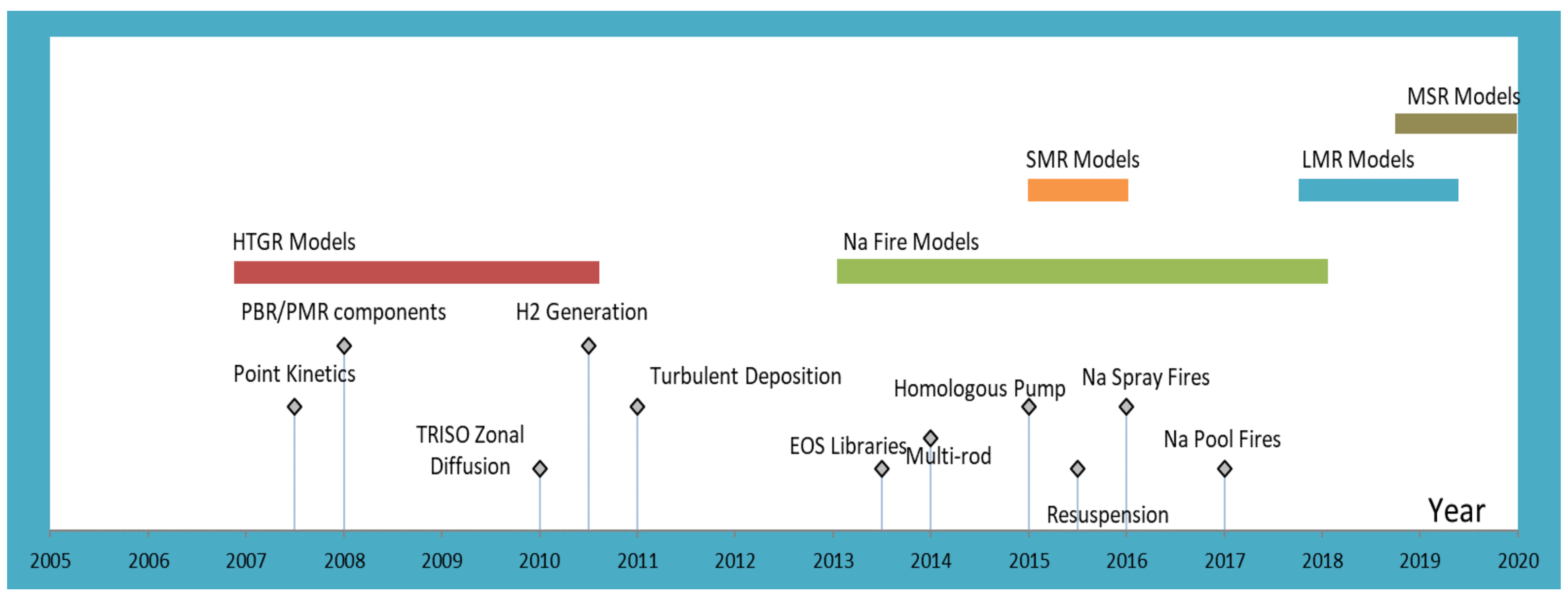
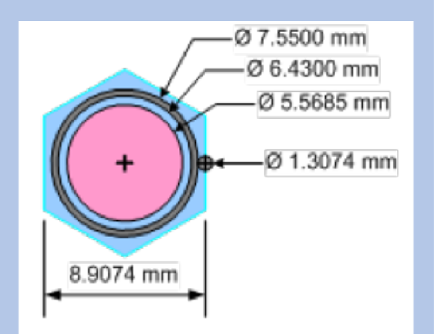
SAND2022-7757D

SFR Modeling



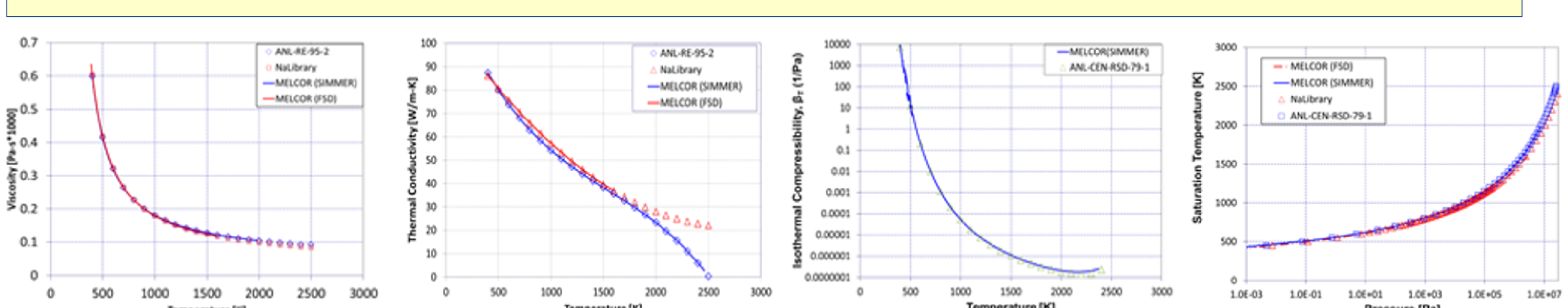
SFR Components (under development)

- SFR to use fuel, clad, cannister, and support/non-support structure
- Bond sodium gap not its own component as of now
  - Existing gap modeling capabilities
  - New models for gap closure, sodium migration to plenum, and attending FP transport
- Pin plenum not its own component as of now
  - Initialization
  - Volume accounting and ideal gas treatment
  - Attending FP transport
  - Pressure calculation
- Expect reflector component could factor into SFR designs
- May revise some intracell and intercell component-wise heat transfer models



Sodium Equation of State (EOS)

- Two alternatives: Fusion Safety Database (FSD) and SIMMER-III
  - FSD uses a soft-sphere EOS model fit to an experimental database
  - SIMMER-III supplemented with experimental data (Fink & Leibowitz)
- Verified EOS on a wide range of thermodynamic conditions
- Enthalpy, heat capacity, heat of fusion, vapor pressure, heat of vaporization, density, thermal conductivity, thermal diffusivity, and thermal expansion
- Demonstration calculations reproduce the experimental database



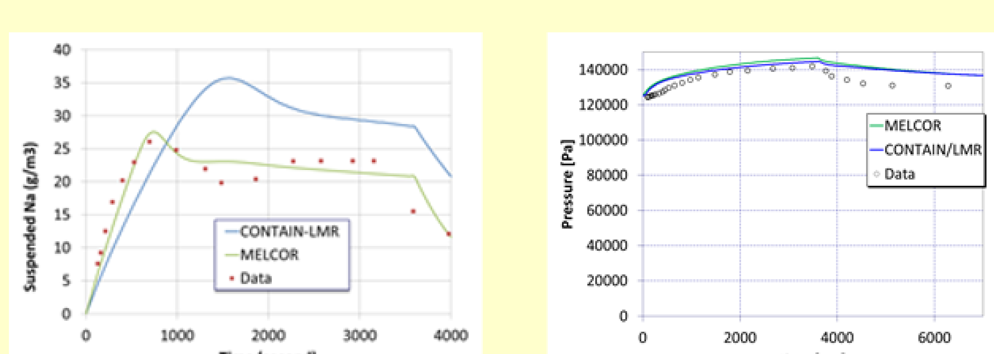
SFR Containment (Ex-Vessel) Models

- Spray and pool fire models from CONTAIN/LMR
- Pool fire
  - Pool fire model from SOFIRE-II based on pool fire tests
  - Predicts rate of oxygen and sodium consumption plus heat evolved from reaction

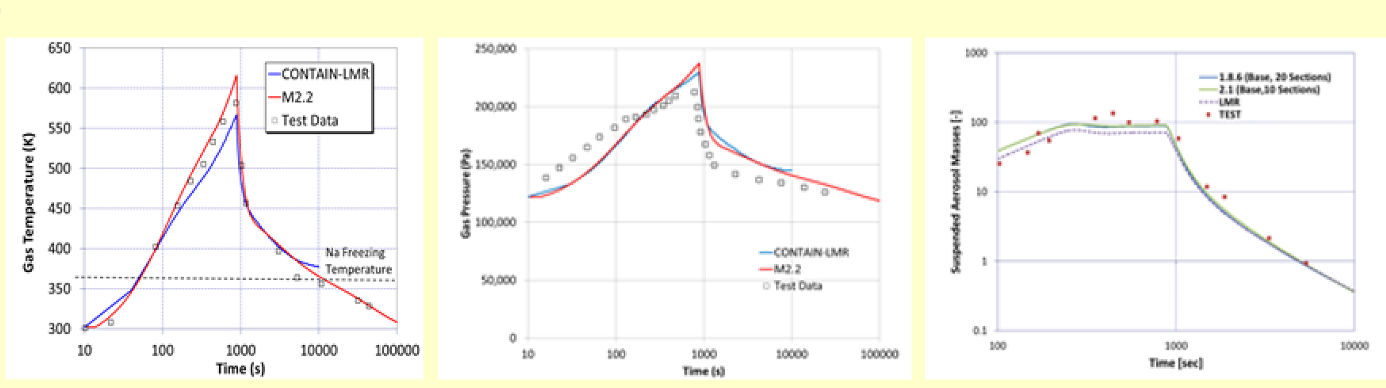
$$(1+f_1)\cdot 2\cdot Na + O_2 \rightarrow 2\cdot f_1\cdot Na_2O + (1-f_1)\cdot Na_2O_2 + q(reaction)$$

- Spray fire
  - Spray fire model from NACOM
  - Predict total burned sodium mass as function of droplet size and fall velocity
  - Integrate combustion rate over droplet fall height

- Fire model validation – ABCOVE AB1/AB5
  - AB1 (pool)



  - AB5 (spray)



- Atmospheric chemistry
  - Aerosol/atmosphere
  - Aerosol on surfaces
  - Sodium/water in atmosphere
  - Reactions in hierarchical order
  - Affected through NAC package
  - New RN classes
  - New sensitivity coefficients

$$Na(l) + H_2O\,(l) \rightarrow NaOH(a) + \frac{1}{2}H_2$$

$$2\,Na(g,l) + H_2O\,(g,l) \rightarrow Na_2O(a) + H_2$$

$$2\,Na(g,l,a) + \frac{1}{2}O_2\,or\,O_2 \rightarrow Na_2O(a)\;or\;Na_2O_2(a)$$

$$Na_2O_2(a) + 2\,Na(g,l) \rightarrow 2\,Na_2O(a)$$

$$Na_2O(a) + H_2O\,(g,l) \rightarrow 2NaOH(a)$$

$$Na_2O_2(a) + H_2O\,(g,l) \rightarrow 2NaOH(a) + 0.5O_2$$

Transient/Accident Solution Methodology

Stage 1: Thermal Steady State

Establish COR, CVH, & HS temperatures

Establish steady flow patterns

Initialize any RN form mass outside fuel

Assume thermal hydraulic conditions hold constant over pre-transient stage

Stage 2: Steady/Pre-Transient Mechanics and Fission Product Transport

Option 1) – User Input
- *Fuel and Clad geometry changes*
- *Pin plena initialization*
- *Fuel swelling/porosity distribution*
- *DCH/RN class mapping to gaseous and solid fission products*
- *End-of-burnup RN class inventory*
  - *Gaseous and solid in fuel*
  - *Solid in bond sodium gap*
  - *Gaseous in pin plena*

Option 2) – Calculated (coming soon)
- *Mechanical response of fuel pins*
  - *Algebraic formulation*
  - *Stress, strain, and displacement*
  - *Bond sodium gap dynamics*
- *Fission gas transport in-pin*
  - *Volume accounting methods*
  - *Ideal gas assumptions*
  - *Empirical models for fuel swelling and porosity dynamics*

Stage 3: Transient Diffusion & Transport calculation

In-pin dynamics (coming soon)
- *Up to and including pin failure*
- *Fuel molten cavity formation*
- *Fuel and clad dimensional changes*
- *Clad dynamics*
  - *Eutectic thinning*
  - *Mechanical failure*
  - *Candling and conglomerate debris*
  - *Assembly peripheral area (CN,CL)*
- *Clad/pin failure*

RN release from COR to CVH/RN in GRTR

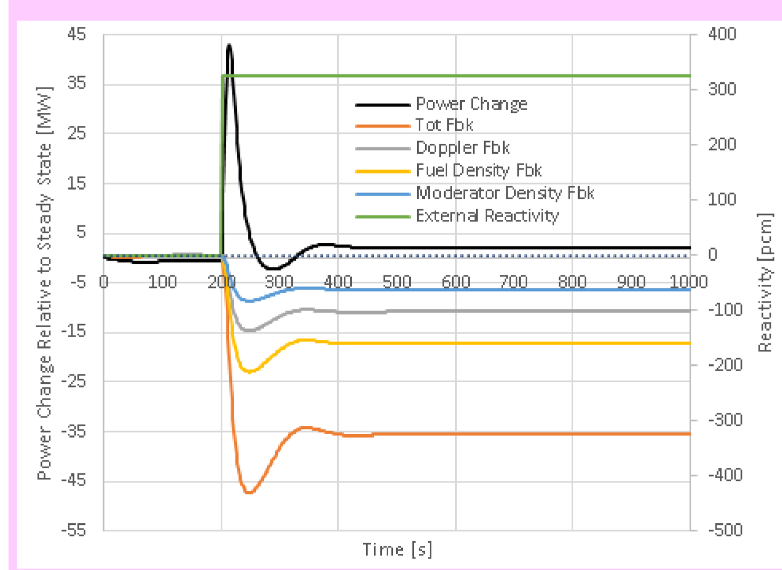
Severe accident phenomena (coming soon)
- *Clad relocation (conventional candling)*
- *Clad relocation (reverse candling)*
- *Fuel relocation in a candling mode*
- *Pin effluents ejection*
  - *Solid (particles, chunks, streamers)*
  - *Molten material and pin gases*

Standard Point Reactor Kinetics Equations

Standard 6 group treatment

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

$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right)P - \lambda_i C_i, \qquad for\ i = 1\ldots6$$



Kinetics data accessible by sensitivity coefficients

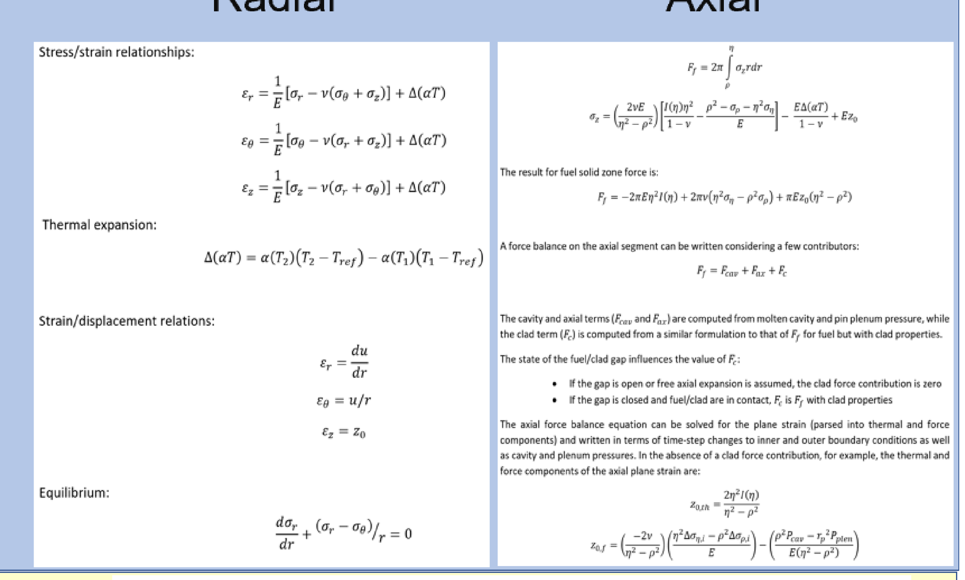
Feedback models
- Control function-specified external
- Doppler
- Fuel and moderator density
- New for SFRs (under development)
  - Dimension changes and rod bowing
  - Molten fuel/clad
  - Sodium void

Define core cell ranges over which component average temperatures are taken to inform feedback models

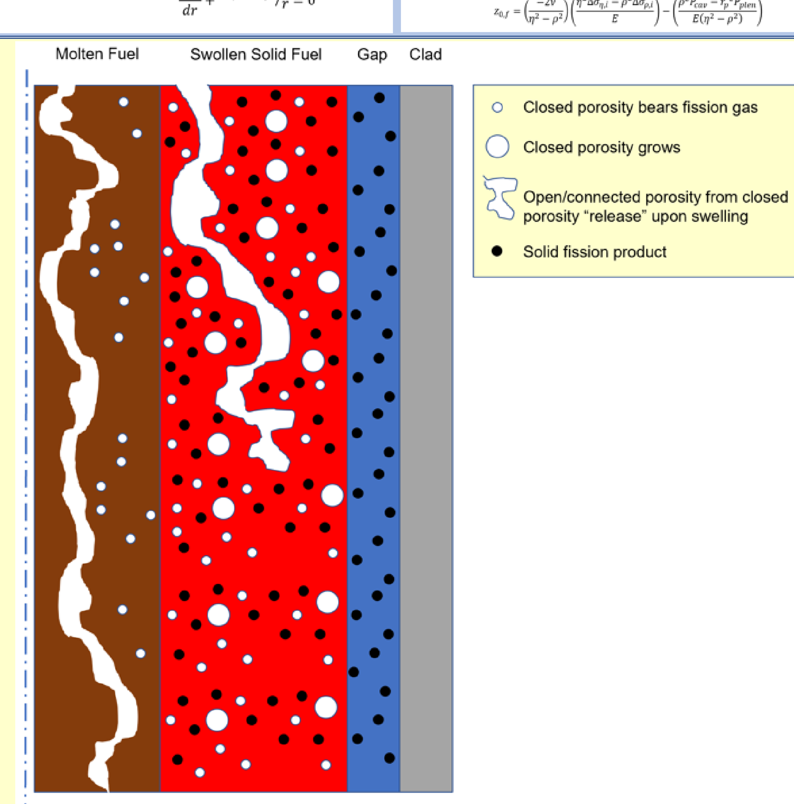
SFR Expanded In-Vessel Modeling

- Pin Mechanics
  - Radial stress/strain/displacement
  - Axial stress/strain
  - Solve iteratively
- Miscellaneous models
  - Fuel swelling
  - Fuel molten cavity formation
  - Pin pressurization
  - Reactivity effects

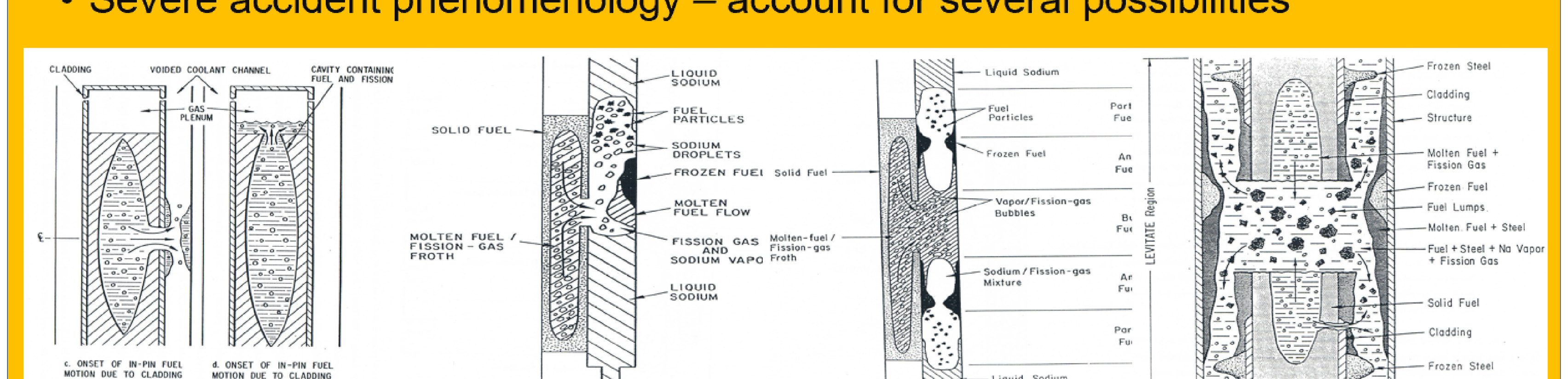
Radial | Axial



- Fission gas dynamics in-pin
  - Forms closed porosity in solid fuel
  - Closed porosity grows
  - Closed porosity "releases" – swelling
  - Open/connected porosity
    - Forms from closed porosity release
    - A "free volume" in pin
    - Communicates with pin plenum
    - At pin plenum pressure
  - Molten fuel
    - Forms as solid melts
    - Subsumes open/closed porosity
  - RN class inventory migrates as volume



- Severe accident phenomenology – account for several possibilities



MSR Modeling

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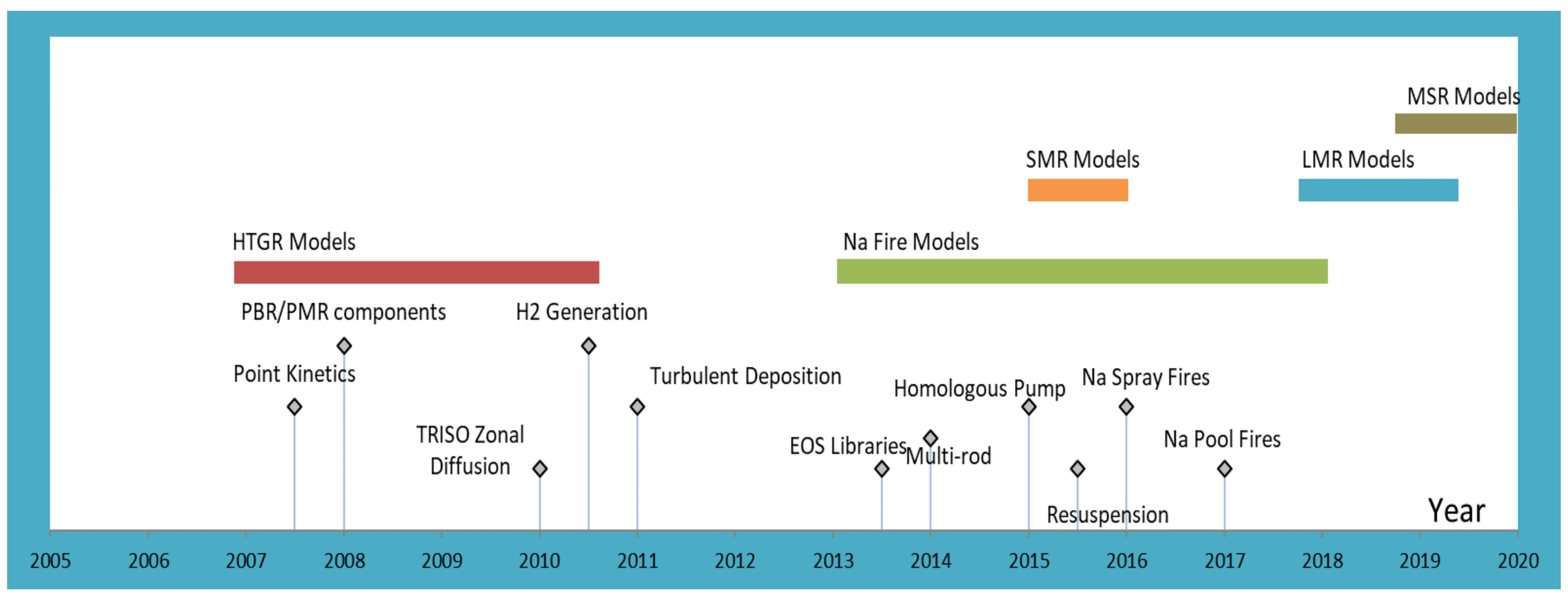


Transient/Accident Solution Methodology

Stage 1: Thermal Hydraulic Steady State

Establish COR, CVH, & HS temperatures

Establish steady flow patterns

Initialize or source in RN form-wise mass

Stage 2: Pre-Transient

Fluid fuel point kinetics

GRTR framework governs form-wise transfer to some steady distribution of RN class mass across user-defined RN forms

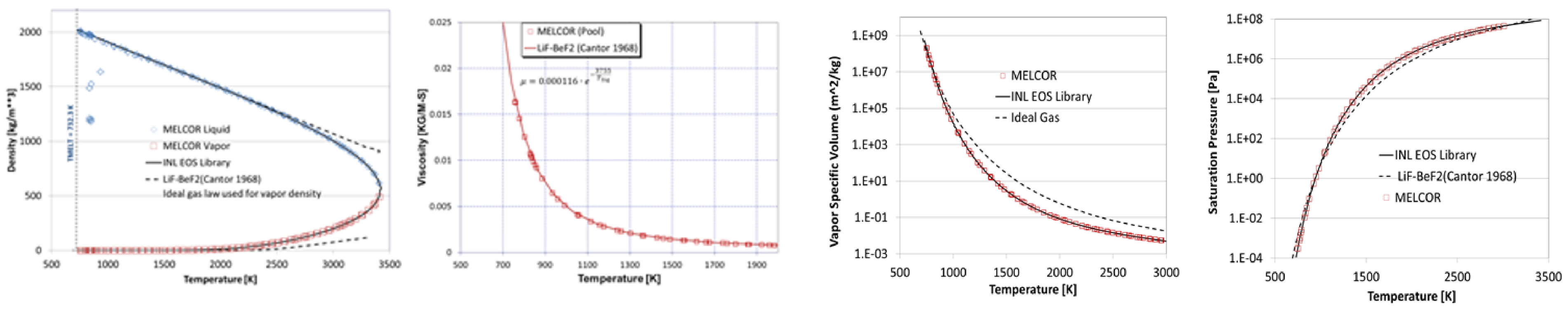
Stage 3: Transient

Fluid fuel point kinetics governs power according to flow reactivity excursions

GRTR moves RN class mass between forms
- *Thermodynamic conditions evolve*
- *Vapors, aerosols, and RN package physics are still in play within GRTR*
- *User-directed transfers between user-defined forms or internal models*

FLiBe Equation of State (EOS)

- Property database based on ORNL publication
- Verified EOS on a wide range of thermodynamic conditions
- Demonstration calculations reproduce the experimental database
- Provisions exist for salt freezing (solid phase) from liquid phase



Fluid Fuel Point Reactor Kinetics Equations

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

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

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

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

Where:

$P(t)$= Thermal power due to fission 0

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

A – In-Vessel DNP gain by fission
B – In-Vessel DNP loss by decay, flow
C – In-Vessel DNP gain by Ex-Vessel DNP flow
D – Ex-Vessel DNP gain by In-Vessel DNP flow
E – Ex-Vessel DNP loss by decay, flow

Under these assumptions, the steady form of the FFPRK equations is:

$$\frac{dP(0)}{dt} = 0 = \left(\frac{\Delta\rho_0 - \bar{\beta}(0)}{\Lambda}\right)P_0 + \sum_{i=1}^{6}\lambda_i C_{i,0}^C = \left(\frac{\Delta\rho_0 - \beta + \beta_{lost}(0)}{\Lambda}\right)P_0 + \sum_{i=1}^{6}\lambda_i C_{i,0}^C$$

$$\frac{dC_i^C(0)}{dt} = 0 = \left(\frac{\beta_i}{\Lambda}\right)P_0 - \left(\lambda_i + {}^2/_{\tau_C}\right)C_{i,0}^C + \left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^2/_{\tau_L}\right)C_{i,0}^L, \quad i = 1 \dots 6$$

$$\frac{dC_i^L(0)}{dt} = 0 = \left(\frac{V_C}{\tau_C V_L}\right)C_{i,0}^C - \left(\lambda_i + {}^1/_{\tau_L}\right)C_{i,0}^L, \quad i = 1 \dots 6$$

Solving for DNP cohorts:

$$C_{i,0}^C = \alpha_i P_0, \quad i = 1 \dots 6$$

$$C_{i,0}^L = \gamma_i \alpha_i P_0 = \gamma_i C_{i,0}^C, \quad i = 1 \dots 6$$

$$\gamma_i = \left(\frac{V_C}{\tau_C V_L}\right) \Big/ \left(\lambda_i + {}^1/_{\tau_L}\right), \quad i = 1 \dots 6$$

$$\alpha_i = \left(\frac{\beta_i}{\Lambda}\right) \Big/ \left[\left(\lambda_i + {}^2/_{\tau_C}\right) - \gamma_i\left(\left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^2/_{\tau_L}\right)\right)\right], \quad i = 1 \dots 6$$

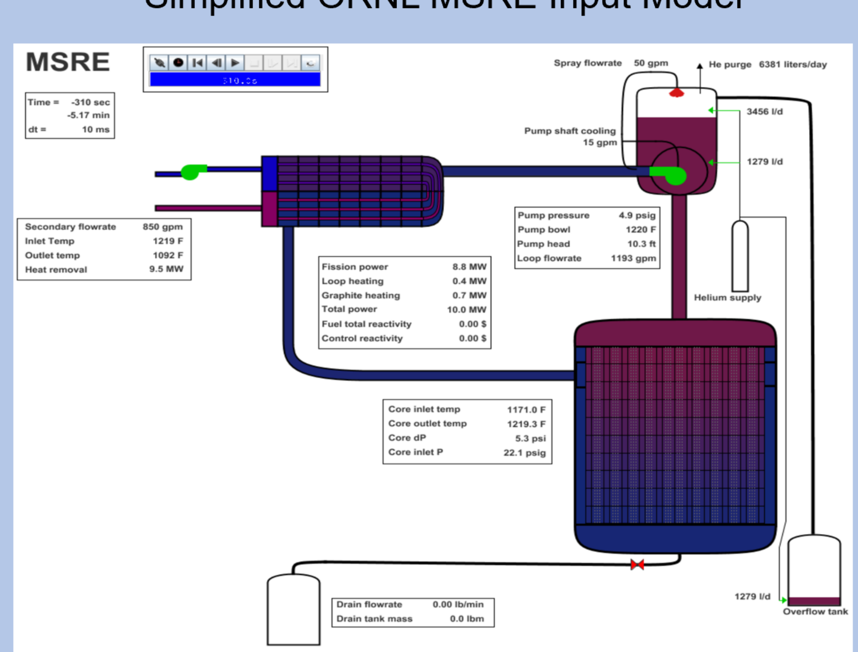
Solving for the bias reactivity and the time-zero effective delayed neutron fraction:

$$\Delta\rho_0 = \beta - \Lambda\sum_{i=1}^{6}\lambda_i\alpha_i(1+\gamma_i)$$

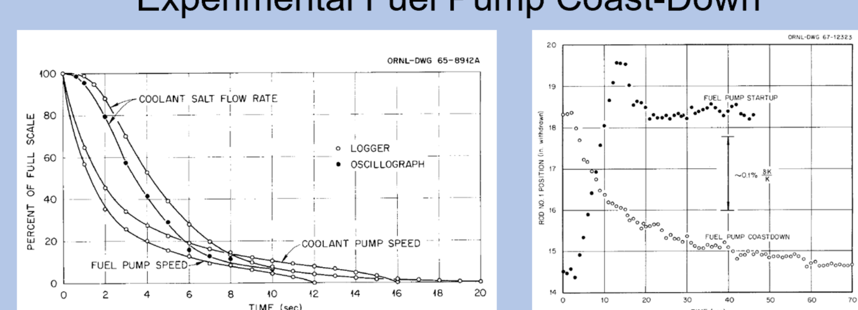
$$\bar{\beta}(0) = \beta - \beta_{lost}(0) = \beta - \Lambda\sum_{i=1}^{6}\lambda_i\gamma_i\alpha_i$$

ORNL MSRE Zero-Power Flow Coast-Down Benchmark

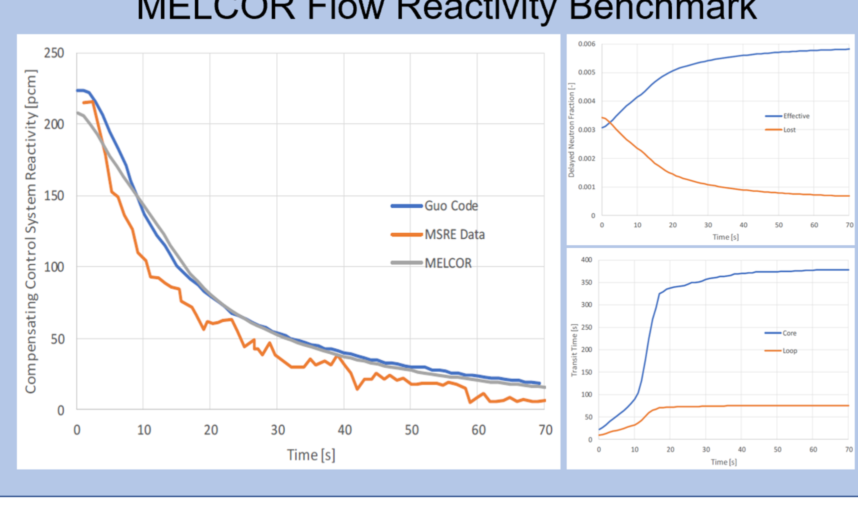
Simplified ORNL MSRE Input Model



Experimental Fuel Pump Coast-Down



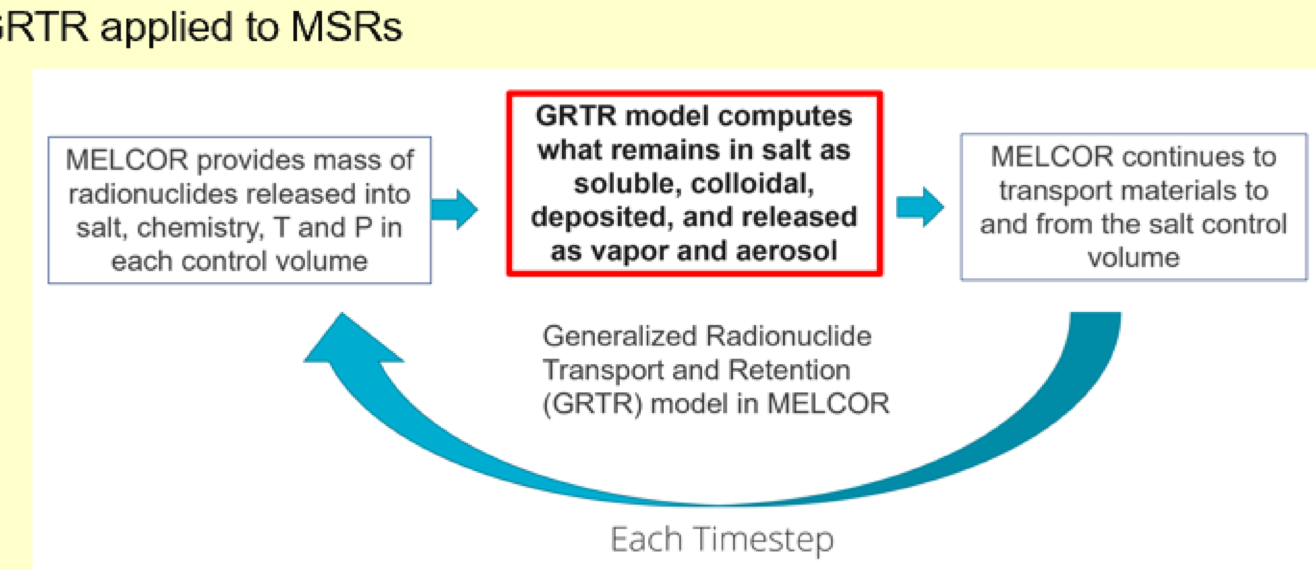
MELCOR Flow Reactivity Benchmark

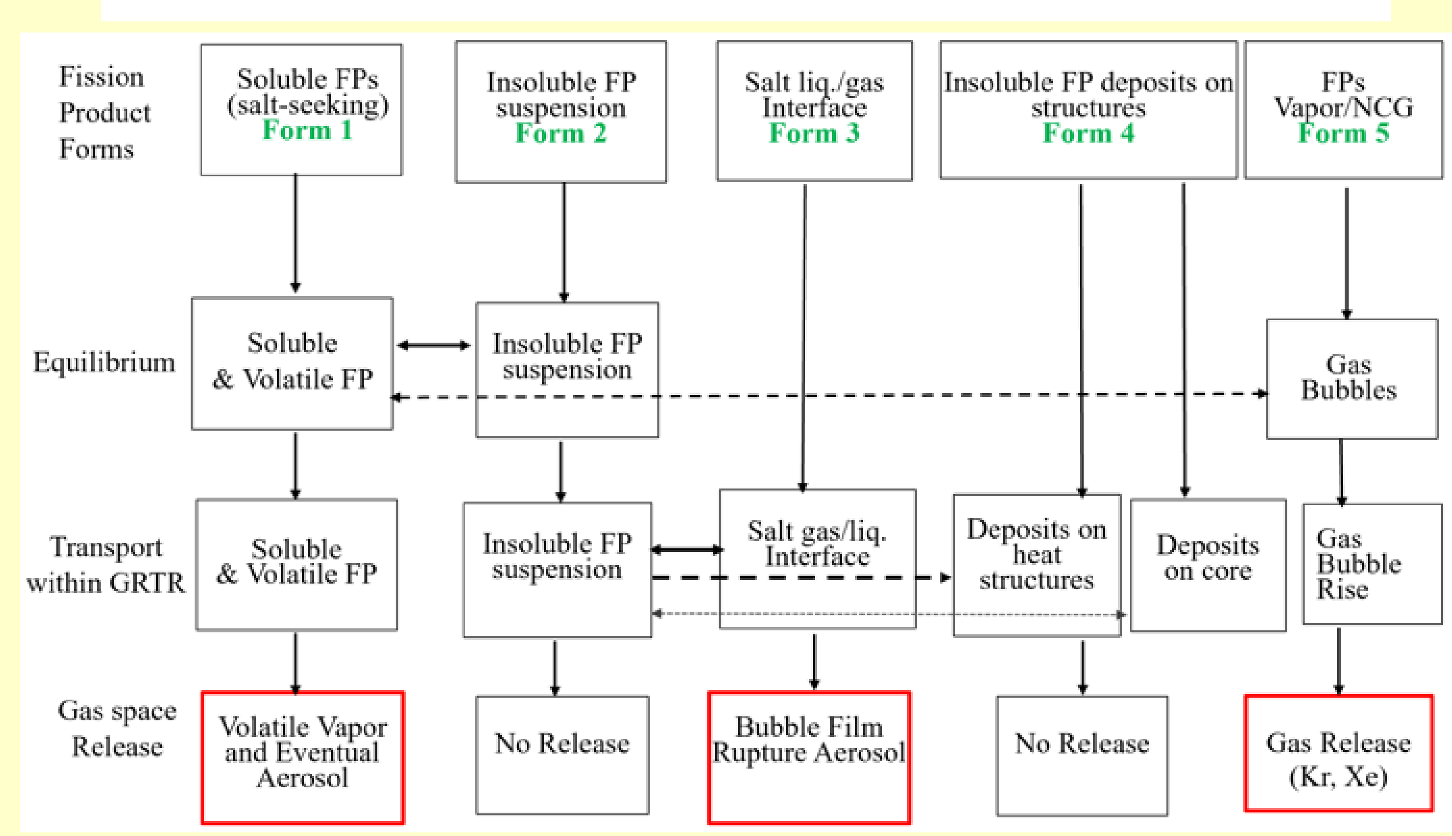


GRTR Modeling Framework

- GRTR affected through CVH and RN1
  - CVH input declares:
    - User-defined forms and their characteristics (sectionwise, nonsectionwise, HS deposition)
    - Transfers between user-defined forms and from user-defined forms to built-in forms
    - Control functions can direct transfers
    - Limited built-in form-wise transfer physics models
    - Limited ability to employ Gibbs Energy Minimization tools like Thermochimica
  - RN1 input declares:
    - Initial user-defined form-wise mass by class and control volume
    - Sources for user-defined form-wise mass by class and control volume
  - If COR package is active, require a mapping for user-defined form-wise release

- GRTR applied to MSRs



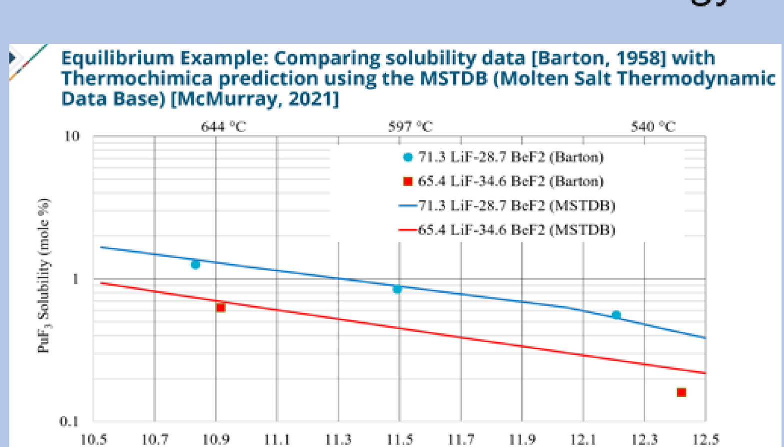


- In MSR context, GRTR can account for:
  - Dissolved mass and its coming out of solution
  - Colloidal (insoluble) mass and its transport
  - Generation of aerosol at a free surface as bubbles burst
  - Vaporization
  - Aerosol dynamics according to conventional MELCOR physics models
  - HS deposition of any of the above forms
  - Advection of any of the above with CVH/FL flows
  - Use of control functions or built-in models or Thermochimica for form-wise transfers

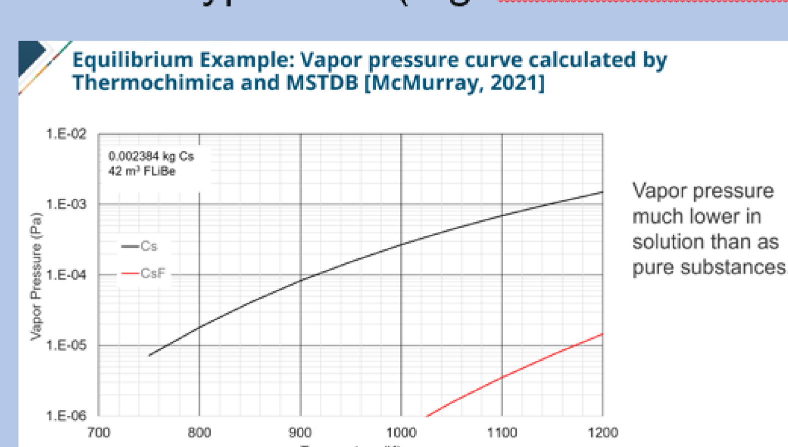
Thermochemistry and Data Needs

- MELCOR capabilities are in place to use data as available
- MELCOR can utilize Gibbs Energy Minimization type tools (e.g. Thermochimica)

Equilibrium Example: Comparing solubility data [Barton, 1958] with Thermochimica prediction using the MSTDB (Molten Salt Thermodynamic Data Base) [McMurray, 2021]

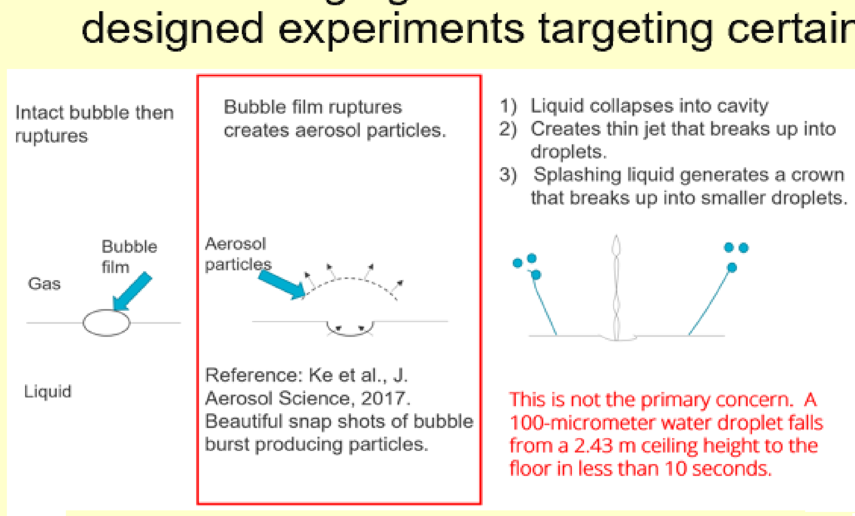


Equilibrium Example: Vapor pressure curve calculated by Thermochimica and MSTDB [McMurray, 2021]

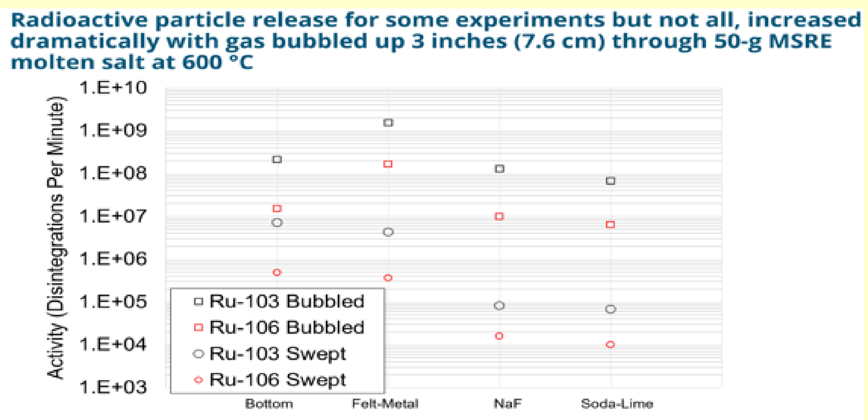


- Thermo databases available in FactSage format:
  - MSTDB w/ 2 systems:
    - Fluoride: Pu-U-Th-Nd-Ce-La-Cs-Rb-Ni-Ca-K-Na-F-Be-Li
    - Chloride: Pu-U-Ce-Cs-Rb-Ni-Fe-Cr-Ca-K-Cl-Al-Mg-Na-Li
  - JRC database: Pu-U-Th-Ce-La-Cs-I-Zr-Rb-Ca-K-Cl-Mg-Na-F-Be-Li
- Databases under active development, needs for severe accidents include:
  - High temperatures (beyond normal operating range)
  - Fission product elements in row 5 of periodic table (Sr, I, Ag, etc.)
  - Species introduced during possible severe accidents (air, water vapor)

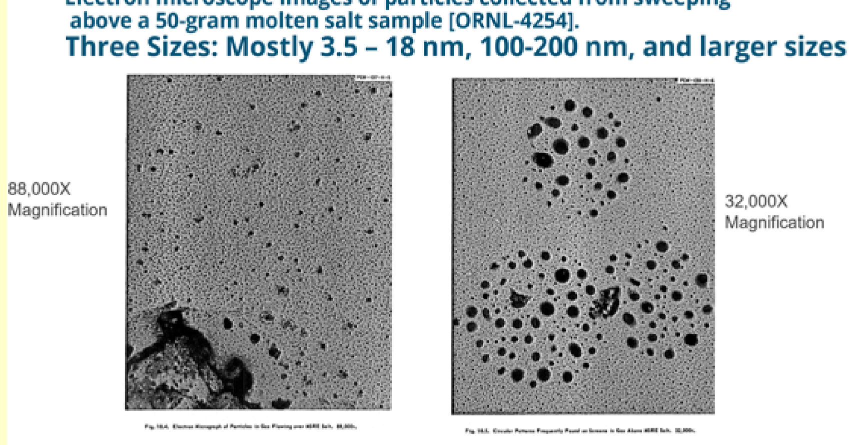
- Gas bubbling/agitation and burst in molten salt is a case-in-point that well-designed experiments targeting certain data needs are valuable



Radioactive particle release for some experiments but not all, increased dramatically with gas bubbled up 3 inches (7.6 cm) through 50-g MSRE molten salt at 600 °C

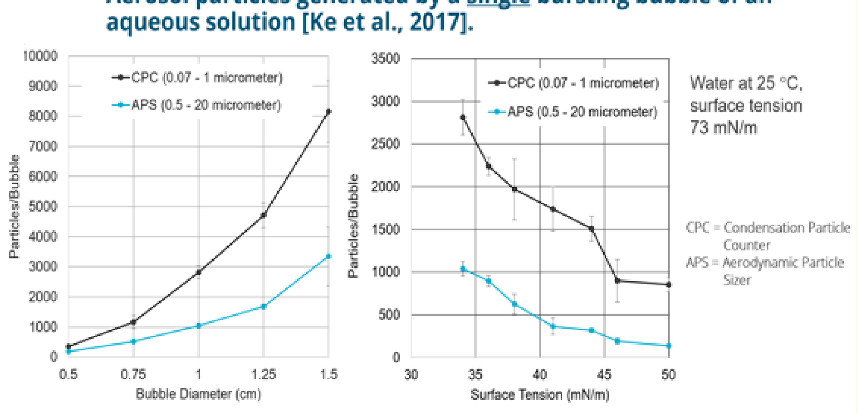


Electron microscope images of particles collected from sweeping above a 50-gram molten salt sample [ORNL-4254].
Three Sizes: Mostly 3.5 – 18 nm, 100-200 nm, and larger sizes



Respirable (< 10 micron aerodynamic diameter) particles released from molten salt during benign operations. This is important!

Aerosol particles generated by a single bursting bubble of an aqueous solution [Ke et al., 2017].



- Larger bubbles rupture with thousands more respirable aerosol particles per bubble.
- Higher surface tension results in thousands fewer respirable aerosol particles.