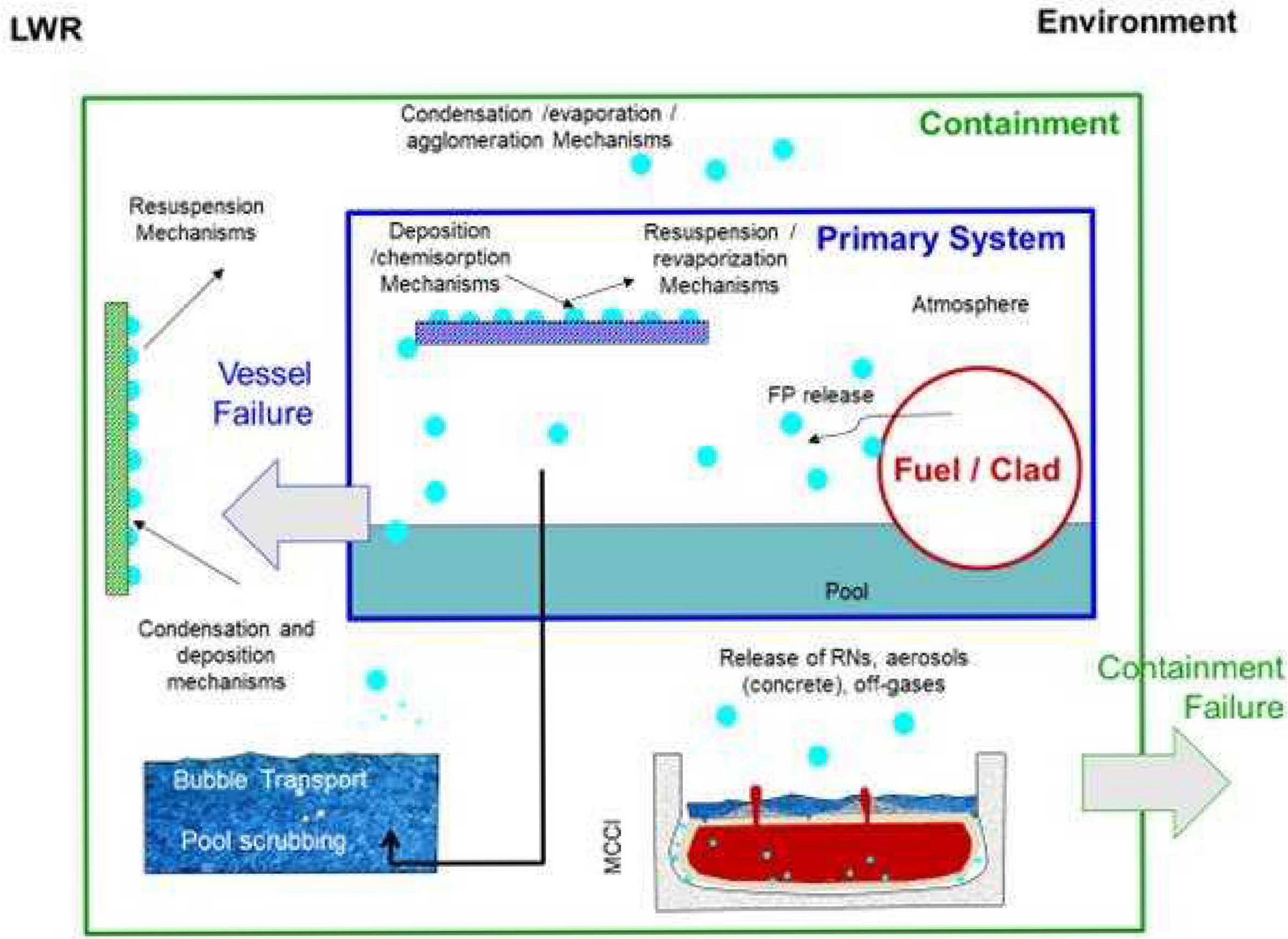
	Gap Release***	In-vessel	Ex-vessel	Late In-vessel
Duration (hours)	0.5	1.3	2.0	10.0
Noble Gases**	0.05	0.95	0	0
Halogens	0.05	0.35	0.25	0.1
Alkali Metals	0.05	0.25	0.35	0.1
Tellurium Group	0	0.05	0.25	0.005
Barium, Strontium	0	0.02	0.1	0
Noble Metals	0	0.0025	0.0025	0
Lanthanides	0	0.0002	0.005	0
Cerium Group	0	0.0005	0.005	0

* Values shown are fractions of initial core inventory.
** See Table 1 for a listing of the elements in each group.
*** Gap release is 3% if long term fuel cooling is maintained.

The MELCOR RN Package

- Originally intended to treat behavior (release, transport, interactions) of RadioNuclides in nuclear reactor accidents
- Some models (and some coding) are extracted from other codes, but implemented in a more-consistent form
- RN materials are “traces”, hosted by other materials or objects
  - Fuel and/or debris
  - Hydrodynamic materials Surfaces of heat structures
- Mass, volume, heat capacity, are negligible
  - Temperature, when needed, taken as host’s
- Give some understanding of a few within-volume models in MELCOR RN1 Package
  - **MAEROS**: Aerosol physics
  - **TRAP-MELT**: Condensation and evaporation involving aerosols and surfaces
  - **Water aerosol models**: CVH “fog” & Hygroscopic model
- **RN1:** models mainly within-volume processes, calculated before hydrodynamic advancement (Releases, interactions)
- **RN2:** models mainly between-volume processes, calculated during or after hydrodynamic advancement (Advection with fluids, removal by filters)
- The RN package distinguishes RN *classes*, groups of materials with properties that are “similar enough” to treat together
  - “Actual” radionuclides (see next slide)
    - Ideal gases, alkali metals (Cs, Rb), etc. (~17 classes)
    - Important compounds (CsI, Cs_2MoO_4)
  - Boron (from reactor control elements)
  - Concrete (oxides from MCCI)
  - Water (water aerosols that interact w/other aerosols)
  - Other trace materials (solid or vapor)
    - Species in Iodine pool model
    - User-defined materials

RN Transport Paths



MAEROS - Multicomponent AEROSol model

- Calculates time history of aerosol particle size distribution and chemical composition
  - Calculates changes in masses of each component (material) in each section as a function of time. Prior to this development, material composition of aerosol was unavailable and all particles were assumed to be of the same chemical composition regardless of particle size (e.g., CONTAIN modeling)
  - Currently limited to requiring that all aerosol components (materials), have the same material density.
  - Solves multi-sectional, multi-component formulation of aerosol dynamics equations for deposition and agglomeration
- Basic Approximations
  - Total mass of a particle determines how the particle deposits, agglomerates, and grows.
  - (Currently) All component material densities are the same.

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Phenomena Treated by MAEROS

- Deposition on surfaces
  - Traditionally modeled as always adhering to surfaces contacted, but new resuspension model was implemented taking it into account
  - Mechanisms that drive aerosols to surfaces
    - Gravity usually dominates
    - Brownian diffusion to surfaces
    - Migration to cooler surfaces by thermophoresis
    - Migration to surfaces by diffusiophoresis (i.e., condensation)
    - Turbulent deposition
- Agglomeration of aerosols
  - Several mechanisms cause collisions and sticking to produce larger particles
    - Brownian diffusion (relative motions)
    - Differential gravitational settling
    - Turbulent agglomeration
- Condensation and evaporation treated in TRAP-MELT model
- Disposition of particles that grow larger than computational domain (to conserve mass)
  - Ordinarily "settle" immediately
  - This requires at least one available surface in each volume
- MELCOR adds additional "settling surfaces" to represent common boundaries of volumes
  - Treated as deposition surfaces
  - Allows aerosols to fall from one volume to another
  - Can also provide destination for oversize particles

TRAP-MELT

- Models condensation and evaporation of RN vapors involving aerosols and surfaces (replaces treatment in stand-alone MAEROS)
- Volatile radionuclides (e.g., CsOH, I_2, CsI, Cs_2MoO_4) have finite vapor pressures that increase with temperature
  - Concentration in atmosphere limited by vapor pressure at T_{atm}
  - Mass can be transported to/from condensed phase on aerosol surfaces and/or structural surfaces
    - Aerosols are at atmosphere temperature,
    - Structure surfaces may be hotter or colder,
    - Rate limits apply

$$\frac{dM_a}{dt} + \sum_i \frac{dM_i}{dt} = 0 \qquad \frac{dM_i}{dt} = A_i k_i \left(C_a - C_i^s\right)$$

- Structural materials can be volatile too (e.g. Zr and SS in-vessel)
- Conservation of mass, and rate equations are
  - *M* is mass, *C=M/V* is concentration, subscript *i* refers to surface, superscript *s* is saturation at surface temperature (Surfaces include aerosols, section by section)
- Model evaluates closed-form solution for full MELCOR timestep, Δt
  - Iteration may be needed if any surface mass falls to zero

$$C_a = M_a / V = \frac{\beta}{\alpha} - \left(\frac{\beta}{\alpha} - C_{a0}\right) e^{-\alpha\Delta t} \qquad M_i = M_{i0} + A_i k_i \left(\frac{\beta}{\alpha} - C_i^s\right) \Delta t - A_i k_i \left(\frac{\beta}{\alpha} - C_{a0}\right)\left(\frac{1 - e^{-\alpha\Delta t}}{\alpha}\right)$$

$$\alpha = \sum_i A_i k_i / V \qquad \frac{\beta}{\alpha} = \frac{\sum_i A_i k_i C_i^s}{\sum_i A_i k_i}$$

Water Aerosols

Overview

- Water also forms aerosols, but water vapor is a hydrodynamic material
- Mass, volume, heat capacity of RN vapors and aerosols is ignored by hydrodynamics
- Condensation/evaporation for water aerosols need to be solved separately

Hygroscopic model

- RN "takes possession of" all liquid water in atmosphere
  - Necessary to account for hygroscopic and Kelvin effects that modify vapor pressure of water in aerosol form so different from water in the rest of MELCOR (CVH, HS, …)
- Condensation taken from CVH steam, evaporation returned to CVH steam
- Water aerosols deposited on pool and HS surfaces as ordinary water
- Mass/energy conservation accounting in CVH and HS adjusted for these transfers

Original Model

- Water aerosol identified with CVH "fog" (liquid water in atmosphere)
- RN Package accepts new fog mass (after CVH) as new total water aerosol mass, then imposes the change in size distribution
  - Uses MAEROS coefficients based on sectional integration of Mason equation

$$\frac{dQ_{\ell,k}}{dt} = \ldots + {}^{1}\overline{G}_{\ell,k} Q_{\ell} - \sum_{i=1}^{N_a} \left[{}^{2}\overline{G}_{\ell,k} Q_{\ell,k} - {}^{2}\overline{G}_{\ell\pm1,i} Q_{\ell\pm1,k} \right]$$

- Calculate condensation explicitly, normalized so that sum over sections matches net change

$$\Delta m_w = \sum_{\ell} Q_{\ell} \, {}^{1}\overline{G}_{\ell,w} \, X \, \Delta t$$

- Calculate sectional transfers implicitly, using post-condensation masses
  - Condensation, particles grow—only have up-transfers
  - Evaporation, particles shrink—only have down-transfers

Release Mitigation Modeling

- Very important to accurately represent the system
- Pool scrubbing
  - Covered by SPARC90 in MELCOR2.2
  - Older model, not set-up for stratified pools
- Decontamination factors
  - User-defined options
- Impact of release significant components
  - MSIVs
  - SRVs
- Integrity of the containment
  - DW head flange and penetration failure criteria
- Deposition structures in containment and reactor building
  - Surface area dependent

RN Potential Improvements

- The basic assumptions (same density, same shape factors) for all particles in a section could be relaxed, but:
  - General theory for shape factors for all particle sizes and all events needs further research
  - Can include separate material densities of different materials. This will increase aerosol computation, but computer time for this is no longer limiting.
- New numerical methods can sharpen results
  - Can upgrade numerical technique for particle growth by vapor condensation due to hygroscopic effect (incorporate better algorithm for speed and accuracy) – *In progress*
- Conclude that (at this time) MAEROS formulation is mostly adequate

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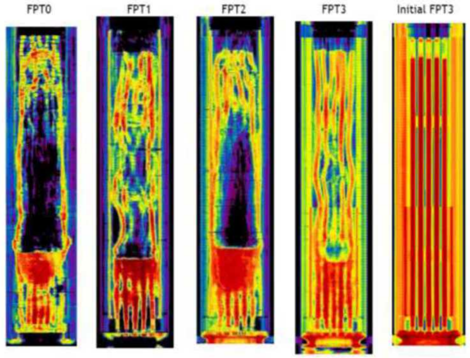
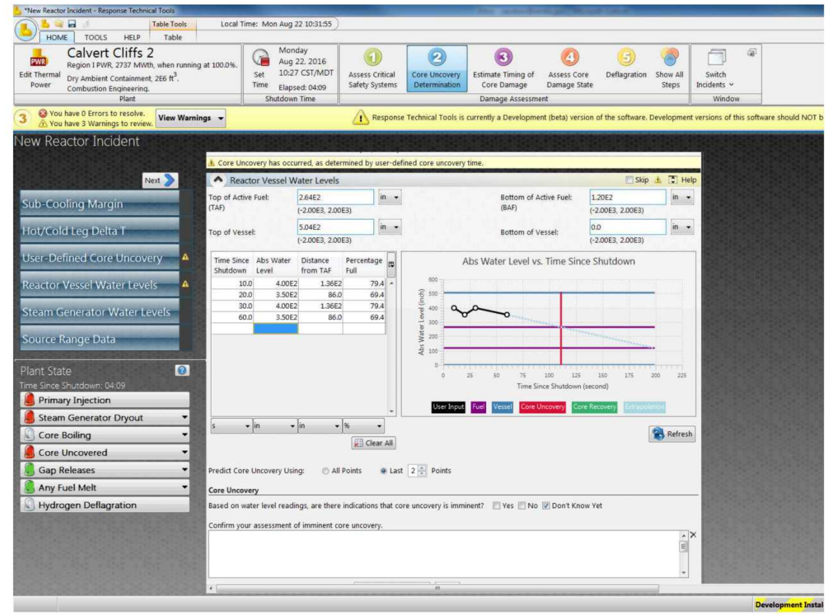
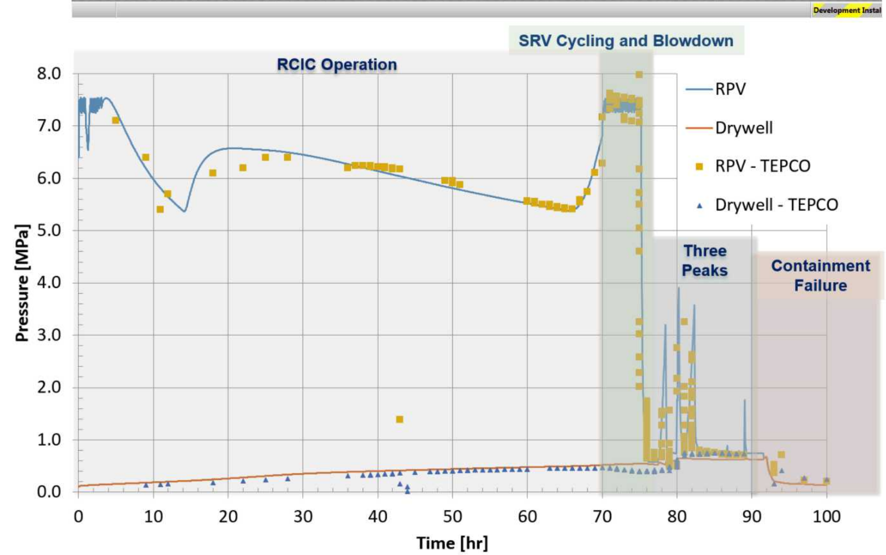


APPROACHES AND TOOLS

Source Term Code Framework

- Before an Accident
  - ORIGEN/SCALE
    - Build radionuclide inventory
  - FAST
    - Fission gas inventories, early gap releases
  - MELCOR
    - System level behavior
    - Core degradation
    - Radionuclide transport to environme
  - MACCS
    - Dispersion within the environment
- Accident Response
  - Response Technical Tools
    - Assess accident scenario
  - RASCAL
    - Radionuclide dispersion



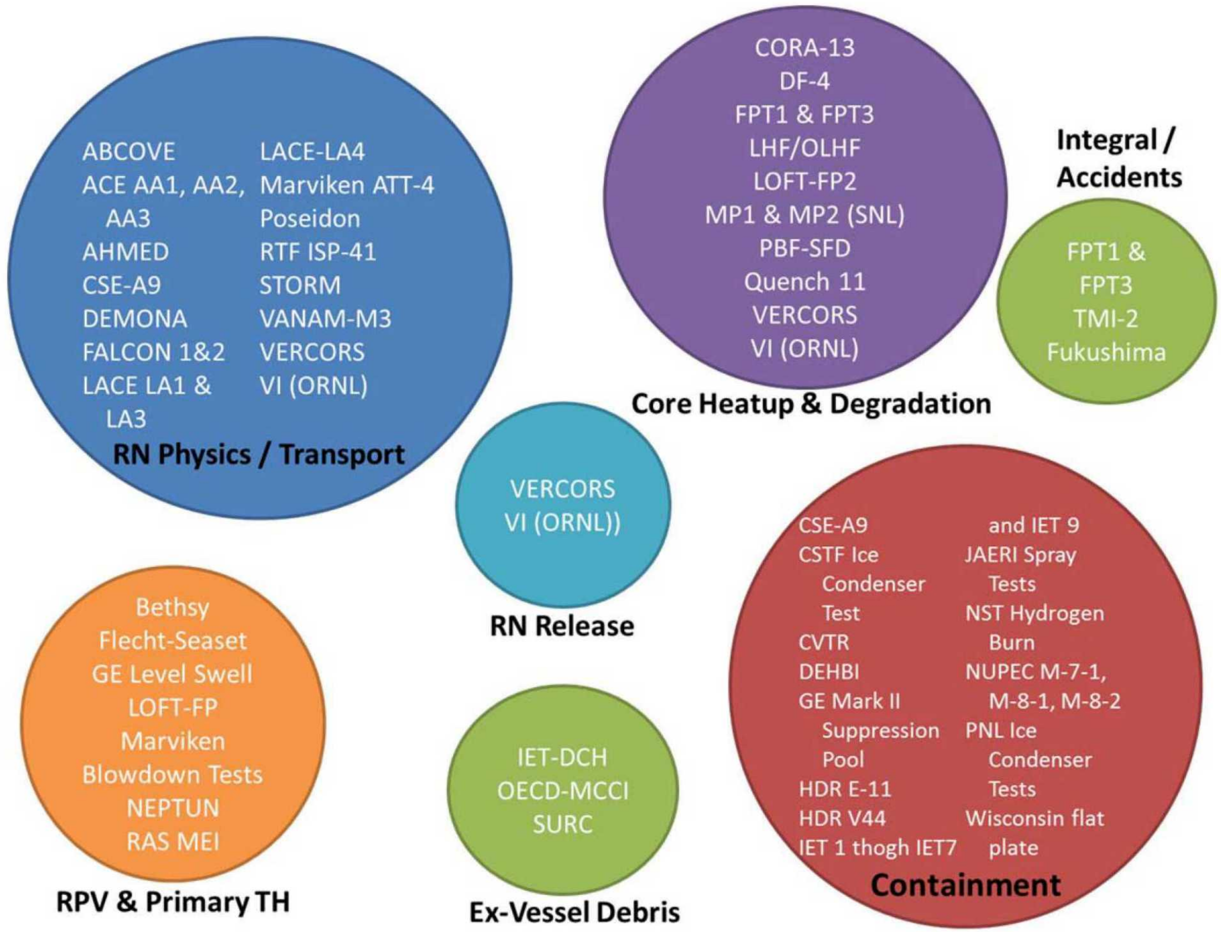


Capturing Uncertainties

- Accurately capturing system and phenomenological uncertainties can ensure that all potential RN behavior is captured
- Core degradation uncertainties
  - Eutectic interactions, radial relocation, blockage, etc.
- System uncertainties
  - Scrubbing efficiencies, leakage locations, valve behavior, etc.
- Aerosol uncertainties
  - Deposition rates, local conditions, etc.
- SOARCA UA
  - Peach Bottom
  - Surry
  - Sequoyah

MELCOR Validation

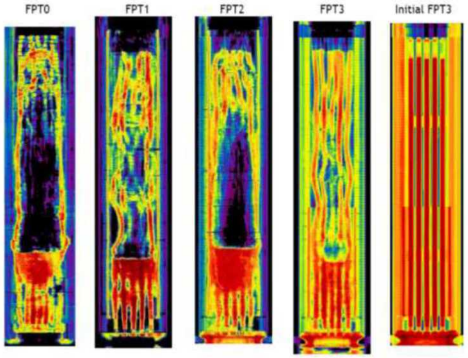
- Analytic results
- Code-to-code comparison with other validated programs
  - xWalk activities
- Experimental results
- Comparison to data from real-life accidents
  - TMI
  - 1F accidents



Unanswered Issues for LWRs

- Long-term behavior can have a major impact on total source term
  - Significant uncertainties in the composition and location of corium when it relocates ex-vessel
- MELCOR predicts a failure of the lower head near the bottom-center
  - 1F2 seems to indicate a large amount of metallic debris spread over floor
  - Long-term leakage pathways are not well known, but still have a significant impact of system pressure and source term
- Liner failure through ablation
  - Injection vs. containment breach size
- Injection into containment can increase overall fission product release if debris is not fully submerged and containment is still compromised
- Impact of different in-vessel degradation mechanism and materials failure points
- Progression of MCCI: spreading and cooling
- Operation of plant equipment beyond design basis (e.g. RCIC, SRV)
- Role of CRD structural materials below the lower head in accident progression


Unit 6
Unit 5
Unit 1
Unit 2
Unit 3
Unit 4
Source: Tokyo Electric Power Company


FPT0
FPT1
FPT2
FPT3
Initial FPT3

QUESTIONS?

NUREG 1465 Sequences

Plant	Sequence Description
Surry (Westinghouse 3-loop PWR with large-dry, subatmospheric containment)	Hot leg loss of coolant accident (LOCA), no containment sprays (CS), no fan coolers (FC)
	Loss of Offsite Power (LOOP), no Power Conversion System (PCS), no Auxiliary Feedwater (AFW)
	Interfacing systems LOCA (ISLOCA)
	Station blackout (SBO), reactor coolant pump (RCP) seal LOCA
	Small-break LOCA (SBLOCA), no emergency core cooling system (ECCS), H_2 combustion
	SBLOCA, 6”-equivalent diameter hole in containment
Zion (Westinghouse 4-loop PWR with large-dry containment)	2”-equivalent diameter LOCA, no ECCS, no CS recirculation
	RCP seal LOCA, no ECCS, no CS, no FC, early H_2 burn-induced containment failure (CF)
	22DCF1, except late CF (overpressure or H_2 burn)
	Transient, no power conversion system (PCS), no ECCS, no AFW, CF due to direct containment heating (DCH)
Oconee 3 (B&W PWR with large-dry containment)	SBO, no AFW
	3”-equivalent diameter LOCA, no AFW, no ECCS, no CS, no FC
Sequoyah (Westinghouse 4-loop PWR with ice condenser containment)	RCP seal LOCA, no ECCS, no CS recirculation, reactor cavity flooded
	S3HF1, hot leg creep-rupture before vessel failure (VF)
	S3HF1, dry reactor cavity
	½”-equivalent diameter LOCA, SBO, no AFW
	SBO, hot leg creep-rupture before VF, H_2 burn-induced CF
	Hot leg LOCA, no ECCS, no CS
	SBO, delayed RCP seal failure (4), turbine-driven AFW
	RCP seal LOCA, no ECCS, no CS recirculation
	RCP seal LOCA, no ECCS recirculation

Water Aerosols: Hygroscopic Model

- Based on single-step implicit solution of Mason equation, which accounts for conduction of latent heat (a term) and diffusion of water vapor (b term)

$$\frac{dr}{dt} = \frac{1}{r}\frac{(S - S_r)}{a + b} \qquad a = \left(\frac{\Delta h_f^2 M_w \rho_w}{R T_\infty k_a^*}\right) \qquad b = \left(\frac{R T_\infty \rho_w}{D_v^* M_v p_{sat}(T_\infty)}\right)$$

- *S* is saturation ratio (relative humidity), S_r is effective saturation ratio at particle surface

$$S_r = A_r \cdot \exp\left(\frac{2 M_w \sigma}{R T_\infty \rho_w r}\right) \qquad A_r = \exp\left[-\sum_i \frac{\nu_i n_i}{n_w}\right]$$

  - Activity factor A_r accounts for ionization of dissolved soluble aerosols. This *reduces* equilibrium vapor pressure over solution (usually below saturation)
  - Exponential multiplier accounts for Kelvin effect, where surface tension effects “resist” condensation. This *increases* equilibrium vapor pressure (can be greater than saturation)
- Solution requires double iteration to determine end-of-step partial pressure and saturation pressure for water