Sandia National Laboratories

Securing the future of Nuclear Energy

MELCOR

MELCOR MSR Modeling Capabilities for Licensing and Severe Accident Analysis

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U.S. DEPARTMENT OF ENERGY NNSA

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MELCOR for Advanced Nuclear Energy Technologies

MELCOR

Fully integrated, engineering-level code

- Thermal-hydraulic response of reactor coolant system, reactor cavity, rector enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

Level of physics modeling consistent with

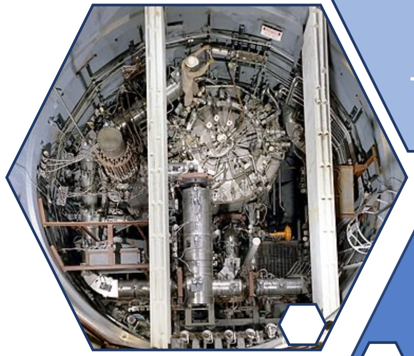
- State-of-knowledge
- Necessity to capture global plant response
- Reduced-order and correlation-based modeling

Traditional application

- Models constructed by user from basic components (control volumes, flow paths and heat structures)
- Demonstrated adaptability to range of reactor designs – LWR, LWR-SMR, FHR, HPR, HTGR, MSR, SFR, ATR, VVER, SFP…

Molten Salt Reactor Modeling

- MELCOR Molten Salt Reactor source term modeling strategies revolve around3 primary areas:
  1. Control
  2. Cool
  3. Contain
- MELCOR capabilities have been tested using models for the Molten Salt Research Experiment (MSRE) and Molten Salt Breeder Reactor



Control

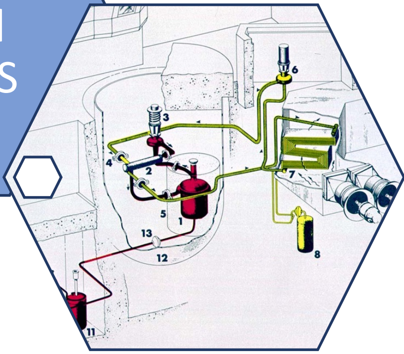
Fluid point kinetics, transmutation

Cool

Generalized EOS, CVH, HS

Contain

Radionuclide species, transport, and retention



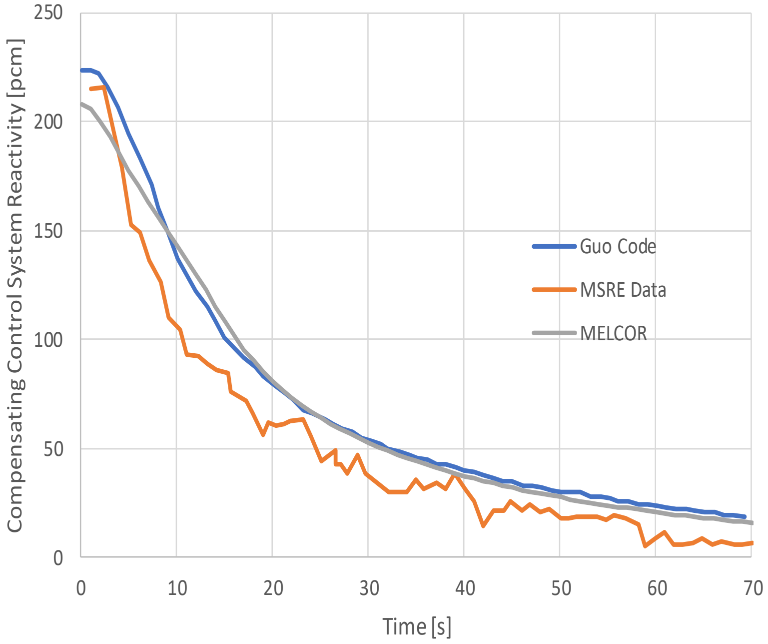
Control Neutrons

- Fuel point kinetics – Derived from standard PRKEs and solved similarly
  - Feedback models
    - User-specified external input
    - Doppler
    - Fuel and moderator density
    - Flow reactivity feedback effects integrated into the equation set

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

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

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



- Transmutation – Depletion Module (under development)
  - Treats transmutation of the initial radionuclide inventory (radioactive decay and neutron interactions) during severe accidents including mass transfer between radionuclide classes

$$\frac{dN}{dt} = \left(A_\lambda + A_\phi \Phi\right) N(t) + S(t)$$

$N(t)$: vector of isotope number densities

A_λ: radioactive decay transition matrix

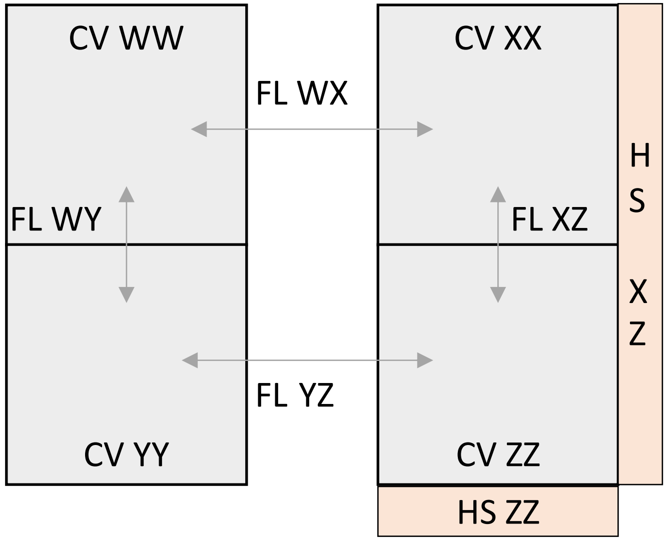
A_ϕ: neutron interaction transition matrix

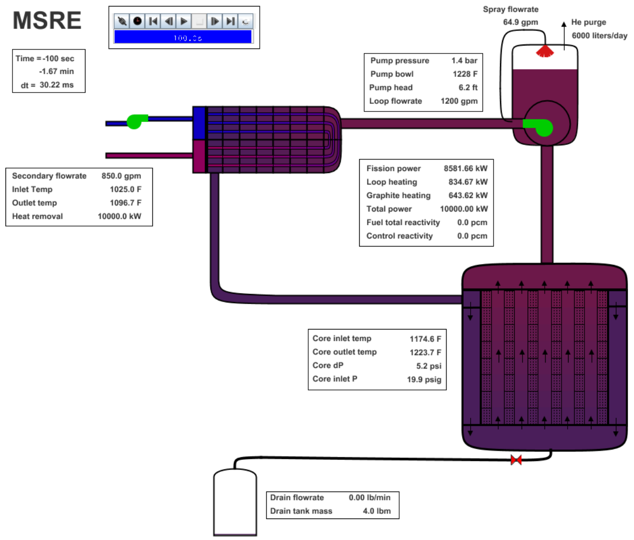
Φ: scalar neutron flux

$S(t)$: eternal isotope source

Keep the Reactor Cool

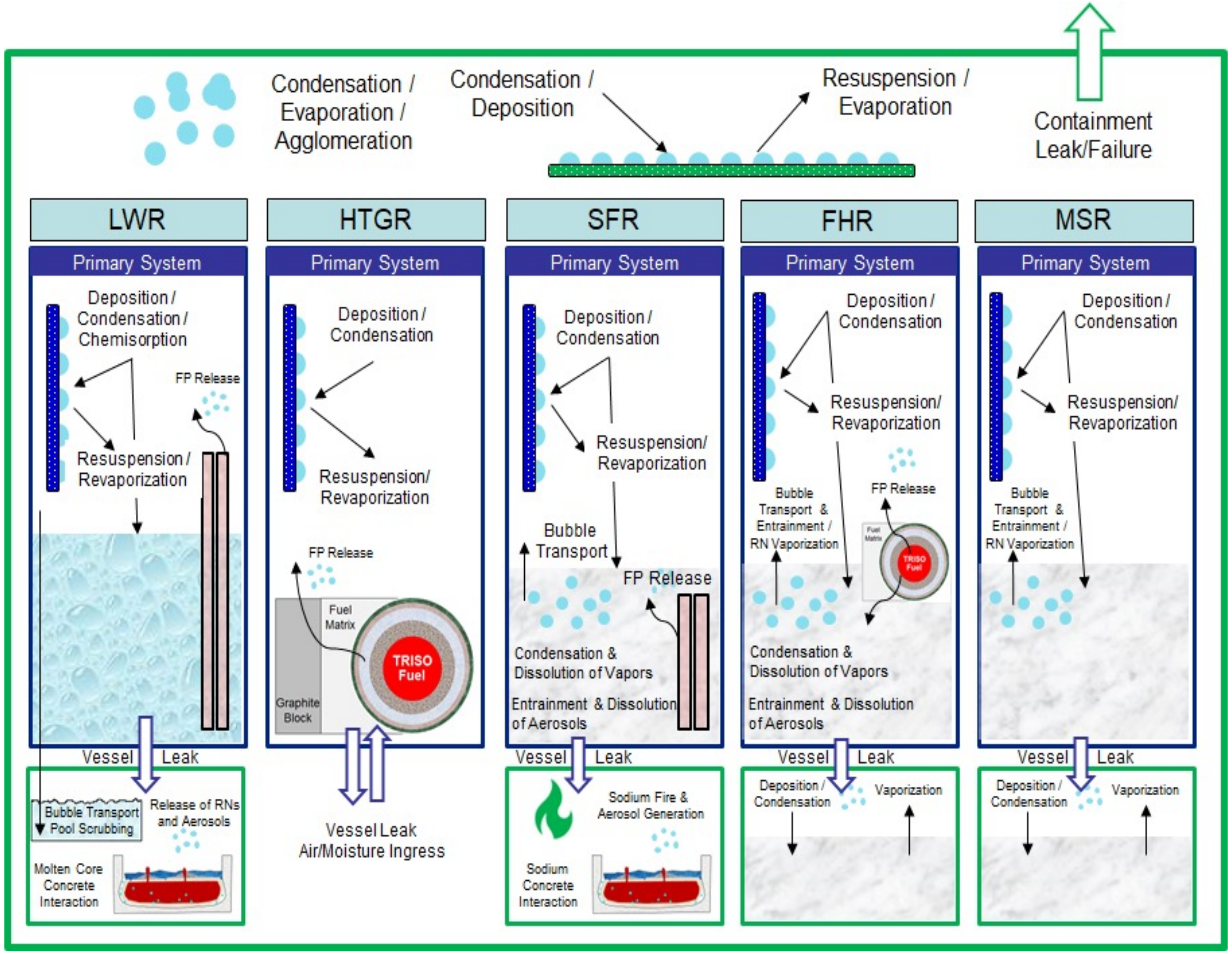
- Generalized EOS – Equations of state for multiple working fluids are presently available in MELCOR including water, sodium, and FLiBe.
  - MELEOS can generate equations of state for any fluid with the necessary data
- Thermal hydraulics – CVH/FL Packages
  - The CVH package defines control volumes (CV)
  - The FL package defines flow paths (FL)
- Heat Transfer – HS/CVH/COR Packages
  - The HS package defines heat structures (HS) that model radiative and conductive heat losses
  - The CVH package manages convective heat losses
  - The COR package controls heat losses of heat bearing and other core structures





Contain Radionuclide Release

- Radionuclide Species – DCH/RN1
  - Default 17 representative radionuclide species/elements (RN classes)
  - Species categorized by similar transport and retention mechanisms
  - Each species represents a set of elements and the corresponding collapsed isotopic masses
  - Does not currently model RN class masses at the isotopic level or mass transfer between RN classes
  - Users have the ability to redefine/add RN classes
- Radionuclide Transport and Retention
  - Transport and retention of RN classes modeled by various physiochemical processes
  - New MELCOR structure allows rapid implementation and benchmarking for models



RN Package Generalized Representation Degrees of Freedom

- Generalize RN package for species transport modeling
  - RN package initially intended to model radionuclide transport
  - Has evolved with MELCOR to generally characterize transport of any trace species

Generalized mathematical representation in software

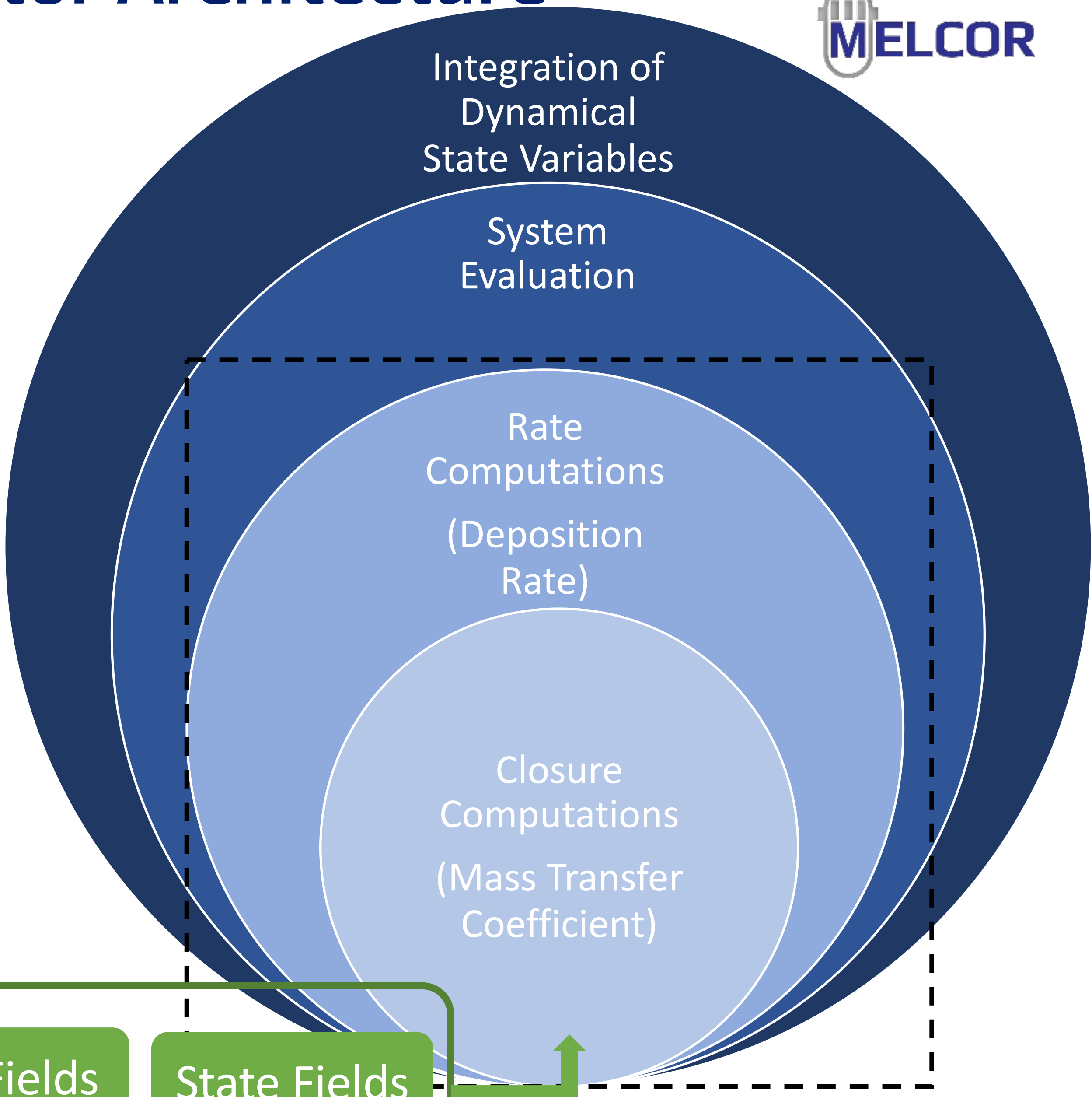
- *Degrees of freedom designed to be expanded*

- Hazardous Trace Species "State"
  - Nuclear State
  - Chemical State
  - Hosting Volume
    - Free to transport to other hosting volumes
    - Trapped within hosting volume
  - Species phase
    - Vapor
    - Particle
      - Aerosol particle size
  - ...

- Species have number of possible degrees of freedom
  - Chemical state (Speciation)
  - Nuclear State (Isotope)
  - Phase/Location

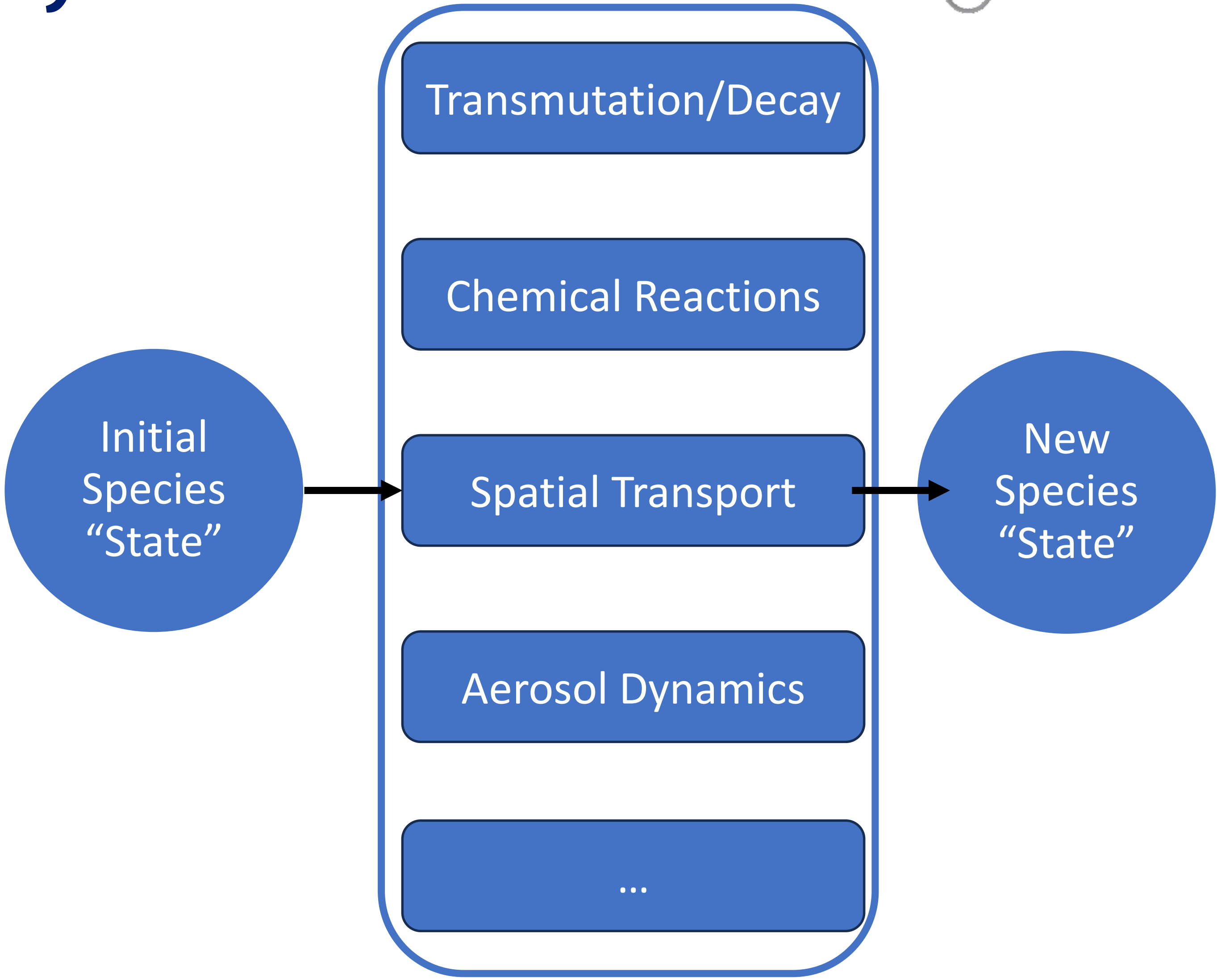
MELCOR's New Generalized Reactor Architecture

- MELCOR modernization established a new software platform
- Rapid capability implementation through physics/chemistry generalizations
- Generalized means re-using physics equations but changing system state variables
- Numerics **separated** from physics



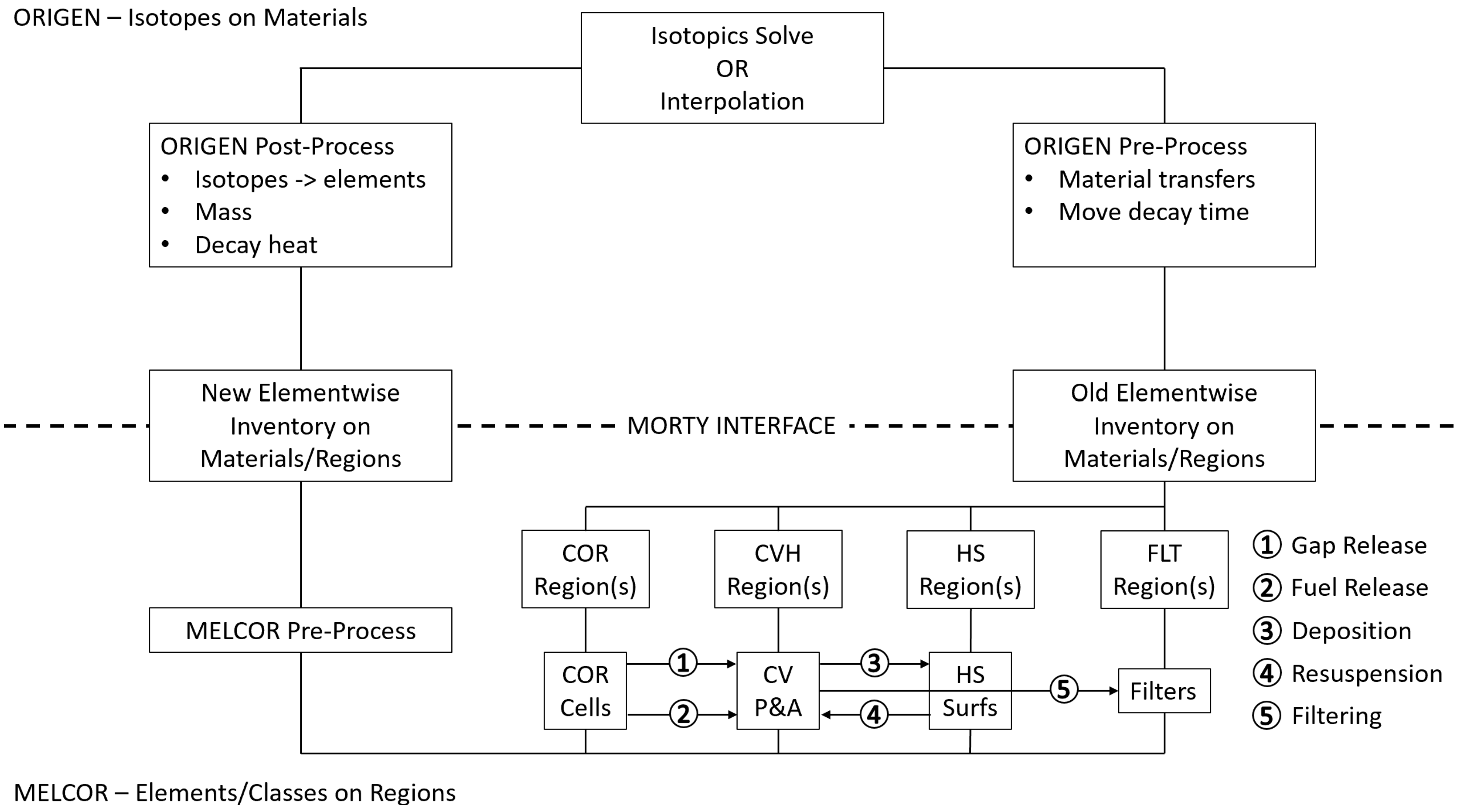
RN Package Generalized Dynamics

- Species transport is formulated as mass fluxes
- **Interfacial Transport:** Transport of species between "volumes"
- **Aerosol Dynamics:** Transformation of species within volumes associated with vapor and aerosol dynamics
- **Nuclear Processing:** Transformation of species within hosting volumes due to nuclear transmutation and decay
- **Chemical Processes:** Transformation of species within hosting volumes due to chemical reactions



ORIGEN-MELCOR Integration for Radionuclide Decay

ORIGEN provides isotopic analysis and computation of radionuclide transmutation, fission, and decay



ORIGEN-MELCOR Integration Updates Species Concentrations

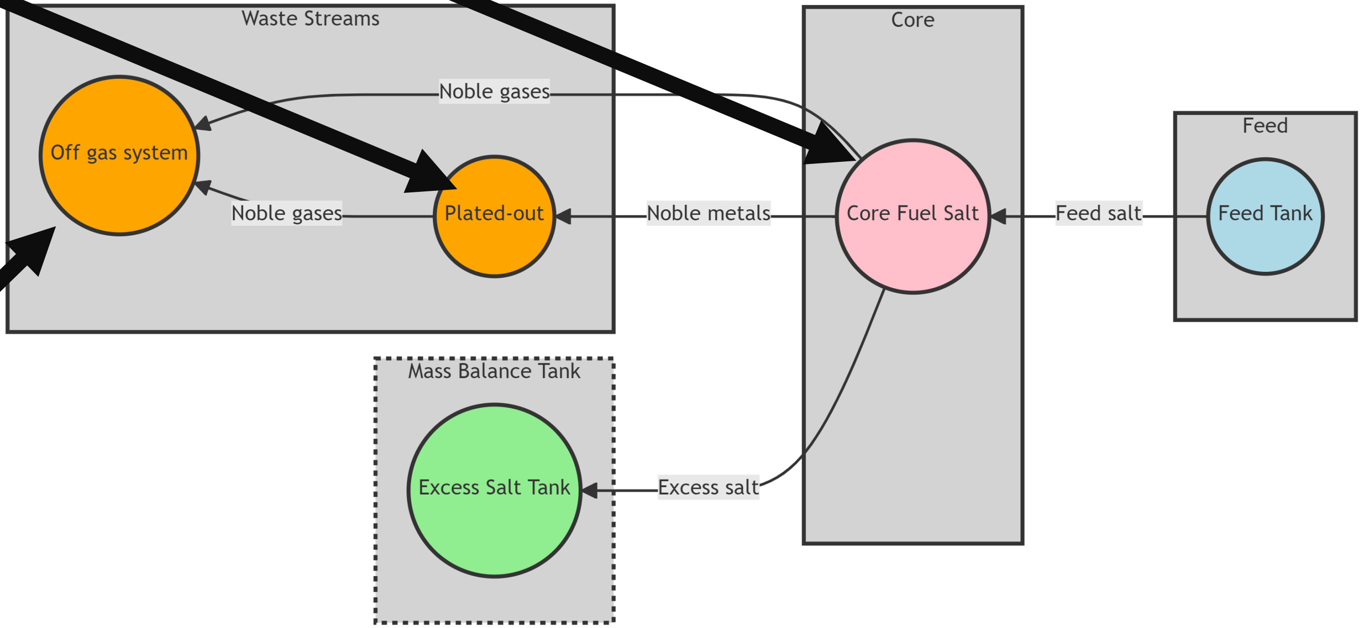
- Primary system radionuclides circulate through the core and exposed to neutron fission environment until shutdown

- Corrosion products and noble metals deposit and decay with transmutation to other elements and possibly change in solubility or phase

- Off-gas hold-up systems designed to decay Xe & Kr but also include transmutation to other elements and possibly change in phase (i.e., gas→ aerosol)

Radionuclide form (aerosol or gas) and nuclide decay impact the source term and health consequences

ORIGEN/MELCOR integration allows independent tracking, decay, and transmutation of nuclides in multiple locations and their impact on radionuclide transport and the source term



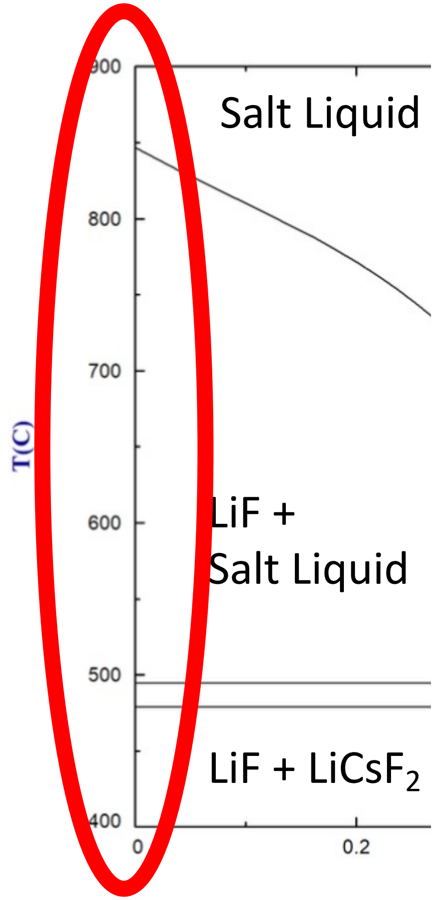
[ORNL/SCALE MSBR drawing]

MELCOR's MSR Chemistry SCOPE

- MELCOR models chemistry in COR, EOS (fluid) and in RN packages
- "Like" species are grouped to reduce computational time (e.g. Rb and Cs)
- Chemical reactions considered if equilibrium constant is $O(10^0\text{-}10^5\text{s})$
- Molten Salt Thermodynamic Database helps to model reactor's chemical speciation and create fluid files
- Can define a chemical reaction model in RN if not in MSTDB
- Models events:
  - Halogen potential control
  - Environmental contamination
  - Reactor Refueling
  - Salt Spill

Assume Radionuclide Masses Minimally Affect Bulk Salt Thermochemical Properties

- Carrier and fuel salt mass is thousands of kgs while radionuclides (RNs) will be a few kgs
- RNs will quickly form products related to phase speciation, having little affect on bulk properties
- RN species will be driven largely by temperature, not mass changes
- RNs in salt can be treated in system with classical mass-transport equations (frozen chemistry)



1% CsF mol frac with LiF

Report: "Investigation of Frozen Chemistry for Molten Salt Reactors (MSRs)" SAND-2024-13136

Chemical Databases and Gibbs Energy Solvers can model Molten Salt Properties

- The Molten Salt Thermochemical Database (MSTDB-TC) contains fitted Gibbs energy functions for salt systems
- Thermochimica uses databases, like MSTDB-TC, to model thermochemical properties (equilibrium speciation, melting point, speciation…)
- Thermochemical properties of multiple molten salt compositions can be modeled (limited by database systems)
- Common fluoride and chloride carrier, fuel and fission product systems available; iodine increasing

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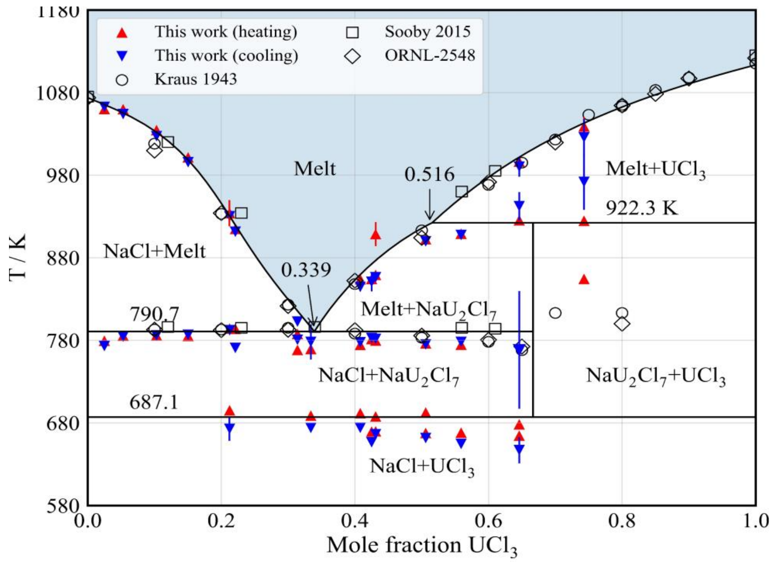
Molten Salt Thermal Properties Database - Thermochemical

MSTDB-TC

T. Besmann (USC)



Yingling et al., J Chem. Thermo 2023, 179, 105974

Thermochimica

M. Piro (McMaster)

MSTDB-TC and Thermochimica can be used to probe MSR chemistry

Thermochemica + MSTDB-TC Allow Investigation of how Reactor Chemistry affects Mass Transfer

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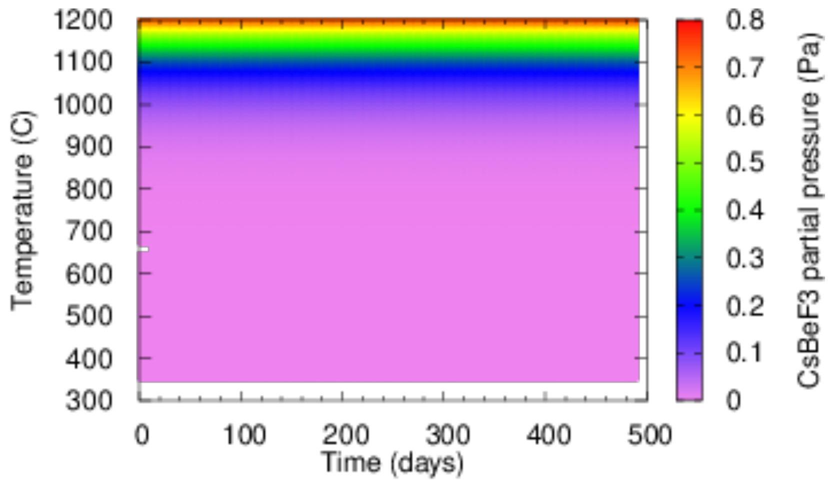
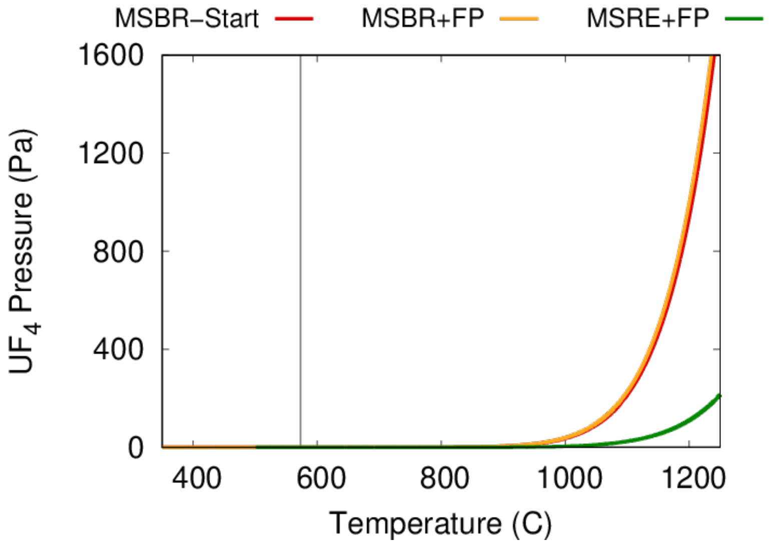
- MSR related topics that can be investigated are:
  - Fission product speciation for different reactor operations
  - Fuel cycle operation design
  - Corrosion control
  - **Parameterize mass transport coefficients in MELCOR**



$CsBeF_3$ Pressure in MSRE 500 Days After Shutdown

- Note: MSTDB-TC contains finite salt systems (e.g., Pb, Ti, S); use wisely

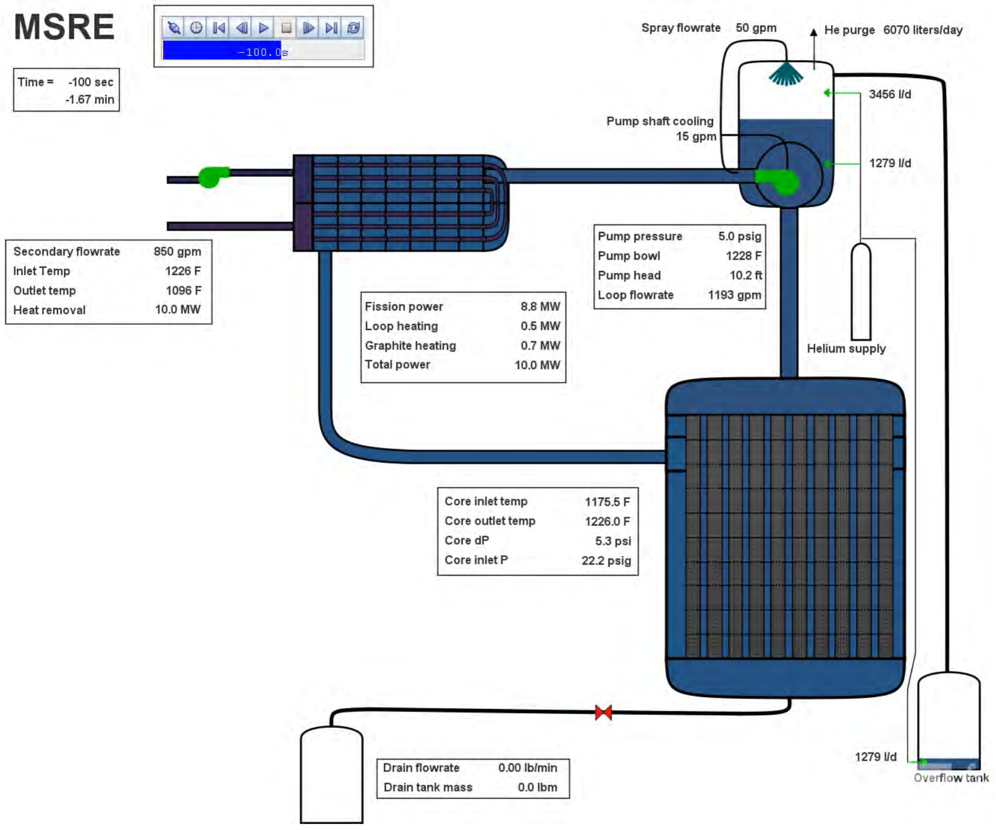
- New classes in RN can be created for off gas modeling from Thermochimica results



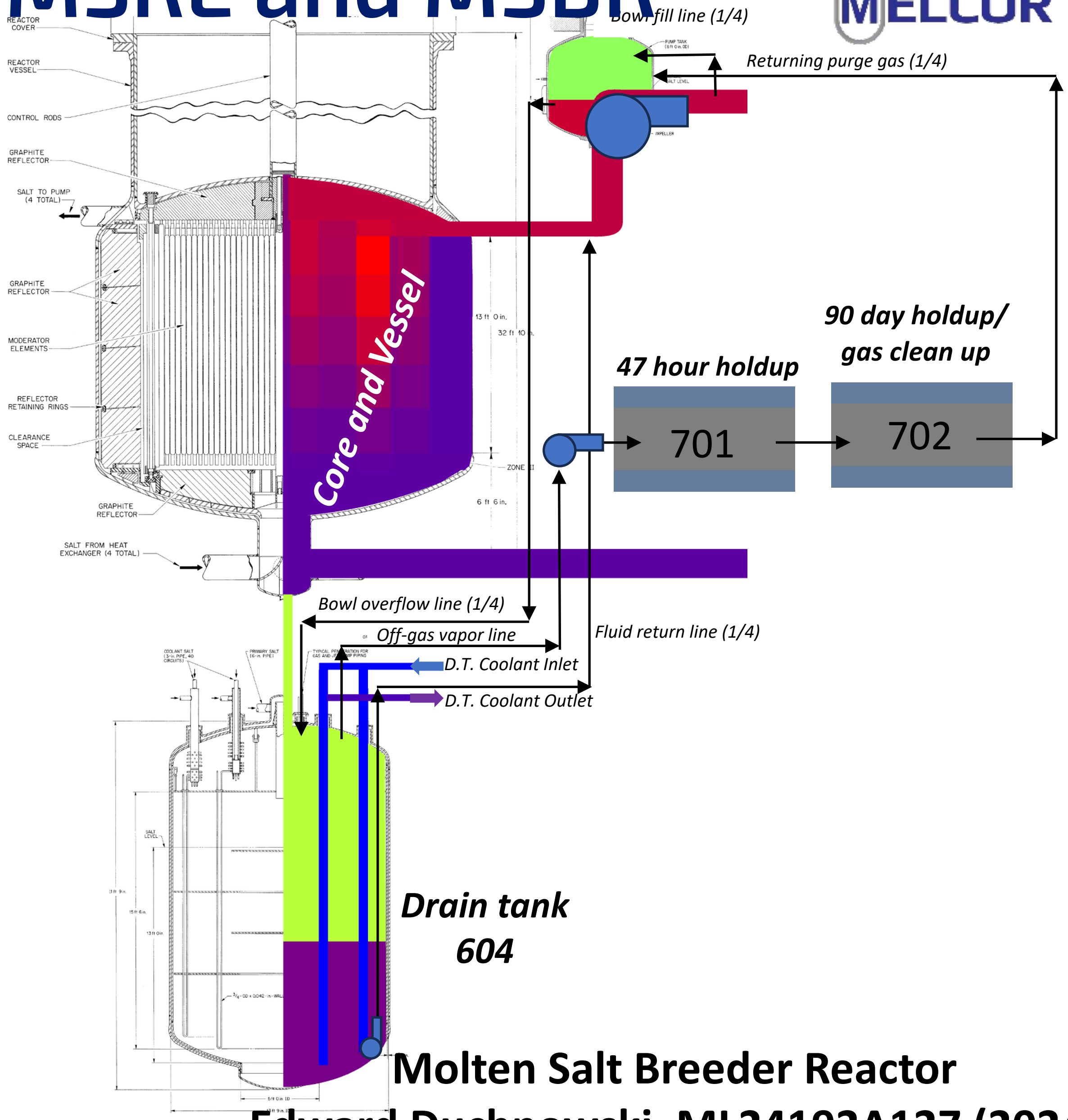
UF_4 Pressure in Different Systems

Use Thermochimica + MSTDB-TC to fit parameters, such as Antoine coefficients, RN transport

MELCOR Demonstrations of MSRE and MSBR



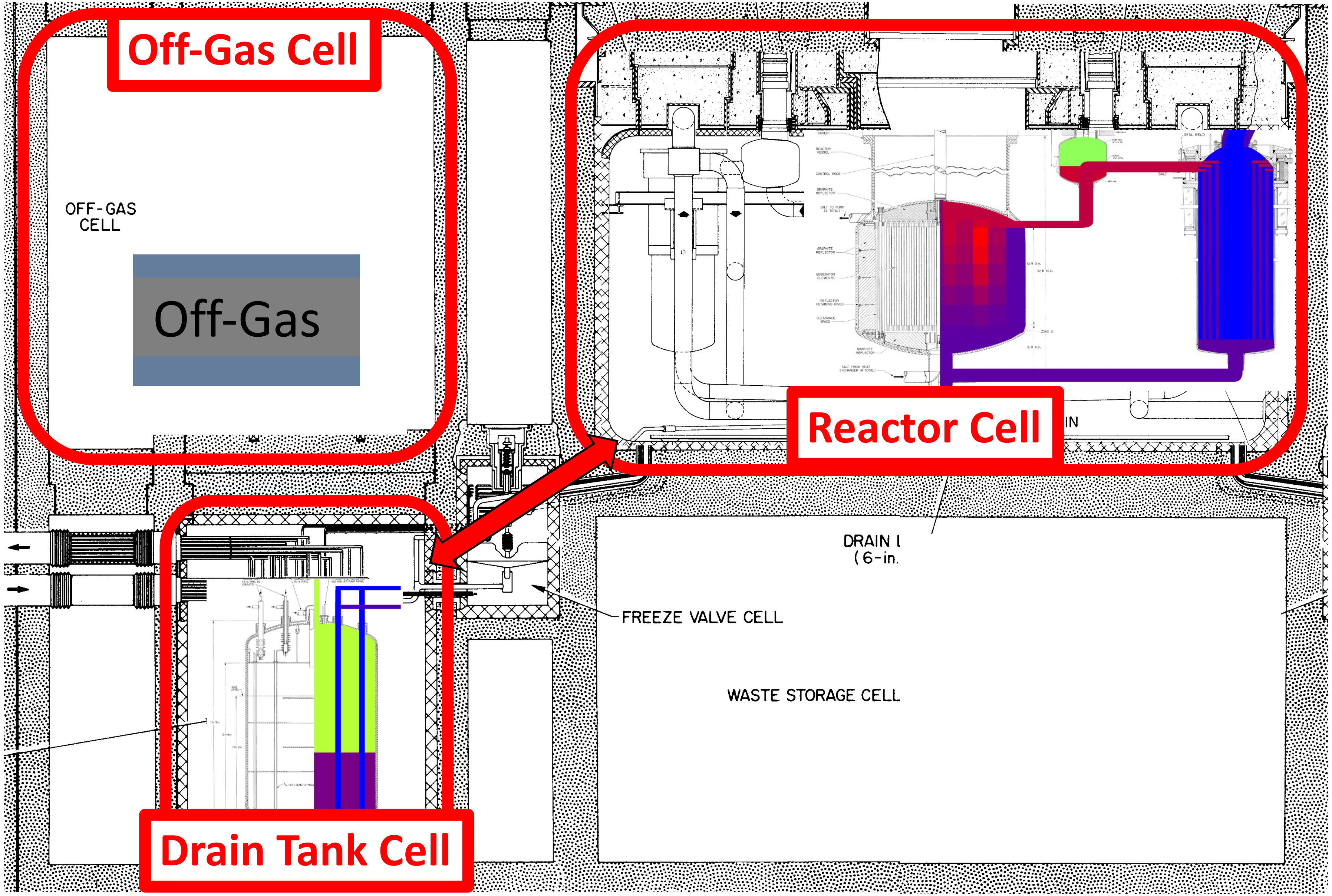
Molten Salt Reactor Experiment
Casey Wagner, SAND2022-12146PE (2022)



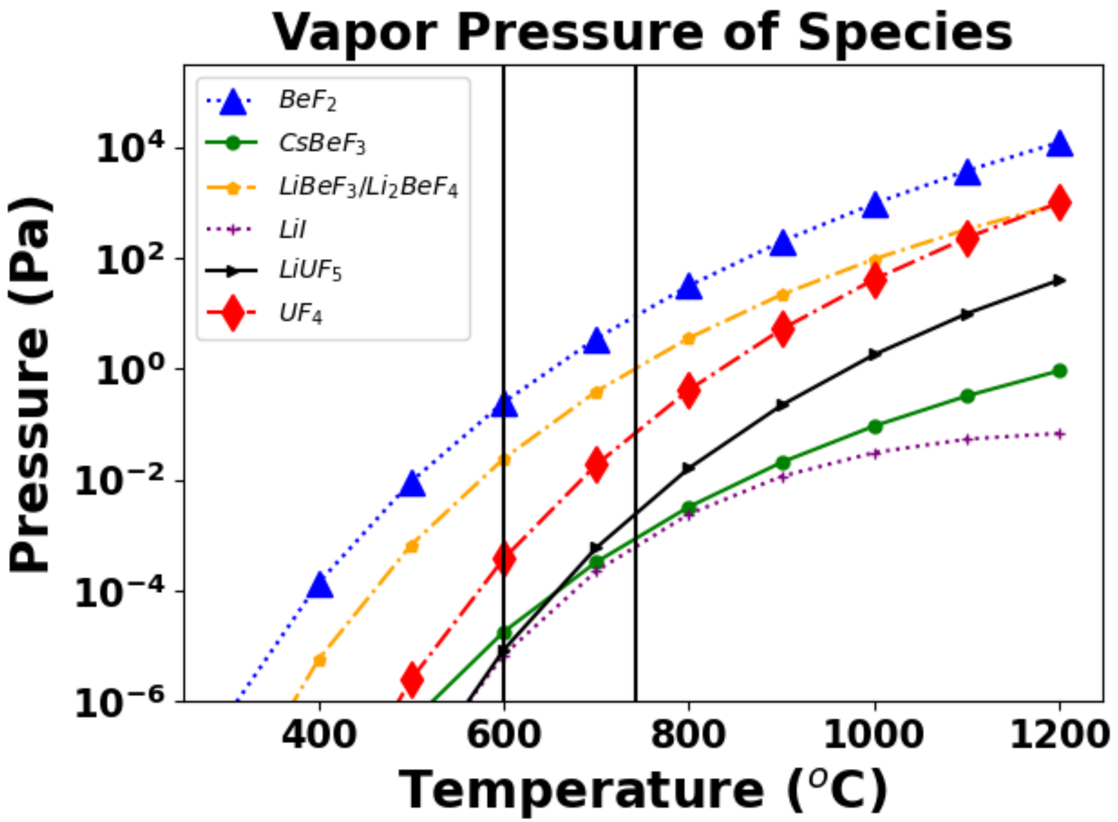
Molten Salt Breeder Reactor
Edward Duchnowski, ML24192A127 (2024)

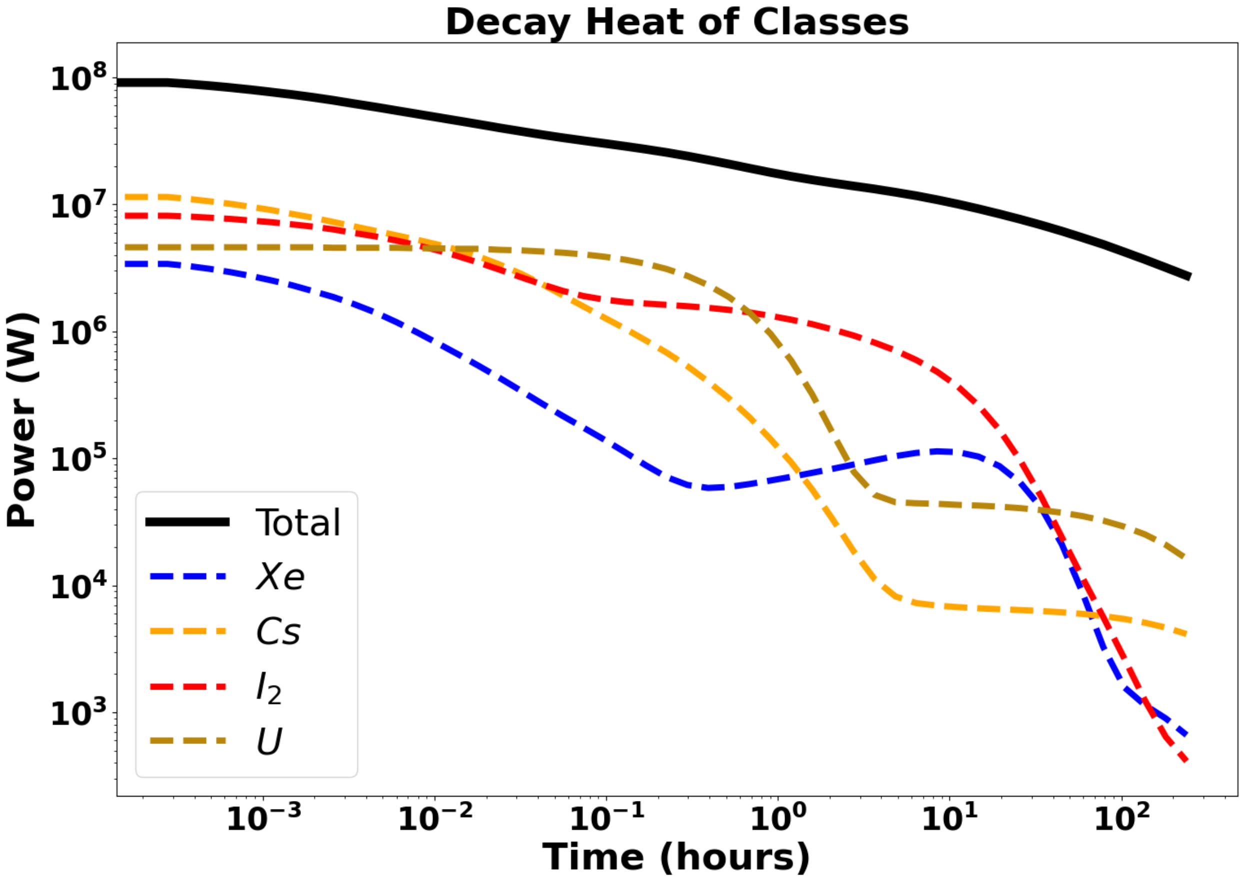
MELCOR MSBR Nodalization

- Off-gas, drain tank, and primary loop in respective containment
- Drain tank cell and reactor cell connected through freeze valve cell
  - Essentially maintain equivalent environments during steady state operation



SCALE and Thermochimica Results Used for MELCOR



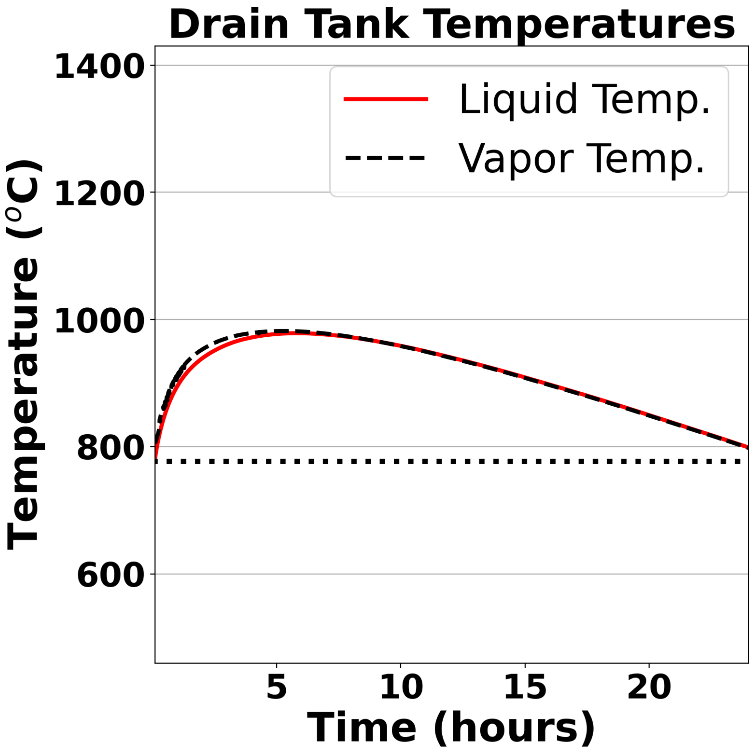


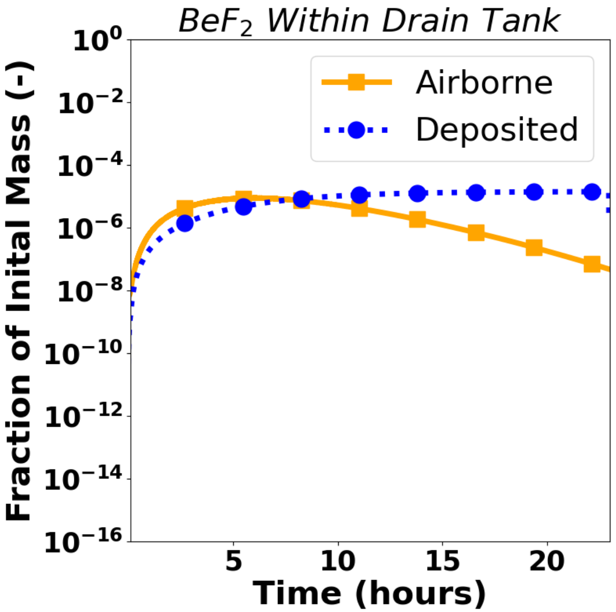
Thermochemica calculated vapor pressures using SCALE calculated RN inventories

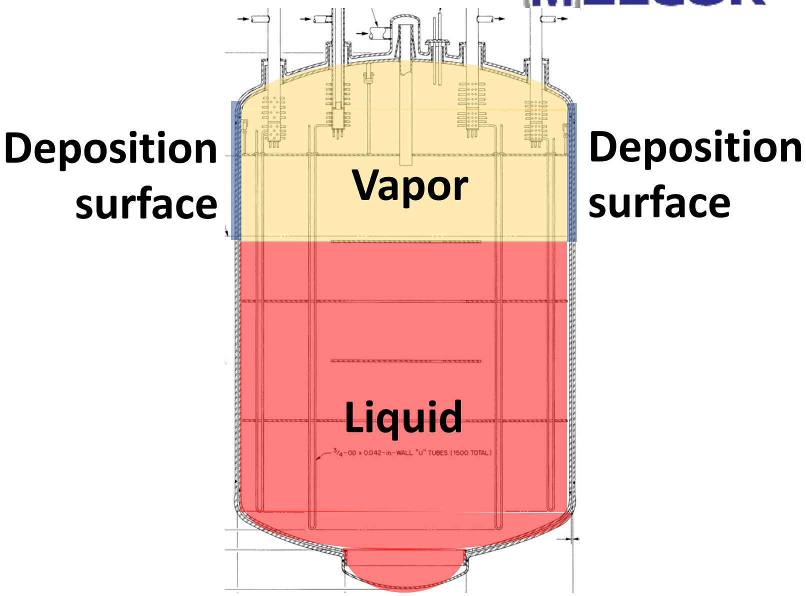
Element decay heat from SCALE calculations

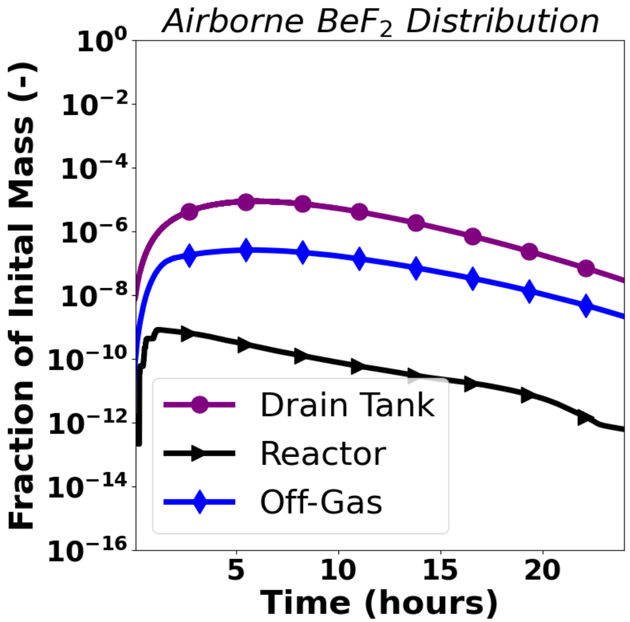
Emergency Drain: BeF_2 and UF_4 Distribution

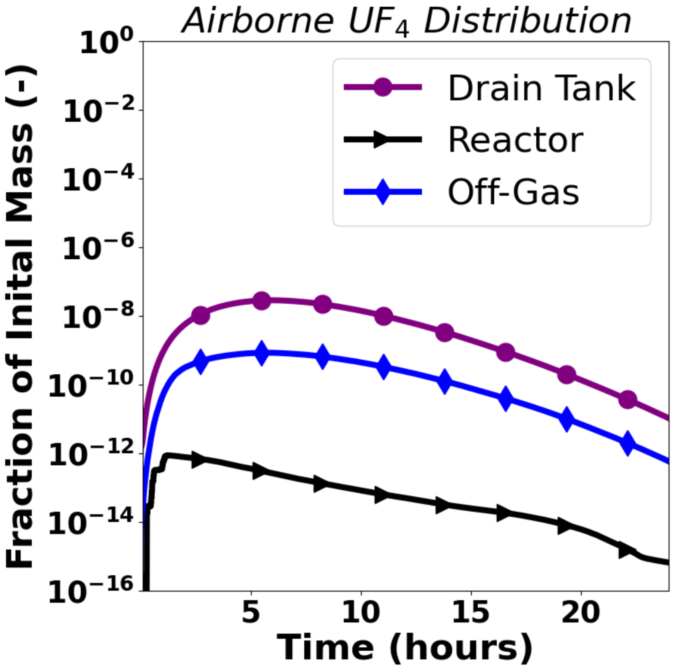
- Small amounts of BeF_2 and UF_4 continuously released
- Release rates vary as function of fuel salt temperature
- Airborne species condense back into pool and deposit on cool drain tank wall





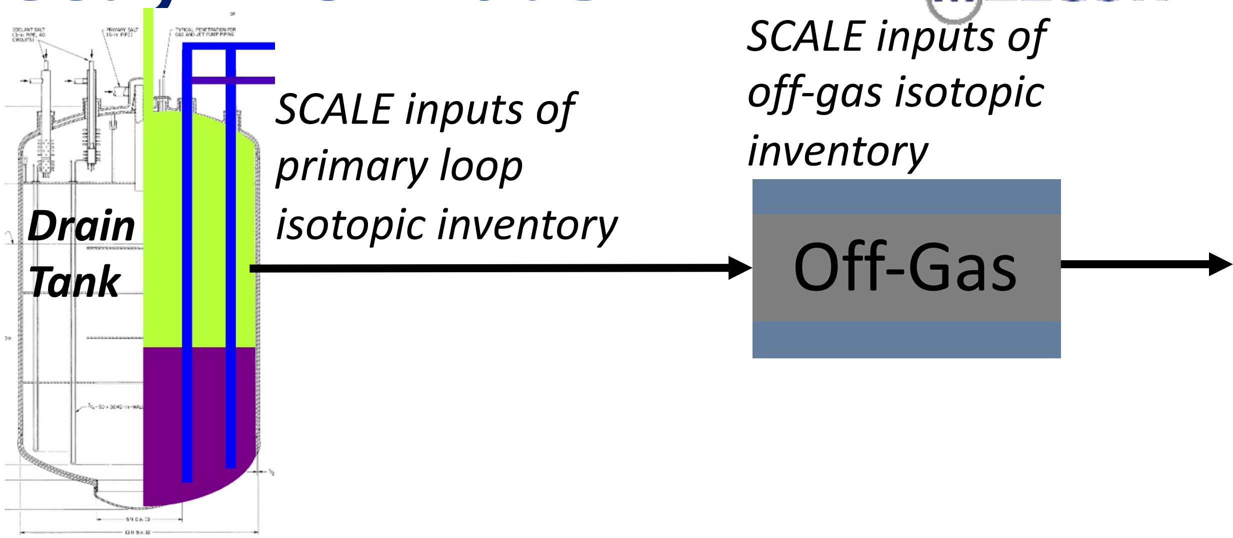


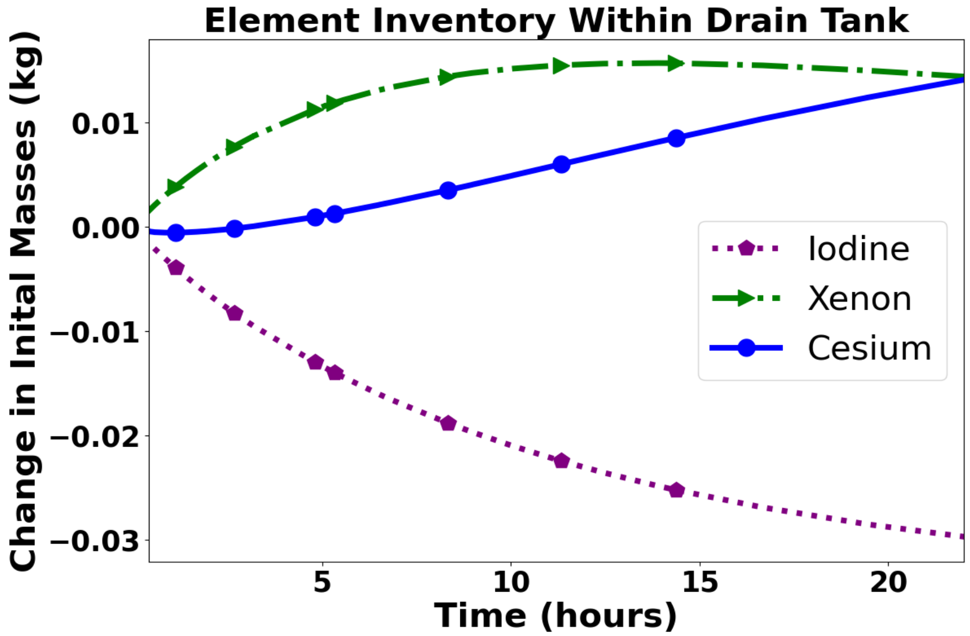


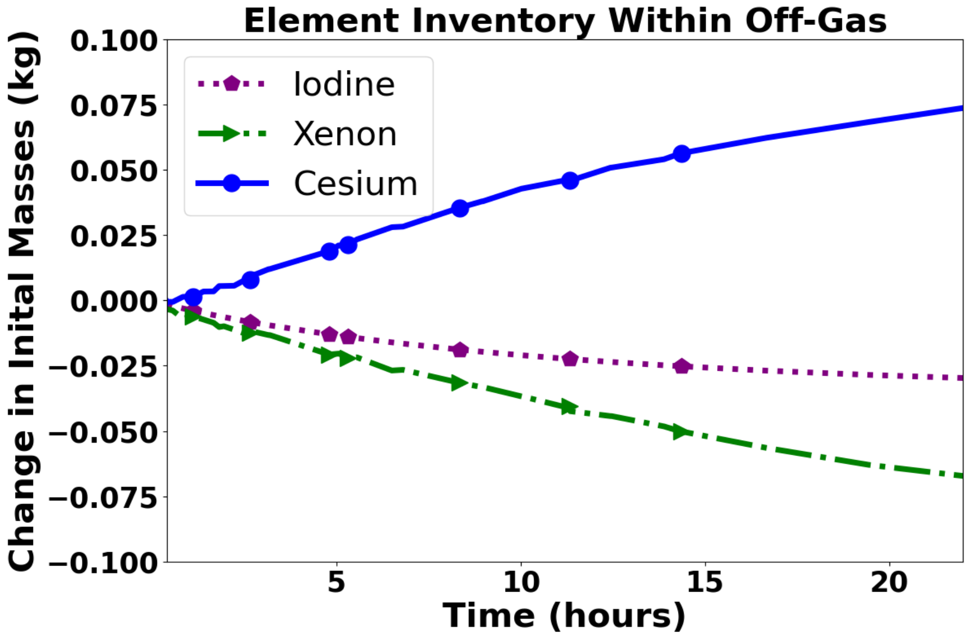


Emergency Drain: Radioactive Decay In Off-Gas

- Noble gases lumped into 'Xe' class
  - Common methodology to describe gaseous fission products
- Coupling of SCALE/ORIGEN with MELCOR allows for investigation of specific elements
  - Can **track the transport, production, and decay** of isotopes such as xenon-135 within the 'Xe' class

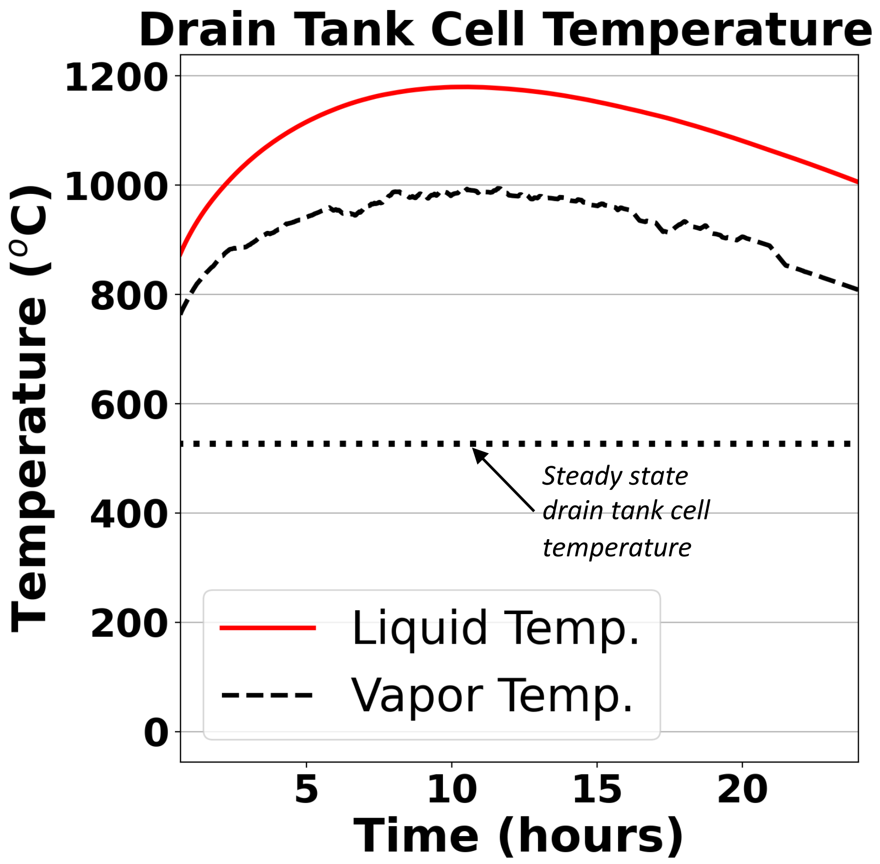


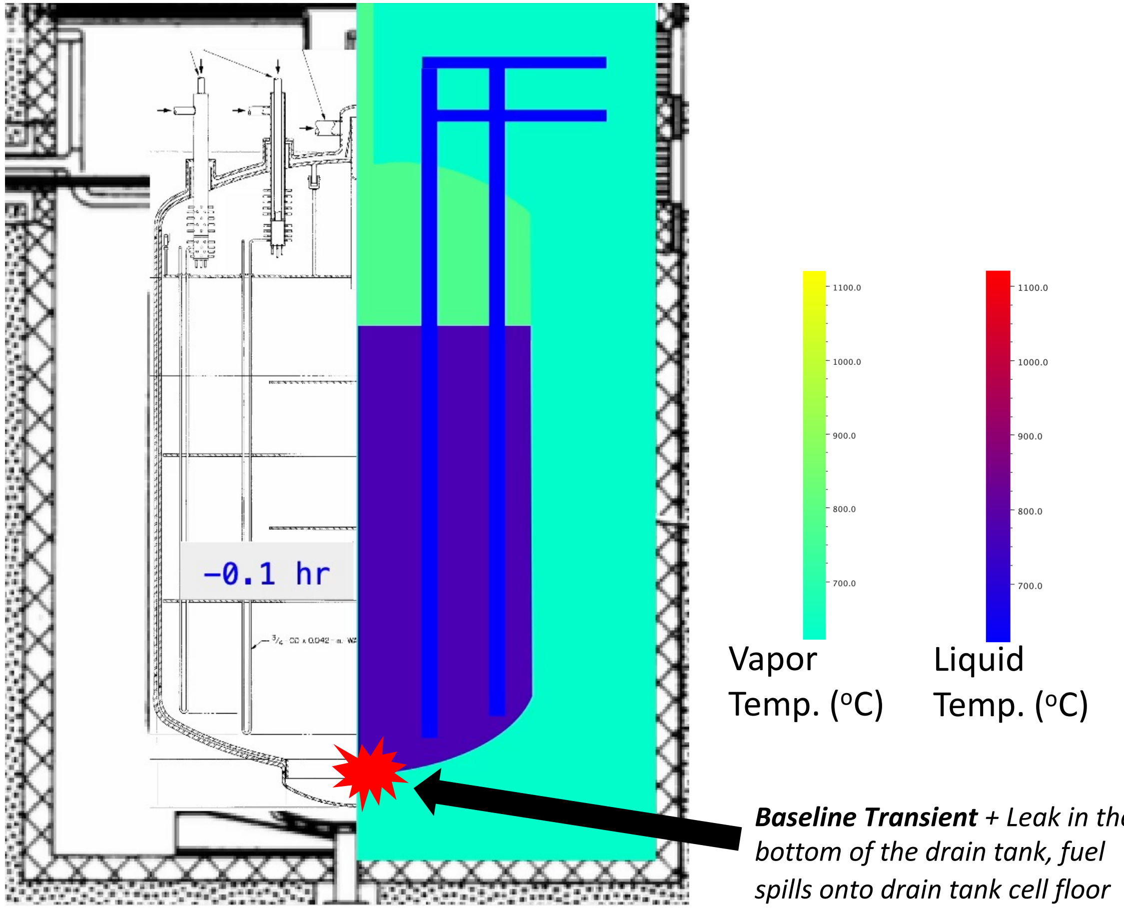




Drain Tank Leak Accident

- Leak in bottom of drain tank
  - Allows for all liquid to drain into drain tank cell
  - Liquid no longer cooled by drain tank heat removal system
  - Passive heat removal from drain tank cell floor and walls

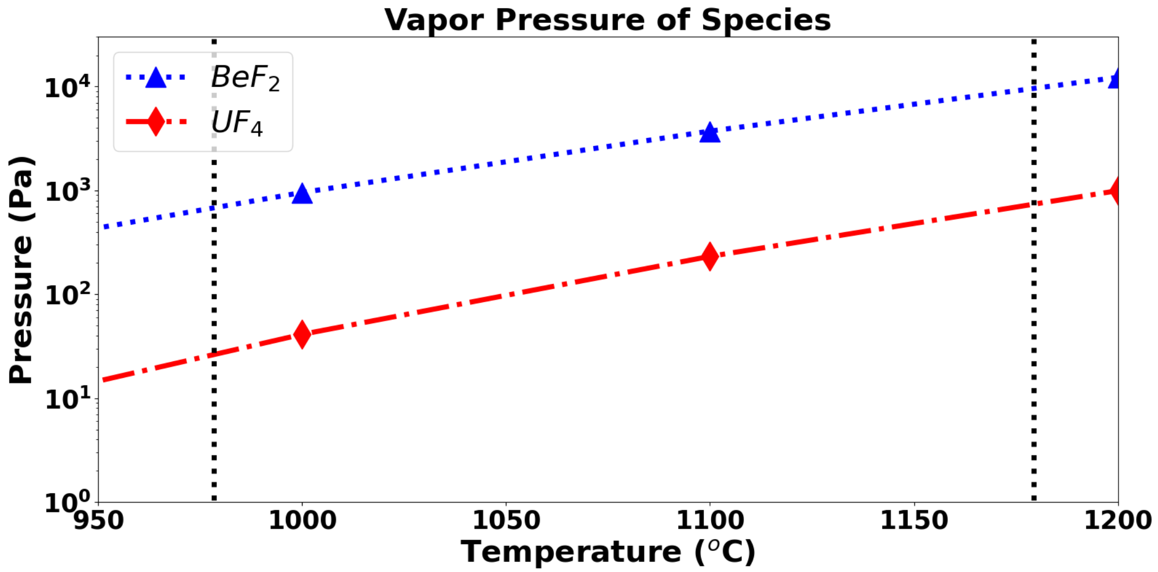


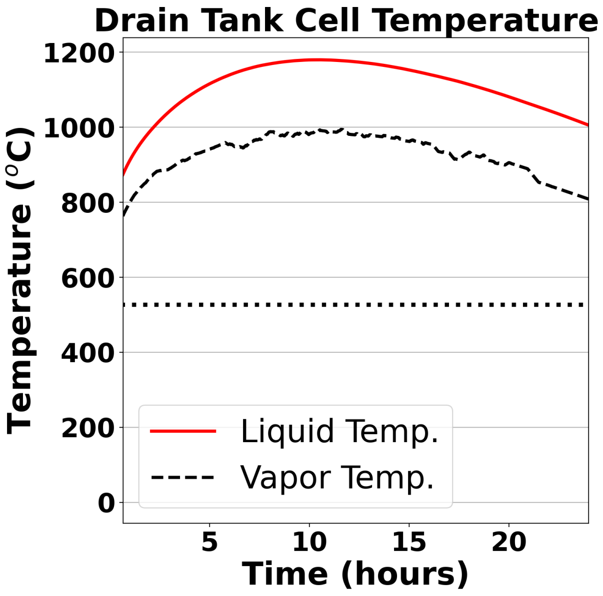


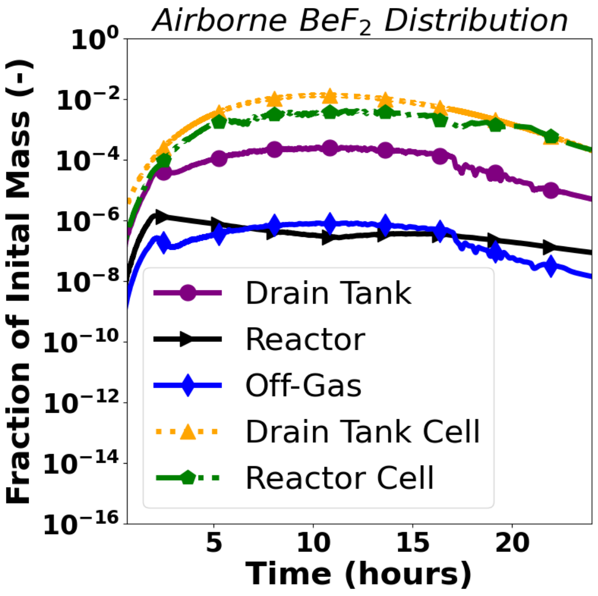
Baseline Transient *+ Leak in the bottom of the drain tank, fuel spills onto drain tank cell floor*

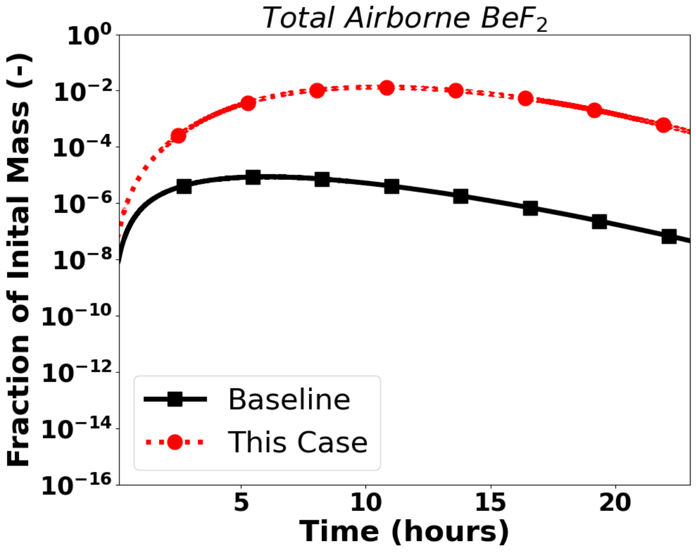
Drain Tank Leak Accident

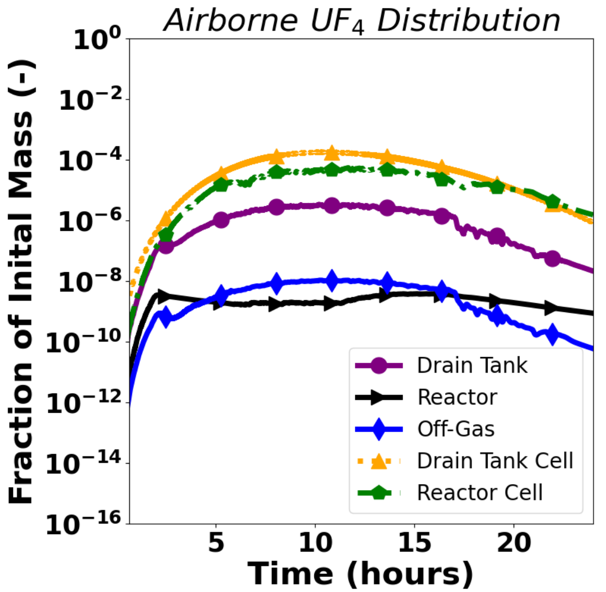
- Higher liquid temperatures due to insufficient cooling, around an order of magnitude higher vapor pressure
- Initially lower atmosphere pressure in drain tank cell than drain tank
- **Much larger fraction of airborne BeF_2 and UF_4 than in baseline case**
  - Significant fraction of airborne species escape fron drain tank cell to reactor cell











MELCOR Chemistry Road Map

- **Particle Deposition**
  - Solids (Noble metals, corrosion products, oxides)
  - Aerosols
- EOS thermophysical property sensitivity studies
  - Viscosity
  - Density
  - Heat Capacity
- Bubble formation and dynamics (Daniel Orea, Oak Ridge National Lab)
  - Bubble size/shape
  - Diffusion through liquids and solids, such as Xe into graphite
  - Bursting transfer from liquid to vapor phases
- MSR/Super-Critical CO_2 Heat exchanger failure

Summary

- MELCOR MSR modeling centers around “Control, Cool and Contain” ethos
- New Generalized MELCOR architecture allows for rapid implementation and evaluation for physical models
- SCALE integration into MELCOR allows for evaluation of radionuclide decay during system analysis
- Chemistry is informed through SCALE radionuclide calculations and MSTDB-TC calculations
- Demonstrations have been carried out for MSRE and MSBR designs
- MELCOR is being continuously developed to add important chemistry/physics models and to reduce uncertainties in MSR modeling.

Assume Radionuclide Masses Minimally Affect Bulk Salt Thermochemical Properties

- Sandia MELCOR Team
- Ted Besmann/Juliano Schrone-Pinto and tea
- Joanna McFarlane, Daniel Orea, Kevin Robb… (ORNL)
- Patricia Paviet (PNNL)
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