SCALE & MELCOR non-LWR Fuel Cycle Demonstration Project

Molten Salt Reactor Fuel Cycle

NRC's Volume 5 – Public Workshop #3

July 11, 2024

U.S. Nuclear Regulatory Commission

Office of Nuclear Regulatory Research

Office of Nuclear Reactor Regulation

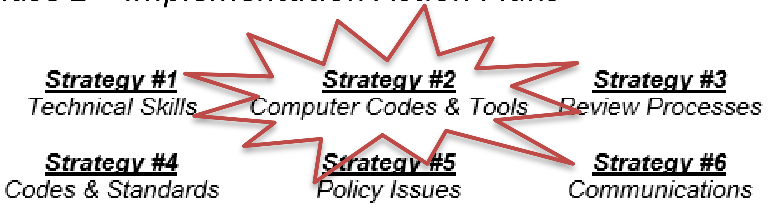
Office of Nuclear Material Safety and Safeguards

Outline

- NRC Strategy for non-LWRs Readiness
- MSR Nuclear Fuel Cycle
- Overview of the Simulated Accidents
- Demonstration of SCALE for MSR Fuel Cycle Analysis
- Molten Salt Reactor Modeling using MELCOR
- Summary & Closing Thoughts

NRC's Strategy for Preparing for non-LWRs

- *NRC's Readiness Strategy for Non-LWRs*
  - *Phase 1 – Vision & Strategy*
  - *Phase 2 – Implementation Action Plans*



- *IAPs are planning tools that describe:*
  - *Required work, resources, and sequencing of work to achieve readiness*

- *Strategy #2 – Computer Codes and Review Tools*
  - *Identifies computer code & development activities*
  - *Identifies key phenomena*
  - *Assess available experimental data & needs*

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What's in Volume 5?

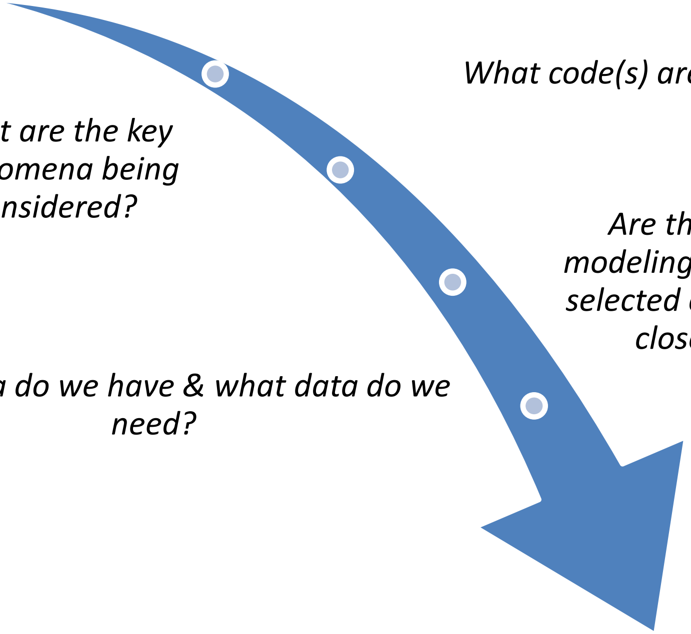
What system(s) are we analyzing?

What are the key phenomena being considered?

What code(s) are we using?

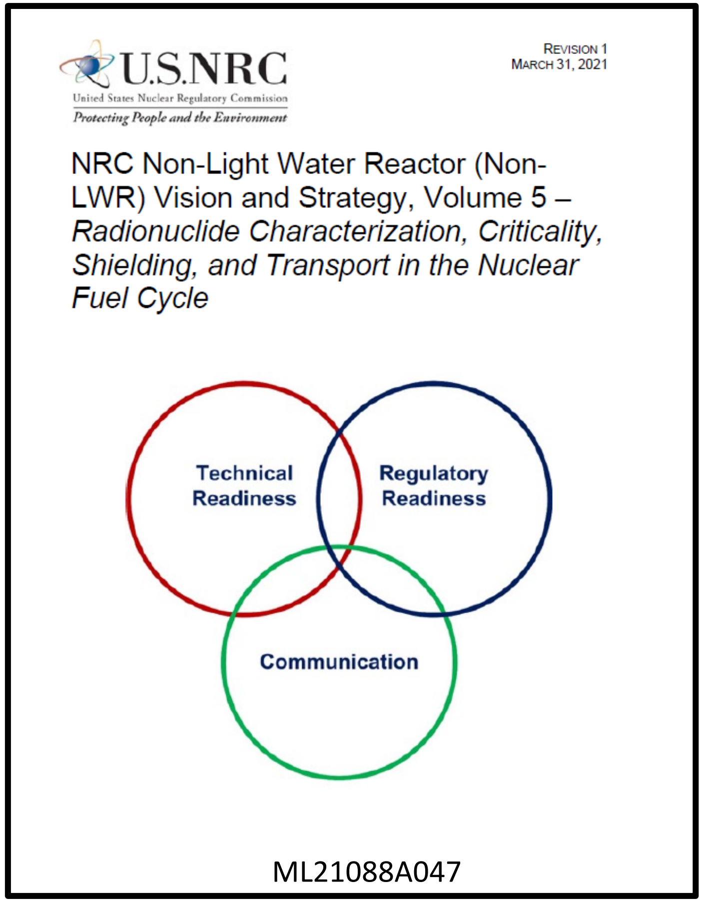
Are there any gaps in modeling capabilities of the selected codes? How do we close these gaps?

What data do we have & what data do we need?



IAP Strategy 2

Volume 5



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REVISION 1
MARCH 31, 2021

NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 5 – *Radionuclide Characterization, Criticality, Shielding, and Transport in the Nuclear Fuel Cycle*

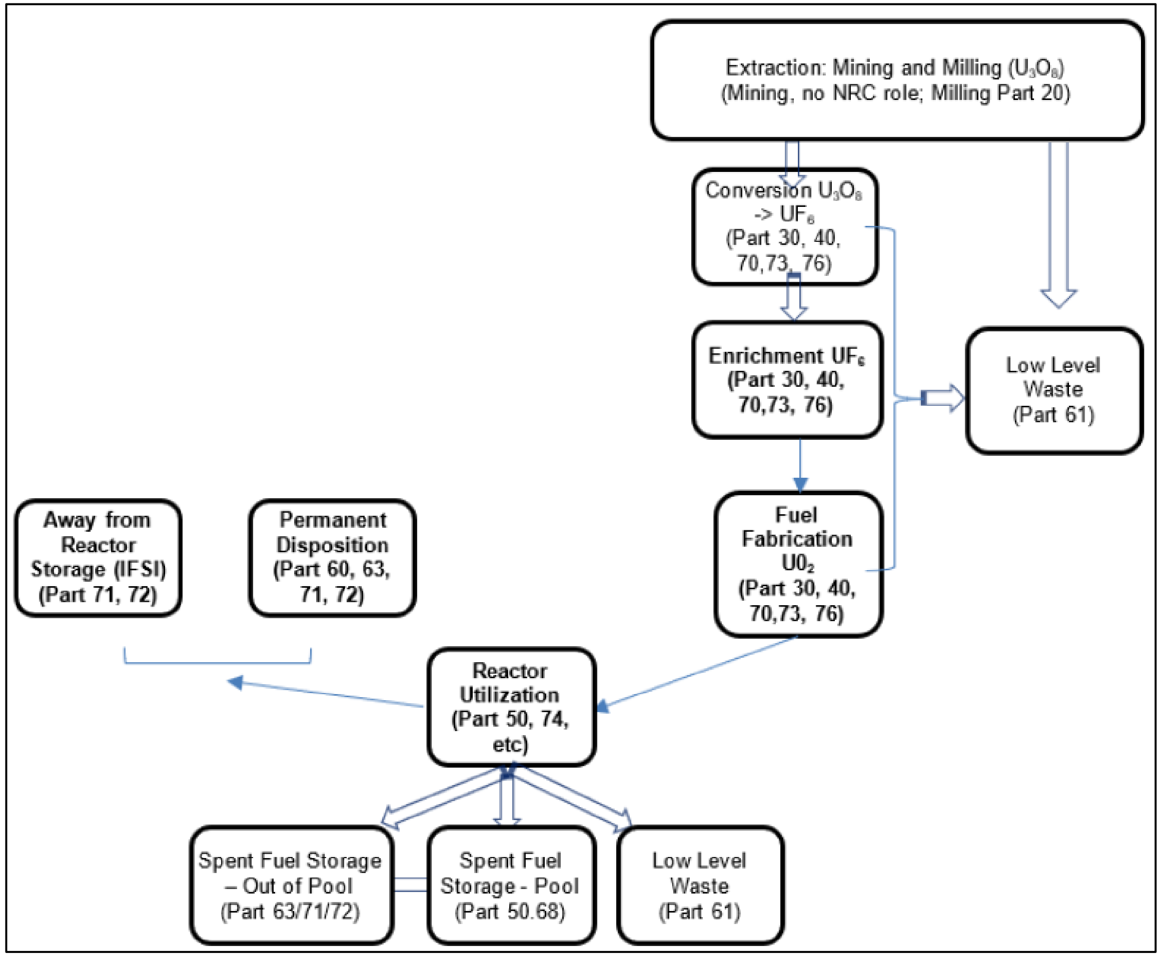
ML21088A047

LWR Nuclear Fuel Cycle

Regulations for the Nuclear Fuel Cycle

- *Protects onsite workers, public and the environment against radiological and non-radiological hazards that arise from fuel cycle operations.*
    - *Radiation hazards*
    - *Radiological hazards*
    - *Non-radiological (i.e., chemical) hazards*

- *Applicable Regulations*
    - *Uranium Recovery / Milling – 10 CFR Part 20*
    - *Uranium Conversion – 10 CFR Parts 30, 40, 70, 73 and 76*
    - *Uranium Enrichment – 10 CFR Parts 30, 40, 70, 73 and 76*
    - *Fuel Fabrication – 10 CFR Parts 30, 40, 70, 73 and 76*
    - *Reactor Utilization – 10 CFR Parts 50 & 74*
    - *Spent Fuel Pool Storage – 10 CFR Parts 50.68*
    - *Spent Fuel Storage (Dry) – 10 CFR Parts 63, 71, and 72*



Project Scope - Non-LWR Fuel Cycle

- *Stages in scope for Volume 5*

  - Enrichment: *UF_6 enrichment*
  - UF_6 Transportation
  - Fuel Fabrication
  - Fresh Fuel Transportation
  - Fuel Utilization (including on-site spent fuel storage)

- *Stages out of scope for Volume 5*

Uranium Mining & Milling	• *Not envisioned to change from current methods.*
Power Production	• *Successfully completed and leveraged from the **Volume 3 – Source Term & Consequence work***
Spent Fuel Off-site Storage & Transportation	• *Large amount of uncertainties for non-LWR concepts & lack of information*
Spent Fuel Final Disposal	• *Large amount of uncertainties for non-LWR concepts & lack of information*

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Codes Supporting non-LWR Nuclear Fuel Cycle Licensing

- NRC's comprehensive neutronics package
  - Nuclear data & cross-section processing
  - Decay heat analyses
  - Criticality safety
  - Radiation shielding
  - Radionuclide inventory & depletion generation
  - Reactor core physics
  - Sensitivity and uncertainty analyses

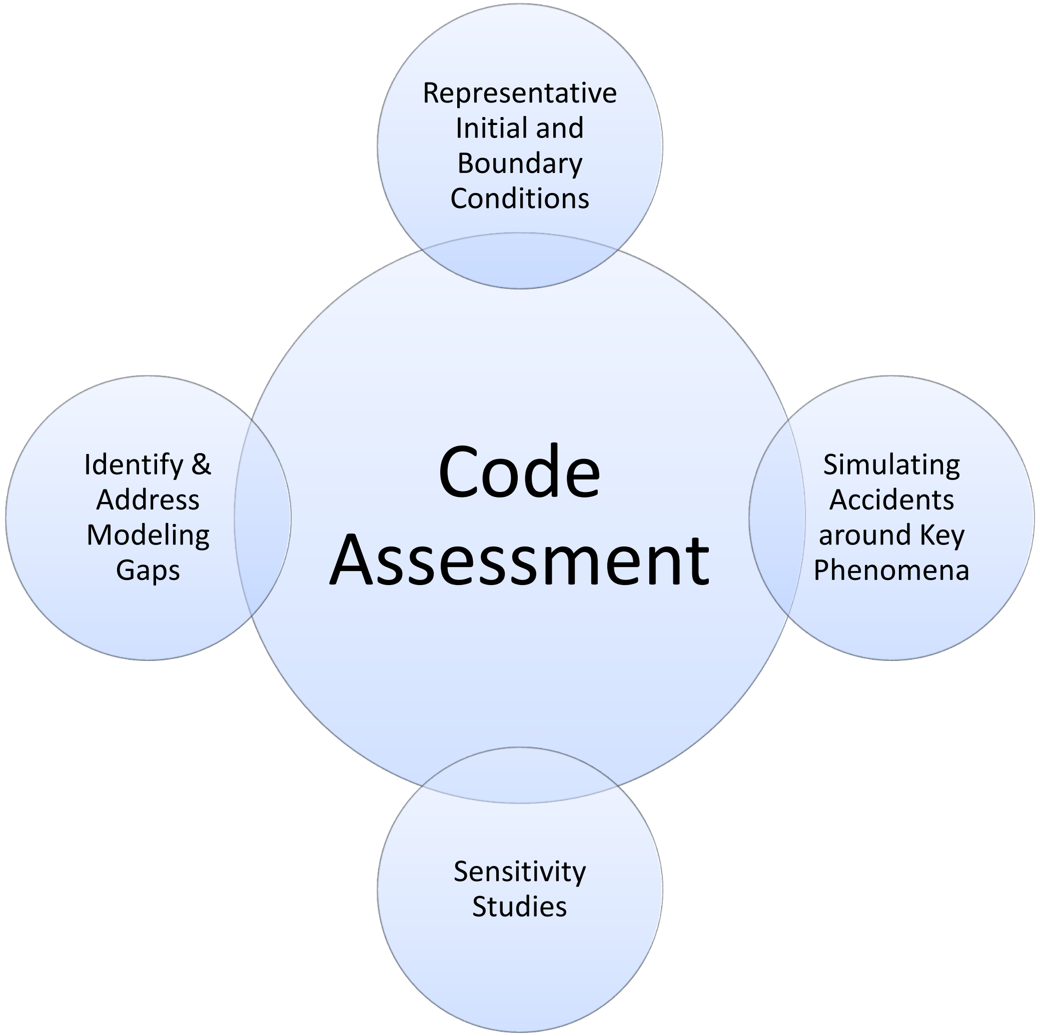
- NRC's comprehensive accident progression and source term code
  - Characterizing and tracking accident progression,
  - Performing transport and deposition of radionuclides throughout a facility,
  - Performing non-radiological accident progression

Project Approach

- Build representative fuel cycle designs **<u>leveraging</u>** the Volume 3 reactor systems designs (where appropriate)

- Identify key scenarios and accidents exercising key phenomena & models

- Build representative SCALE & MELCOR models and evaluate

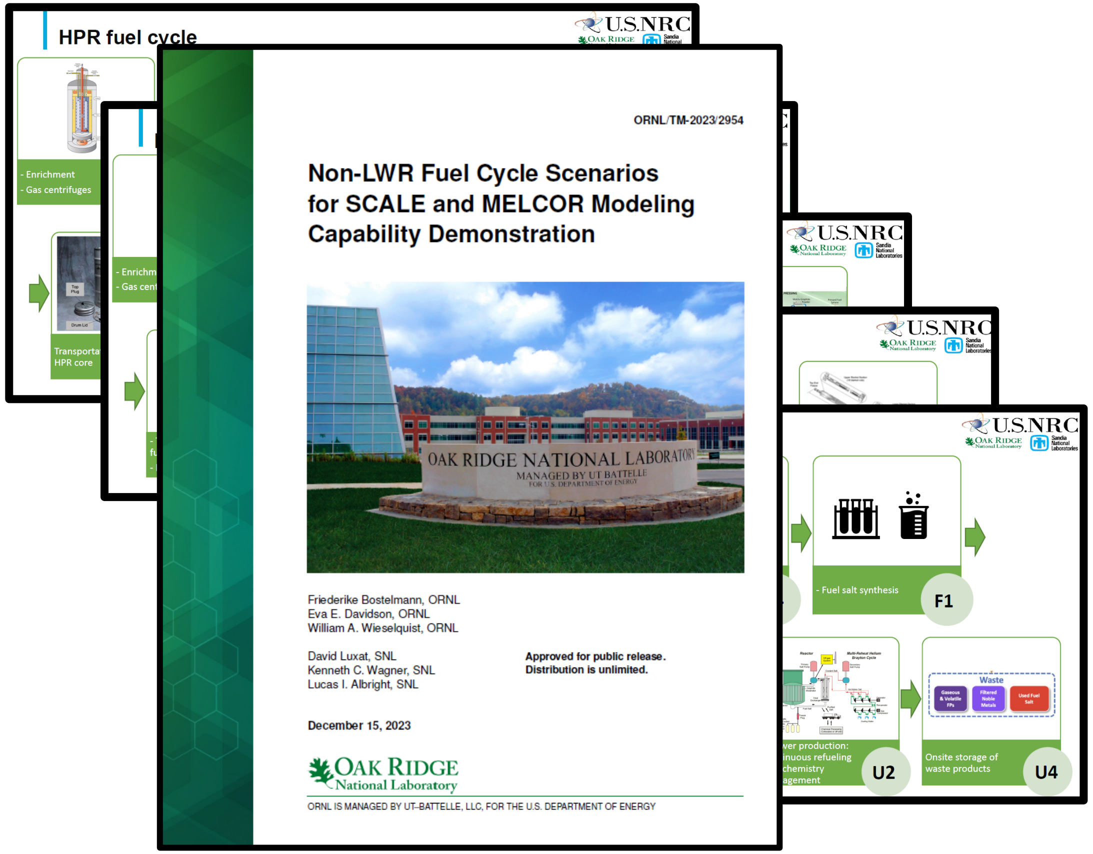


Representative Fuel Cycle Designs

- Completed 5 non-LWR fuel cycle designs for –
  - *Heat Pipe Reactor (HPR)– INL Design A*
  - *High Temperature Gas Reactor (HTGR) – Pebble Bed Modular Reactor (PBMR)-400*
  - *Fluoride-Salt Cooled Hight Temperature Reactor (FHR) – University of California, Berkeley (UCB) Mark 1*
  - *Molten Salt Reactor (MSR) – Molten Salt Reactor Experiment (MSRE)*[1]
  - *Sodium-Cooled Fast Reactor (SFR) - Advanced Burner Test Reactor (ABTR)*

- Identifies potential processes & methods, for example:
  - *What shipping package could transport HALEU-enriched UF6? What are the hazards associated?*
  - *How is spent SFR fuel moved? What are the hazards associated?*
  - *How is fissile salt manufactured for MSRs? What are the various kinds of fissile salt that may be used? What are the hazards?*

Informed Initial and Boundary Conditions for the SCALE & MELCOR Analyses



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[1] *The basis for the MSR fuel cycle design is based upon the MSRE, a small thermal spectrum reactor. Analyses showcased in this workshop utilized the MSR fuel cycle, but the facility and reactor input files were based on the geometry of the MSBR.*

Overview of the MSR Fuel Cycle

L. Kyriazidis (NRC)

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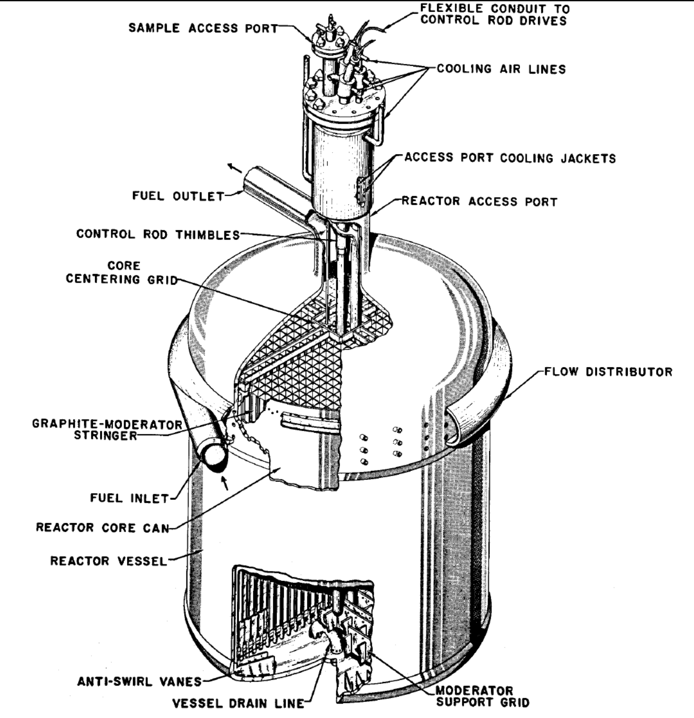
MSBR – Selecting a Large Thermal Spectrum MSR

- MSRE was analyzed during the in-reactor non-LWR demonstration project (Volume 3).

- Today's workshop considers MSBR
  - Large thermal spectrum reactor
  - Fuel salt considered is $LiF\text{-}BeF_2\text{-}UF_4$
  - Fuel salt composition & enrichment informed by SNL & ORNL chemistry & neutronics analyses

- MSBR Characteristics
  - Power – 2250 MW_{th} (MSRE – 10 MW_{th})
  - Total Salt Inventory – 1074 ft^3 (MSRE – ~71 ft^3)
  - Fuel Salt – $LiF\text{-}BeF_2\text{-}ThF_4\text{-}UF_4$
  - ThF_4 not considered in this work, as breeding fuel is out of scope.



MSRE

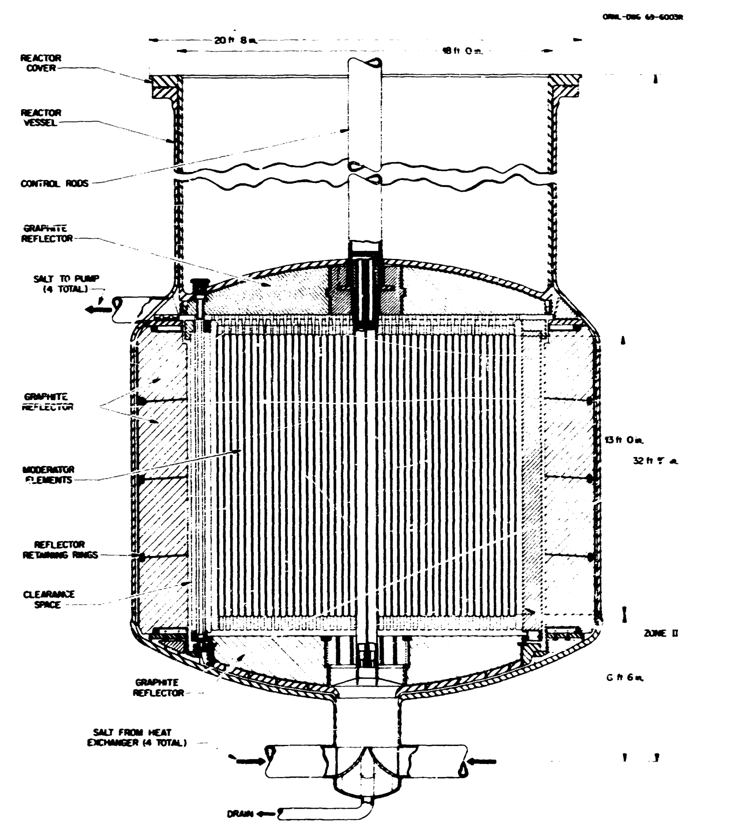
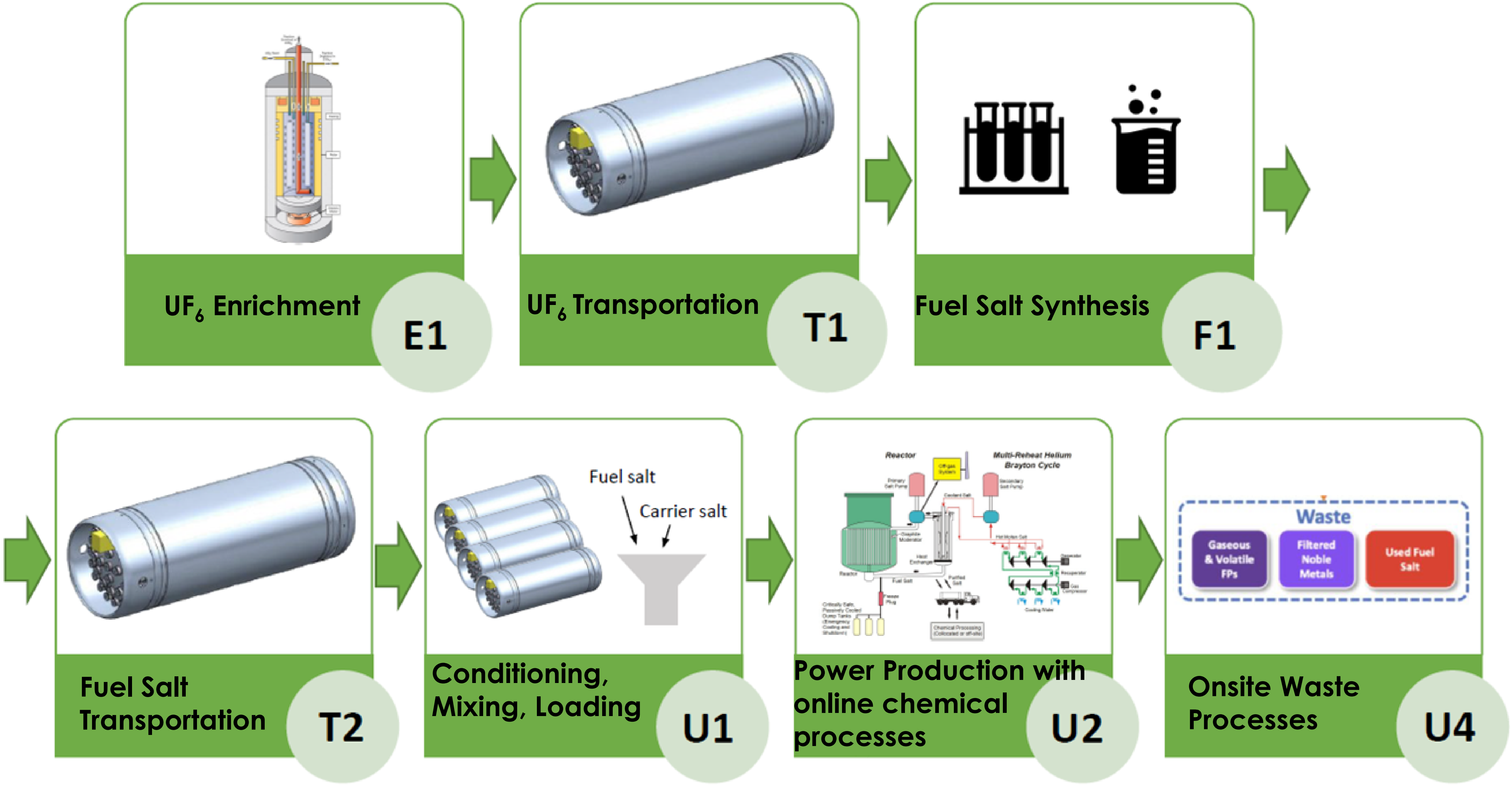


Fig. 3.2. Sectional elevation of MSBR vessel.

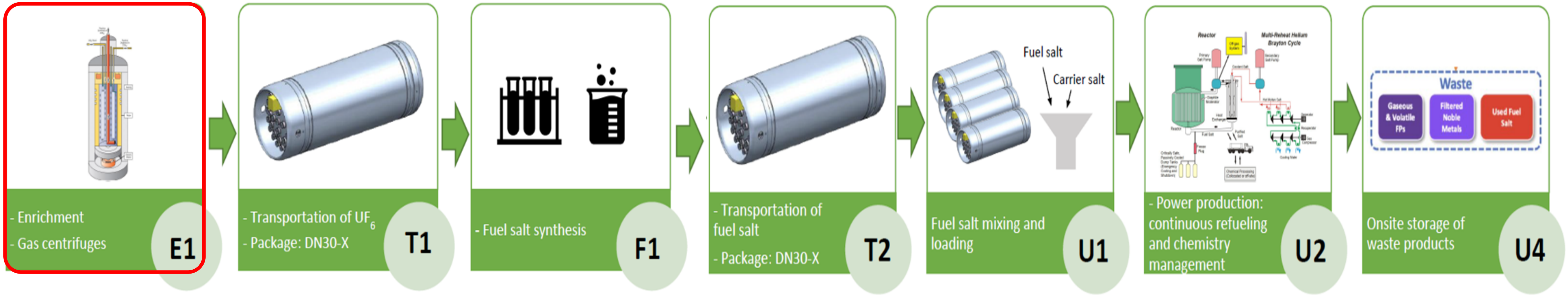
MSBR

MSBR was selected due to the size, fuel salt volume, power level, and burnup.

Overview of the MSR Fuel Cycle



E1: Enrichment



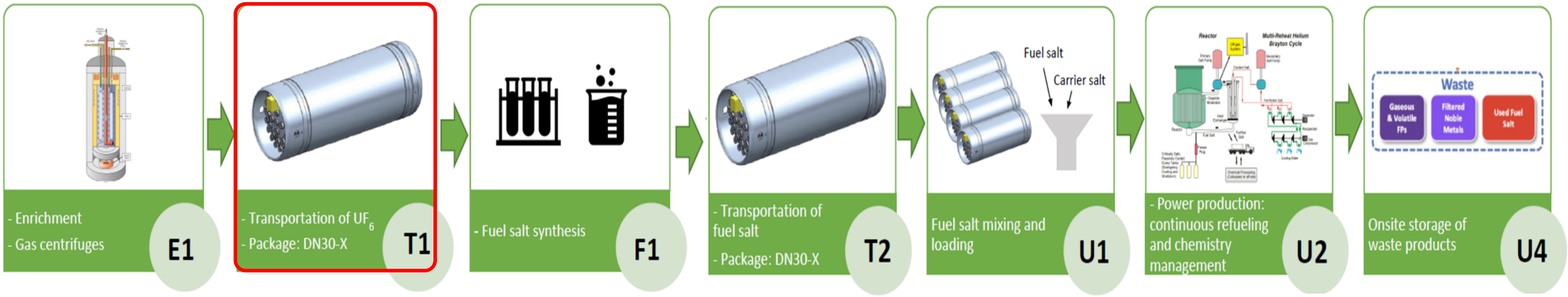
- Non-LWRs seek to use HALEU fuel designs, consisting of UF_6 up to 19.75 wt.% ^{235}U.
- E1 considers:
  - Chemical and processes for conversion of U_3O_8 to UF_6
  - Enrichment of UF_6 through gas centrifuging

Scenarios & Initiating Events Associated with E1

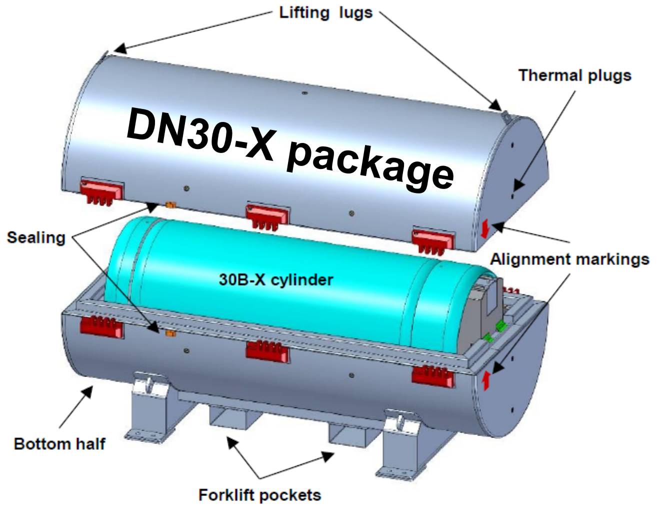
- Criticality – Unintended accumulation of enriched U
- Release – exposure to hazardous material (e.g., UF_6) due to fire, seismic events, tank ruptures, etc.

T1: Transportation of UF_6

Demonstration analyses related to fresh UF_6 transport covered in the Volume 5 HTGR workshop.



- Transportation of enriched UF6 to fuel fabricators.
- ORANO's DN30-X –NRC-approved UF6 package for up to 20 wt.% 235U

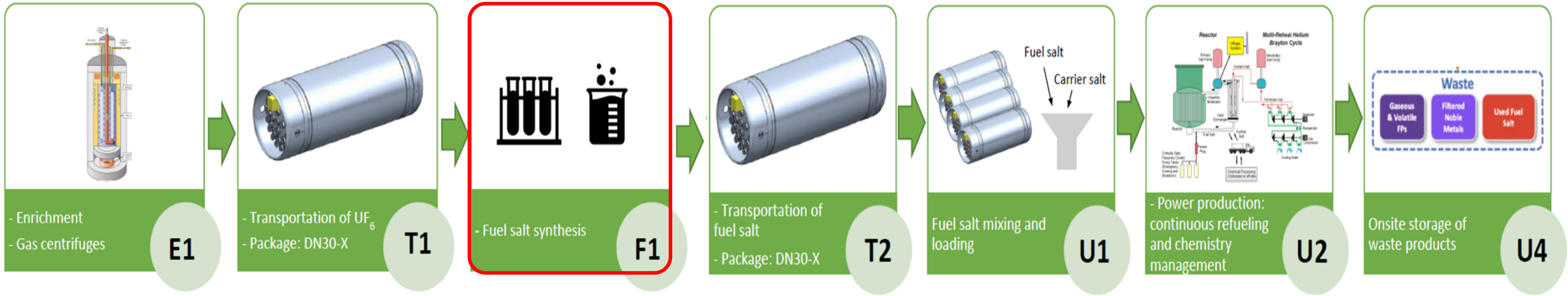


Ref.: ORANO Safety Analysis Report for the DN30-X Package
https://www.nrc.gov/docs/ML2232/ML22327A183.pdf
Certificate of Compliance, Certificate number 9388
https://rampac.energy.gov/docs/default-source/certificates/1019388.pdf

Scenarios & Initiating Events Associated with T1

- Criticality – impact of optimal water / moderator conditions, low temperature, unfavorable geometric changes
- Release – exposure to hazardous material (e.g., UF_6) due to fire, seismic events, tank ruptures, etc.

F1: Fuel Salt Synthesis – Fissile & Carrier Salts



Fuel Salt = Fissile Salt & Carrier Salt

- Two main classes of fissile salts; F1 considers fabrication of fissile salt only.
  - Fluoride-based salts for thermal spectrum systems (covered today)
  - Chloride-based salts for fast spectrum systems (described in ML24004A270)

MSBR
Thermal Spectrum Reactor

Fissile salt – UF_4
Carrier Salt – LiF, BeF_2, ThF_4
Fuel Salt – LiF-BeF_2-ThF_4-UF_4

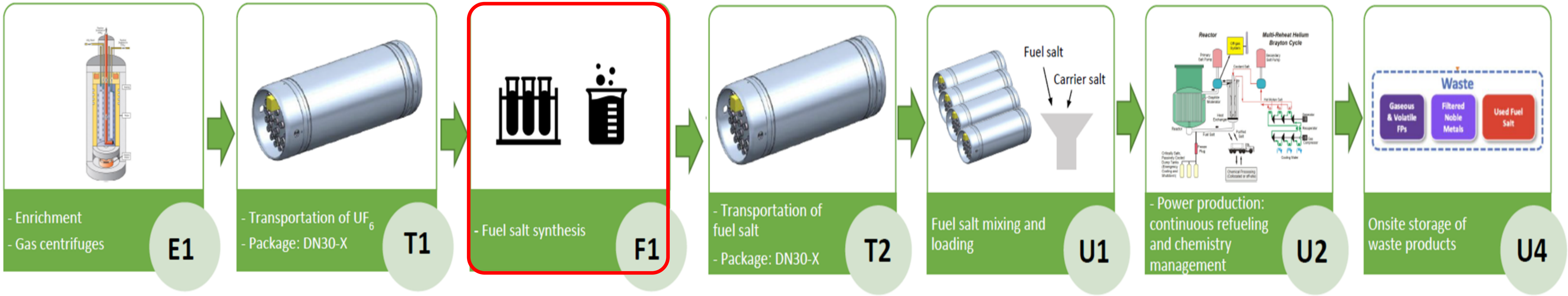
MSRE
Thermal Spectrum Reactor

Fissile salt – UF_4
Carrier Salt – LiF, BeF_2, ZrF_4
Fuel Salt – LiF-BeF_2-ZrF_4-UF_4

MCRE
Fast Spectrum Reactor

Fissile salt – UCl_3
Carrier Salt – NaCl
Fuel Salt – UCl_3-NaCl

F1: Fabrication of Fissile Salt (UF_4)



Four Processes for UF_4 Fissile Salt Manufacturing

Carbon Tetrachloride
- Toxic & corrosive off-gases
- Potential carcinogens

Hydrogen Process
- Toxic & corrosive off-gas
- Combustible reactive gas

NO_x Process
- Toxic & corrosive off-gas

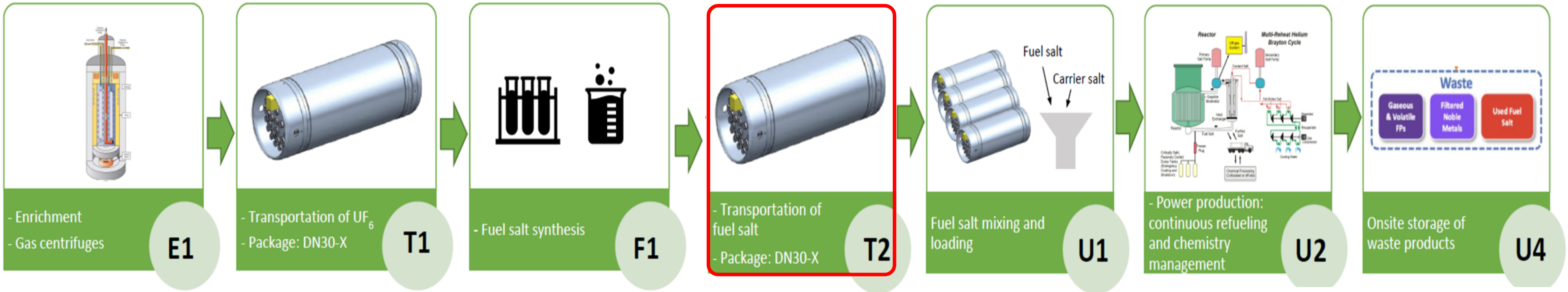
HBr, HCl, HI Process
- Toxic & corrosive off-gas

Scenarios & Initiating Events Associated with F1

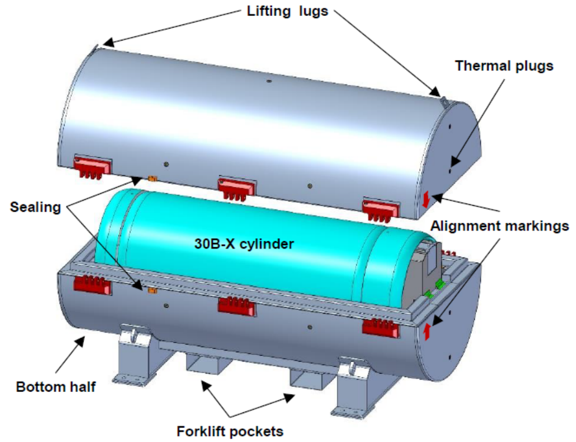
- Criticality – accumulation of U source & final product in reaction vessel or off-gas system, misload of fissile salt during fuel salt synthesis.
- Release – exposure to hazardous & radiological material due to fire, seismic events, tank ruptures, supply /exhaust line breaches, etc.

T2: Transportation of Fuel Salt to Plant

Demonstration analyses related to fresh fuel transport (fresh TRISO pebbles) covered in the Volume 5 HTGR workshop.



- Considers the transportation of freshly manufactured fuel salt and/or fissile salt.
  - No identified or currently-approved container for transporting fissile (UF4) or fuel salt.
  - For analyses purposes, assumes DN30-X package & 30B cylinder for transporting fissile & fuel salts



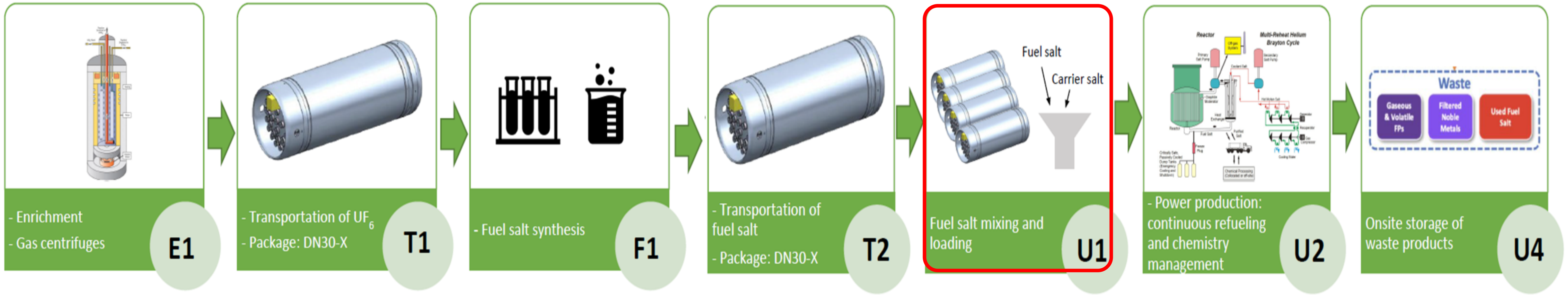
DN30-X package

Scenarios & Initiating Events Associated with T2

- Criticality – moderatior / water surrounding containers, geometric changes of containers (fire, damage, loss of overpack, corrosion).
- Release – exposure to hazardous & radiological material due container release (UO_2F_2, HF, Be, etc.)

Ref.: ORANO Safety Analysis Report for the DN30-X Package
https://www.nrc.gov/docs/ML2232/ML22327A183.pdf
Certificate of Compliance, Certificate number 9388
https://rampac.energy.gov/docs/default-source/certificates/1019388.pdf

U1 – Fuel Conditioning, Mixing, Loading

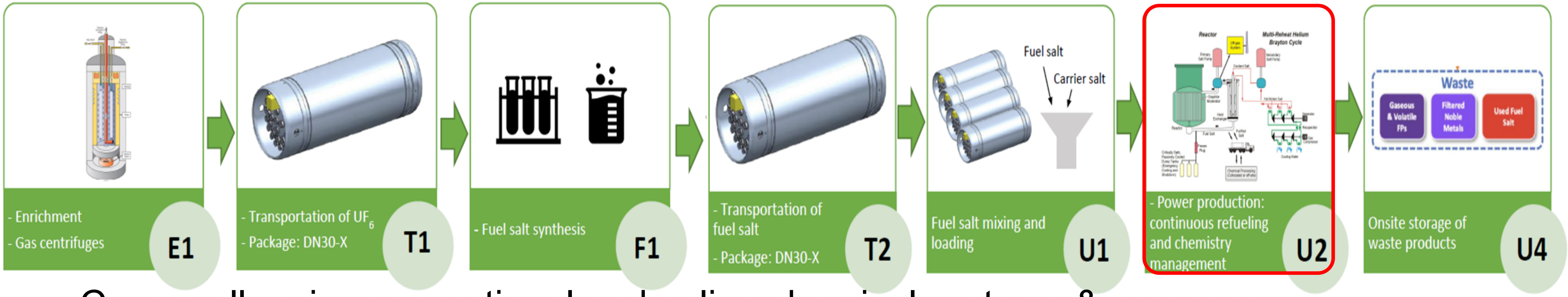


- Covers all the various pre-operational processes:
  - Storage & staging of salts
  - Mixing,
  - Salt conditioning (heating & melting),
  - Conditioning (oxygen & sulfur removal)

Scenarios & Initiating Events Associated with U1

- Criticality – moderatior / water surrounding containers, water ingress into containers, geometric changes of containers (fire, damage, loss of overpack, corrosion).
- Release – exposure to hazardous & radiological material due container release, spills, breaches due to corrosion

U2 – Power Production with Online Chemical Processes



- Covers all various operational and online chemical systems & processes
  - Cover-gas & off-gas systems, drain & hold tanks, and online monitoring systems

Important Phenomena related to U2

- Plating Out – noble metal fission products plate out onto structures or precipitate from the fuel salt.
- Gas Diffusion – diffusion of tritium (and helium) through metal at high temperatures

Scenarios & Initiating Events Associated with U2

- Criticality – release of reactor inventory (criticality outside of reactor), misload of fissile salt, control rod misalignment, injection of fuel salt at incorrect temperature, etc.
- Release – hydrolysis in salt / steam generation, breach of off-gas system, water ingress in reactor, air ingress in reactor, tritium release, drain tank breach
- Heat Removal – reduced salt pump flow rate (accumulation of FPs),
- Other – overcooling / salt freezing, core flow blockage

U4 – Onsite Discharged Fuel Waste Forms

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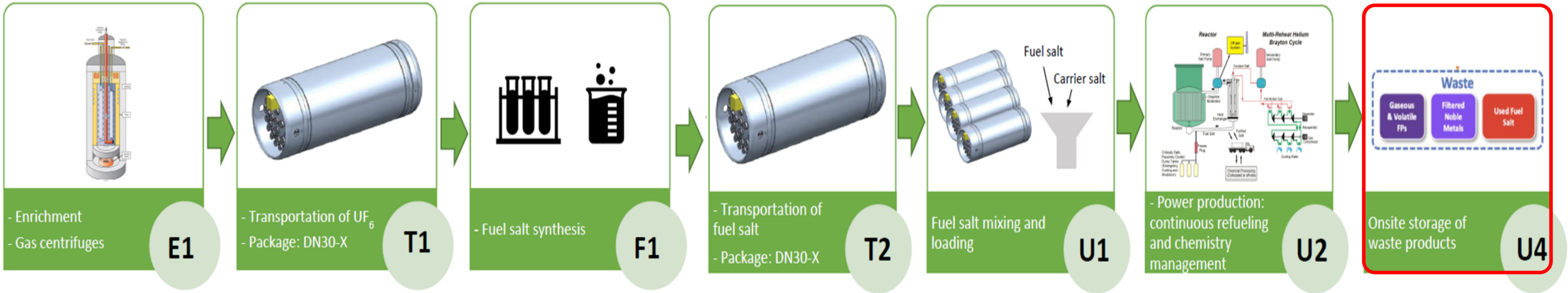
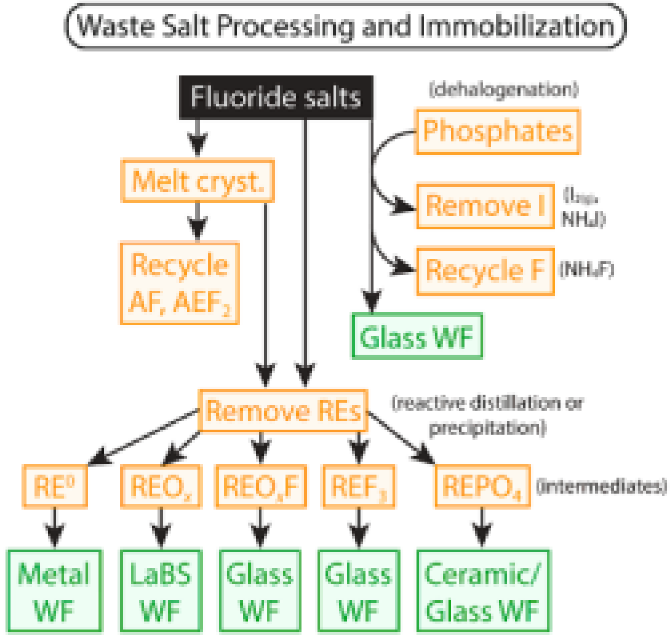


- Salts are highly soluble in water and pose a risk of migrating into groundwater (resulting from spills, releases, loss of confinement, etc.).
    - Immobilization of salt is expected (e.g., vitrification). Hazards and processes associated with waste immobilization considered. Waste forms consist of glasses and ceramics.



Scenarios & Initiating Events Associated with U4

- Criticality – water surrounding the storage container .
- Release – air ingress into storage container yielding a buildup of HF (corrosive agent).
- Heat Removal – Failure of active & passive cooling resulting in increase in temepraturе,

Summary of the MSR Fuel Cycle

Major differences in the MSR fuel cycle compared to LWR:

- Continuous operations with online loading of material feed and removal of fission gases through the off-gas system.
- MSRs may require strict chemical control (i.e., monitoring the redox potential to mitigate corrosion)
- Many new chemicals and processes throughout the various stages of the fuel cycle (e.g., fissile salt synthetic, fuel conditioning, cover-gas & off-gas systems, new waste streams, vitrification, etc.)

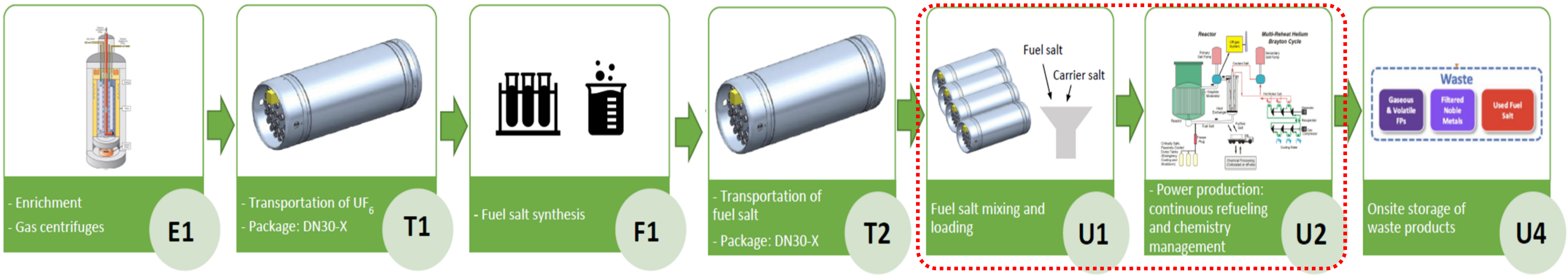
Major identified hazards:

- Higher enrichment impacting criticality during UF_6 and fissile salt (UF_4) storage and transportation
- Hazards from the use of the various chemicals (spills, reaction with water, fire, explosion)
- Interaction of salt with water & air, and the introduction of impurities into the reactor
- Poor control of the redox potential within the salt loop may introduce corrosion of key components

Additional details needed:

- Design & operational details of a full-scale power reactor
- Fuel salt specifications
- Details of the auxiliary systems (e.g., off-gas system, chemical control system, etc.)

Accidents Covered in Today's Workshop



Scenario for this stage studied in this workshop

Upcoming Scenarios Analyzed

<u>Scenario #1 (U1) Excess Fissile Content during Fuel Salt Makeup</u>

Criticality analysis modeling the insufficient mixing of fissile and carrier salt.

<u>Scenario #2 (U2) Release of Fission Product during Operations</u>

Radiological transport & shielding analyses of a tritium release and a breach in the off-gas system.

<u>Scenario #3 (U2) Insufficient Residual Heat Removal of the Drain Tank</u>

MSR drain tank fails due to a failure in decay heat removal. Results in radiological inventory transport throughout the facility.

<u>Demonstrating ORIGEN/MELCOR Coupling</u>

- Removes the need to generate time-dependent decay tables by coupling ORIGEN into MELCOR for on-the-fly generation of decay tables.
- Allows for decay and depletion in MELCOR

Demonstration of SCALE for MSR Fuel Cycle Analysis

D. HARTANTO, G. RADULESCU, F. BOSTELMANN, W. A. WIESELQUIST

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OBJECTIVE AND APPLICATIONS

Objective: Demonstrate use of SCALE for simulating accident scenarios in all stages of the nuclear fuel cycle for molten salt reactors (MSRs)

Scenario 1: Criticality event during fuel salt preparation (U1.5)

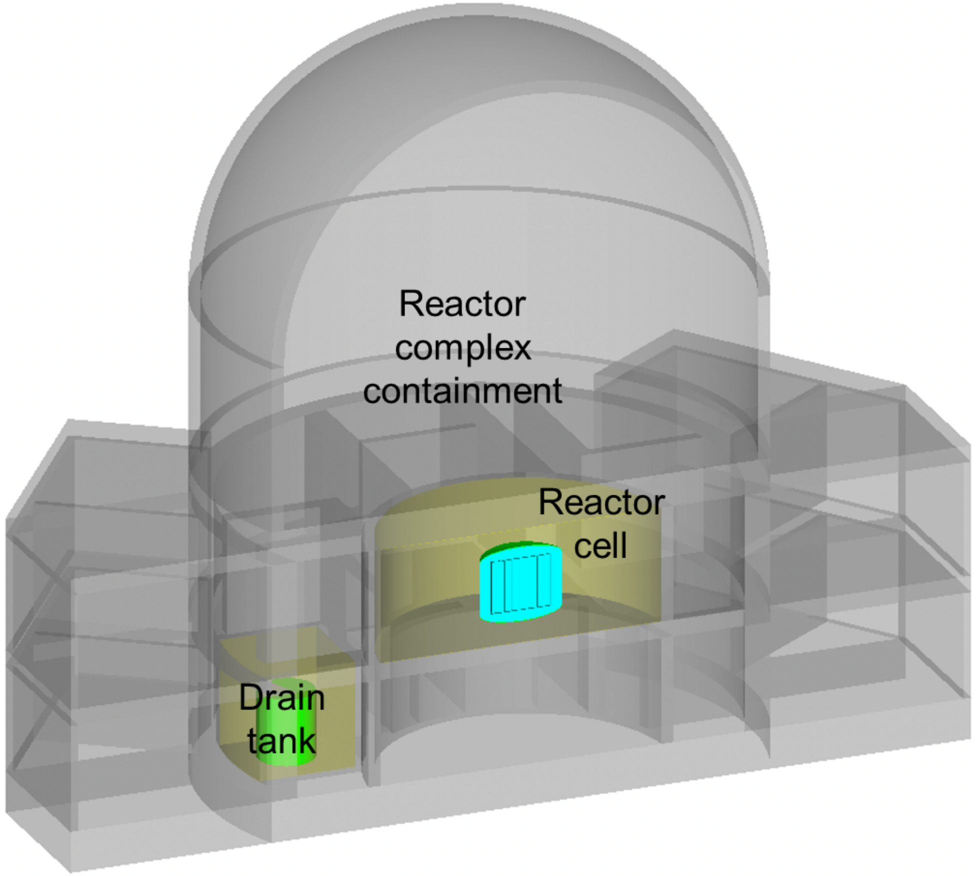
- Accident: Insufficient mixing of fissile and carrier salt leading to batches with high fissile material
- Analysis: 1) Determine fuel salt canister, 2) perform criticality calculations for different compositions, temperature, and configurations

Scenario 2: Release of fission products during operation (U2)

- Accident:
  - Tritium release
  - Breach in the off-gas system leads to release of fission products
  - Dose rate at reactor cell during operation
- Analysis: 1) Determine fuel inventory, and 2) perform radiation dose rate calculation

Scenario 3: Heat removal of drain tank (U2)

- Accident: Failure in heat removal of drain tank
- Analysis: 1) Determine fuel inventory, and 2) perform radiation dose rate and decay heat calculations



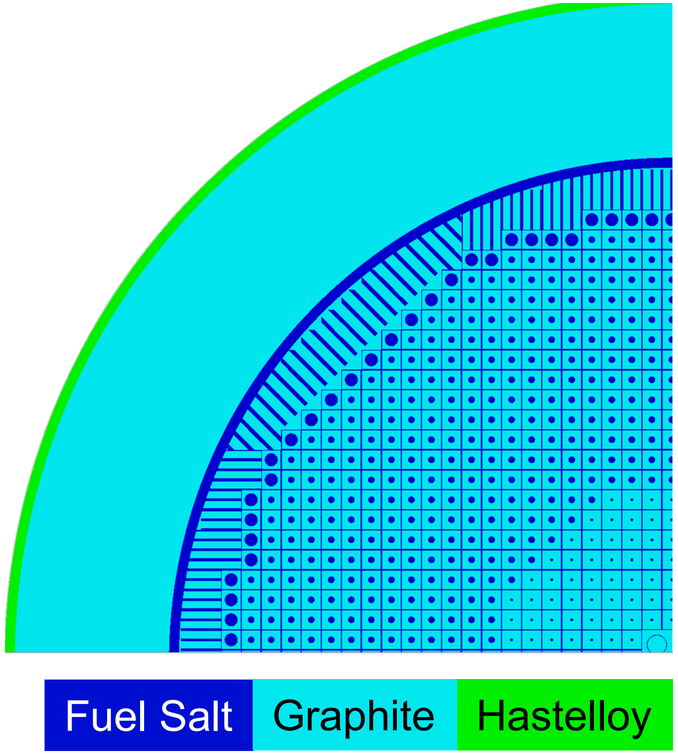
MSR Plant Model

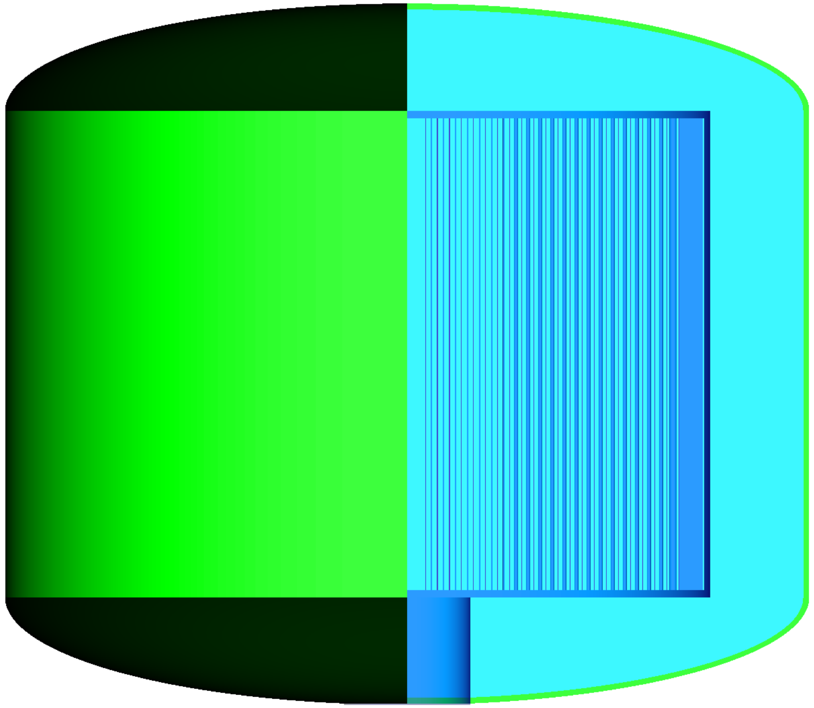
Ref: Robertson, R. C., et al., "Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor," ORNL-4541, Oak Ridge National Laboratory, 1971

REFERENCE MOLTEN SALT REACTOR MODEL

- Reference model based on molten salt breeder reactor (MSBR)
  - SCALE reactor model to obtain reactor physics parameters and nuclide inventory
- Fuel salt was updated to uranium-based fuel salt

Reactor Power	2250 MW_t, 1000 MWe
Fuel Salt	$^{7}LiF\text{-}BeF_2\text{-}ThF_4\text{-}UF_4$ (original) **$^{7}LiF\text{-}BeF_2\text{-}UF_4$ (current)**
Fuel Salt Temperature	838.7 K/977.6 K
Cycle Length	4 years



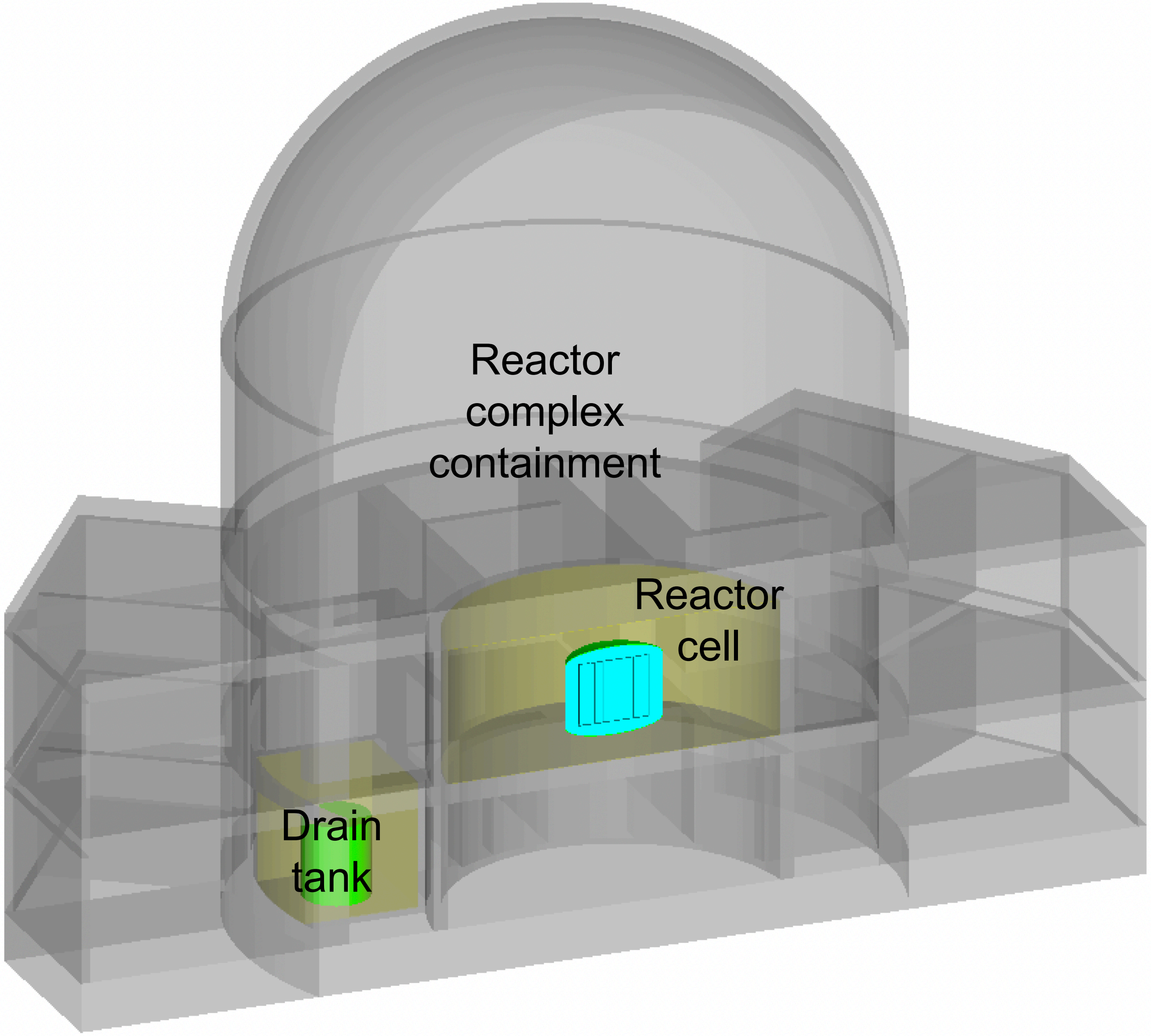


SCALE MSR Model

Refs.:
[1] Robertson, R. C., et al., "Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor," ORNL-4541, Oak Ridge National Laboratory, 1971
[2] Davidson, E. E., et al., "Reactor Cell Neutron Dose for the Molten Salt Breeder Reactor Conceptual Design," Nuclear Engineering and Design 383, 111381, 2021.

REFERENCE MSR PLANT MODEL

- Simplified model for shielding calculations with focus on:
  - Reactor within reactor cell
  - Reactor cell within reactor complex containment at reactor cell elevation
  - Drain tank located in primary salt drain tank cell at waste storage elevation
  - Heat exchangers, pumps, and pipes not considered



APPLIED SCALE 6.3.1 SEQUENCES

Reactor physics burnup calculations with **TRITON**

- Monte Carlo neutron transport code (KENO or Shift) coupled with ORIGEN depletion solver
- **Output**:
  - Multiplication factor
  - Spatial flux and power distributions
  - Nuclide inventory

Shielding & radiation dose calculations with **MAVRIC**

- Monte Carlo photon and neutron transport code (Shift) with automated variance reduction for shielding analyses
- Requires radiation source terms
- **Output**:
  - Spatial flux/dose rate distributions

Criticality calculation with **CSAS**

- Monte Carlo neutron transport code (KENO or Shift) for criticality analysis
- **Output:**
  - Multiplication factor
  - Spatial flux and fission density distributions

Sens. Analysis & Unc. Quantification with **SAMPLER**

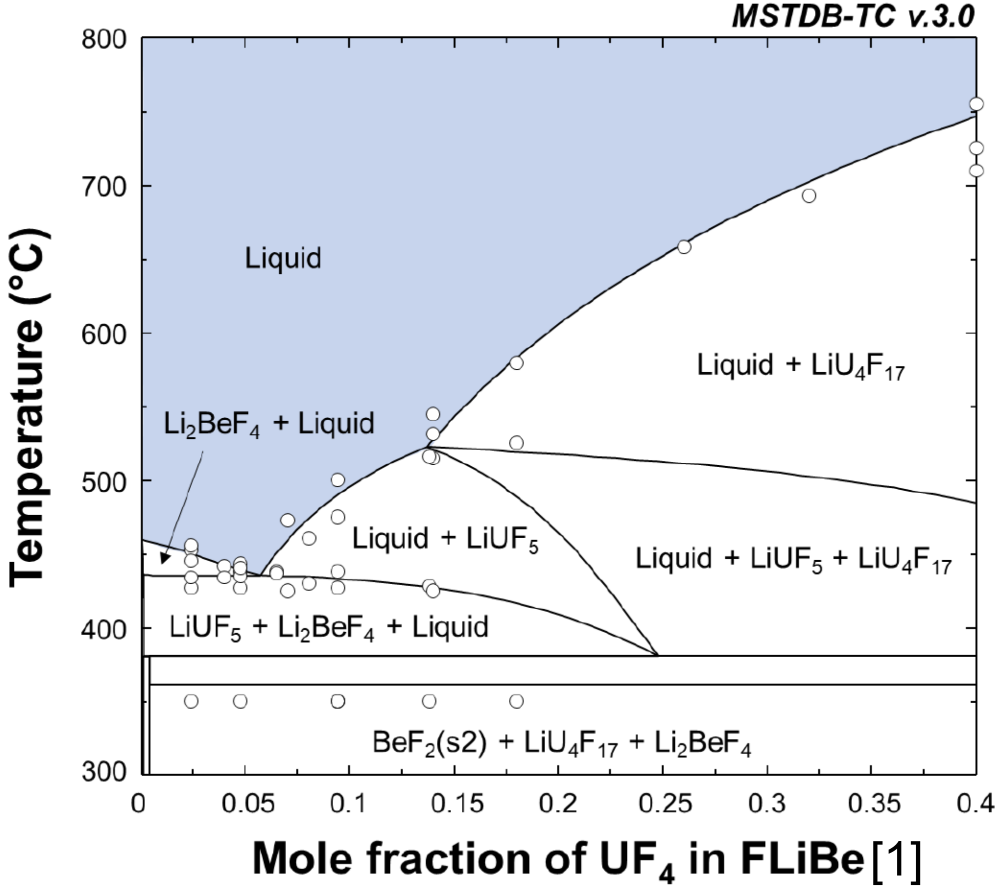
- General uncertainty analysis by statistically sampling the input data
- **Output:**
  - Uncertainty of user-specified results
  - Correlations matrices

ENDF/B-VII.1 nuclear data library used for all calculations

Refs.:
[1] Wieselquist, W. A., Lefebvre, R. A., Eds., SCALE 6.3.1 User Manual, ORNL/TM-SCALE-6.3.1, Oak Ridge National Laboratory, 2023.
[2] Chadwick, M. B., et al. ENDF/B-VII. 1 nuclear data for science and technology: cross sections, covariances, fission product yields and decay data. Nuclear data sheets, 112(12), 2887-2996, 2011.

FUEL SALT CHARACTERISTICS

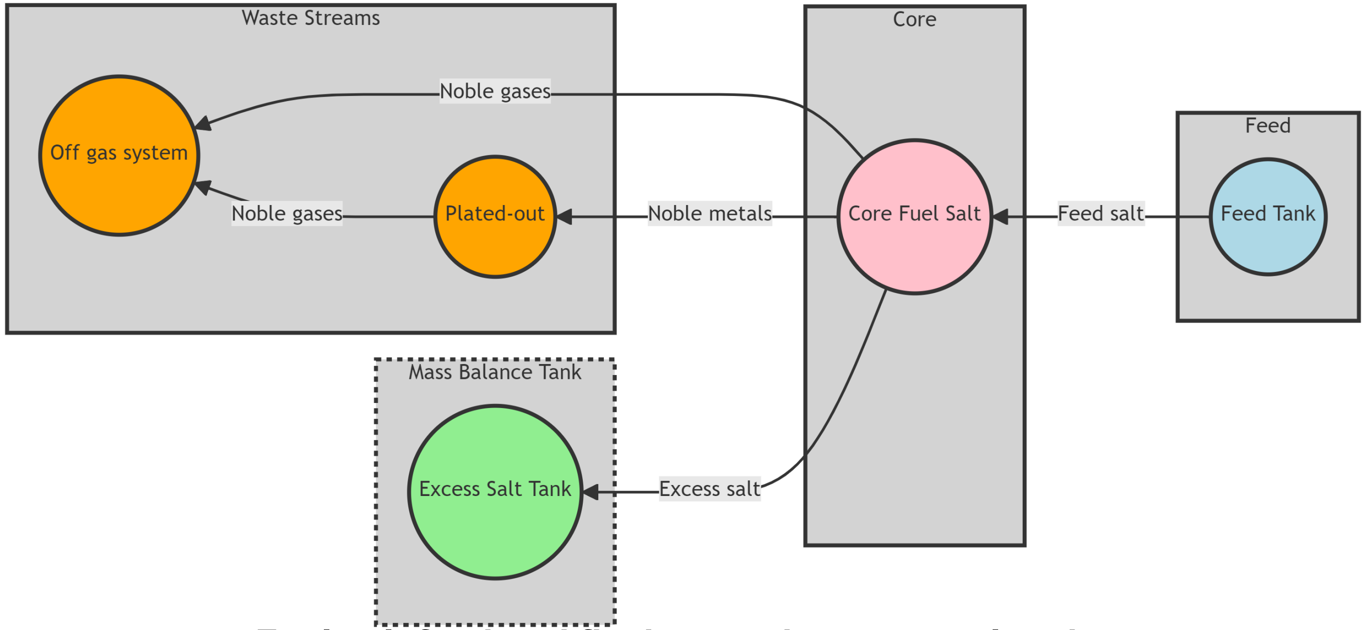
- MSRE fuel salt according to design specifications:
  $^7LiF\text{-}BeF_2\text{-}ZrF_4\text{-}UF_4$
  (4.70-29.38-5.10-0.82 mol%)
  - Fraction of 0.82 mol% UF_4 causes low initial heavy metal mass
  - Given a thermal power of 2250 MWth, the specific power would be unrealistically high
- Instead, this work uses alternative fuel salt specifications:
  $^7LiF\text{-}BeF_2\text{-}UF_4$
  (60-30-10 mol%)
  - Molar fractions chosen to obtain lower melting point while maximizing U loading



Ref:
[1] Private communication with Dr. J. Schorne Pinto, University of South Carolina, February 2024.

BURNUP CALCULATIONS

- TRITON depletion considering fission products removal and continuous feed of fuel salt (FLOW block).
  - Initial and feed ^{235}U enrichment: 2.30 wt.% and 5.00 wt.%, respectively
  - Removal rate of noble gases and noble metals: 0.0333 /s
  - Redox potential control for corrosion mitigation, such as adding Be or F to the primary salt, was not considered in this simulation



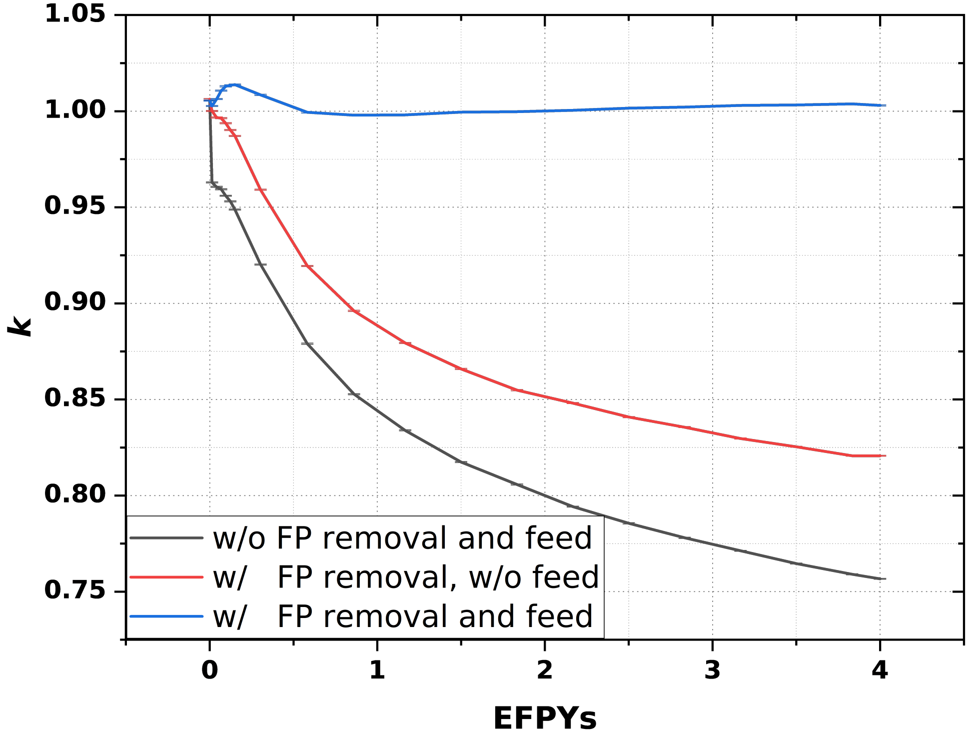
Fuel salt feed and fission product removal paths

```
read timetable
'flow from fuel to OGS'
  flow
    from 1 to 11
    type fractional_removal
    units pers
    nuclides   Xe          Kr          end
    rates      3.33333E-02 3.33333E-02 end
    time       0.0 end
    multiplier 1.0 end
  end flow

'flow from fuel to Noble metal plated out'
  flow
    from 1 to 12
    type fractional_removal
    units pers
    nuclides  Se          Nb          Mo          Tc
              Ru          Rh          Pd          Ag
              Sb          Te          end
    rates     3.33333E-02 3.33333E-02 3.33333E-02 3.33333E-02
              3.33333E-02 3.33333E-02 3.33333E-02 3.33333E-02
              3.33333E-02 3.33333E-02 end
    time       0.0 end
    multiplier 1.0 end
  end flow

'flow from feed, 5% U-235 enrichment'
  flow
    to         1
    type       continuous_feed
    units      gpers
    nuclides   li-6        li-7        be-9
               f-19        u-235       u-238       end
    rates      7.2704E-06  1.4540E-01  9.3390E-02
               1.0500E+00  4.1088E-02  7.8066E-01  end
    time       0.0 end
    multiplier 1.0 end
  end flow

'flow from fuel to drain tank'
  flow
    from       1 to 13
    type       fractional_removal
    units      pers
    nuclides   all   end
    rates      2.8e-8   end
    time       0.0 end
    multiplier 1.0 end
  end flow
end timetable
```

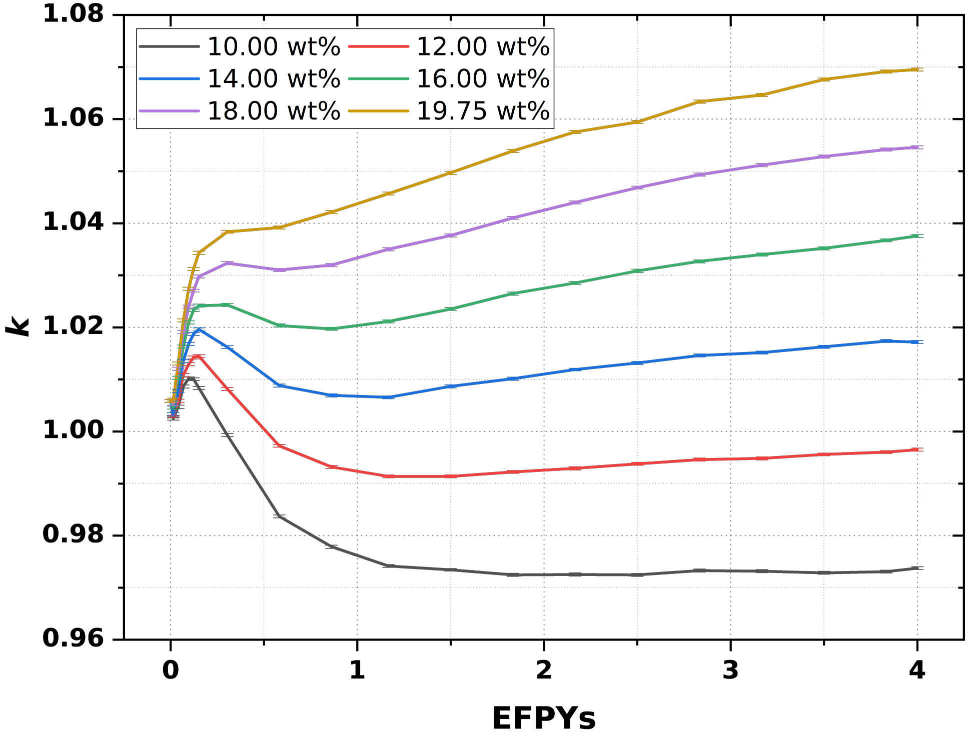
Implementation of FLOW block in SCALE/TRITON

BURNUP CALCULATIONS

- Multiplication factor as function of EFPYs
  - Fuel salt addition was necessary to achieve operating lifetime of 4 years
  - With the feed salt containing 5 wt.% of ^{235}U, the total volume of feed salt was ~3.5 times the volume of the initial primary fuel salt **(used in subsequent calculations)**
  - To obtain a feed salt volume equal to the initial primary salt volume, the ^{235}U of the feed salt would have to be higher than 12 wt.%



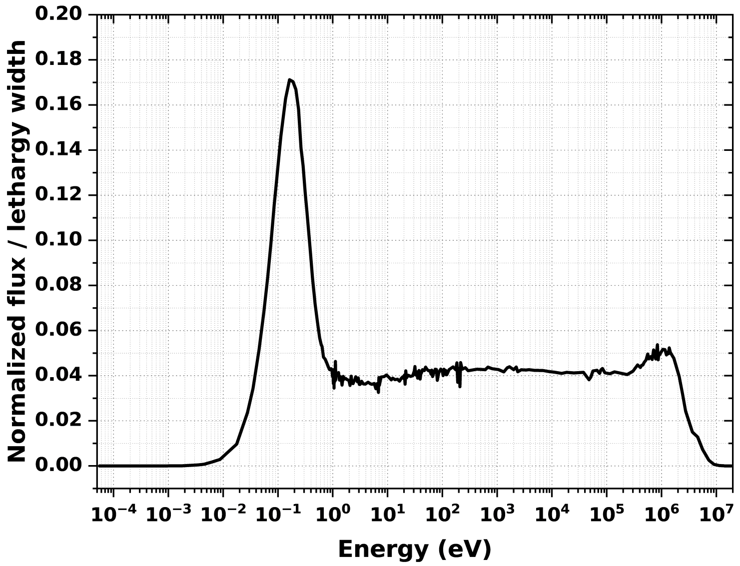
K-eff evolution with and without FPs removal and feed



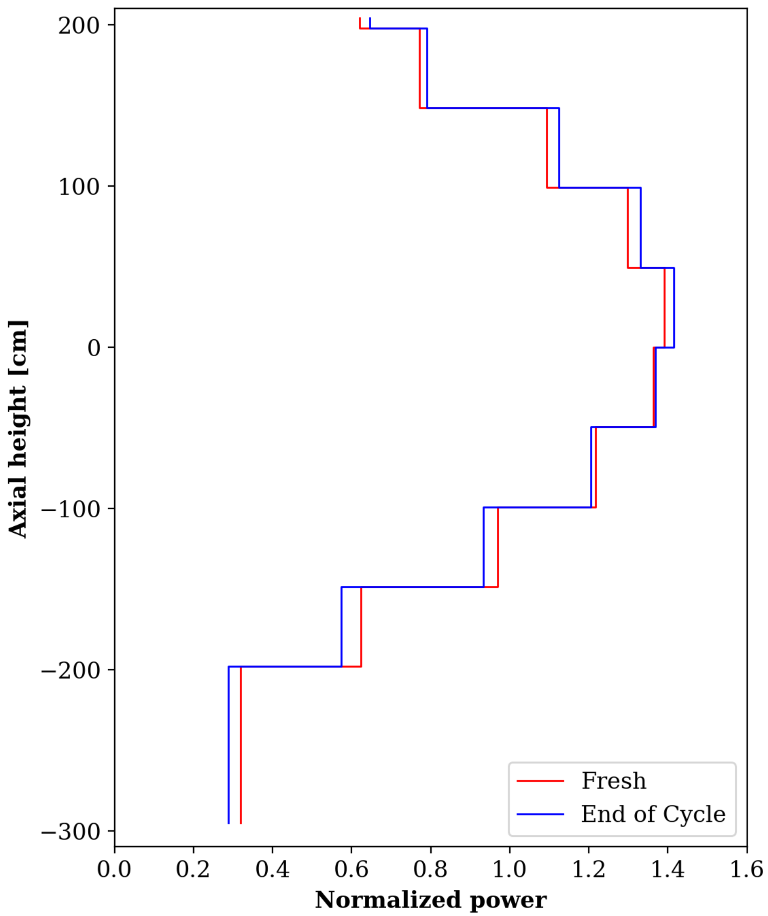
K-eff evolution for different feed enrichment

REACTOR PHYSICS PARAMETERS

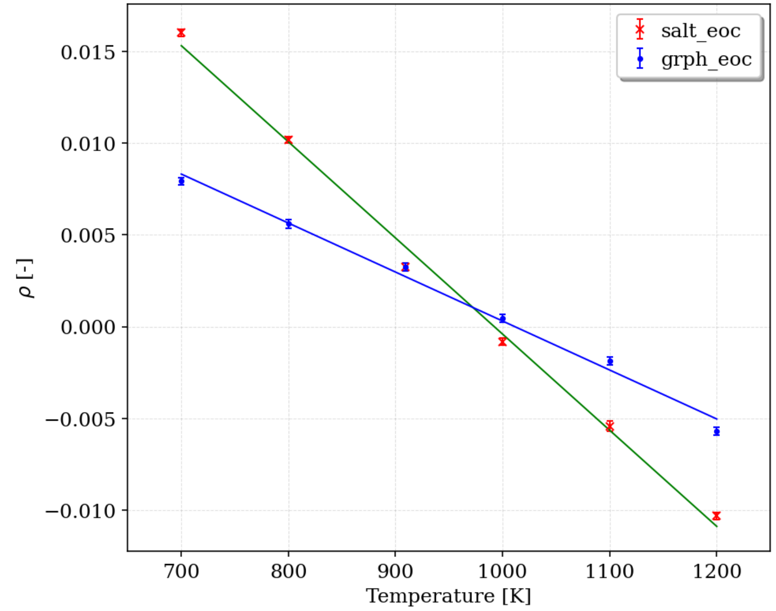
- Flux, power profiles, and reactivity coefficients
  - Power profiles and reactivity coefficients provided to MELCOR



Flux distribution



Axial power distribution



Reactivity as a function of temperature

Reactivity coefficients

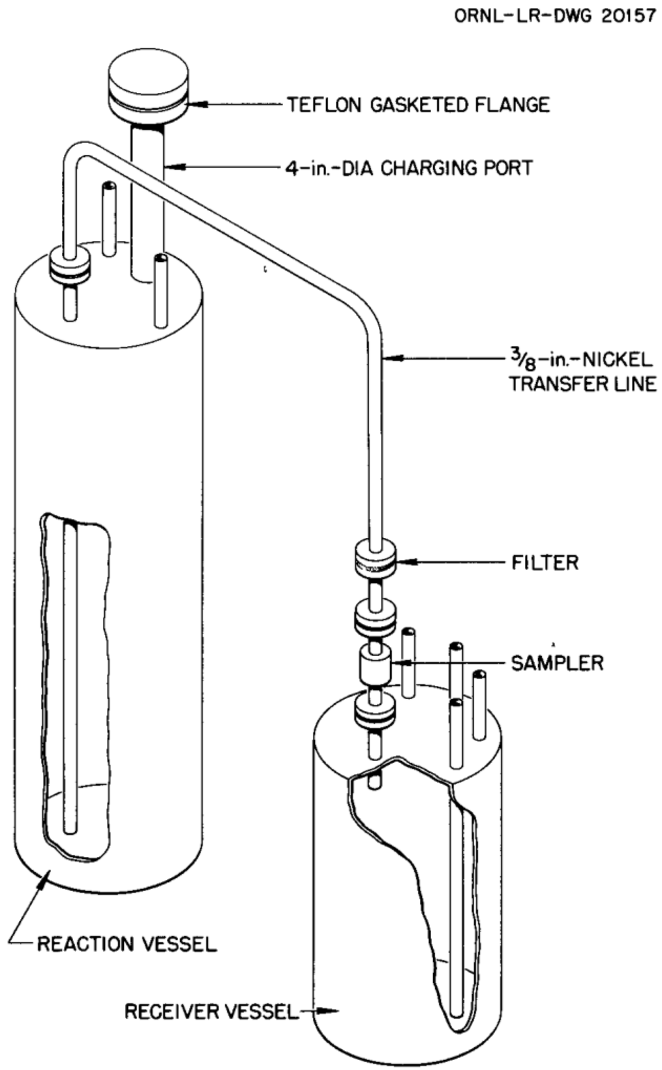
Component	Fresh [pcm/K]	EOC [pcm/K]
Fuel salt	-6.66 ± 0.20	-5.24 ± 0.18
Graphite	-2.42 ± 0.04	-2.67 ± 0.13

Scenario 1

Criticality event during fuel salt preparation

PREPARATION OF ENRICHED FUEL SALT

- Techniques for preparing the enriched fresh fuel salt based on the experience in MSRE [1]
- Batches of melted raw material (carrier salt Flibe and fissile salt UF_4) were mixed in a treatment vessel and transferred to a storage vessel
  - The salt treatment vessel was a 36 in. length of 6 in. IPS sched. 40 SS 304L pipe with an inner liner of 1/8 in. nickel
  - The salt storage vessel was a 36 in. length of 4 in. IPS sched. 40 grade A nickel pipe

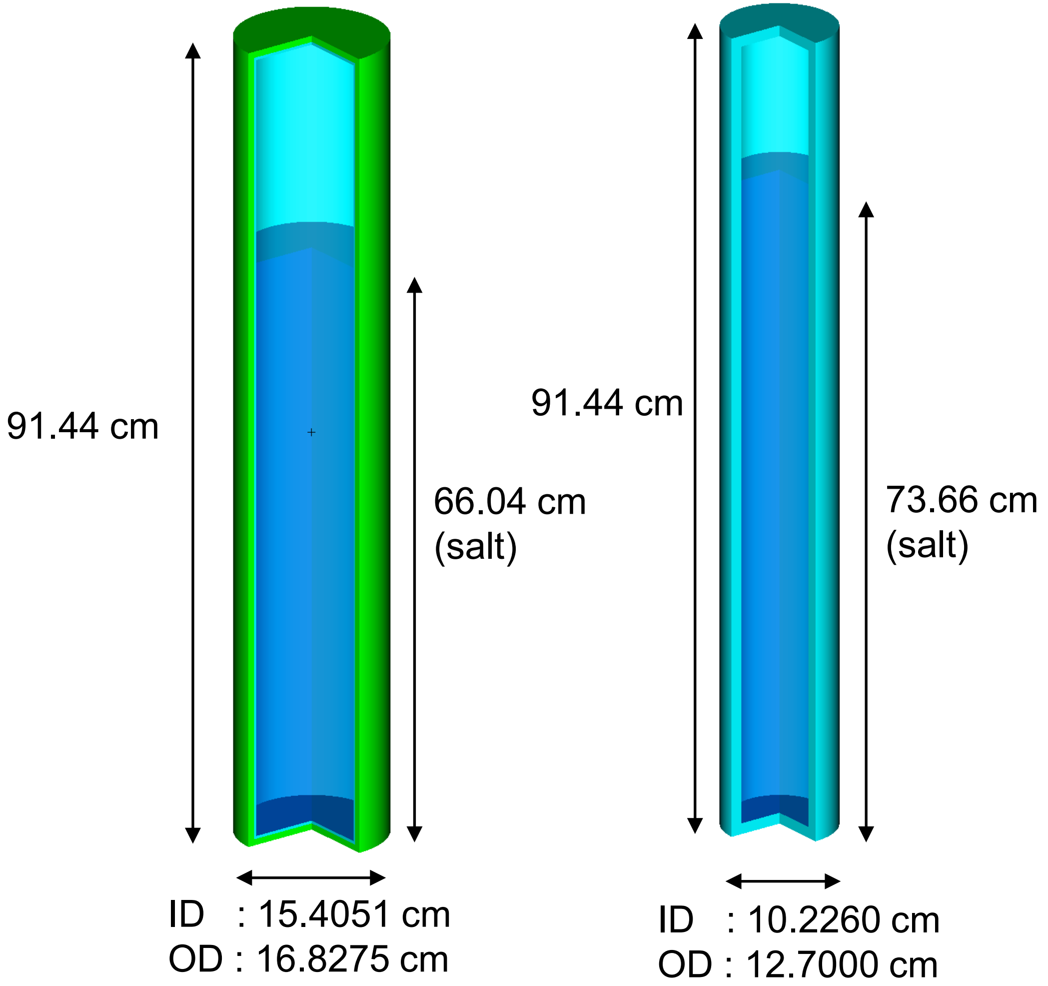


Salt reaction/treatment and storage/receiver vessels

Ref.:
[1] Shaffer, J. H., "Preparation and Handling of Salt Mixtures for the Molten Salt Reactor Experiment," ORNL-4616, Oak Ridge National Laboratory, 1971

PREPARATION OF ENRICHED FUEL SALT

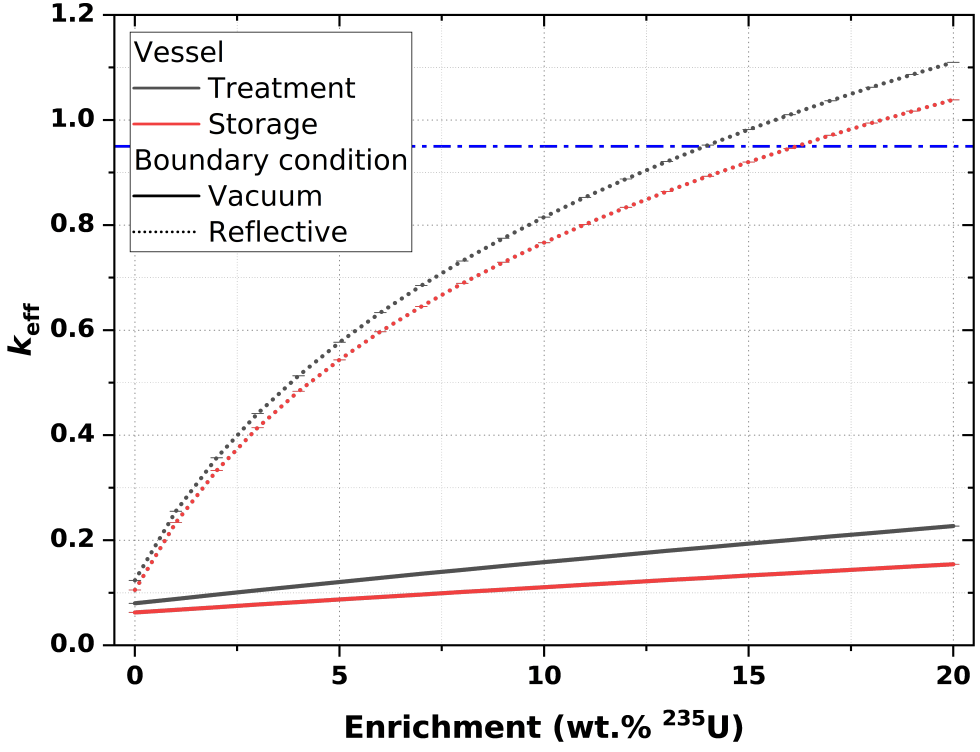
- Criticality calculations were performed using CSAS6-Shift for an infinite lattice of vessels in a tight hexagonal array configuration (touching vessels)
  - Most unfavorable conditions with respect to criticality
- Model perturbations were performed with SCALE/SAMPLER for the following parameters:
  - U-235 enrichment and UF_4 molar fraction
  - Temperature
  - Vessel radius
  - Single vessel (vacuum boundary conditions) vs. infinite array of vessels (reflective boundary conditions)



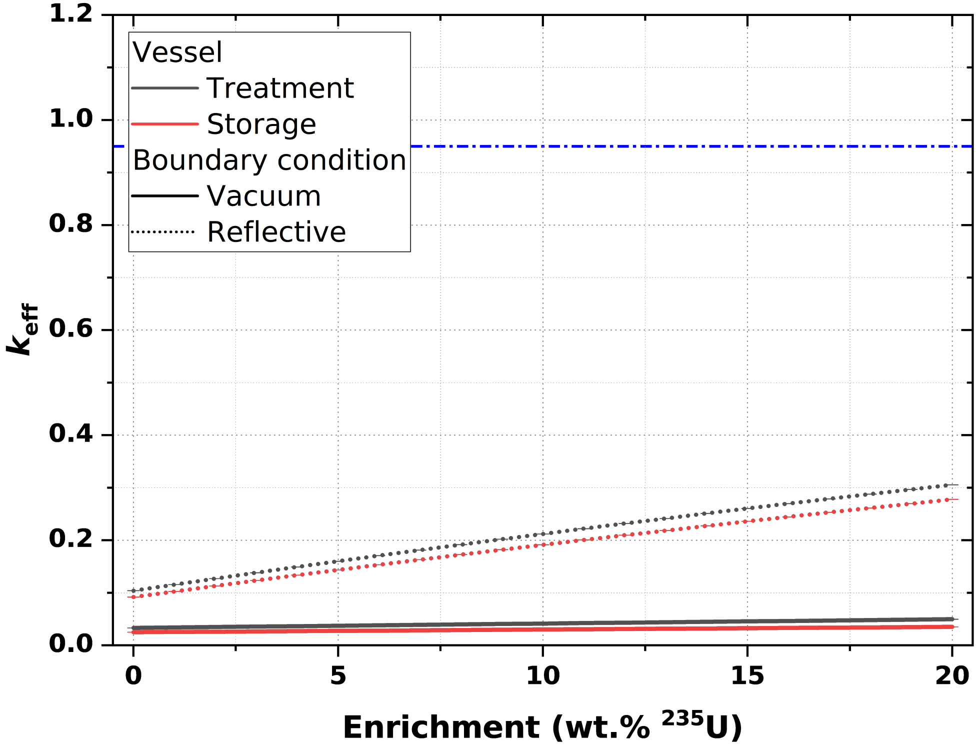
SCALE/CSAS-Shift model for treatment (left) and storage (right) vessels

CRITICALITY ANALYSIS

- Impact of UF_4 enrichment
  - In an infinite array configuration, the vessel containing a pure UF_4 solution can reach k > 0.95 with enrichment > 14 wt.%
  - A looser array configuration would lead to lower k_{eff} values



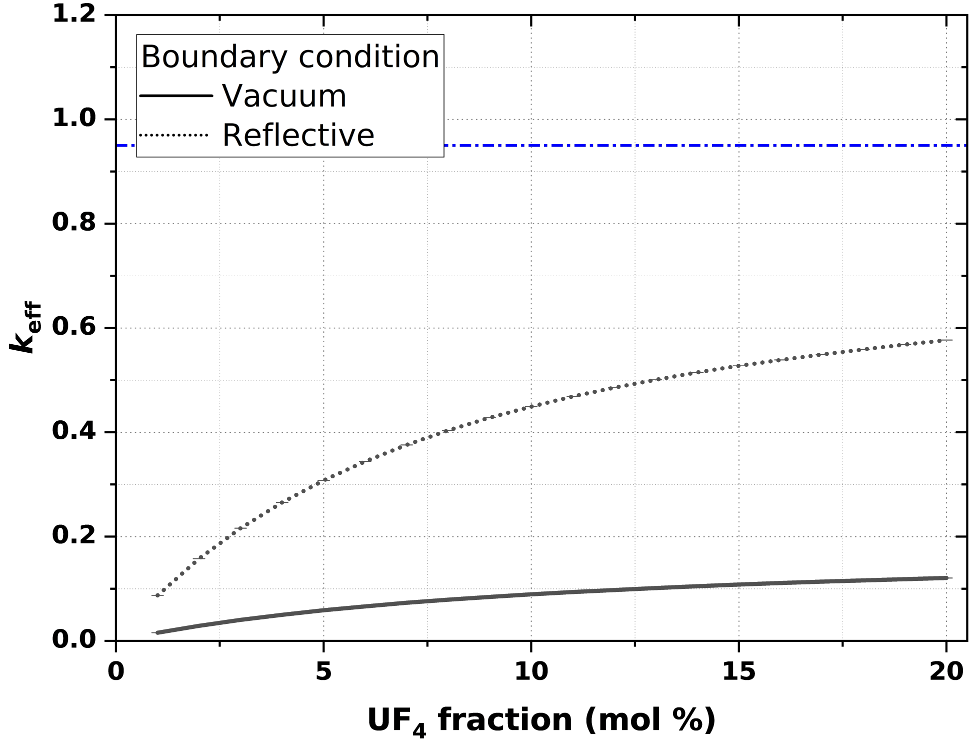
UF_4 only



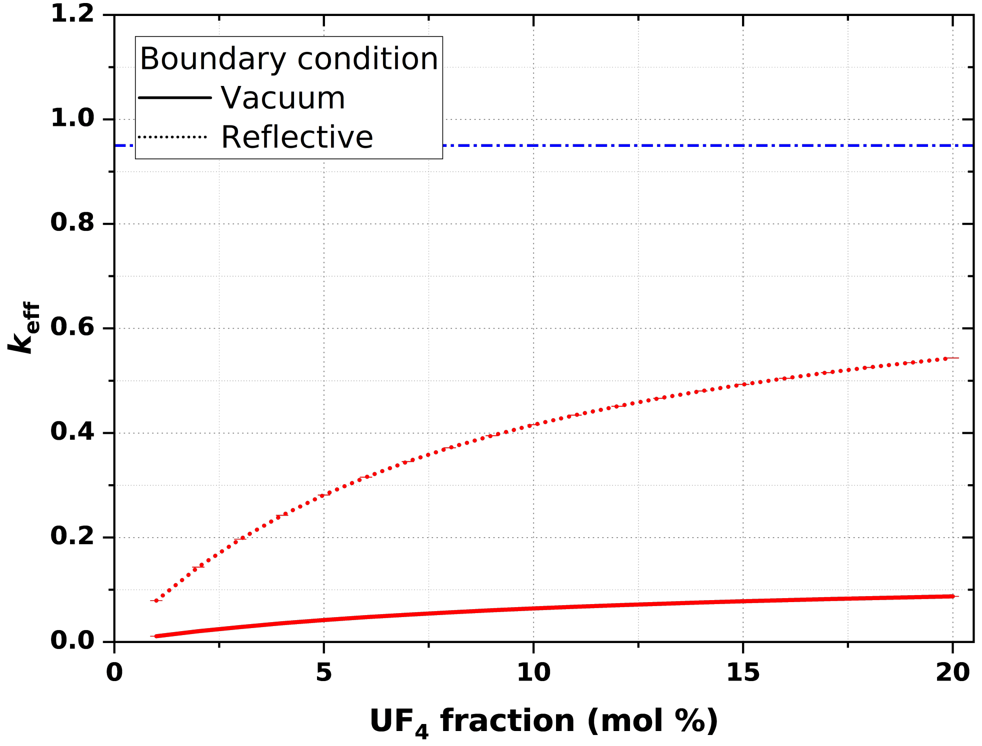
Mixture of FLiBe and UF_4

CRITICALITY ANALYSIS

- Impact of UF_4 molar fraction
  - All cases have k << 0.95



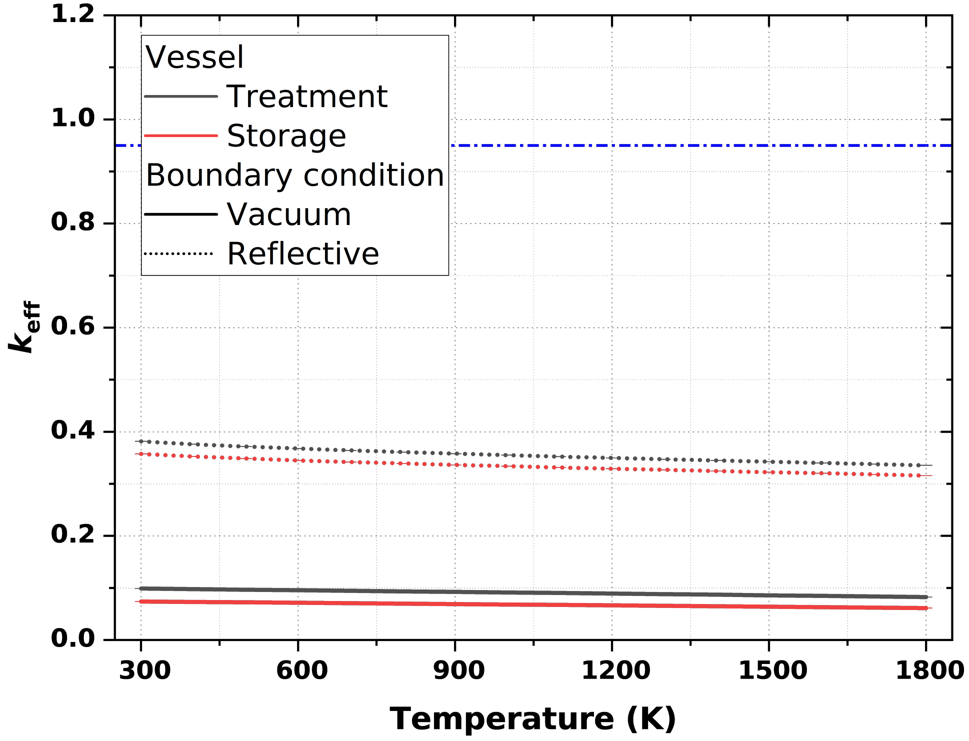
Treatment vessel



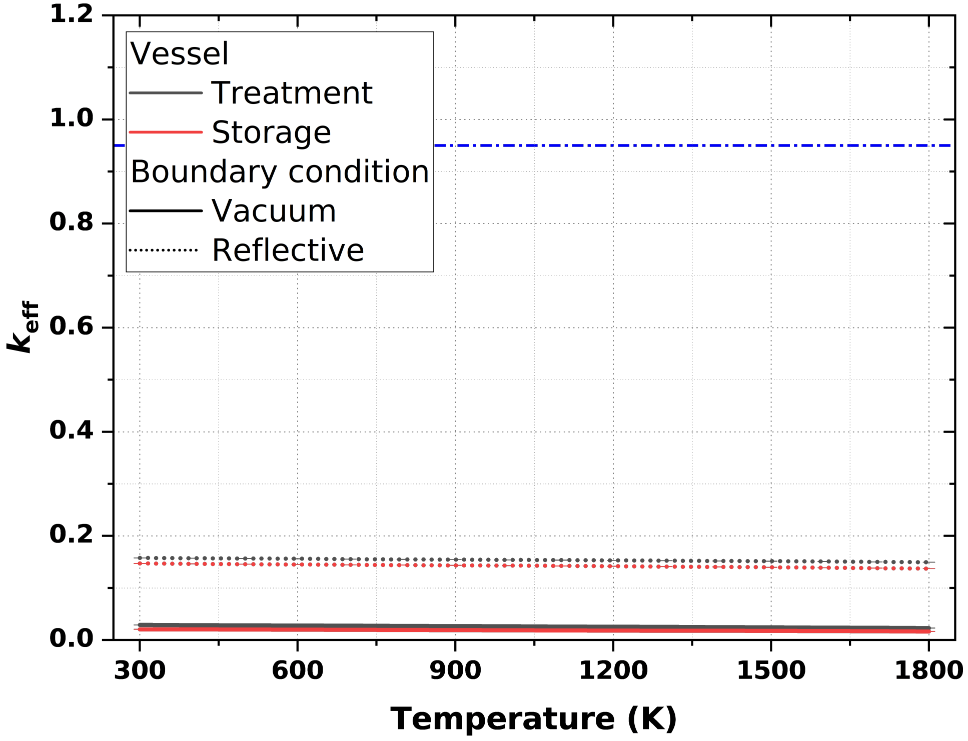
Storage vessel

CRITICALITY ANALYSIS

- Impact of solution temperature
  - The density of the solution was decreased in the calculation as the temperature increases
  - An increase of temperature slightly decreases the criticality; however, all cases have k << 0.95



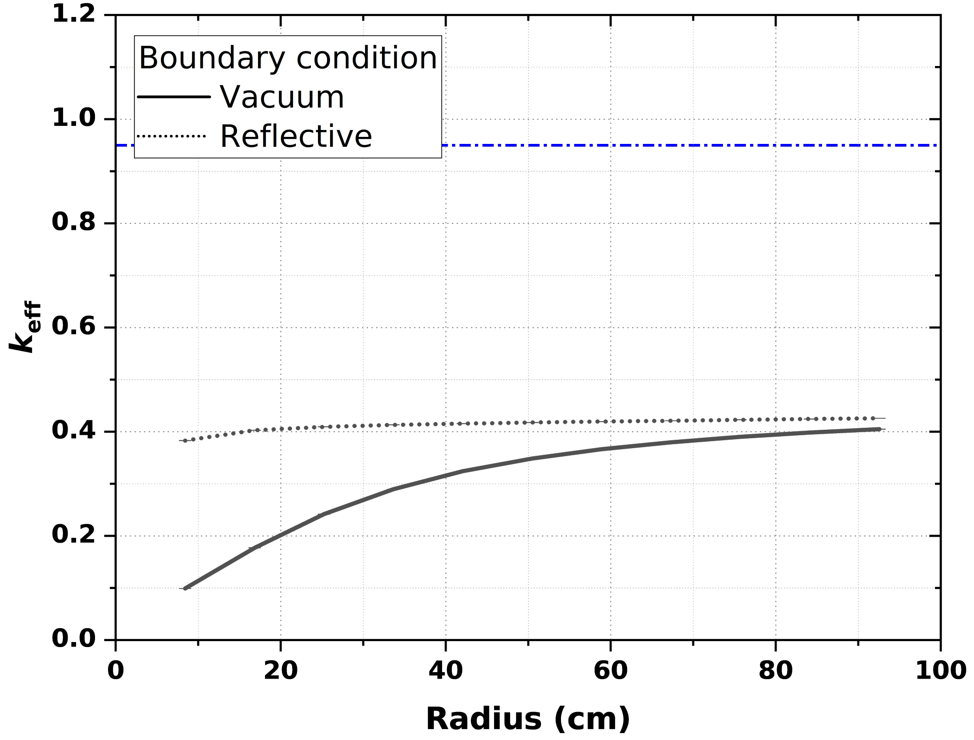
UF_4 only



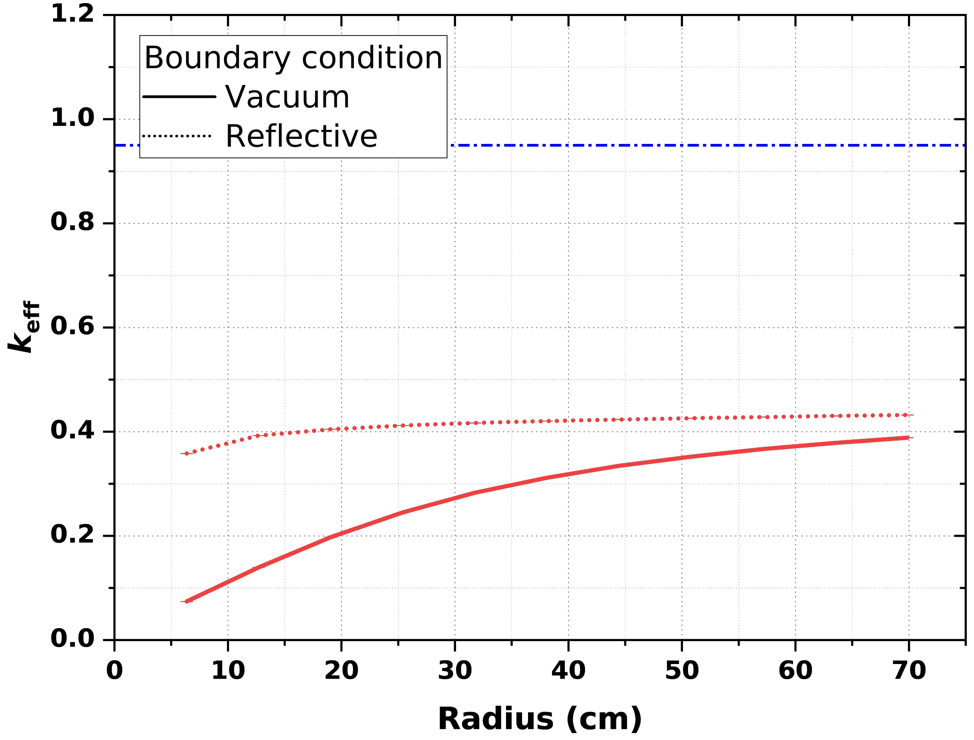
Mixture of FLiBe and UF_4

CRITICALITY ANALYSIS

- Impact of vessel radius
  - Vessel contains UF_4 at its nominal enrichment
  - All cases have k << 0.95



Treatment vessel



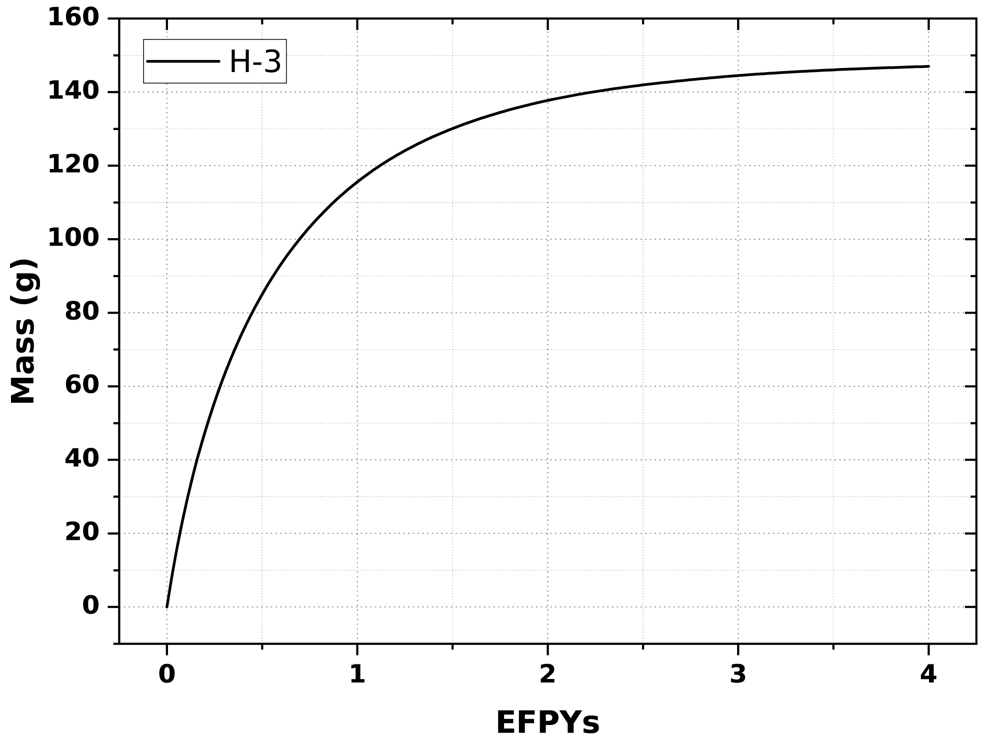
Storage vessel

Scenario 2

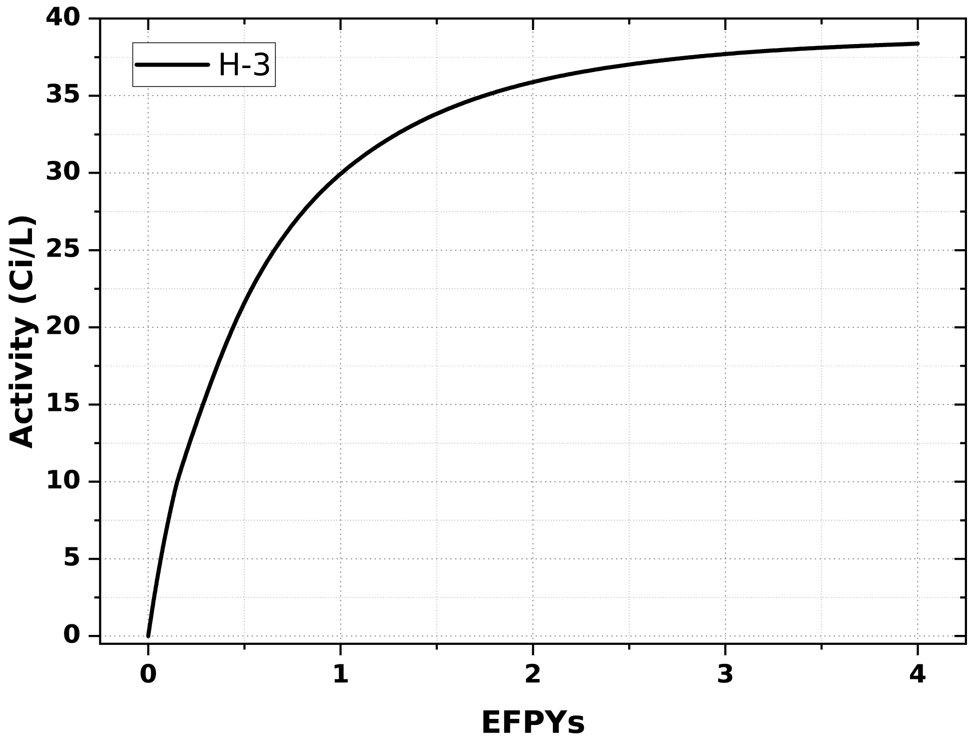
Release of fission products during operation

TRITIUM BUILDUP IN PRIMARY SYSTEM

- In the SCALE/TRITON simulation, no removal path was defined for H-3 produced in the primary fuel salt
- After 4 years, 146.98 g of H-3 with an activity of 38 Ci/L was produced



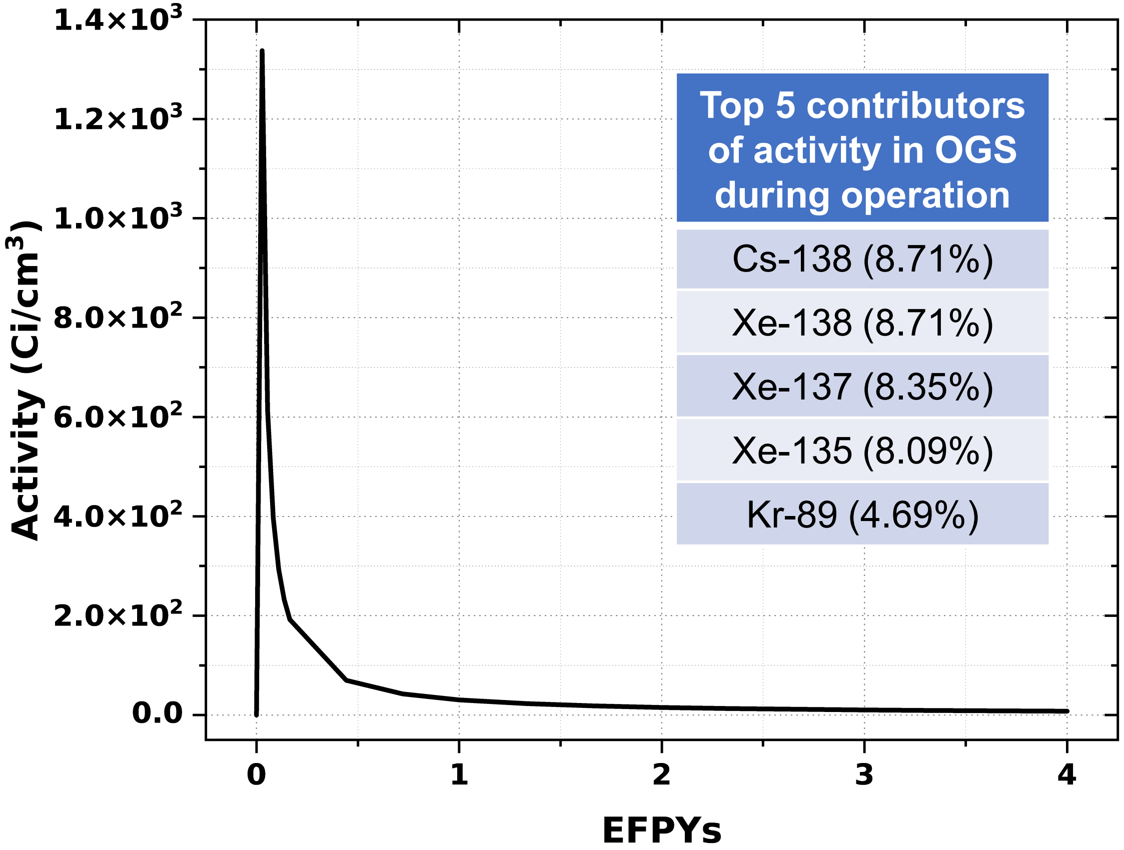
Mass buildup of H-3 in fuel salt



Activity of H-3 in fuel salt

NUCLIDE BUILDUP IN OFF-GAS SYSTEM

- The volumetric activity of the gaseous fission products collected in the off-gas system (OGS) at EOC is ~8 Ci/cm^3
- Using the ideal gas law, the total volume of the gas at EOC is ~147 m^3
  - Assuming room temperature and standard pressure
- In the MSBR conceptual design, the off-gases will be held in the drain tank for about 2 hours, before they go to the short holdup charcoal beds (47 hrs) and the long delay charcoal bed (90 days)
  - Although SCALE/TRITON-Shift can consider all these removal paths, the current calculation did not simulate all removal paths, but only the removal of noble gases from the salt to one mixture representing the OGS



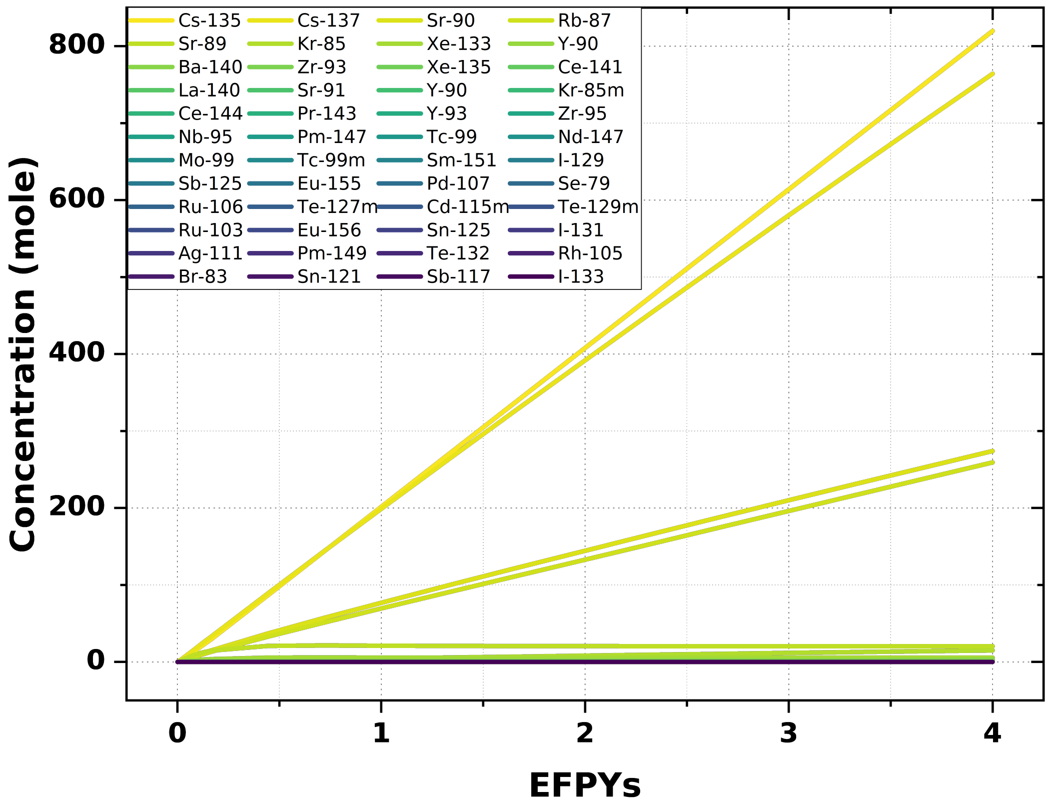
Top 5 contributors of activity in OGS during operation
Cs-138 (8.71%)
Xe-138 (8.71%)
Xe-137 (8.35%)
Xe-135 (8.09%)
Kr-89 (4.69%)

Volumetric activity of all nuclides in the OGS

NUCLIDE BUILDUP IN OFF-GAS SYSTEM

- Concentrations of selected nuclides (48 nuclides [1,2]) in the OGS.
  - They are the fission products ranked in terms of radiotoxicity
  - 26 out of 48 selected nuclides were found in OGS
  - These nuclides contribute to ~22% of the activity in the OGS

Nuclide	Half Life (days)	Dose Factor (mrem/mCi) [1,2]	Concentration after 4 years (mole)
Cs-135	8.39E+08	706.7	819.69
Cs-137	1.10E+04	50.0	764.06
Sr-90	1.05E+04	142.5	274.01
Rb-87	1.76E+13	4.9	259.16
Sr-89	5.05E+01	9.3	20.47
Kr-85	3.93E+03	-	15.04

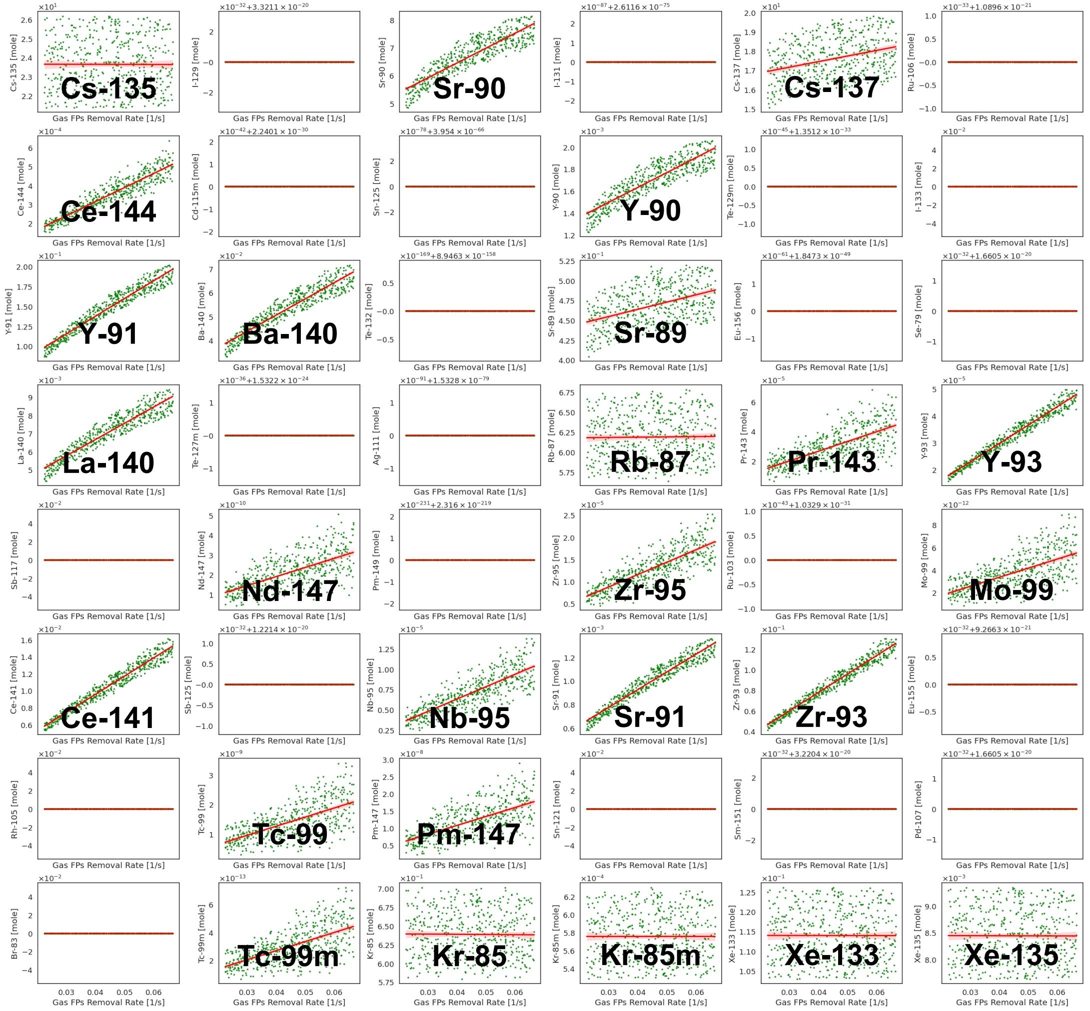


Buildup of selected nuclides in OGS

Refs.:
[1] Thomas, S., and Jerden, J., "Mechanistic Source Term Development for Liquid Fueled MSRs – Model Development Update," ANL/CFCT-20/16, Argonne National Laboratory, 2020.
[2] Eckerman, K., Wolbarst, A., Richardson A., "Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion," EPA-520/1-88-020, 1988.

NUCLIDE BUILDUP IN OFF-GAS SYSTEM

- SCALE/SAMPLER was used to perform uncertainty quantification of the selected nuclides
  - 500 TRITON depletion calculations
  - Axial core slice model
  - Multigroup (MG) mode (56 groups) instead of continuous-energy (CE) mode
    - MG calculation with appropriate self-shielded cross section; small differences were observed to the CE reference results
  - Perturbed parameters: fuel temperature, moderator temperature, fission product removal rate, operating power



The buildup of selected nuclides in the OGS (y-axis) due to perturbation of the removal rate (x-axis)

NUCLIDE BUILDUP IN OFF-GAS SYSTEM

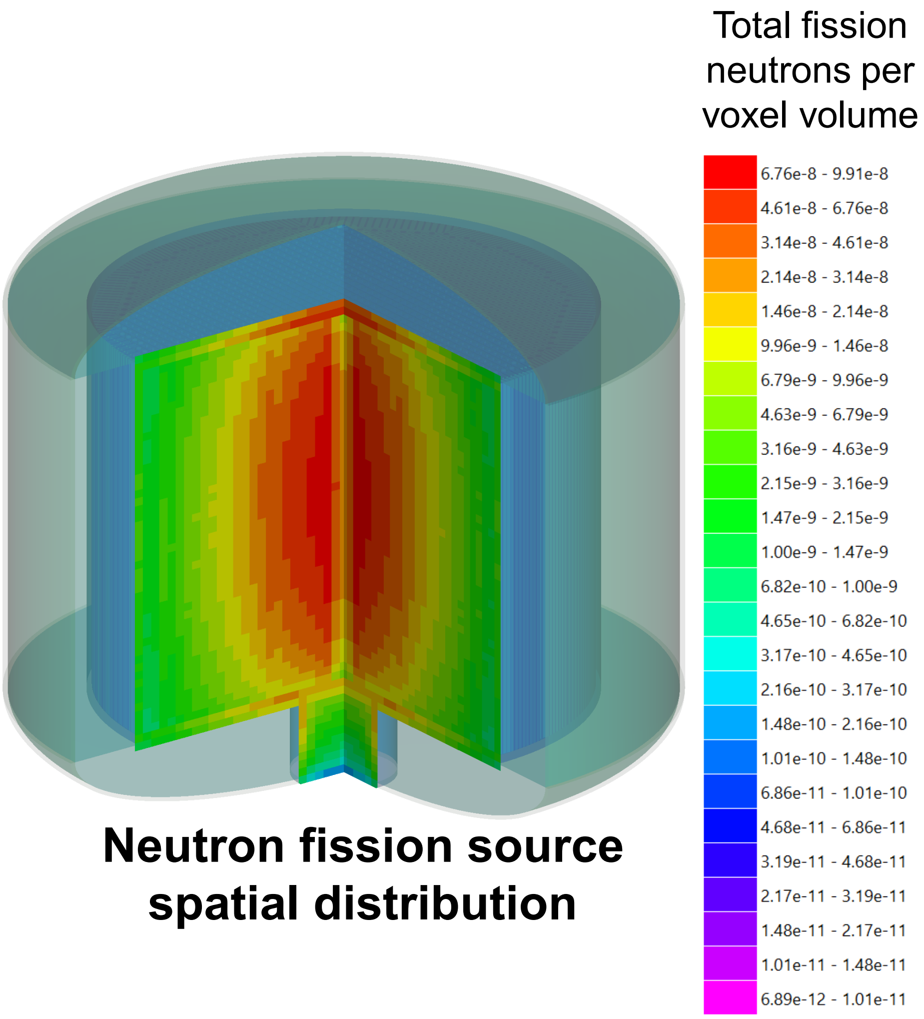
- The gaseous fission products removal rate, and the operating power are the major parameters affecting the buildup of the selected nuclides in the OGS
- Nuclides that have strong correlation with operating power are direct fission products
- Nuclides that have strong correlations with the gaseous fission product removal rate are the decay products of the removed Xe and Kr

	C Temp.	Fuel Salt Temp.	Gas FPs Removal Rate	Noble Metal FPs Removal Rate	Operating Power
Zr-95	-0.097	0.051	0.819	-0.033	0.141
Zr-93	-0.103	0.046	0.982	-0.020	0.152
Y-93	-0.101	0.045	0.983	-0.020	0.150
Y-91	-0.109	0.041	0.968	-0.021	0.220
Y-90	-0.136	0.027	0.894	-0.025	0.400
Xe-135	-0.074	-0.018	-0.004	-0.029	1.000
Xe-133	-0.084	-0.023	-0.002	-0.031	0.999
Tc-99m	0.009	0.100	0.624	-0.065	0.106
Tc-99	0.008	0.099	0.627	-0.065	0.106
Sr-91	-0.109	0.041	0.968	-0.021	0.220
Sr-90	-0.136	0.027	0.894	-0.025	0.400
Sr-89	-0.158	-0.050	0.467	-0.031	0.863
Rb-87	-0.140	-0.076	0.015	-0.034	0.993
Pr-143	-0.071	0.075	0.692	-0.003	0.170
Pm-147	-0.070	0.026	0.636	-0.056	0.140
Nd-147	-0.072	0.027	0.644	-0.056	0.142
Nb-95	-0.097	0.051	0.819	-0.033	0.141
Mo-99	0.009	0.100	0.624	-0.065	0.106
La-140	-0.108	0.045	0.941	-0.023	0.301
Kr-85m	-0.123	-0.073	0.000	-0.027	0.995
Kr-85	-0.126	-0.059	-0.010	-0.031	0.982
Cs-137	-0.103	-0.001	0.339	-0.035	0.930
Cs-135	-0.073	-0.018	-0.003	-0.029	1.000
Ce-144	-0.133	0.063	0.931	-0.020	0.196
Ce-141	-0.097	0.051	0.977	-0.022	0.193
Ba-140	-0.108	0.045	0.941	-0.023	0.301

Pearson Correlation Matrix

OPERATIONAL DOSE RATE

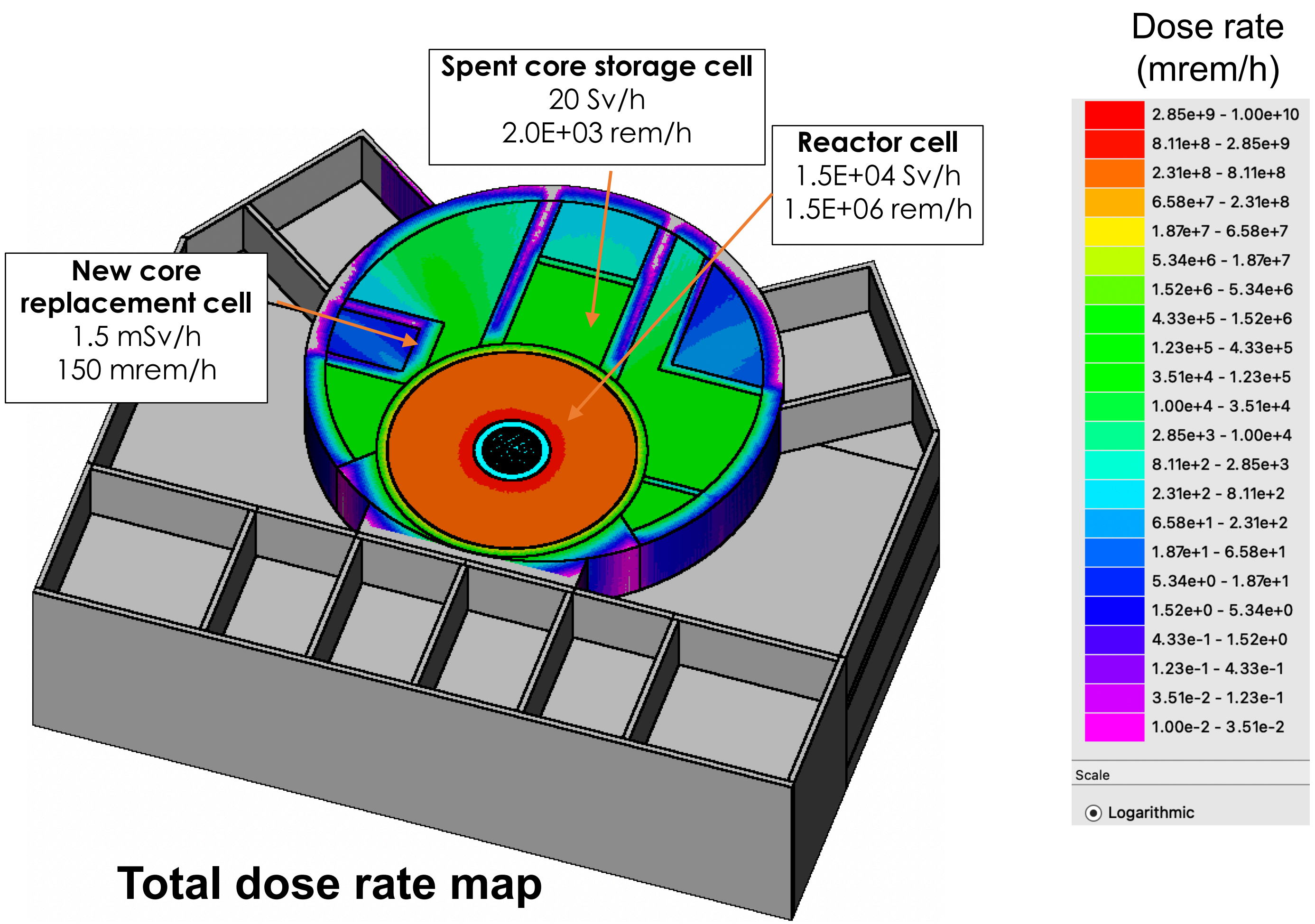
- Radiation source terms
  - Space- and energy-dependent prompt neutron fission source from a CSAS-Shift calculation
    - Tally mesh: 51x51x70 voxels
    - 200 neutron energy groups
  - The neutron source strength calculated using average number of neutrons per fission (2.627) as calculated by CSAS, total reactor power of 2250 MW, and an assumption of 200 MeV recoverable energy from fission
  - Prompt gamma source generated by the MAVRIC-Shift shielding code based on prompt fission neutrons
  - Fission product decay and activation sources not included in the demonstration shielding calculation (source component is lower than the prompt neutron and gamma sources)



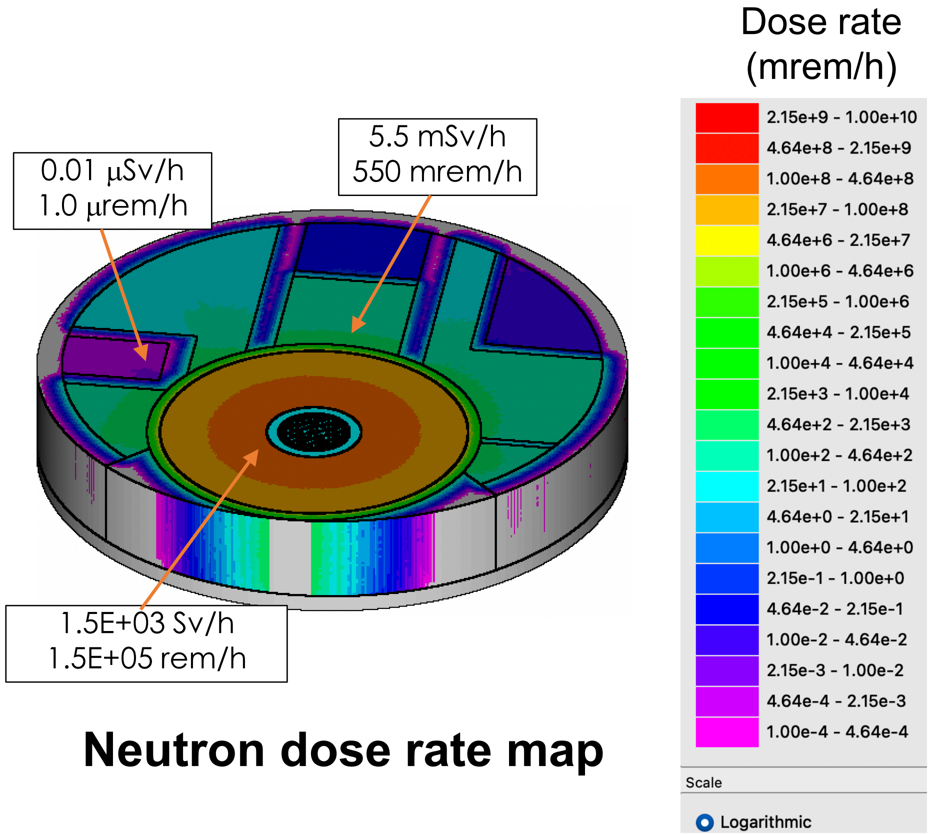
Neutron fission source spatial distribution

OPERATIONAL DOSE RATE

- Dose rates in the reactor cell and reactor complex cell were dominated by gamma radiation
- Adequate building area designation based on radiation levels



Total dose rate map



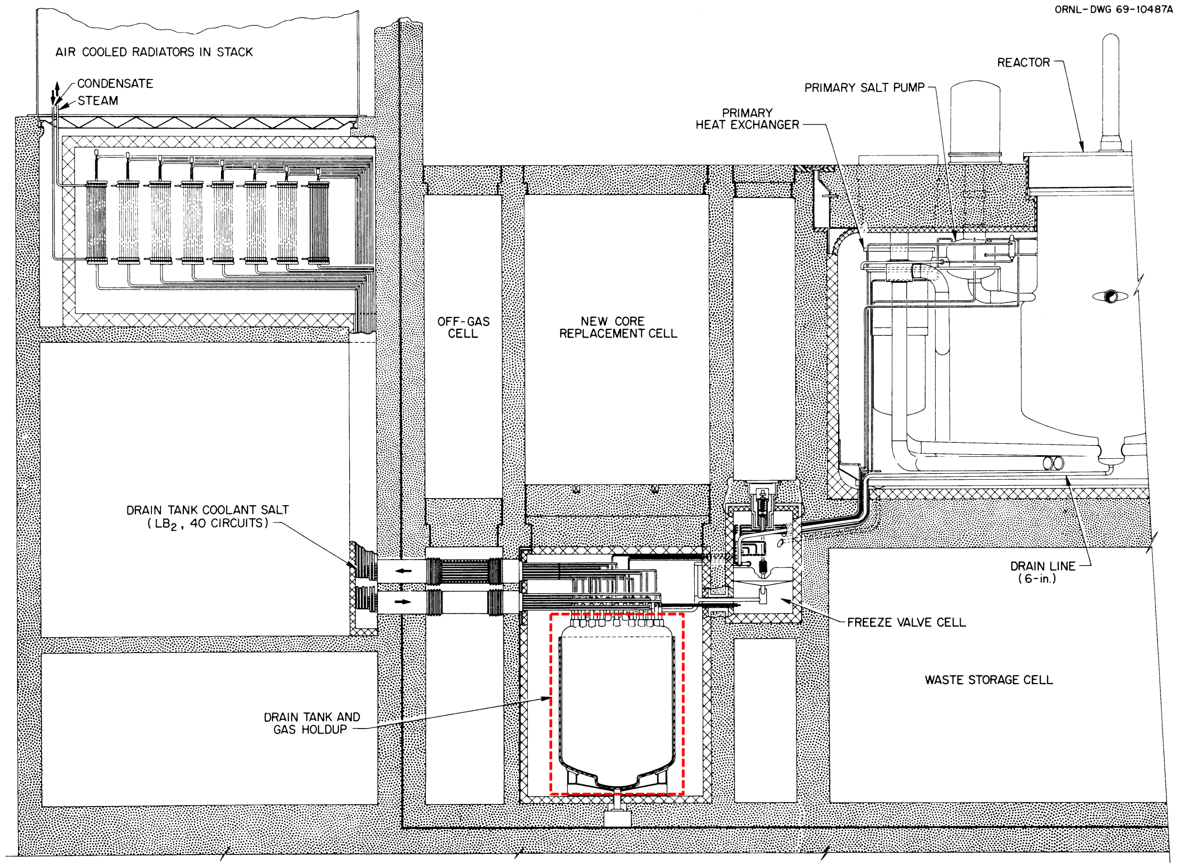
Neutron dose rate map

Scenario 3

Heat removal of drain tank

FUEL SALT DRAIN TANK

- Main function of the drain tank is to safely contain and cool fuel salt under any accidental or intentional situation
- During normal operation, serves as a 2-hr holdup volume for the gaseous fission products
- Assumption for this scenario: complete system fuel salt drained into the tank
- Dimensions and material:
  - Outer diameter: 14 ft (~430 cm)
  - Overall height: 22 ft (~670 cm)
  - Wall thickness: 1 in.
  - Liner thickness: 1 in.
  - Material: Hastelloy N
  - Can store up to 2 times the system fuel salt volume

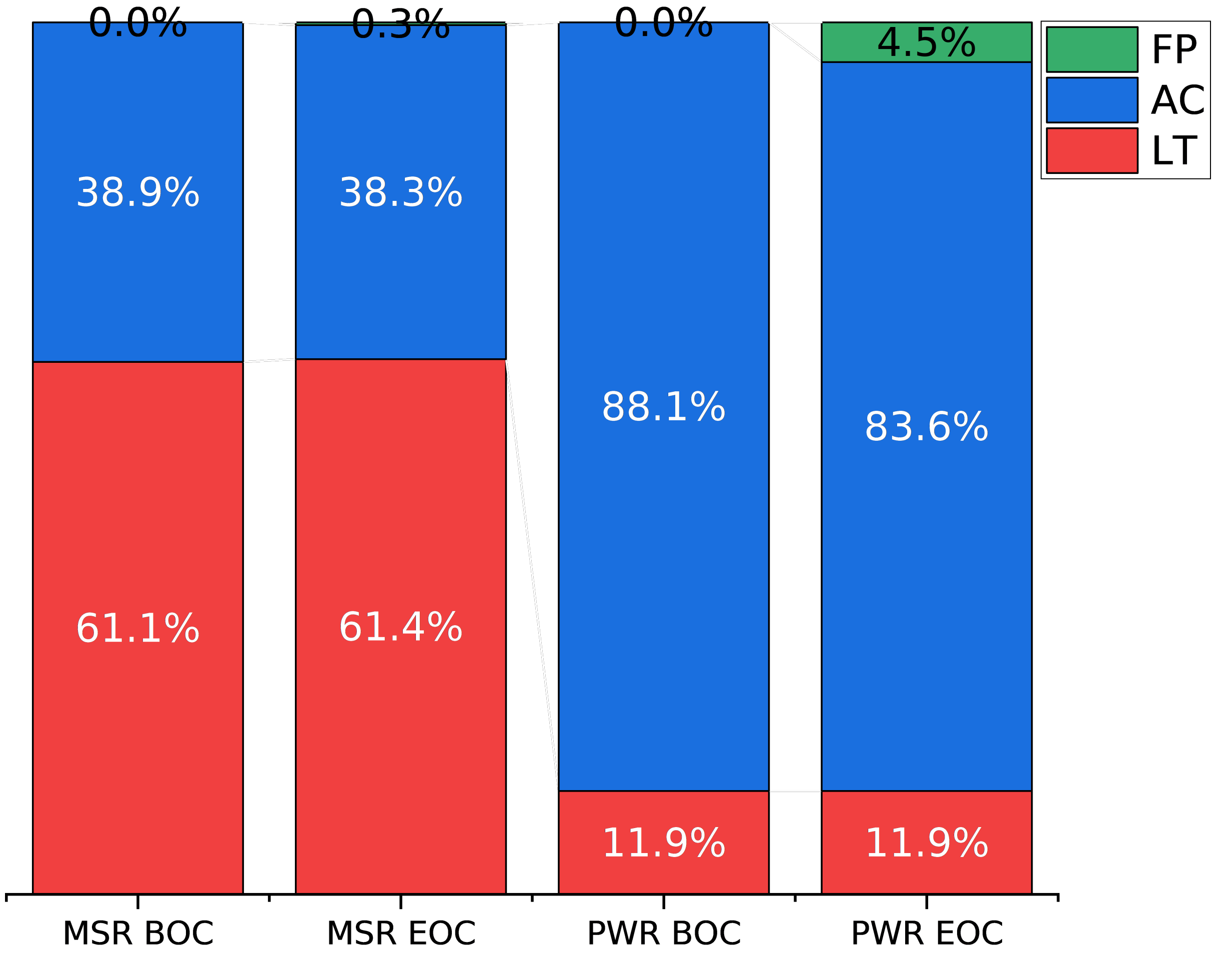


Location of Fuel Salt Drain Tank

Ref.: Robertson, R. C., et al., "Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor," ORNL-4541, Oak Ridge National Laboratory, 1971

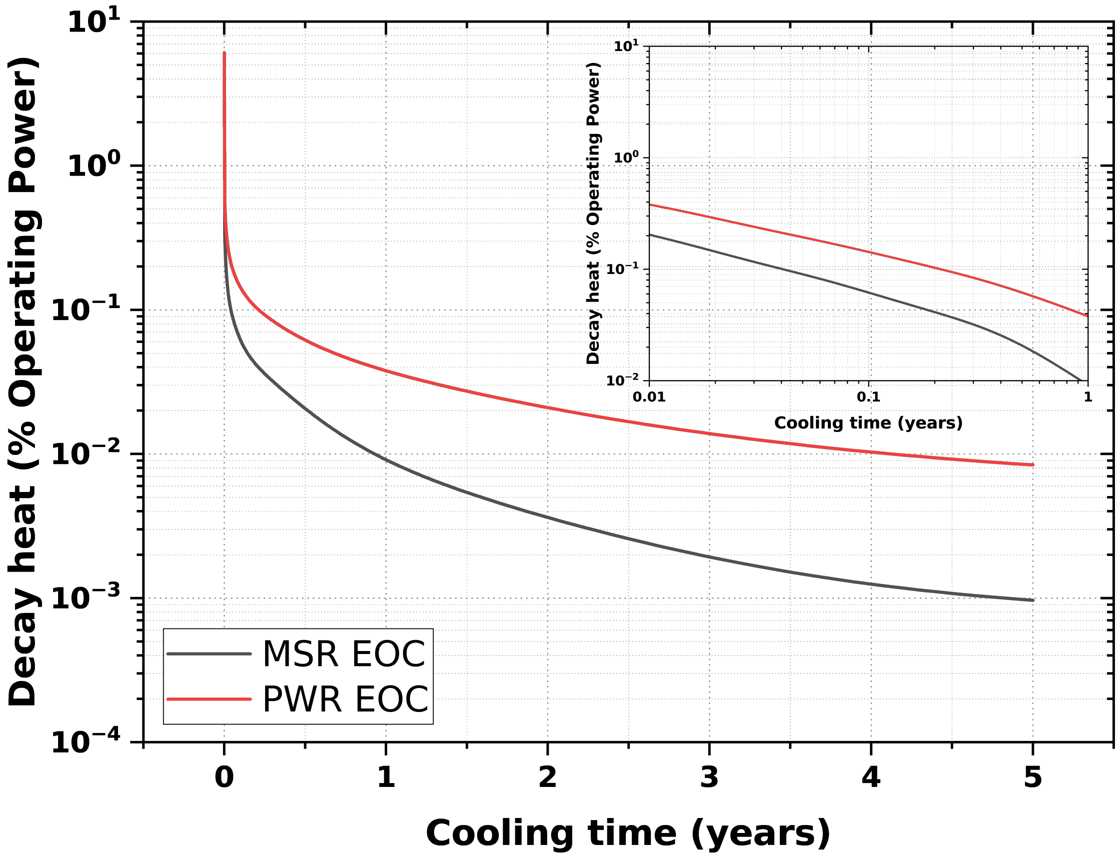
COMPOSITION DISTRIBUTION IN SPENT FUEL

- MSR fuel salt contained more than 60% light elements (LT), and they can be activated during operation.
  - ~1% contribution to the activity at EOC
  - In PWR spent fuel, LT contributions to the activity at EOC are negligible (2.54E-04%)
- Although the MSR spent fuel salt had only ~0.3% of fission products (FPs), the FPs contributed to ~64% of the activity
  - Low number of FPs due to fission product removal (OGS) and plating out
  - In comparison, PWR spent fuel contains about ~4.5% FPs which contribute ~79% of the activity



DECAY HEAT OF DRAIN TANK

- Decay heat at shutdown is ~4% operating power in MSR vs. ~6% operating power in a PWR



Decay heat of MSR and PWR* at EOC

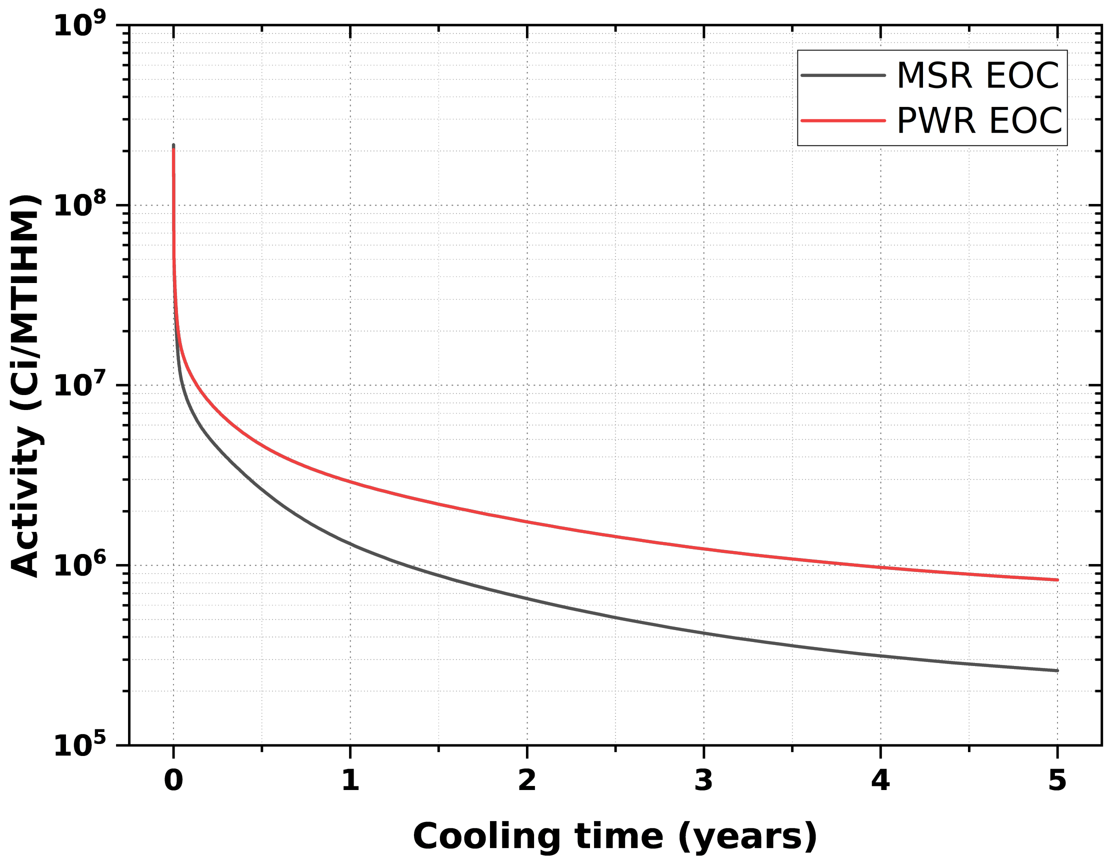
*Burnup of 50 GWd/MTU

Top 5 contributors at shutdown for MSR	Top 5 contributors at shutdown for PWR*
U-239 (4.67%)	U-239 (2.73%)
Np-239 (4.06%)	Np-239 (2.39%)
La-144 (2.21%)	I-134 (1.89%)
Nb-100 (2.01%)	Cs-138 (1.76%)
Rb-92 (1.96%)	Tc-104 (1.64%)

Top 5 contributors after 5 years for MSR	Top 5 contributors after 5 years for PWR*
Y-90 (23.70%)	Cs-134 (18.78%)
Pr-144 (17.48%)	Y-90 (18.54%)
Cm-244 (15.61%)	Ba-137m (18.38%)
Pu-238 (9.12%)	Cm-244 (8.37%)
Am-241 (7.35%)	Rh-106 (7.80%)

ACTIVITY OF DRAIN TANK

- Activity from the drain tank containing the whole volume of fuel salt at EOC
- Comparison between MSR and PWR activity:



Activity of MSR and PWR* at EOC

*Burnup of 50 GWd/MTU

Top 5 contributors at shutdown for MSR	Top 5 contributors at shutdown for PWR*
U-239 (17.51%)	U-239 (10.08%)
Np-239 (17.29%)	Np-239 (10.04%)
Zr-97 (1.10%)	I-134 (1.01%)
Zr-98 (1.08%)	I-133 (0.91%)
Y-95 (1.08%)	I-135 (0.87%)

Top 5 contributors after 5 years for MSR	Top 5 contributors after 5 years for PWR*
Pu-241 (42.11%)	Pu-241 (17.5%)
Pm-147 (14.37%)	Cs-137 (16.86%)
H-3 (9.31%)	Ba-137m (15.97%)
Y-90 (8.14%)	Y-90 (11.41%)
Sr-90 (8.13%)	Sr-90 (11.41%)

RADIATION SOURCES OF DRAIN TANK

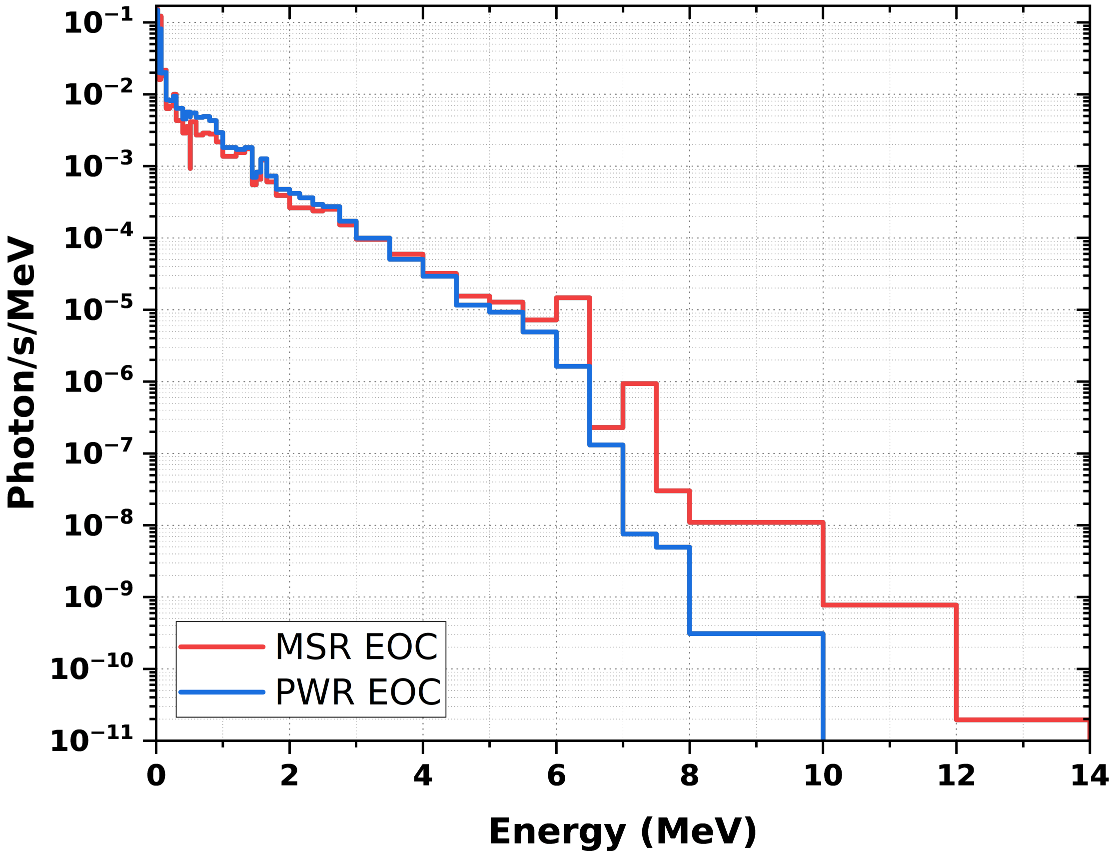
- Gamma sources at EOC:
  - Fission product, actinide, and activation product decay
    - Numerous very short-lived radionuclides ($T_{1/2}$ << 1h) with gamma emissions in the irradiated fuel
  - Bremsstrahlung radiation associated with beta particles from radionuclide decay
- Comparison between MSR and PWR photon source intensities:

	Photons/s per MTIHM**
MSR	1.3690E+19
PWR*	1.3879E+19

*Burnup of 50 GWd/MTU

** MTIHM: metric ton initial heavy metal

- 3000 MWth PWR has ~89 MTIHM.
- MSR has ~44 MTIHM.



Gamma spectra for MSR and PWR at EOC

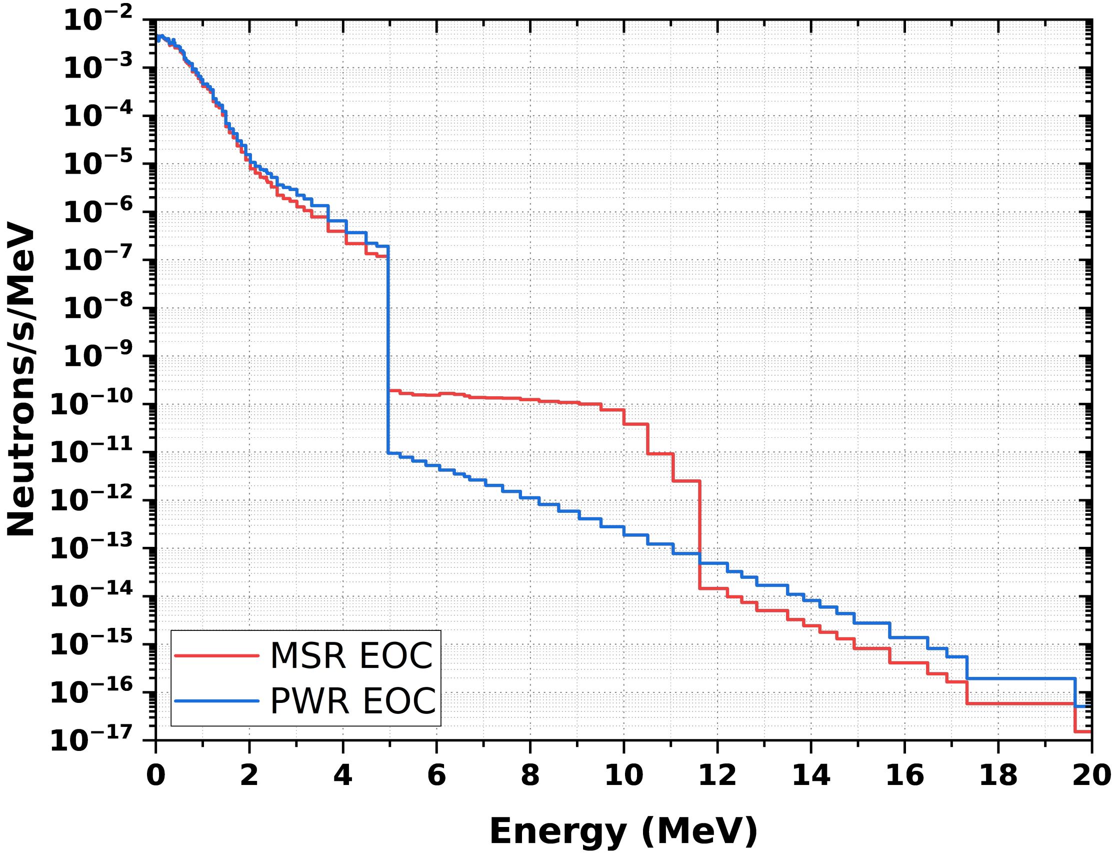
RADIATION SOURCES OF DRAIN TANK

- Neutron source at EOC dominated by delayed neutrons
  - Delayed neutrons
    - Neutrons generated from several milliseconds to several minutes after a fission event
    - Average energy of the delayed neutrons: 200~600 keV
  - Neutrons from (α,n) reactions with light elements in the fuel salt such as Be and Li
  - Neutrons from spontaneous fission
- Comparison between MSR and PWR neutron source intensities (neutrons/s per MTIHM**)

	Delayed neutrons	Neutrons from (α,n) reactions	Neutrons from spontaneous fission
MSR	2.1638E+16	2.9545E+10	5.9075E+08
PWR*	1.4100E+16	1.1928E+08	1.6768E+09

*Burnup of 50 GWd/MTU

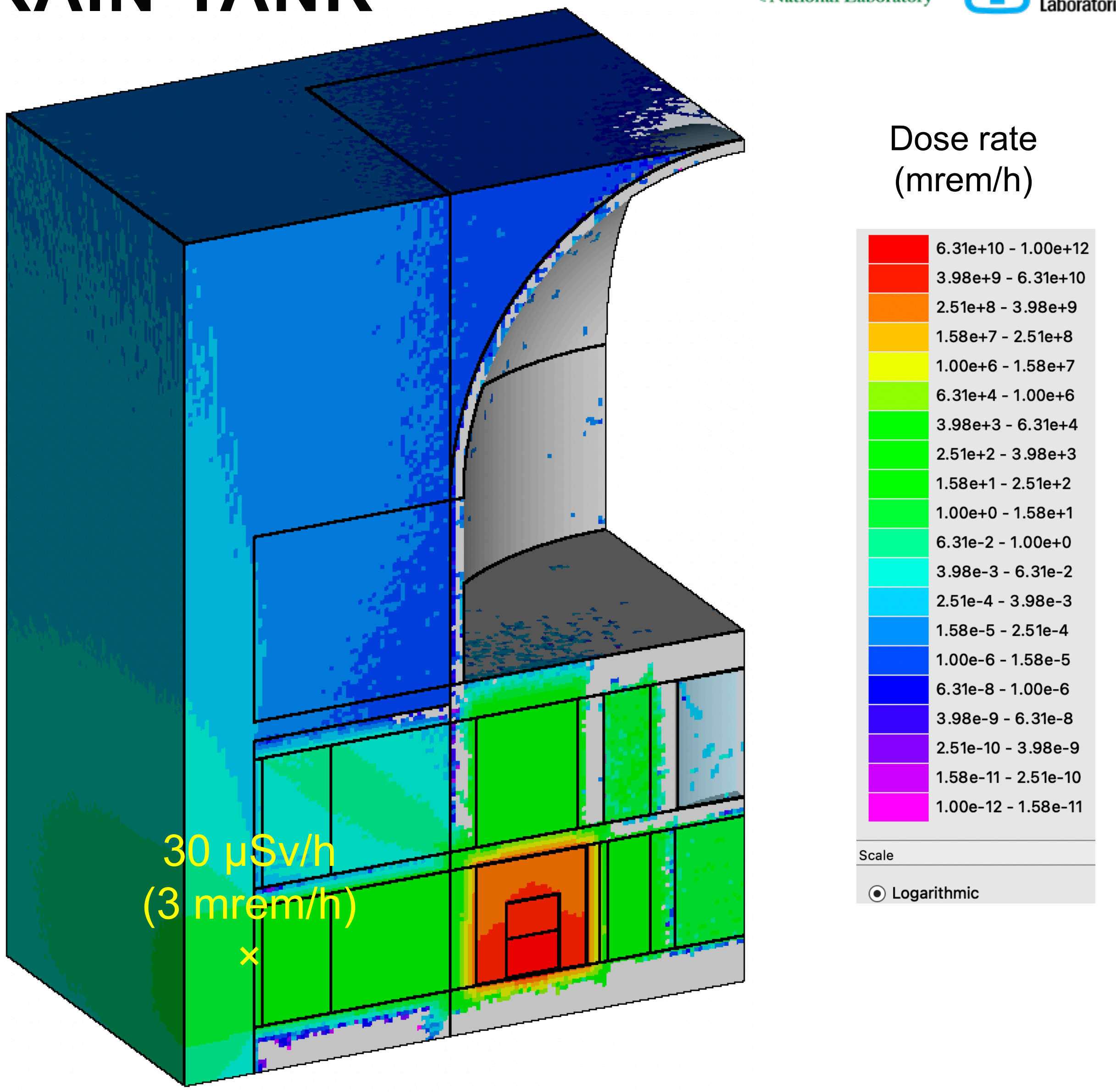
** MTIHM: metric ton initial heavy metal
- 3000 MWth PWR has ~89 MTIHM.
- MSR has ~44 MTIHM.



Neutron spectra for MSR and PWR at EOC

EXTERNAL DOSE RATE OF DRAIN TANK

- Drain tank located in primary salt drain tank cell at waste storage elevation
- Maximum dose rate outside the building
  - Tally mesh voxel size: 30 x 30 x 30 cm^3
  - 30 μSv/h (3 mrem/h) (relative error=1.5%)
  - Very low external dose rate compared to the dose rate at the source, demonstrating adequate MSR building design
  - Negligible external neutron dose rate (~ 5 orders of magnitude lower than the gamma dose rate)



Total dose rate map

Summary

SUMMARY

- SCALE capabilities to simulate different scenarios in the different MSR fuel cycle stages were demonstrated
- The demonstrated capabilities included the calculation of fuel inventory that considered fission product removal and feed addition, decay heat and activity, as well as shielding, radiation dose, and criticality calculations
- Key observations:
  - Criticality analyses of fresh salt preparation show k_{eff} << 0.95 for an infinite array of vessels with pure UF_4 at an enrichment < 14%
  - The selected nuclides in the OGS have a strong correlation to the gaseous fission products removal rate and the operating power
  - The radiation dose rates from operational MSR or the full-core EOL fuel salt drained into the drain tank is dominated by gamma radiation
  - A very low external dose rate compared to the dose rate at the source was observed, demonstrating adequate MSR building design
  - The neutron source per MTIHM from (α,n) reactions in MSRs can be 100 times of that in PWRs because irradiated fuel salt contains light elements (e.g., Be and Li) with high neutron yields

FUTURE DEVELOPMENT

- Recent development efforts in SCALE enable:
  - Additional depletion options with TRITON (e.g., depletion by total power (W))
  - Additional flexibility for mass handling with TRITON (normalized material masses vs. accurate model masses)
- Planned future enhancements:
  - Material mass and volume change in TRITON depletion calculations for improved consideration of material feed
  - Addition of simple delayed neutron precursor drift model for a more accurate prediction of the effective delayed neutron fraction
  - Improve burnup calculation for MSRs with material feed

SAND2024-07835PE

Demonstration of MELCOR for MSR Fuel Cycle Analysis

Edward Duchnowski, Bradley Beeny, Matt Christian, and David L. Luxat

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

OBJECTIVE AND APPLICATIONS

Objective: Demonstrate use of MELCOR for simulating accident scenarios in the nuclear fuel cycle for molten salt reactors (MSRs)

Demonstrate new code models, integrated molten fuel chemistry analysis, and new MSBR model

Integration of MELCOR + ORIGEN:

- High fidelity method of nuclide-level radionuclide and decay chain tracking with MELCOR's thermal-hydraulics models

Application of the Molten Salt Thermal Properties Database (MSTDB) with Thermochimica for MSBR fuel salt properties

- Evaluation of radionuclide and chemical hazards

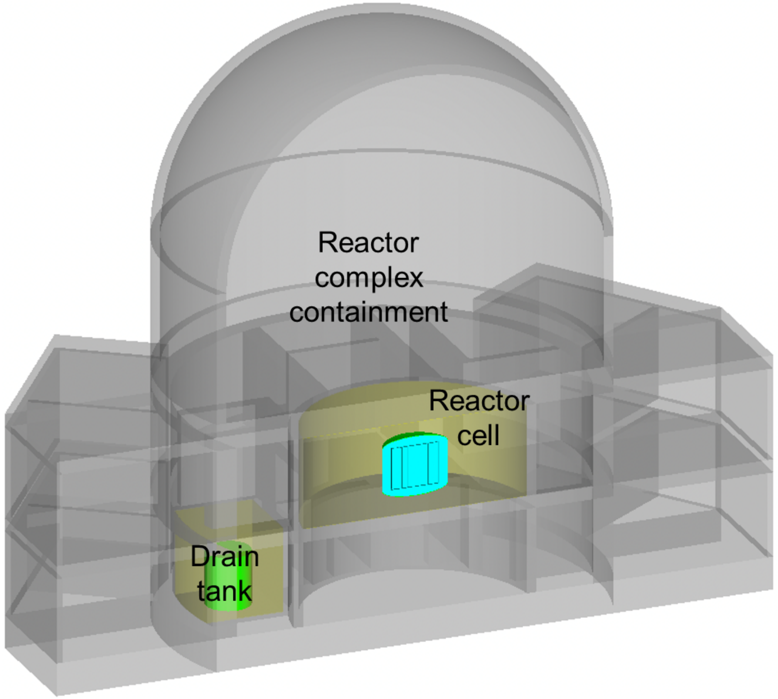
Scenario: Emergency drain from the primary loop into the drain tank

Accident & sensitivities:

- Pump trip with failure to insert shutdown rods
- Emergency fuel salt drain to the reactor cell drain tank with failure of the drain tank heat removal
- Variations in He off gas flow & leakage to the reactor cell

Analysis:

- Thermal-hydraulic response of the reactor system, the drain tank, the off gas system, and the reactor cell,
- Radionuclide vaporization from the molten salt



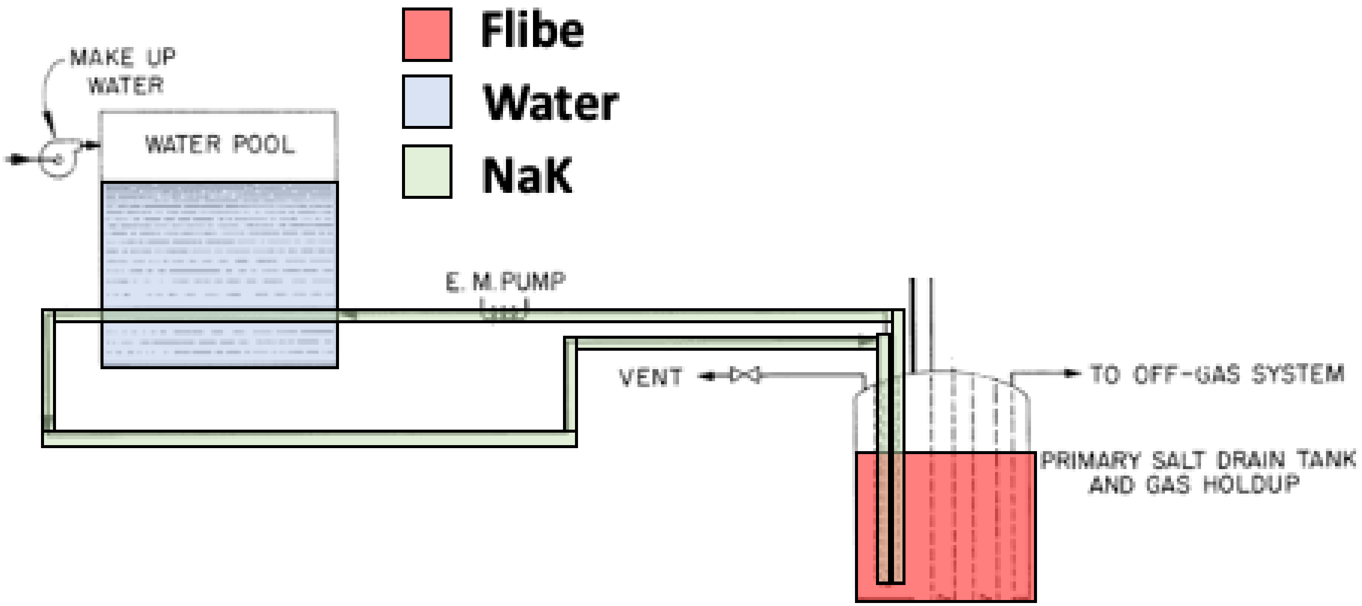
MSR Plant Model

Ref: Robertson, R. C., et al., "Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor," ORNL-4541, Oak Ridge National Laboratory, 1971

Equation-of-State (EOS)

Fluids in MELCOR are modeled with an equation-of-state and the EOS package

- Hydrodynamic, condensable materials occupy control volume pool and/or atmosphere
- Multi-fluid capability (multiple condensable fluids in a calculation) across multiple groups of control volumes with distinct working fluids
- Additional fluids can be readily integrated through flexible database representation



Fluid Name	Database Type	Database Name
Water	Built-in	Water
Water	Auxiliary files	H2O
Hydrogen		H2
Lithium		Li
Potassium		K
Helium		He
Nitrogen		N2
Sodium		Na
Sodium-Potassium		NaK
Lithium-Lead		LiPb
Fluoride-Lithium-Beryllium		Flibe

Capability: Fission Product Release from Fuel Salt

Goal: *Determine magnitude of fission product and chemical hazards released from the molten fuel salt to the environment*

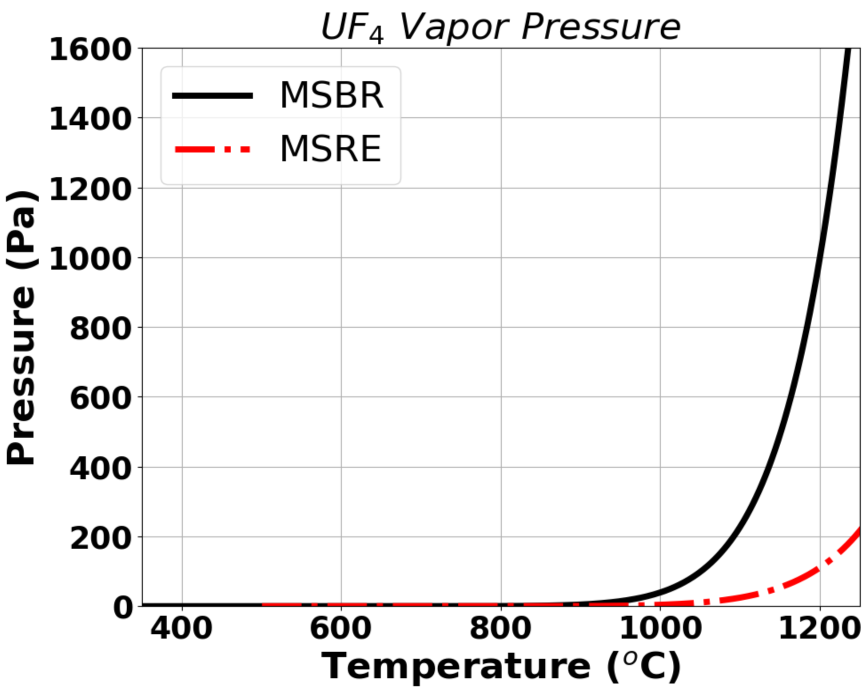
Release from fuel salt coolant

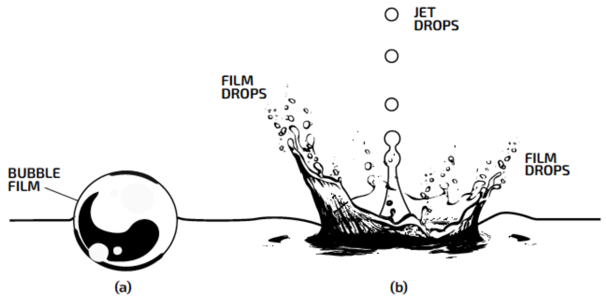
- What compounds exist in the pool? What is their volatility? What rate do they release from the pool?
- Chemical interaction of fission products with fuel salt critical to determine volatility of fission products

Chemical form of the fission products in fuel salt influences transport out of fuel salt

Transport paths out of working fluid like fuel salt being considered in development

- Evaporation influenced by solubility and vapor pressure
- *New* – Radionuclide decay chains changing volatility (e.g., $I^{135} \rightarrow Xe^{135}$)
- Bubble transport and bursting
- Mechanical mobilization through jet breakup and splashing





Thermochemistry modeling demonstrated to determine extent of vaporization of fission products from molten salt

Fluid Fuel Point Reactor Kinetics

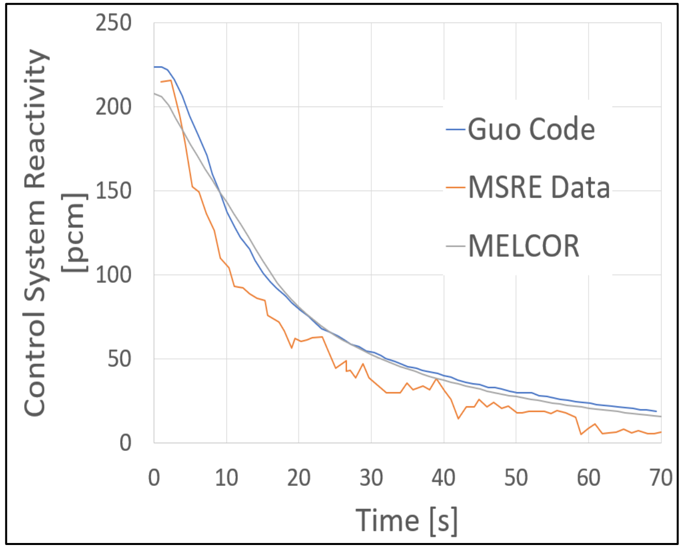
$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \bar{\beta}}{\Lambda}\right) P(t) + \sum_{i=1}^{6} \lambda_i C_i^C + S_0$$

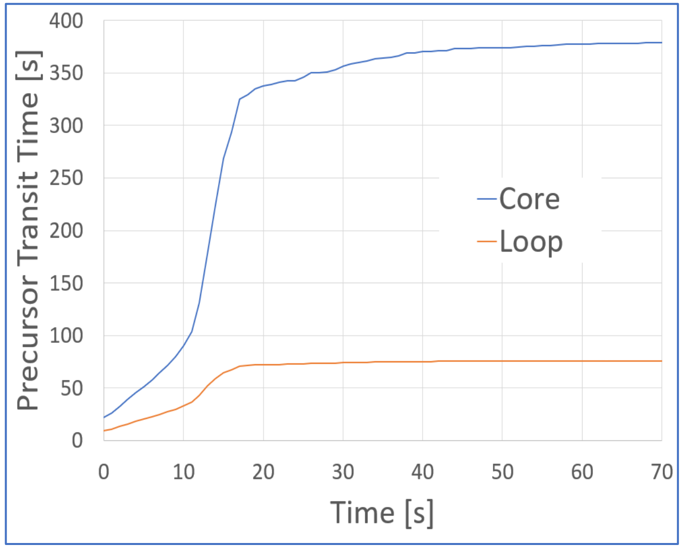
$$\frac{dC_i^C(t)}{dt} = \overset{\text{A}}{\left(\frac{\beta_i}{\Lambda}\right) P(t)} - \overset{\text{B}}{\left(\lambda_i + {}^{1}/_{\tau_C}\right) C_i^C(t)} + \overset{\text{C}}{\left(\frac{V_L}{\tau_L V_C}\right) C_i^L(t - \tau_L)}, \qquad for\ i = 1 \ldots 6$$

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

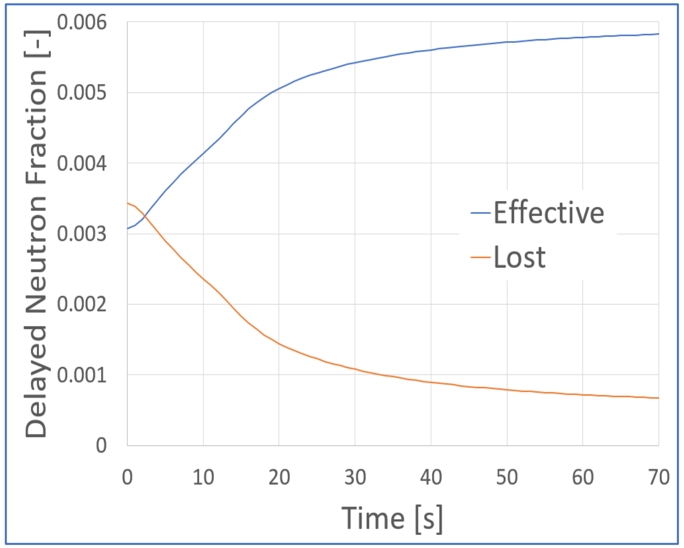
$$\bar{\beta} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum_{i=1}^{6} \lambda_i C_i^L(t)$$

Validation: Zero-Power MSRE Pump Coast-Down





Precursor behavior tracked inside and outside of the core for flowing fuel



Key Processes:

A – In-core delayed neutron precursor gain by fission

B – In-core delayed neutron precursor loss by decay and flow

C – In-core delayed neutron precursor gain by ex-core precursors

D – Ex-core delayed neutron precursor gain by in-core precursors

E – Ex-core delayed neutron precursor loss by decay, flow

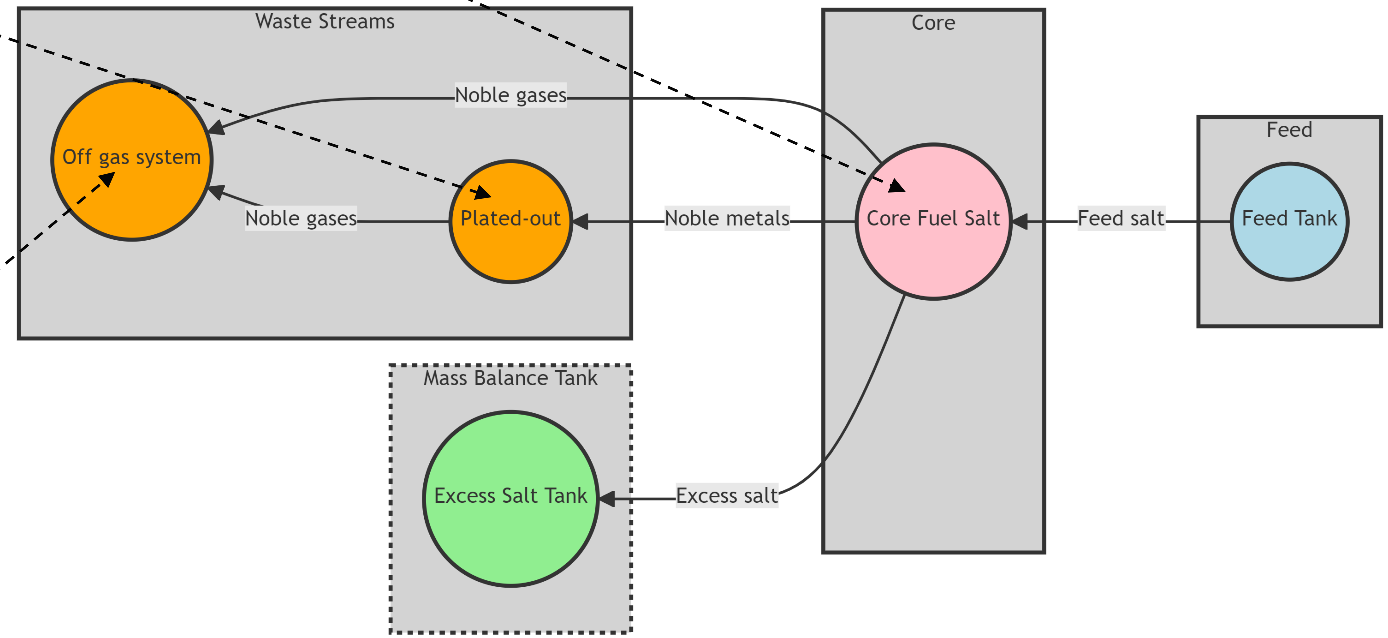
ORIGEN/MELCOR Integration

Why is it important?

- Primary system radionuclides circulate through core
  - Exposed to neutron fission environment until shutdown
- Circulation of radiological material leads to buildup of fission products in different plant regions
  - Contamination of structures due to plate out
  - Off-gas system
- Corrosion products (e.g., noble metals) plate out
  - Radionuclide distribution on structures in reactor system affected by decay
- Migration of fission product gases (Xe & Kr) out of salt handled by off gas system
  - Off-gas hold-up systems designed to decay Xe & Kr
  - Radionuclide distribution in off gas system affected by decay
  - For example, Xe can decay to Cs that could become an aerosol in off-gas system

ORIGEN/MELCOR integration allows

- Independent tracking, decay, and transmutation of nuclides in multiple locations
- Impact of decay and transmutation on radionuclide transport
- Estimation of the potential source term from different regions of the plant



[ORNL/SCALE MSBR drawing]

Approach for ORIGEN/MELCOR Integration

ORIGEN calculates transmutation and decay of isotopes

MELCOR radionuclide species move around a facility due to mass transport processes

MELCOR and ORIGEN have coinciding spatial domains

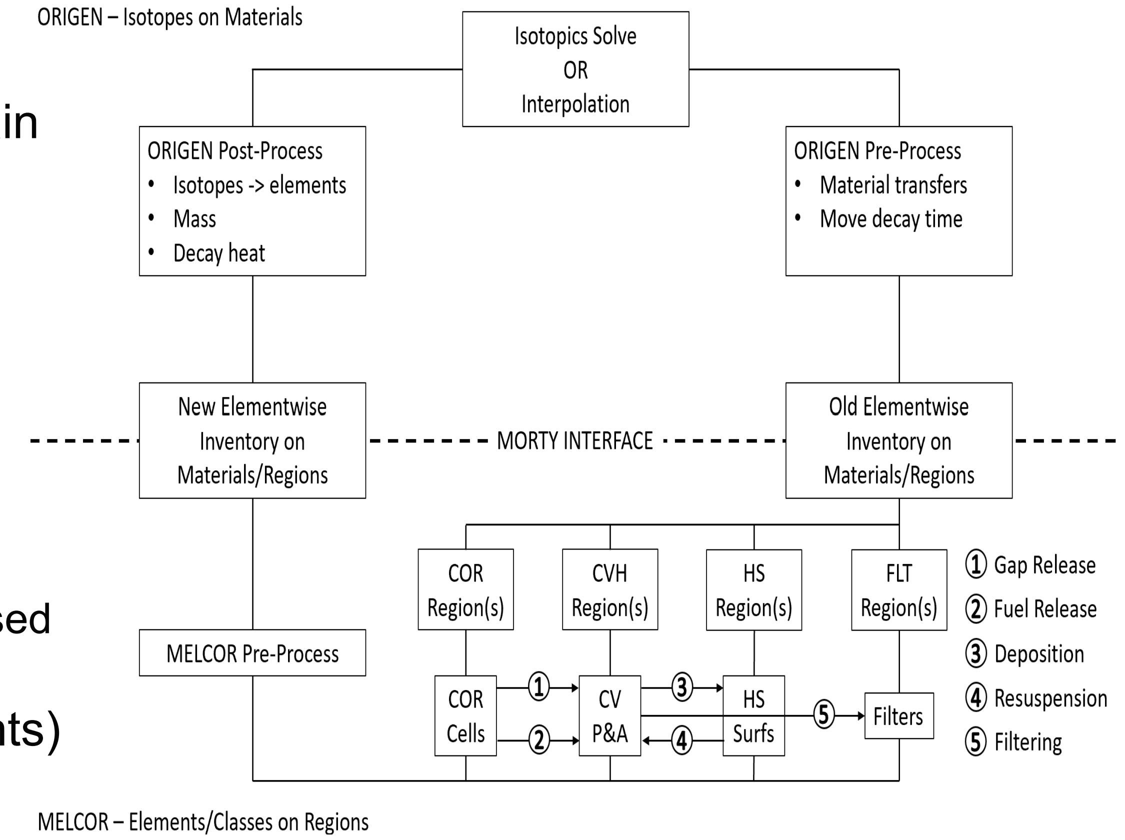
- Spatial fission product distribution assumed uniform over domain

MELCOR initialized using ORIGEN initial distribution from SCALE analysis

MELCOR with ORIGEN simulation steps:

1. ORIGEN decays ~2000 isotopes in each domain
2. MELCOR bins isotopes into classes of chemical compounds representing ~100 elements
   - Chemical classes represent groups of radionuclide species (e.g., $CsBeF_3$) with similar transport behavior (i.e., potential to be released from reactor molten salt)
3. MELCOR moves fission products (and thus chemical elements) within and between spatial domains
4. Element masses in ORIGEN regions are updated
5. ORIGEN updates isotopic distributions in materials based on MELCOR calculation of mass transport between spatial domains

Implementation:



Investigating Reactor Chemistry and Mass Transfer

Question: which fission products will be retained in molten salt?

- Sensitively depends on interaction between salt and fission products → chemical equilibrium of solution

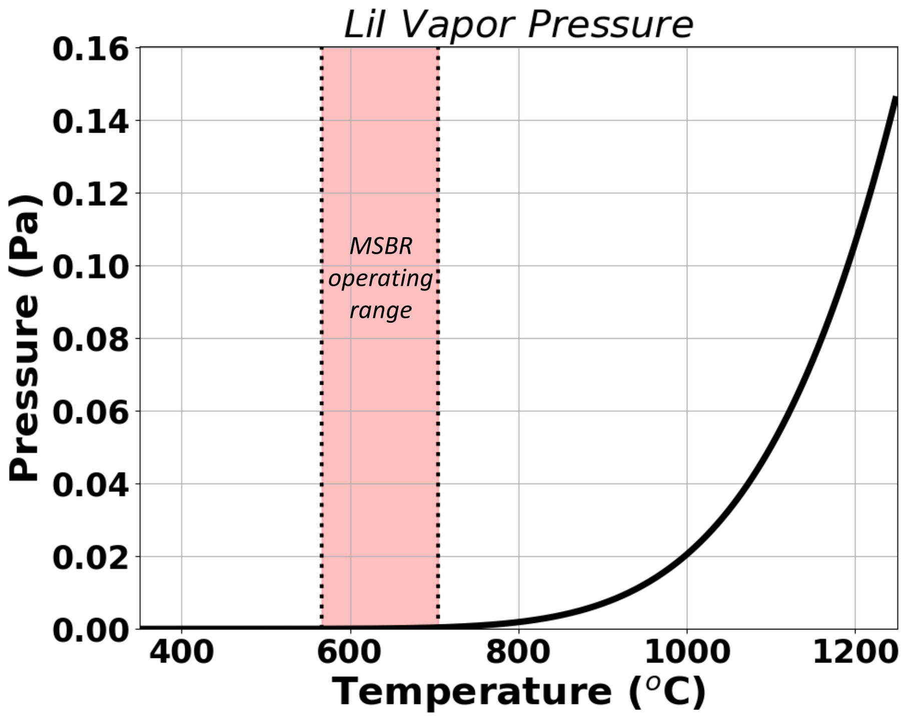
Salt + fission product solution thermochemistry influences chemical speciation, vapor pressure …

MELCOR allows new chemical compounds being added to its species mass transport model (RN package)

- Chemical compounds can represent both radiologically and chemically hazardous materials

Vapor pressure correlations are used by MELCOR to determine fission products that vaporize out of the salt

- Vapor pressures are proportional to “easiness” chemical compounds vaporize out of the salt
- High (low) means chemical compounds are more (less) likely to vaporize out of the salt



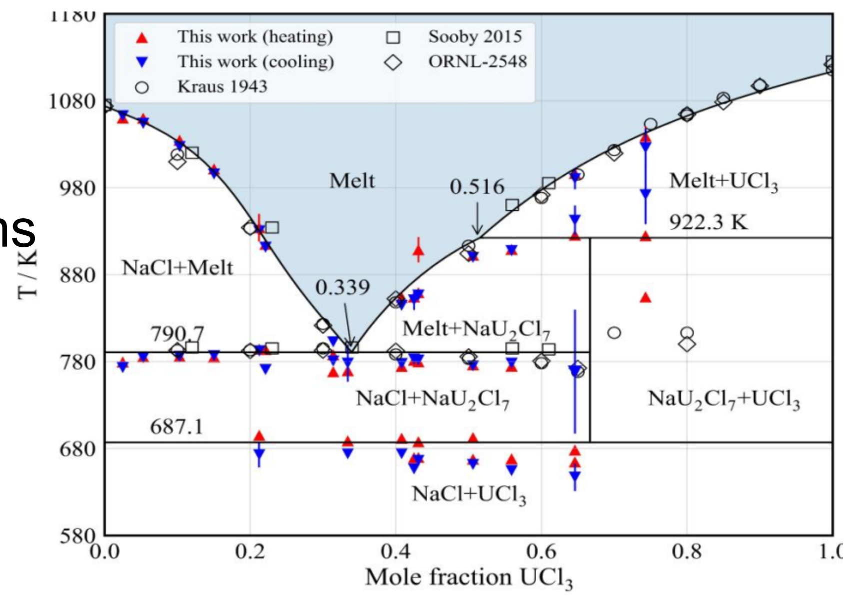
LiI Vapor Pressure in MSBR Model

Thermochemical models combined with MELCOR can parameterize fission product and hazardous chemical migration out of the salt

Thermochemistry Modeling for Molten Salt Systems

- Molten Salt Thermodynamics Database – Thermochemical (MSTDB-TC) contains fitted Gibbs energy functions for salt systems
- Thermochimica uses databases, like MSTDB-TC, to calculate *equilibrium* thermochemical properties
  - E.g., speciation, melting point, vapor pressures…
- Thermochemical properties of multi-component molten salt systems across broad range of temperatures can be modeled
- Common fluoride and chloride carrier, fuel and fission product systems available
  - Data incorporated into MSTDB-TC for iodine limited but increasing
  - Significant gaps for Be compounds due to data sparsity

T. Besmann (USC)



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

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

Thermochimica

M. Piro (McMaster)

Fuel Salt Vapor Pressures

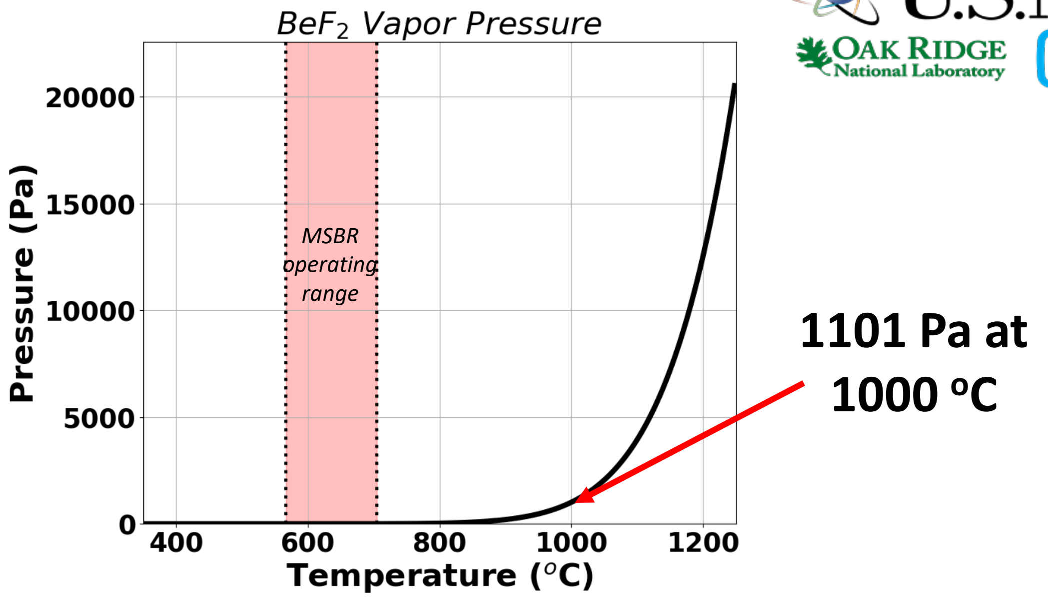
Highest vapor pressures will be for carrier and fuel salt species

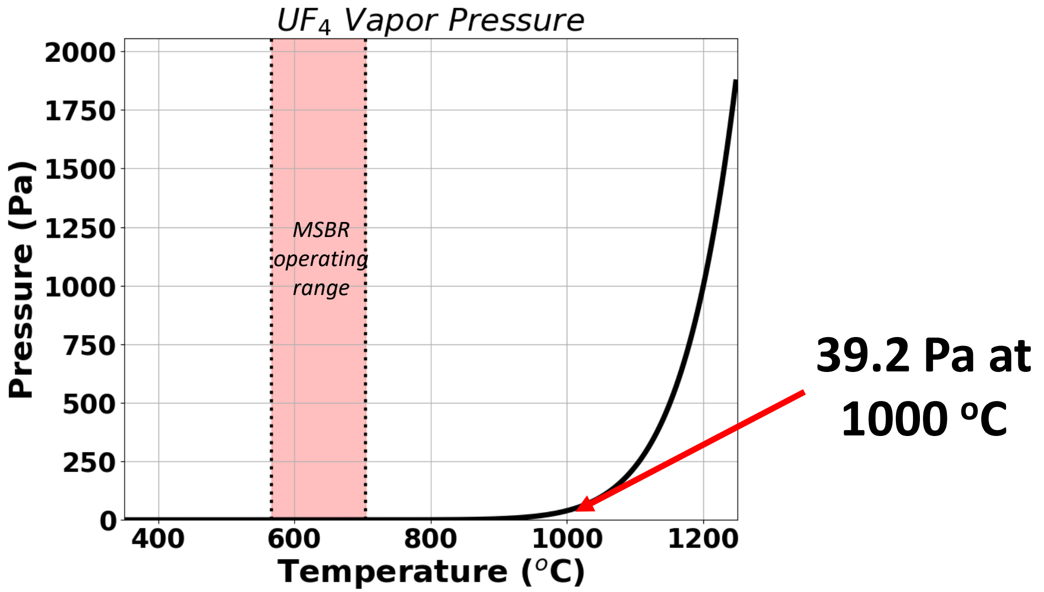
LiF has highest vapor pressure

- Chemical compound does not have hazardous effects on humans

Vapor pressure significantly increases above 1000°C

Other species have negligible vapor pressures

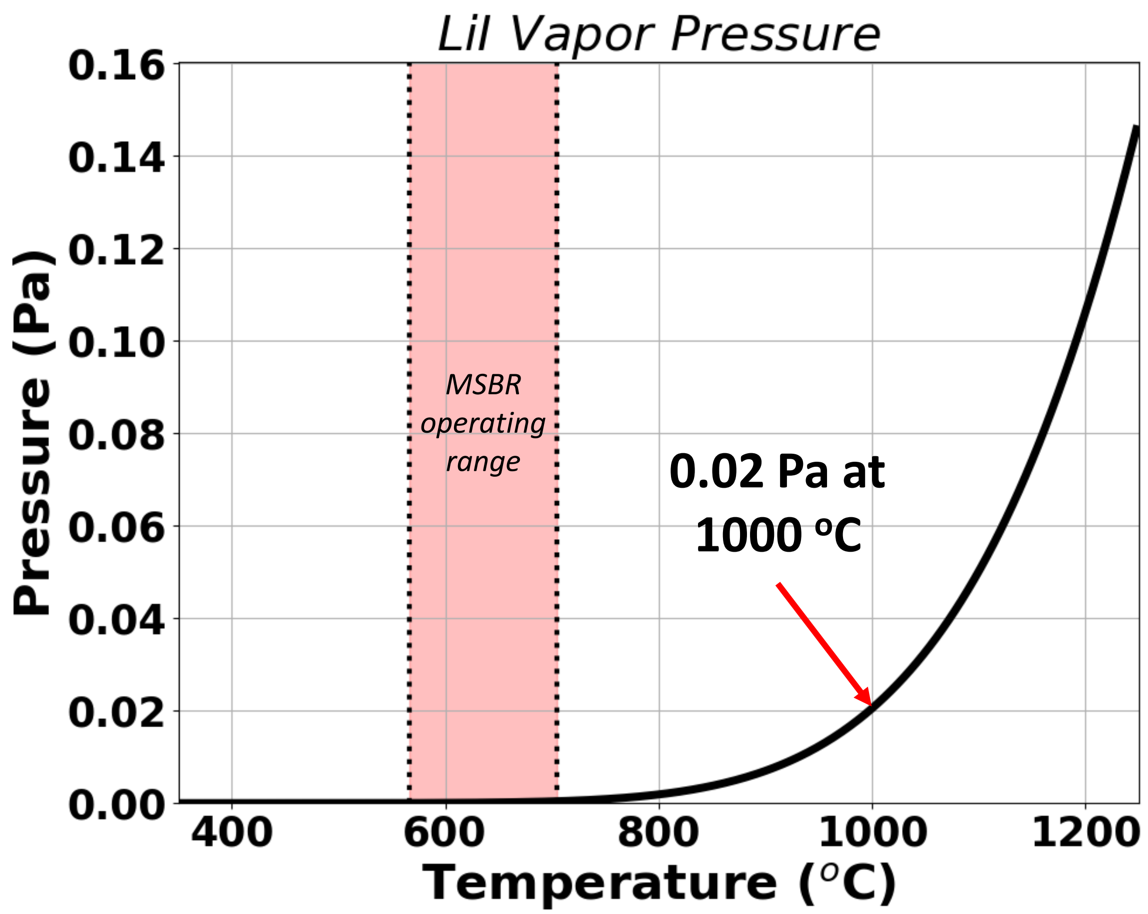


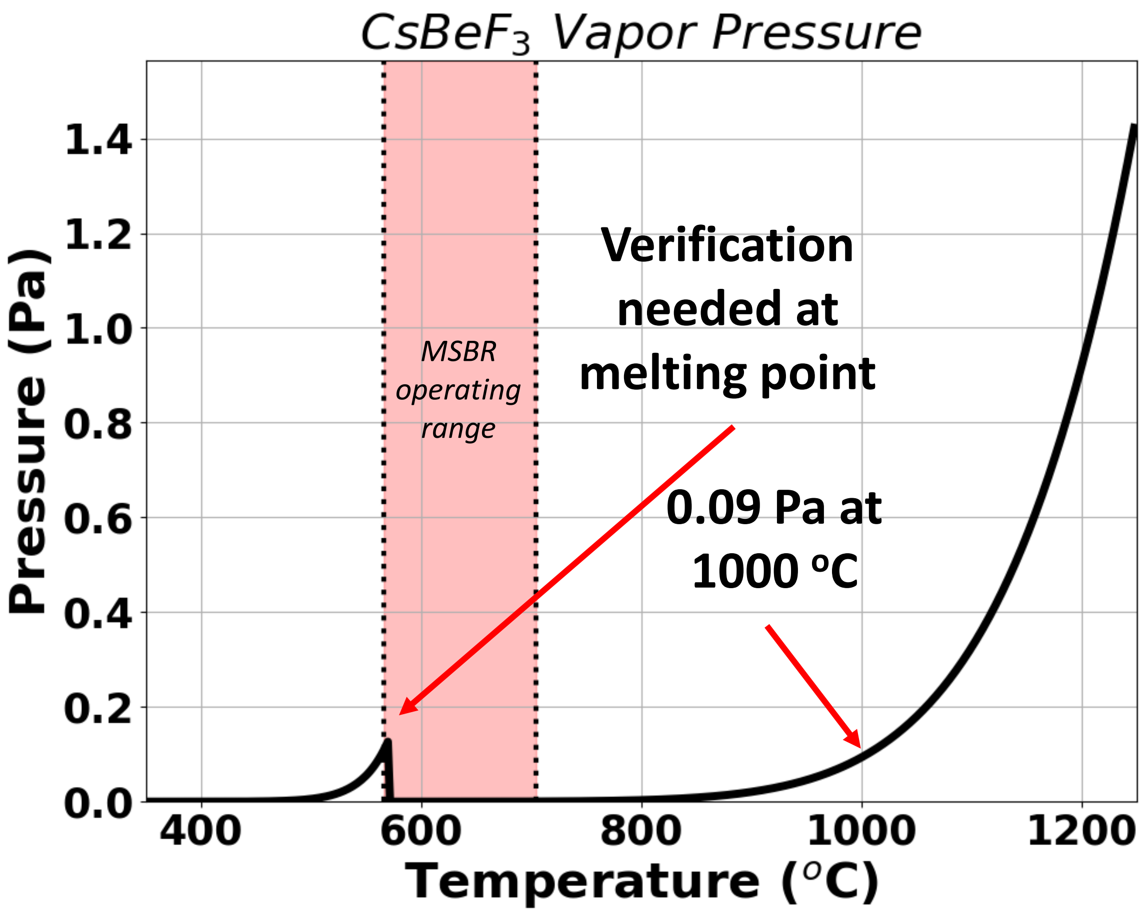


Fission products do not affect fuel salt vapor pressures

Cesium and Iodine Fission Product Compounds

Dominant cesium and iodine compounds shown

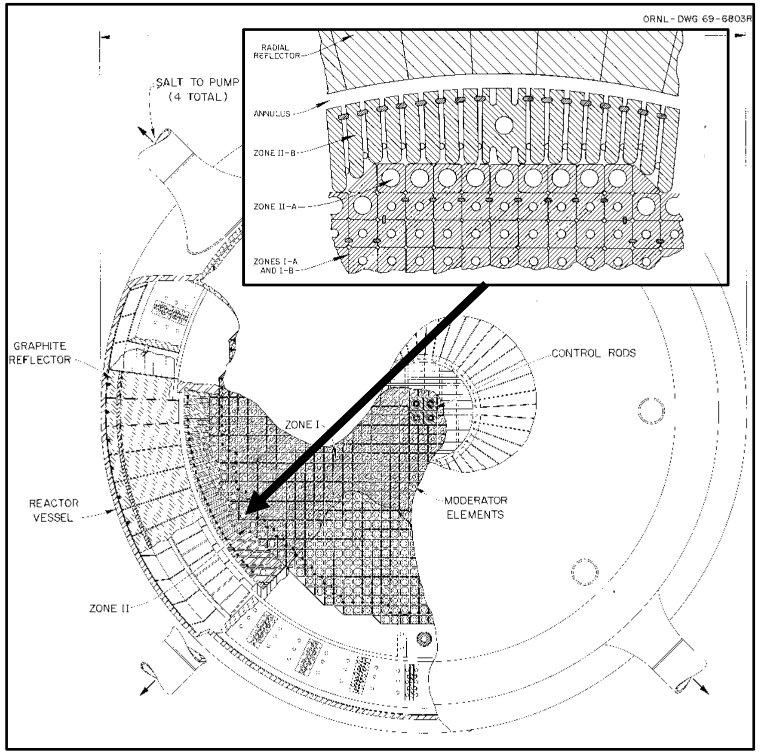


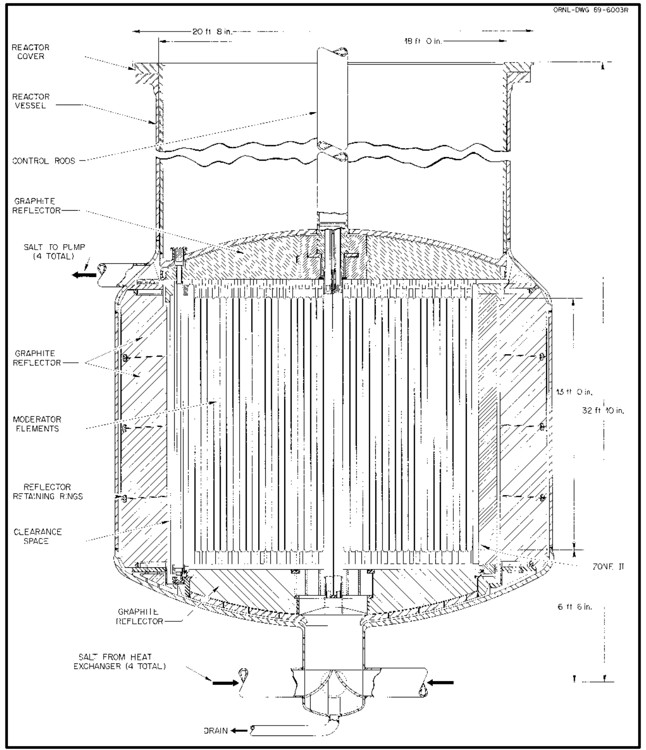


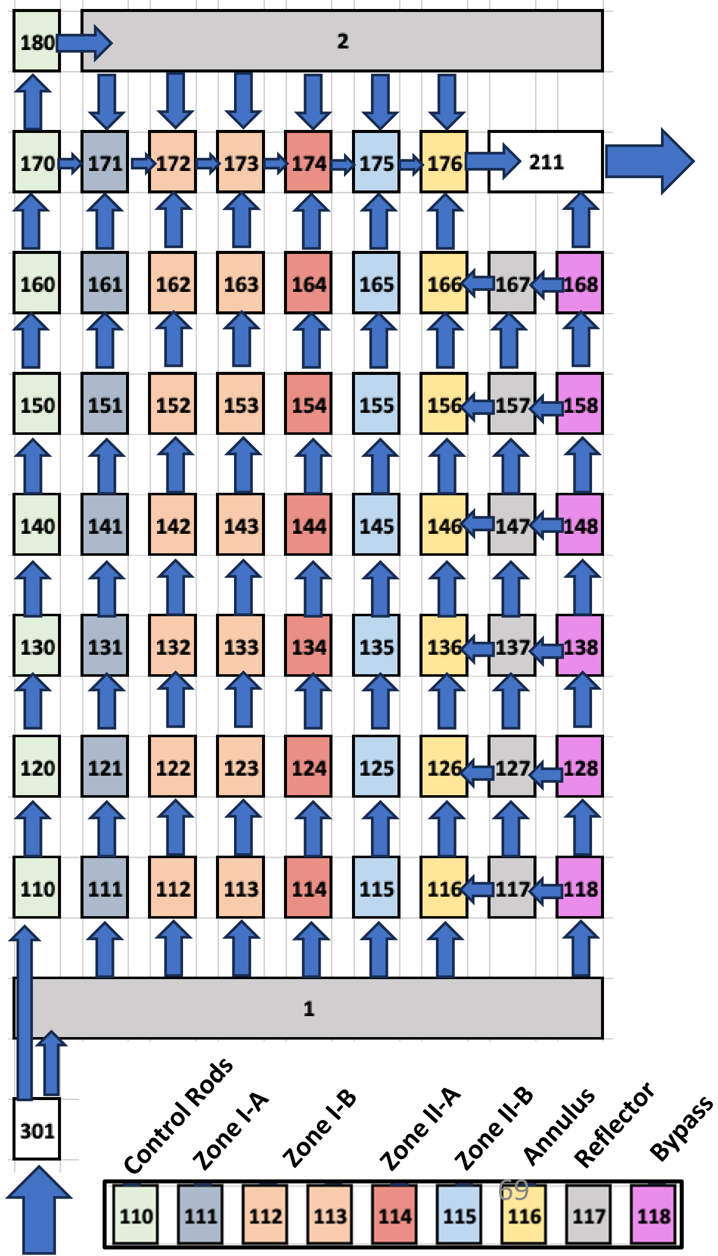
Cesium and iodine not expected to contribute through direct vaporization to the source term in MSBR

MELCOR Nodalization: Vessel and Core

- Salt enters from bottom, exits from top plenum into four loops
  - Four hot legs, primary pumps, and heat exchangers
- Core comprised of various regions/geometries
  - Core split into multiple zones based on geometries

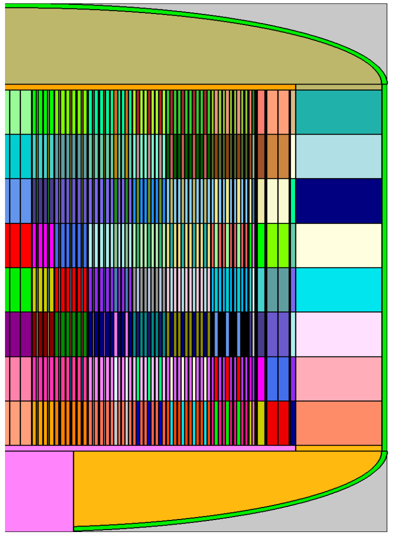


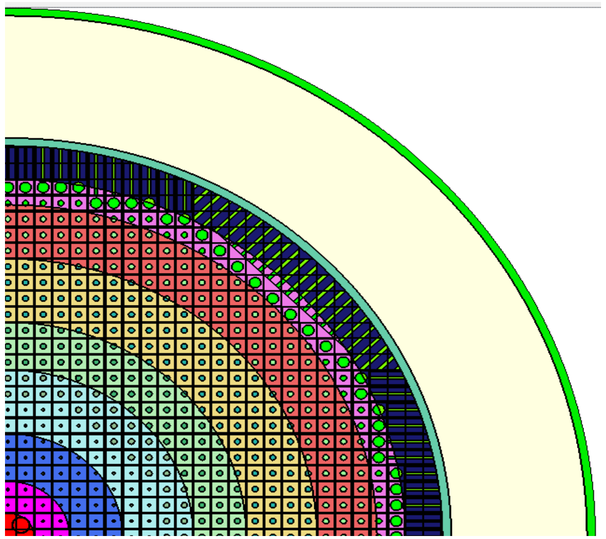


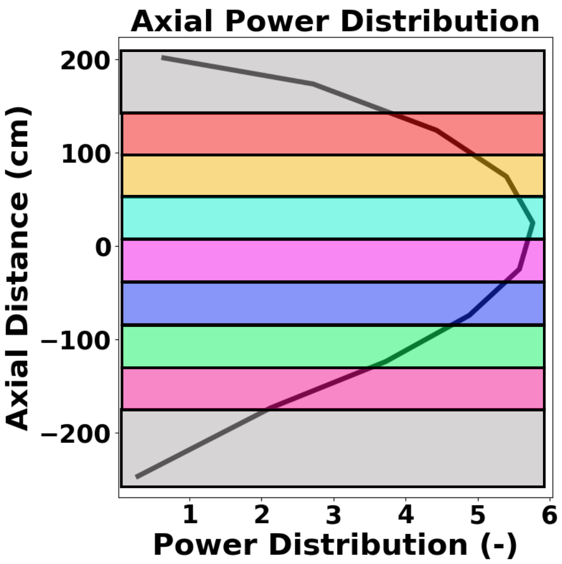


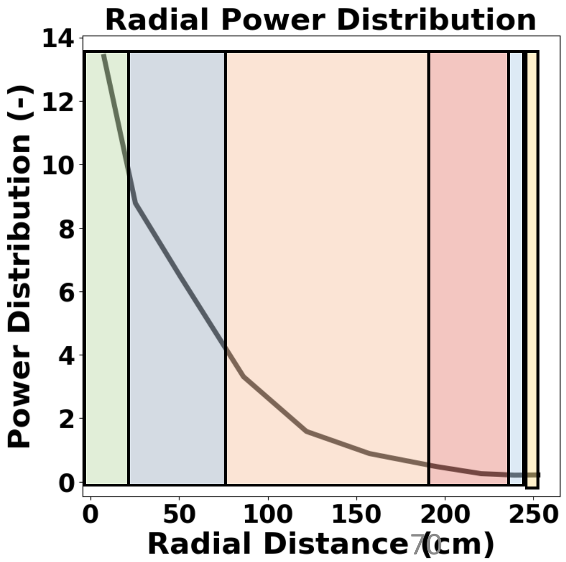
Mapping Power Profile from SCALE

- Two core zones with different graphite element geometries
  - Top and bottom orifices for flow/temperature distribution
  - Outer zone elements with higher fuel to moderator (FTM) ratio due to Region II reflector design
- SCALE nodalization,
  - Average SCALE power within MELCOR node



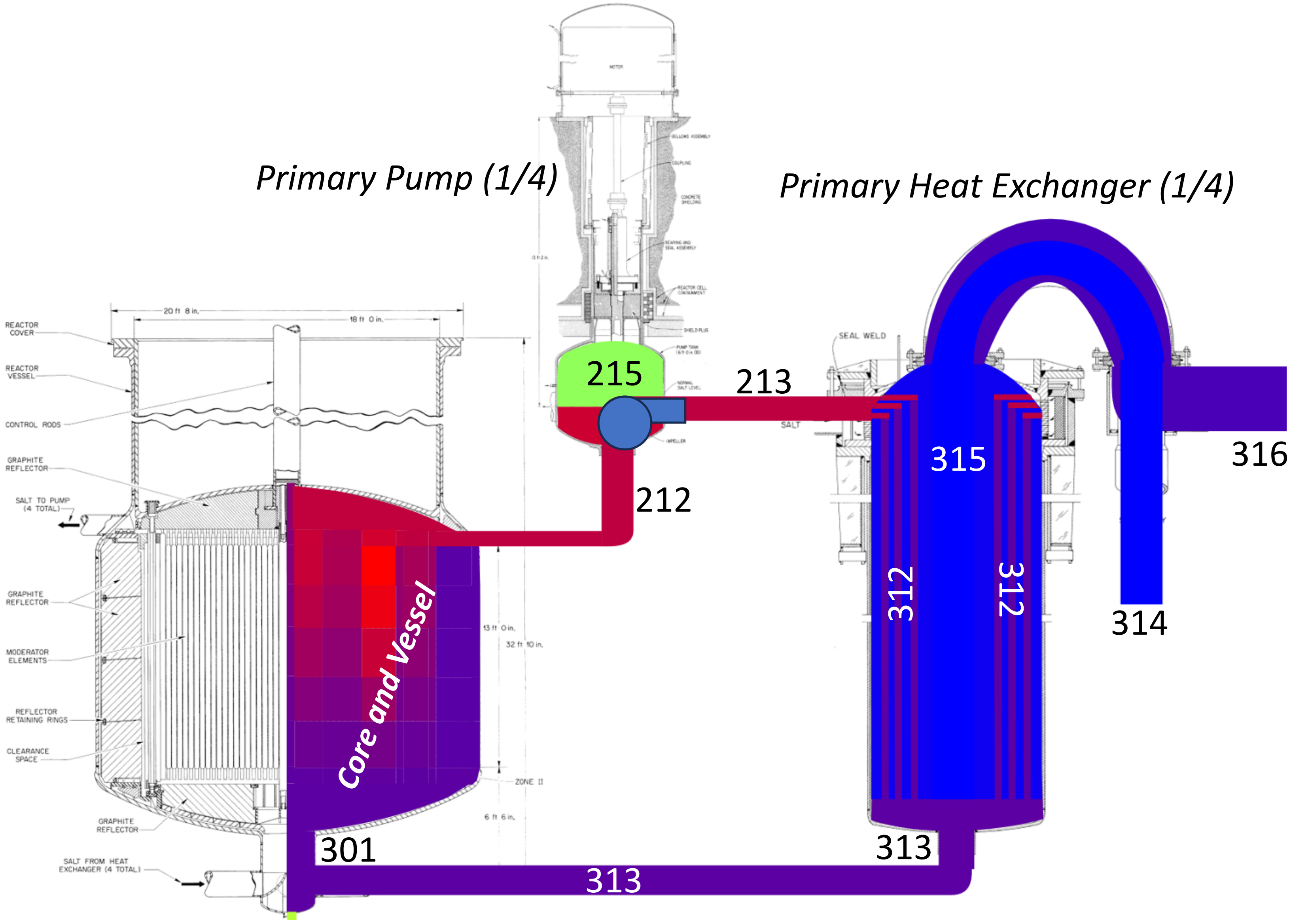






MELCOR Nodalization: Primary Loop

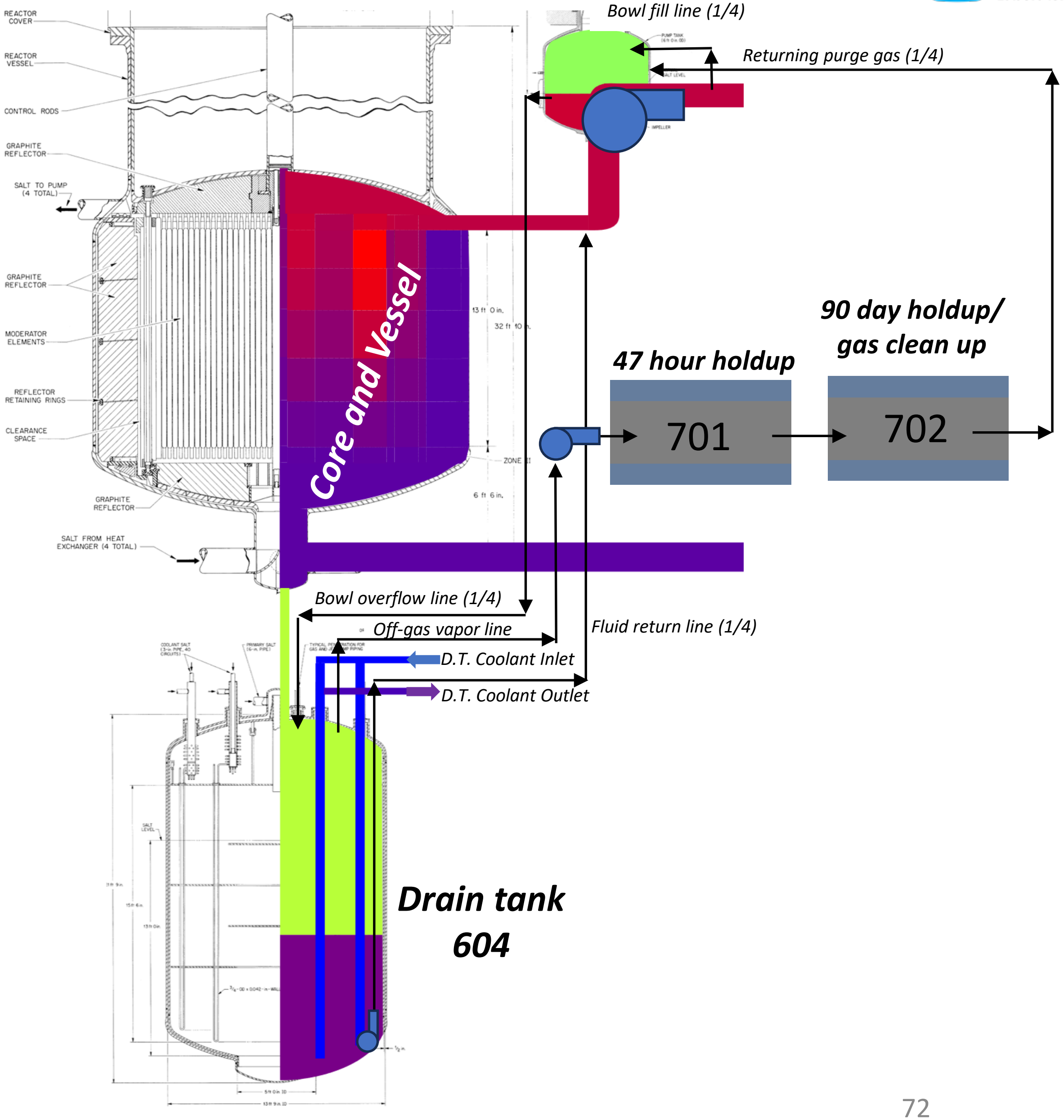
- One out of four identical loops illustrated
  - CV-212, CV-213, CV-312, and CV-313 are one loop
  - All loops recombine at CV-301
- Each hot leg has pump with a pump bowl
- Shell-Tube heat exchangers
  - Secondary side specified using boundary conditions

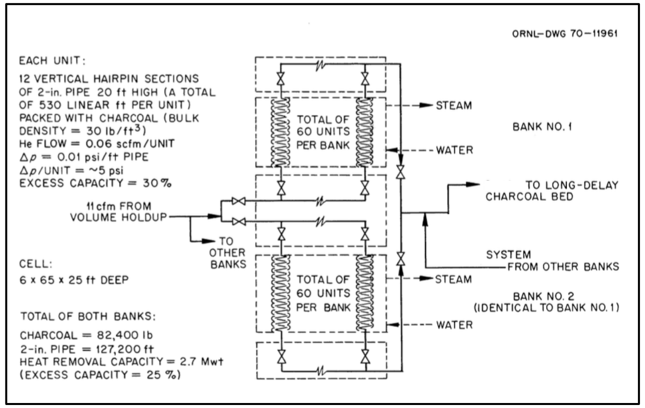


MELCOR Nodalization: Drain Tank & Off-Gas

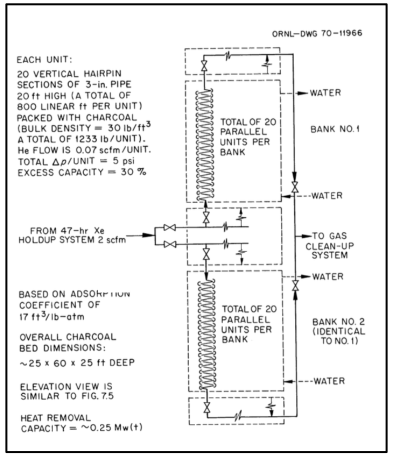
U.S.NRC
Oak Ridge National Laboratory
Sandia National Laboratories

- Off-gas loop:
  - 47 hour hold up tank for xenon decay
  - 90 day hold up tank for long-lived isotope decay
- Drain tank:
  - 2 hour hold up of off-gases from pump bowls
  - Filled from overflow of pump bowl, returned to primary loop
  - Contains active cooling system for heat produced by decay of isotopes
- Circulating fuel and purge gas in/out of drain tank
  - Closed circuit but options for addition of purge gas





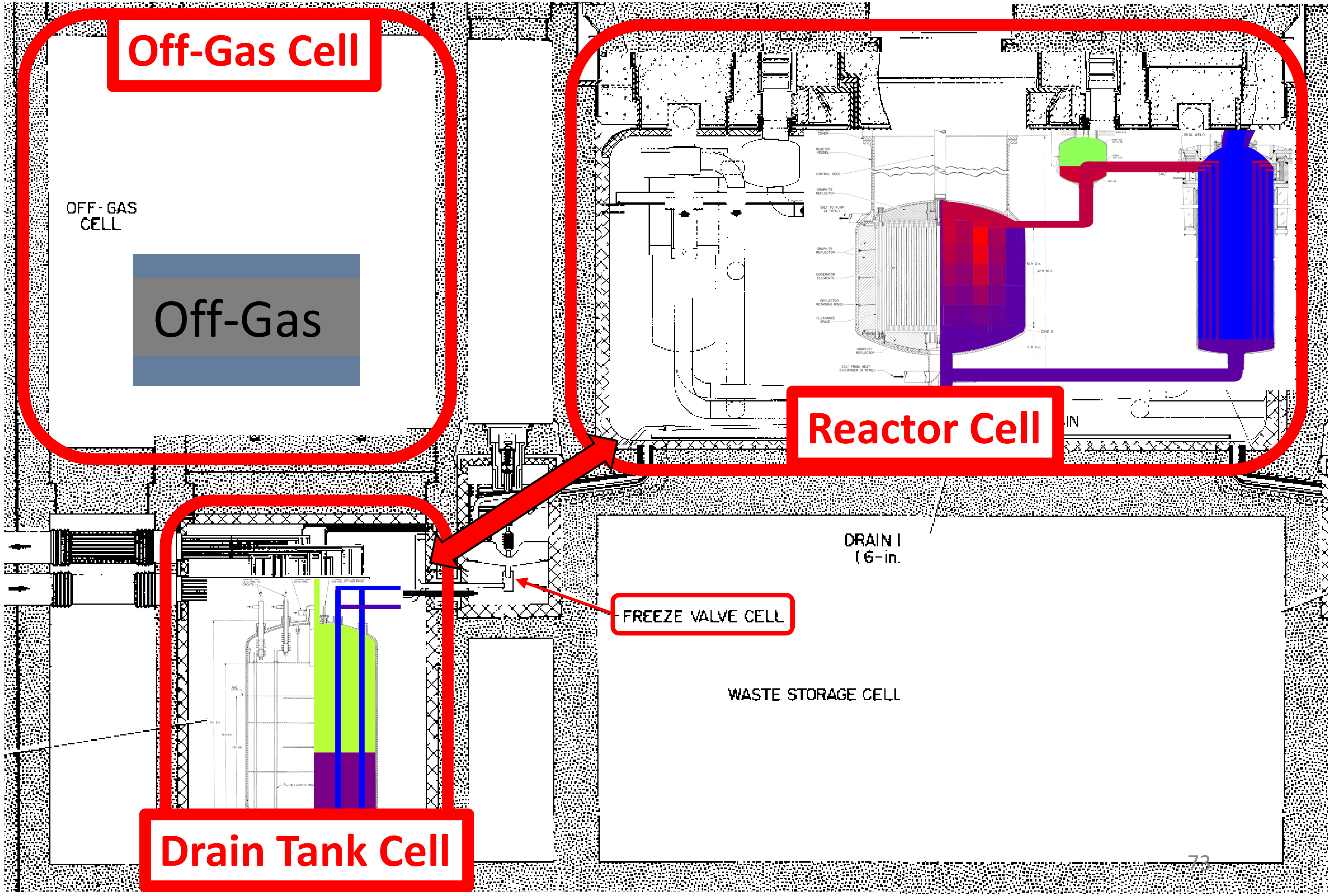
47 hour holdup



90 day holdup

MELCOR Nodalization: Containment

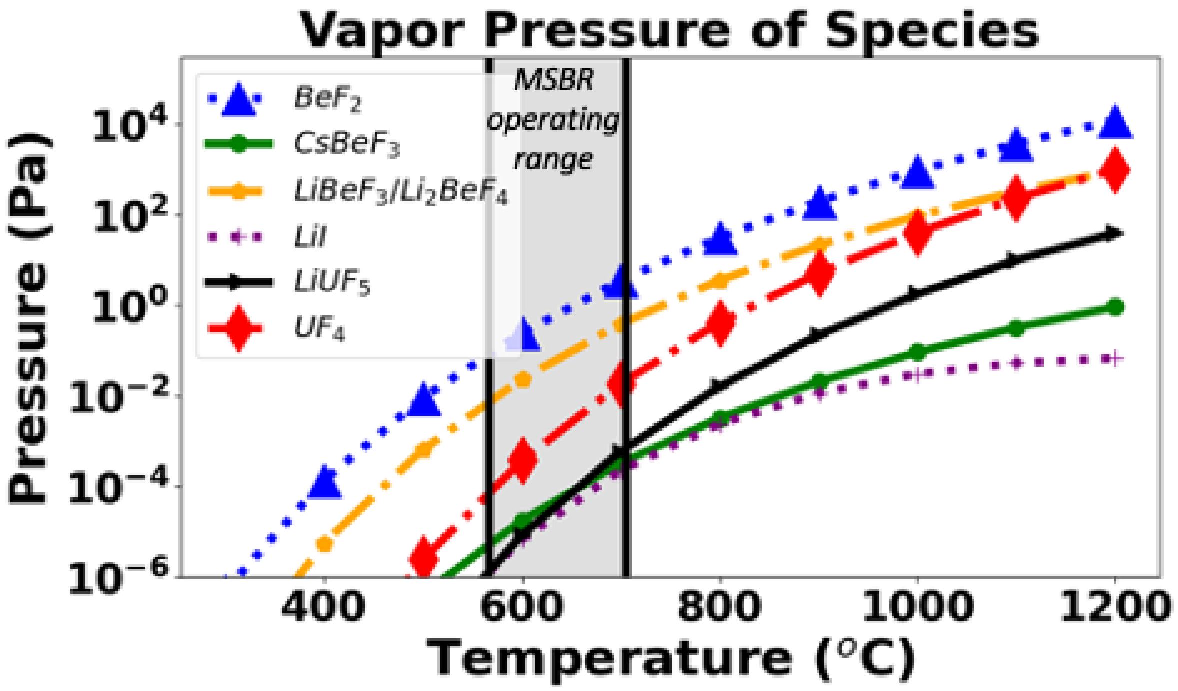
- Off-gas, drain tank, and primary loop in respective reactor cells
- Drain tank cell and reactor cell connected through freeze valve cell
  - Maintains equivalent environments during steady state operation

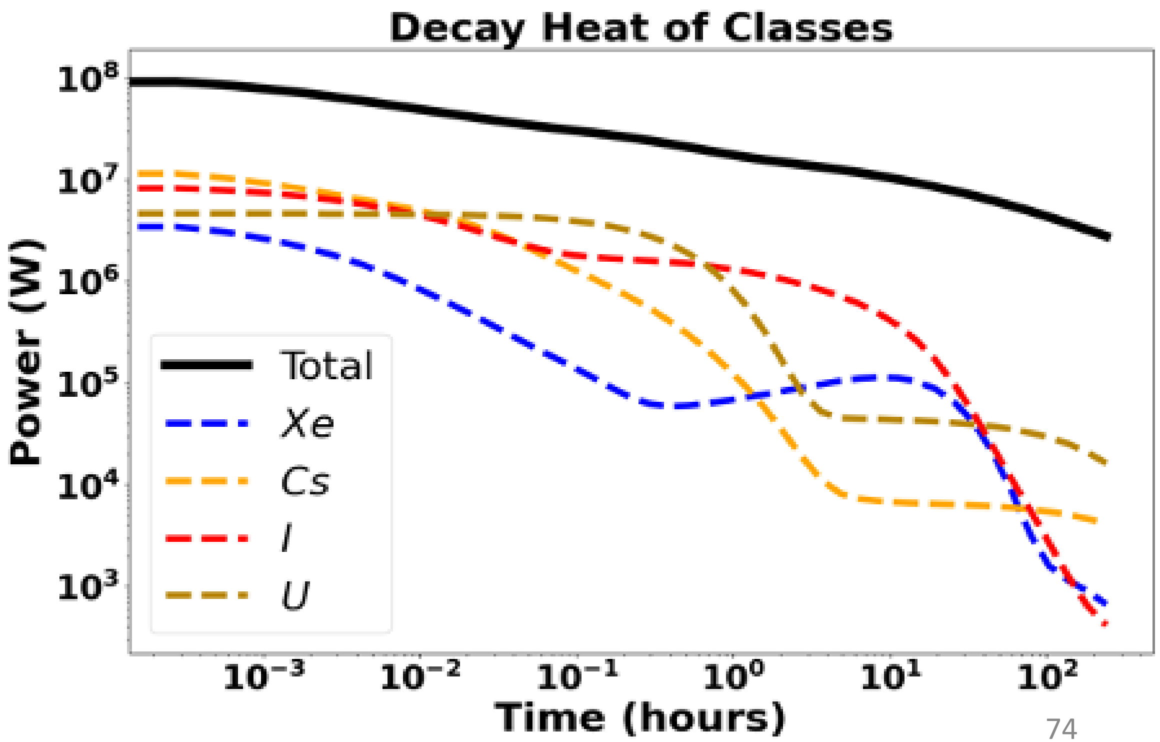


Inputs From Scale and Thermochimica

- MELCOR allows for regrouping of elements into radionuclide classes
  - Default grouping developed for LWRs based on chemical similarity
- The grouping of elements or compounds are changed **for molten salt or chloride reactors**
  - MSR radionuclide **groupings based on solubility and isolating non-soluble corrosion products**

- Due to their higher vapor pressure and potential volatility for release, **BeF_2 and UF_4 are tracked in separate radionuclide classes**

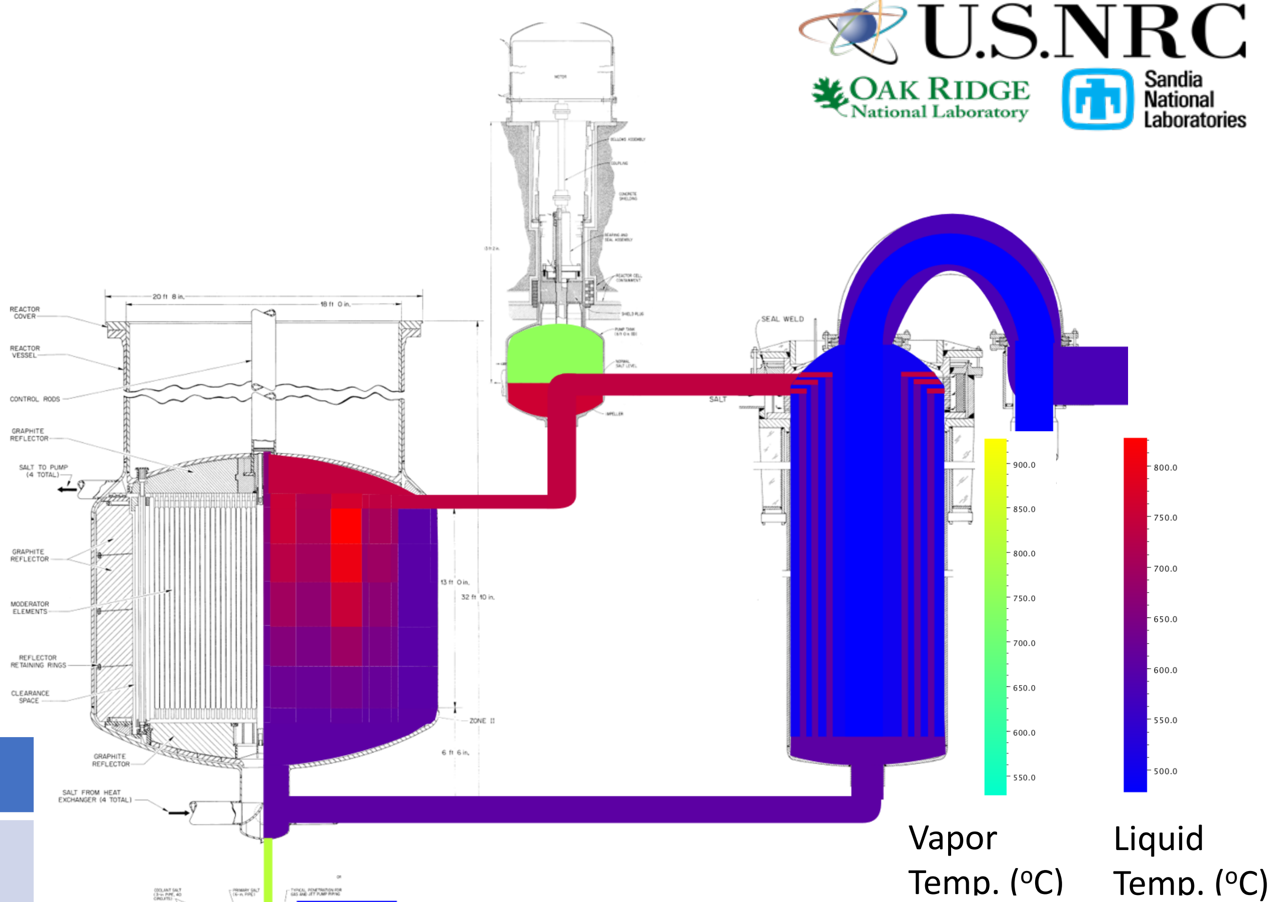


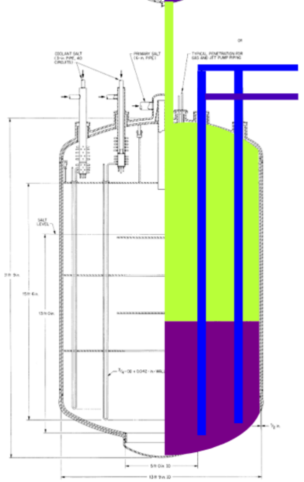


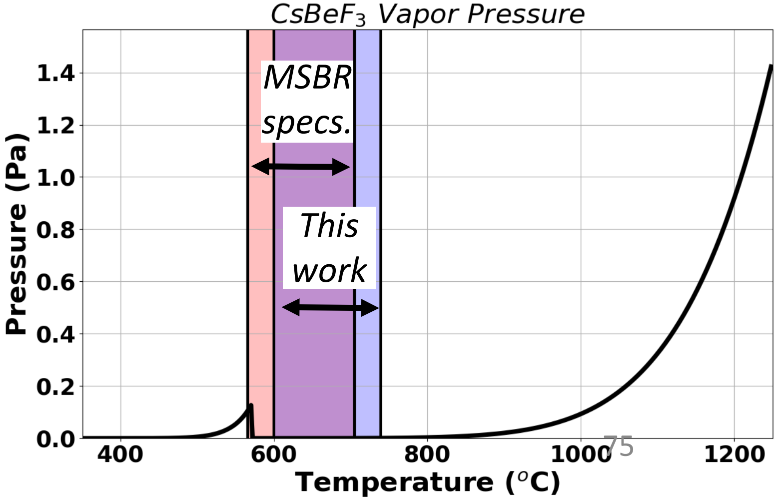
Steady State Results

- Similar operating conditions to MSBR design
  - Inlet temperature increased, avoid freezing, increased safety margin
  - Different thermophysical properties, primary mass flow rate modified to match temperature differential

Parameter	MSBR Specs.	This Work
Fuel density (kg/m³)	3328	1970
Fuel specific heat Capacity (J/kg-K)	1357	2380
Mass flow rate (kg/s)	11820	6801
T_{inlet} (°C)	566	600
T_{outlet} (°C)	705	739



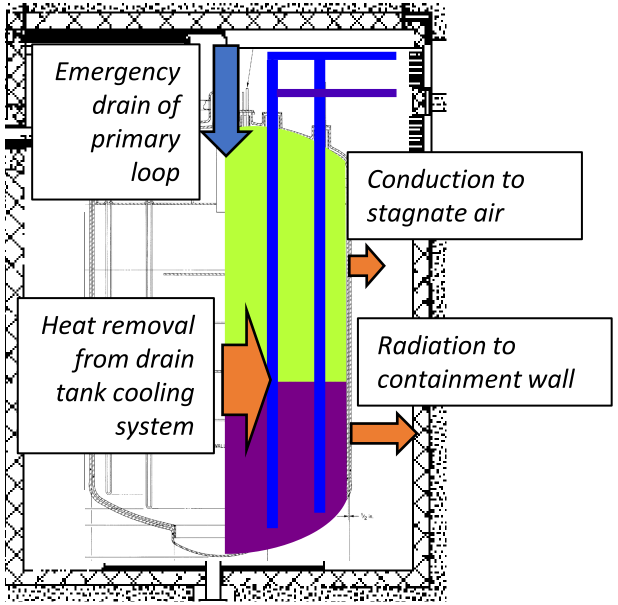




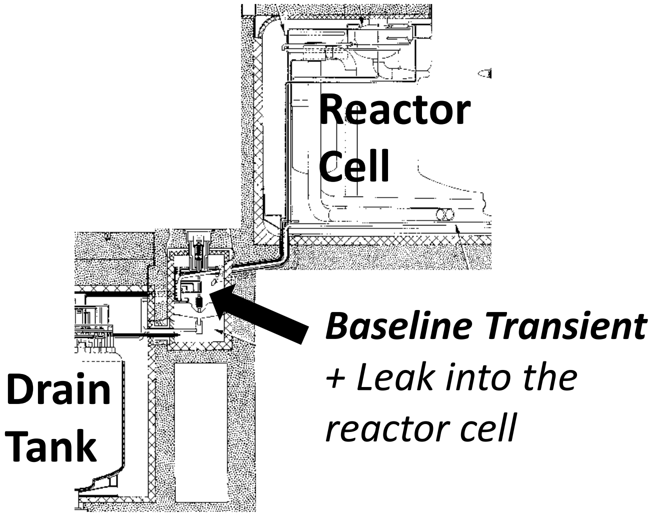
Description of Transients

- **Emergency drain from primary loop into drain tank**
  - Parametric sweep on active heat removal, select one case as baseline
- **Key figures of merit**
  - Thermophysical response
  - Distribution of UF_4 and BeF_2
  - Behavior of radionuclides in the off-gas holdup volumes
- **Sensitivities**
  - Perturb off-gas system
    - Explore production of airborne chemical species
  - Postulated leaks into containment cells
    - Analyze transport of airborne chemical species

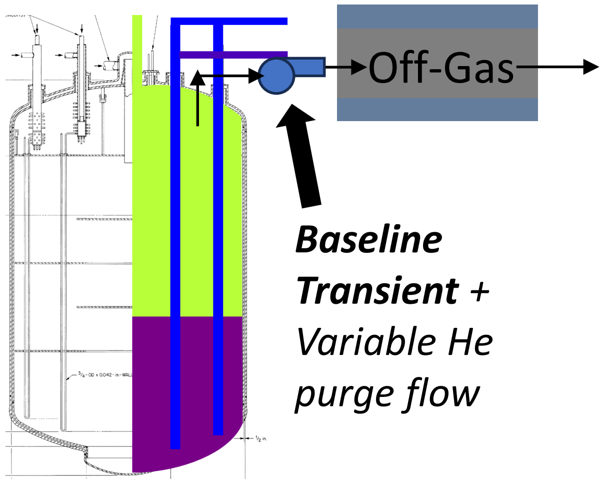
Baseline Transient



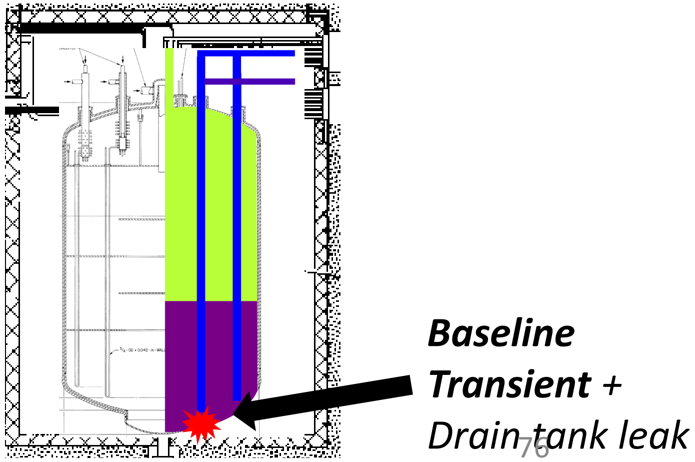
Sensitivity Case 1



Sensitivity Case 2

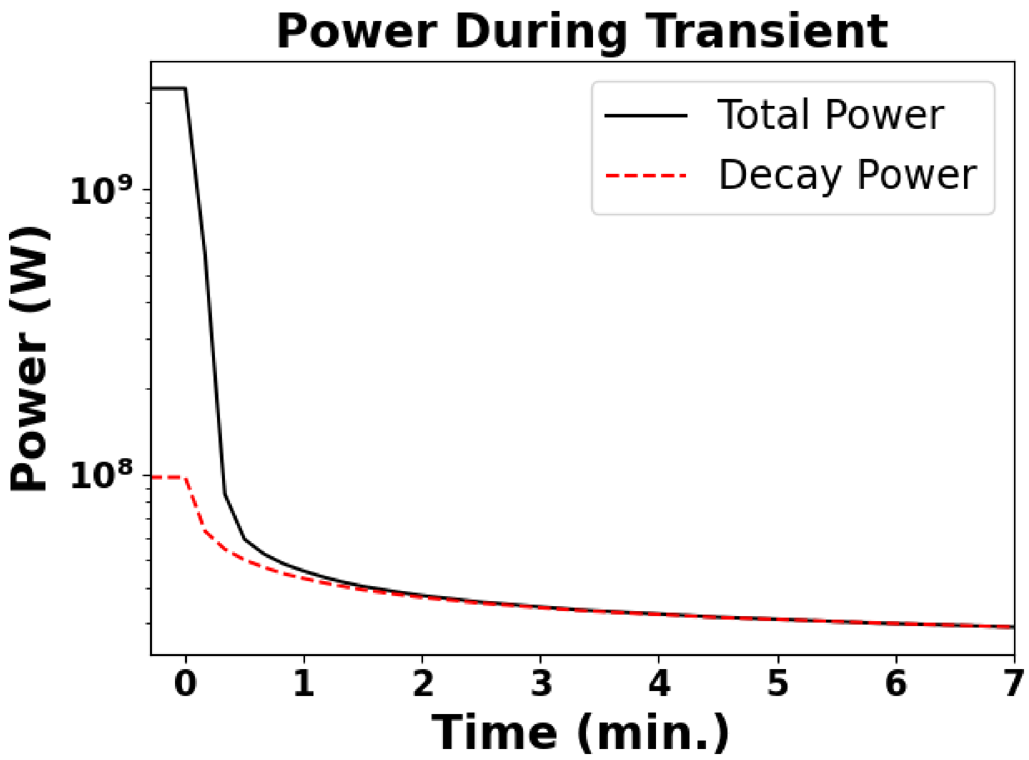


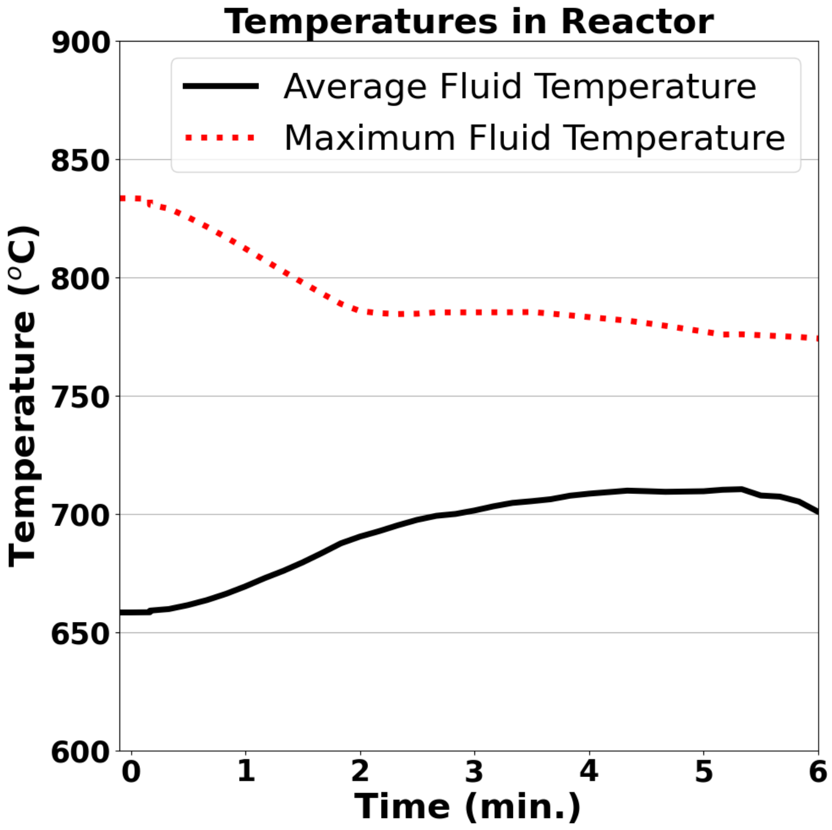
Sensitivity Case 3

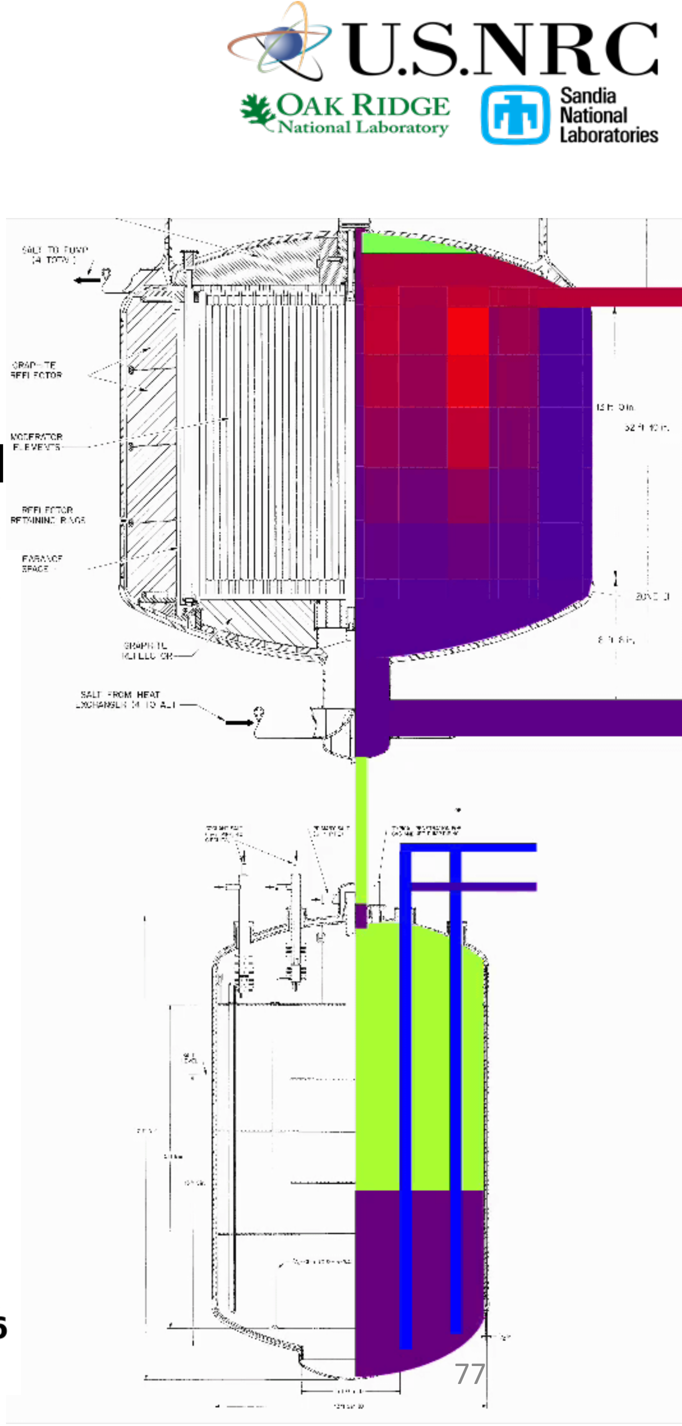


Emergency Drain: Primary System Response

- Core fully drained ~7 minutes
- Shutdown due to fuel draining and reactivity feedback
  - Residual heat reached in ~2 minutes
  - ~97 MW of residual heat during steady state, ~30 MW once fully drained

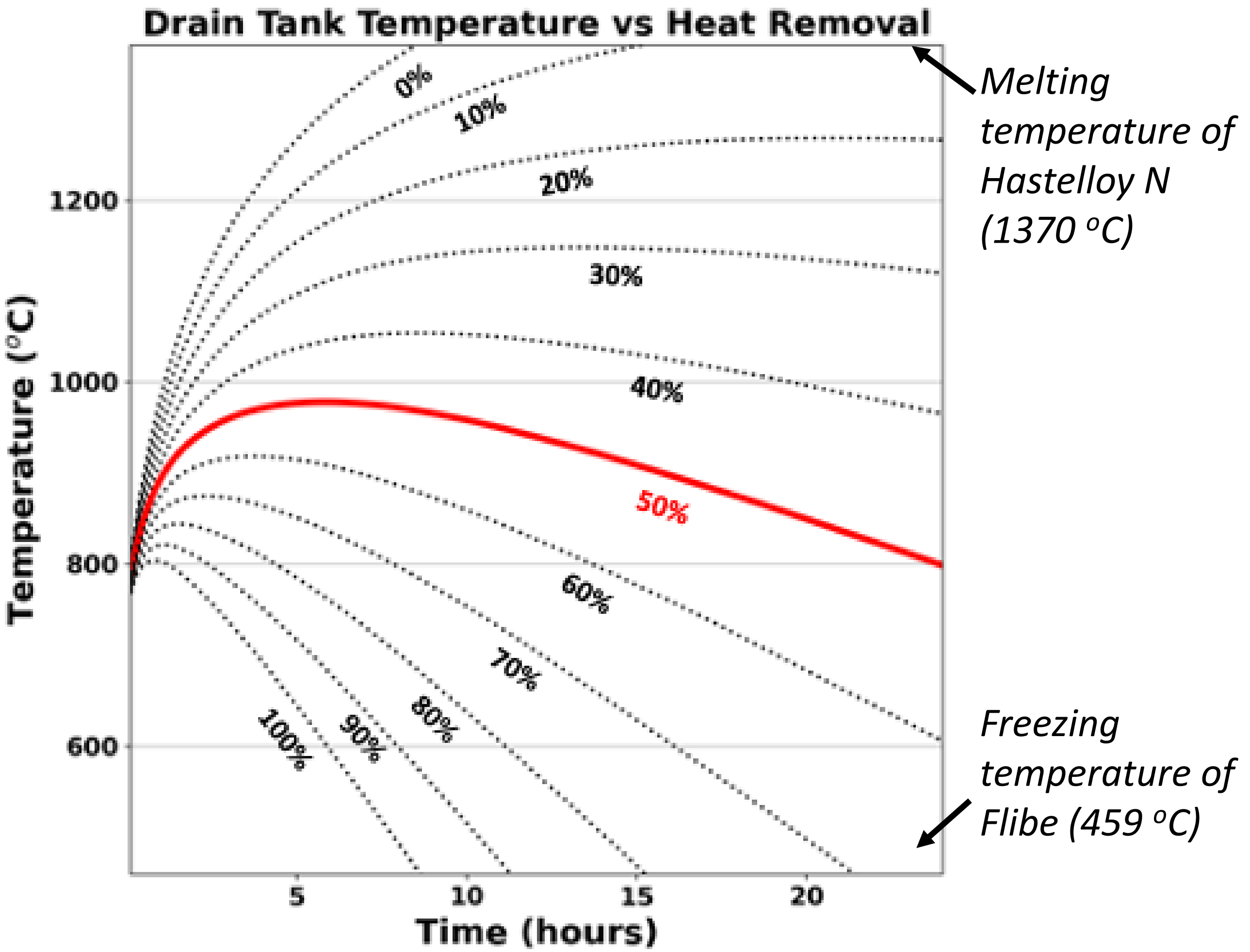


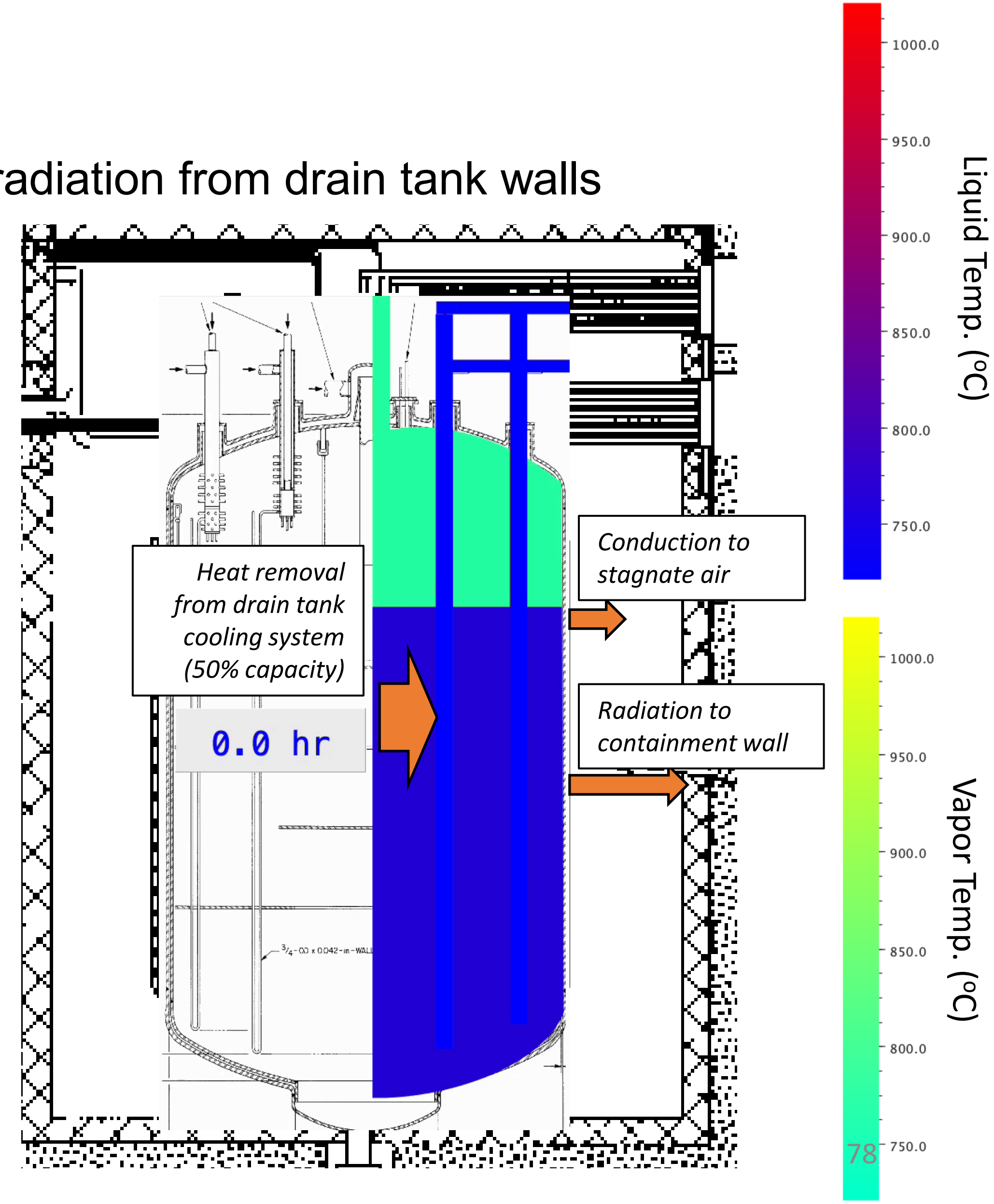




Emergency Drain: Thermal-Hydraulic Response

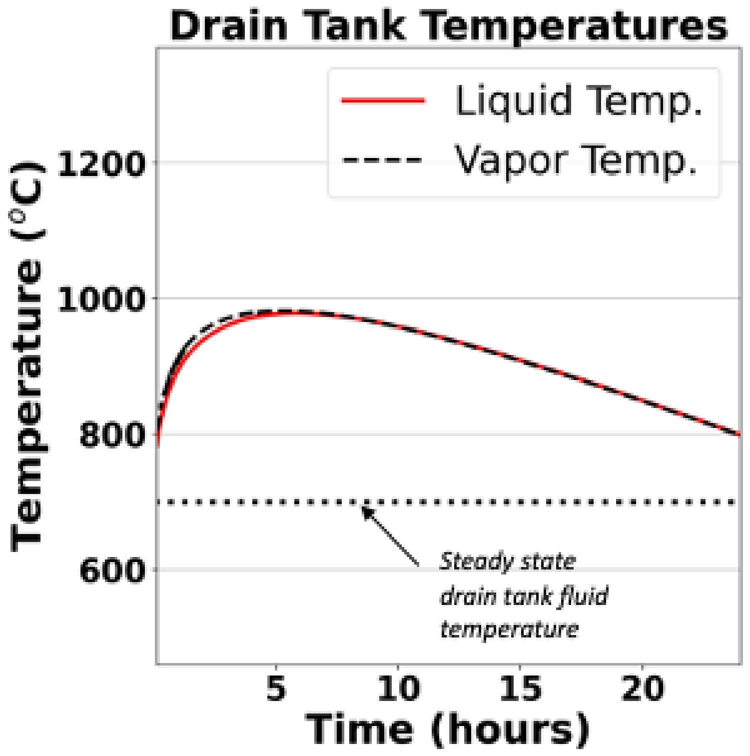
- Variable drain tank cooling system effectiveness
- Fully effective cooling system removes 18 MW
  - Nominal during steady state operation
- Additional passive heat removal through conduction & thermal radiation from drain tank walls

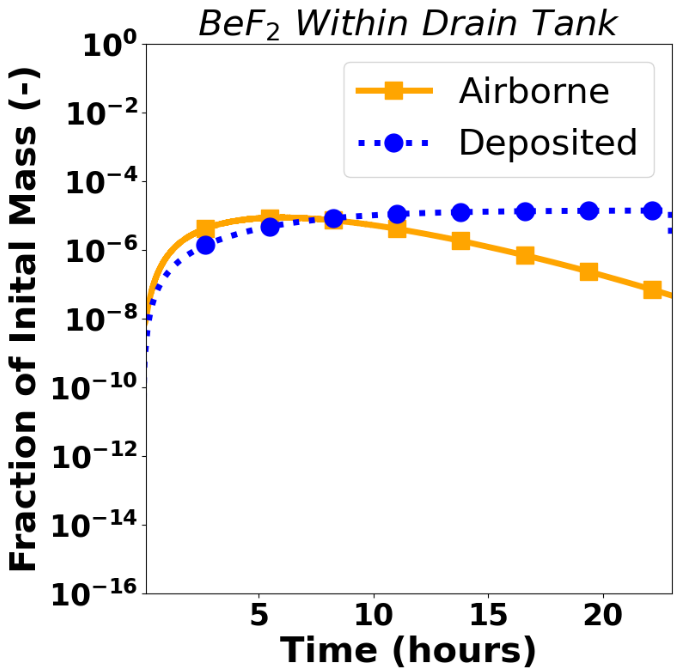


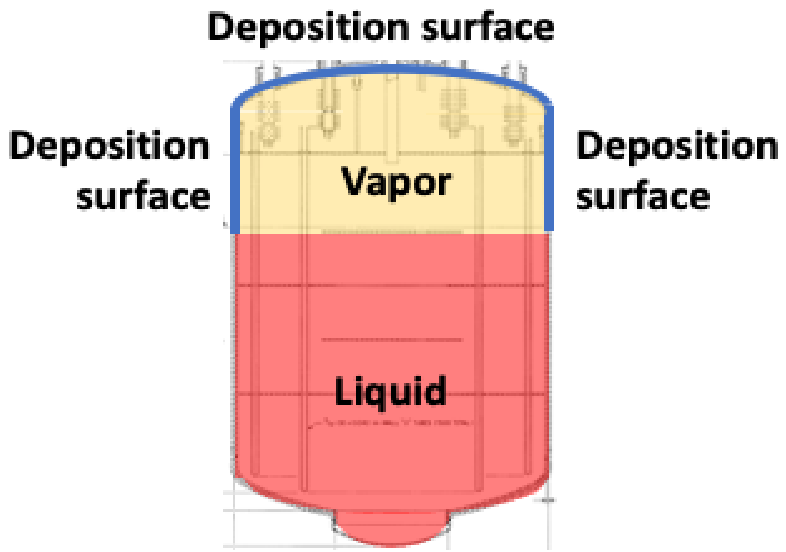


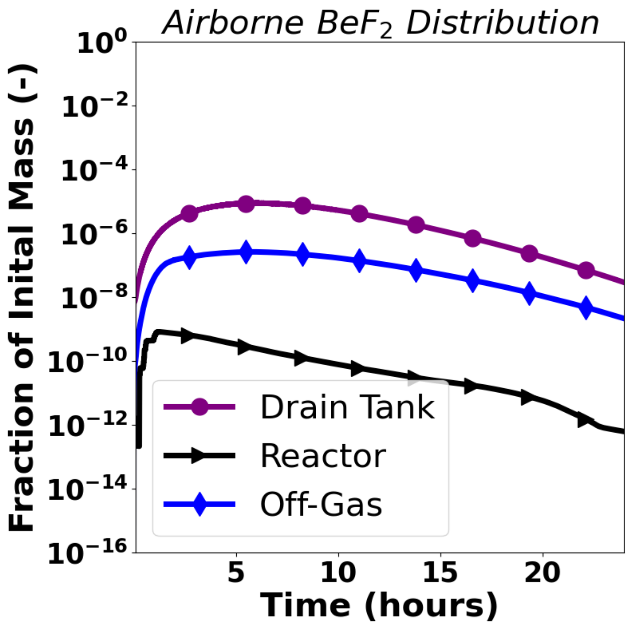
Emergency Drain: BeF_2 and UF_4 Distribution

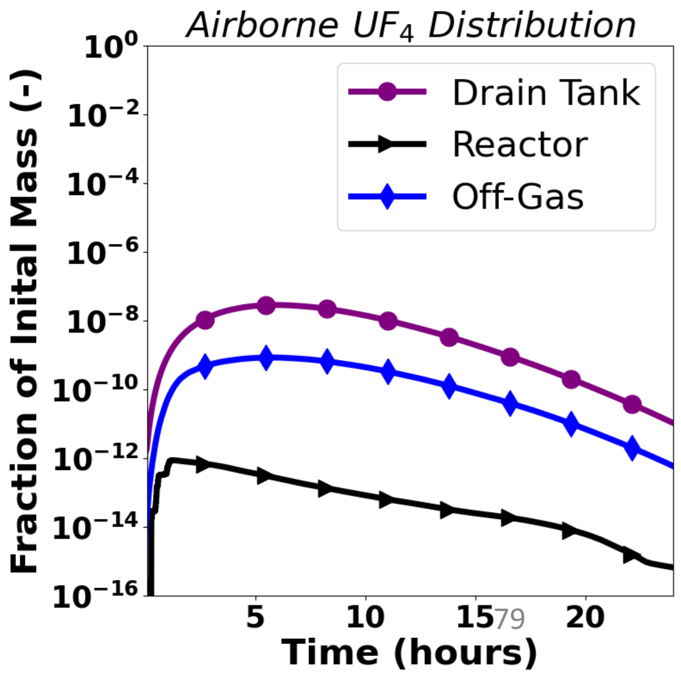
- Small amounts of BeF_2 and UF_4 continuously released
- Release rates vary as function of fuel salt temperature
- Airborne species condense back into pool and deposit on cool drain tank wall







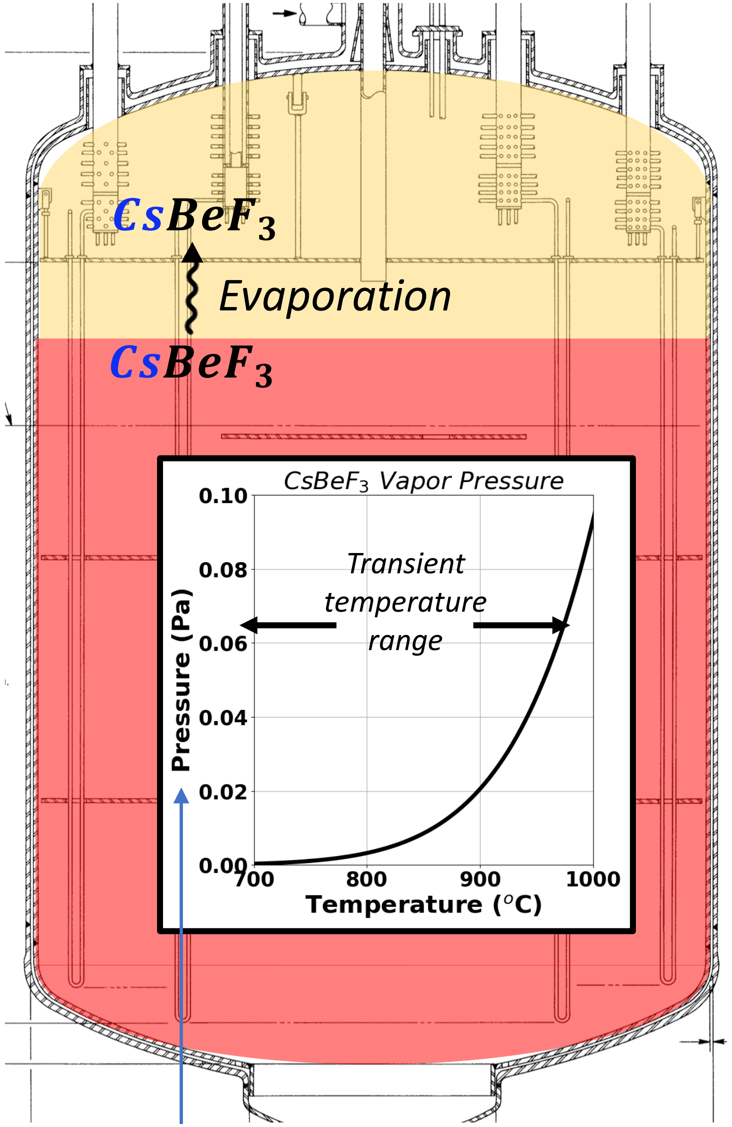




Emergency Drain: Importance of ORIGEN/MELCOR Integration

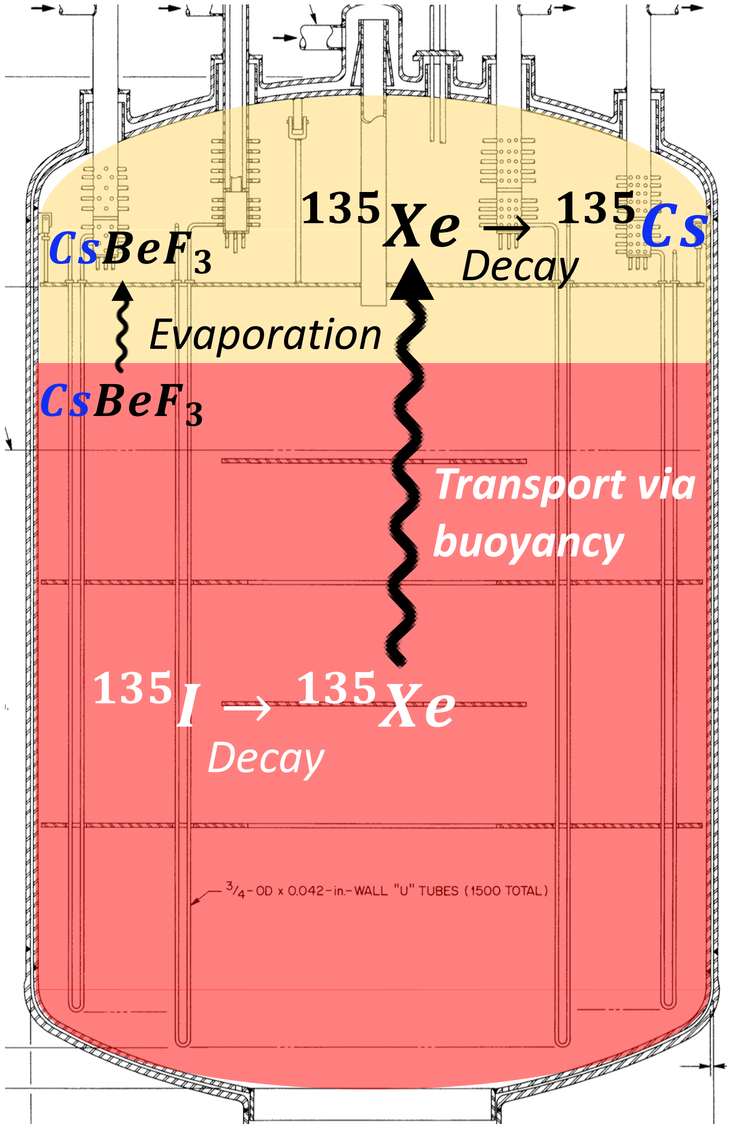
- Elements grouped into representative classes based on particular commonality
  - Solubility and isolating non-soluble corrosion products for MSRs
- MELCOR handles mass transport of classes
  - Advection and evaporation
- With ORIGEN integration, transmutation contributes to mass transfer *between* classes

Without ORIGEN integration



Essentially no Cs release

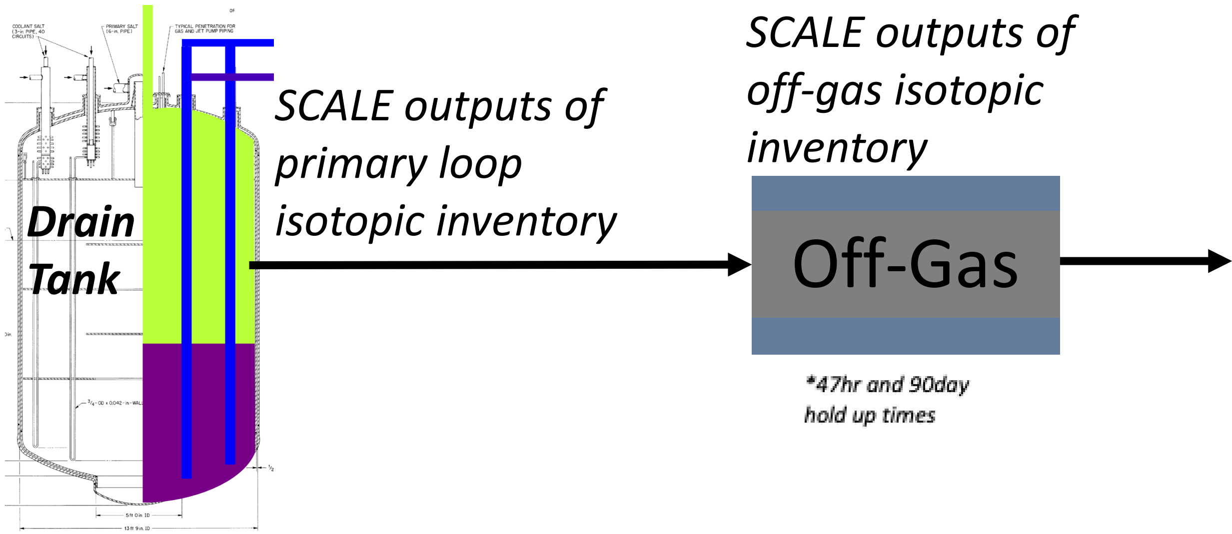
With ORIGEN integration

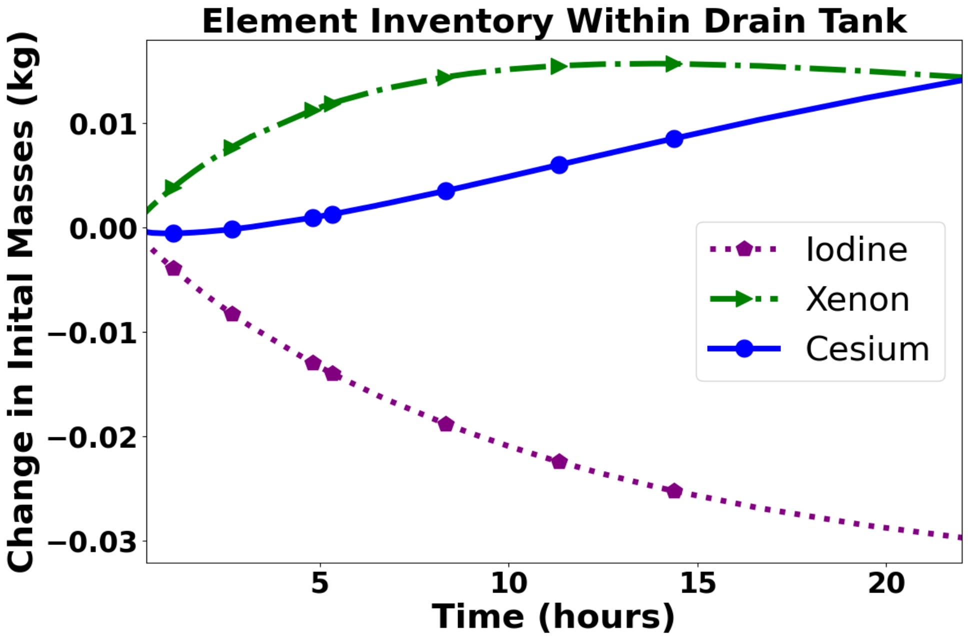


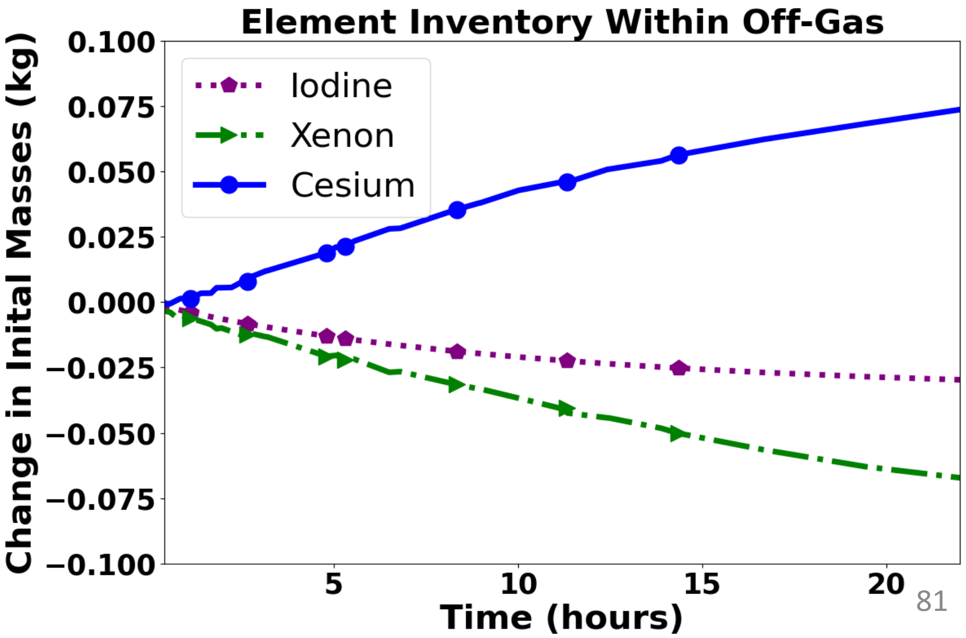
Cs release via iodine decay chain

Emergency Drain: Radioactive Decay In Off-Gas

- Integration of allows for investigation of specific elements
  - Can **track the transport, production, and decay** of isotopes such as xenon-135 within the 'Xe' class
- Region wise isotopic inventories provided by SCALE calculations used as initial conditions for MELCOR

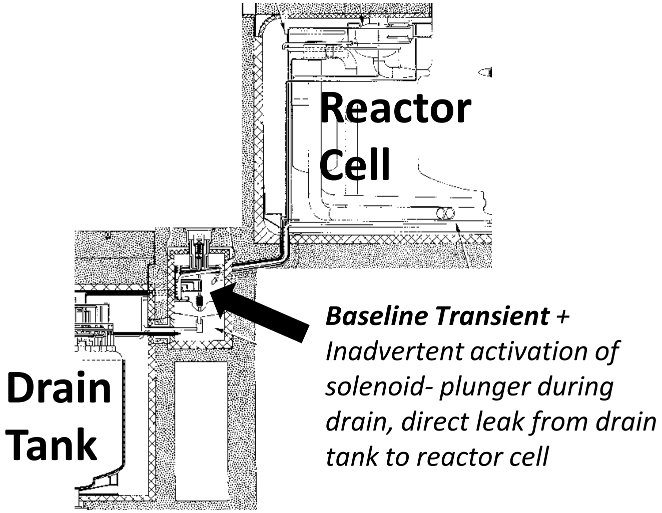


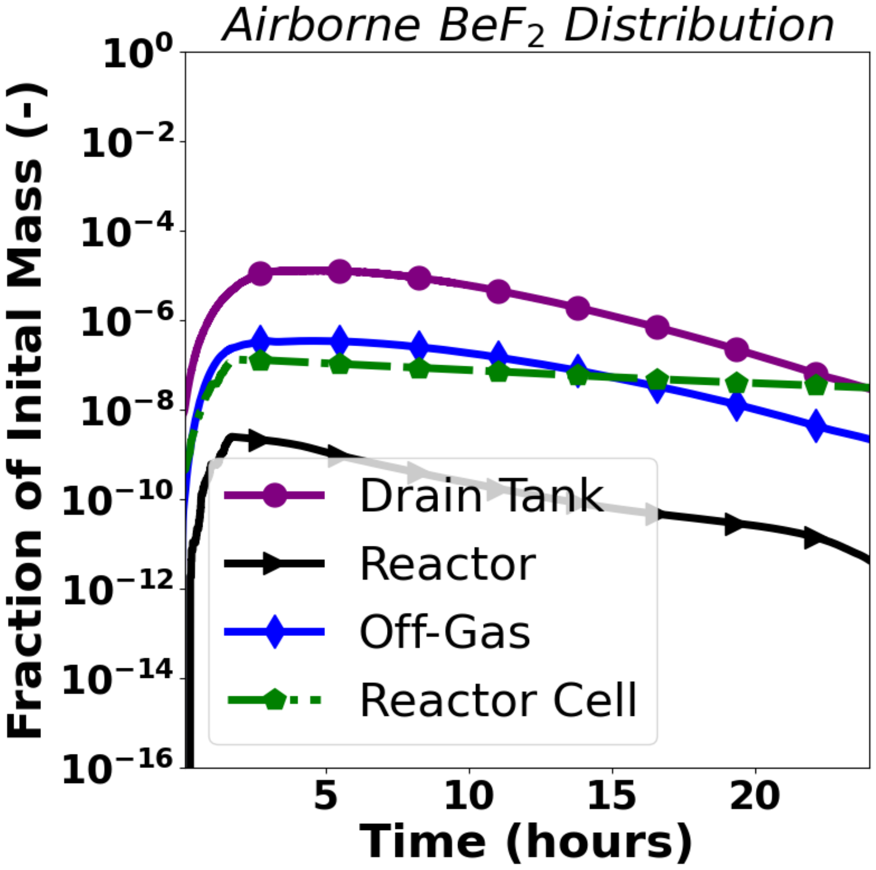


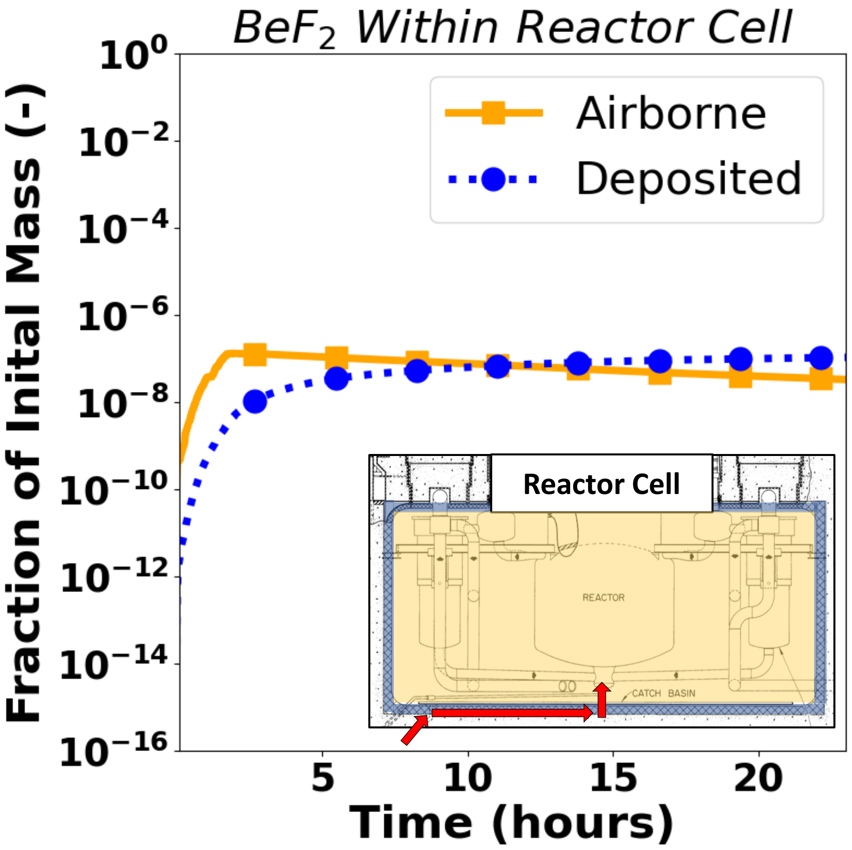


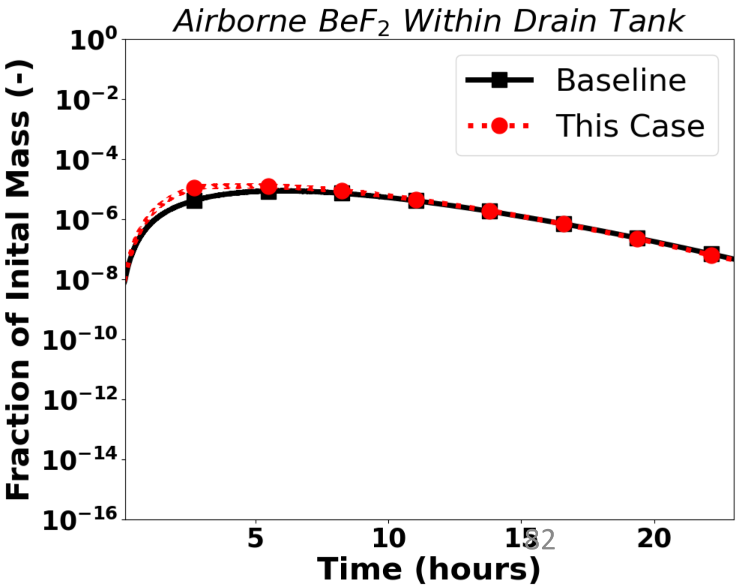
Sensitivity Cases: Case 1

- Postulated activation of solenoid plunger
  - Allows direct flow path from drain tank to reactor cell
- Similar drain tank response to baseline case, temperatures & BeF_2 release
- Fraction of BeF_2 escapes into reactor cell as airborne aerosol
- Condenses onto cooler surfaces within reactor cell



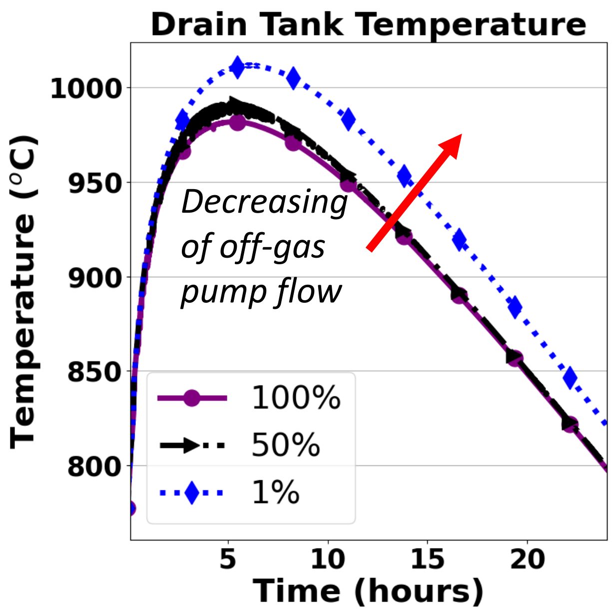


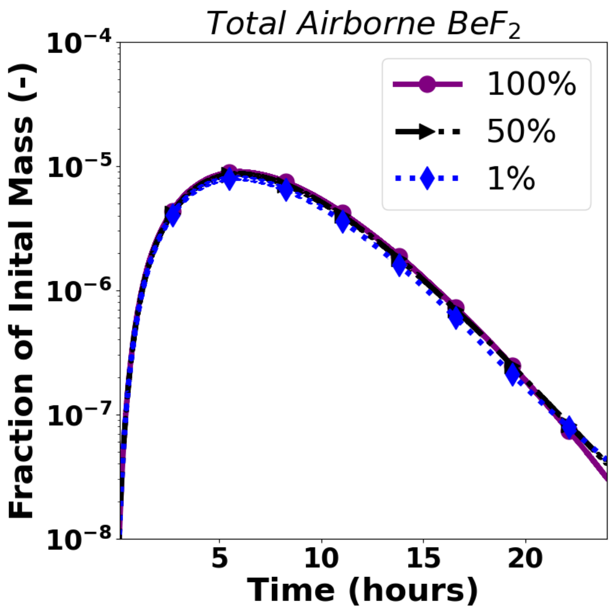


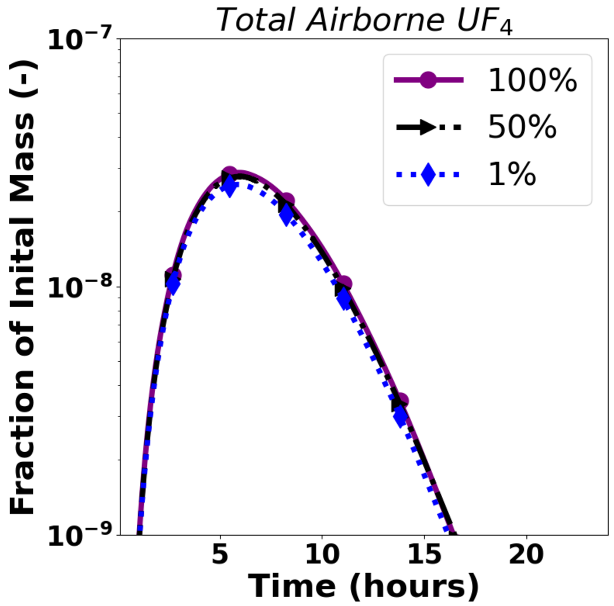


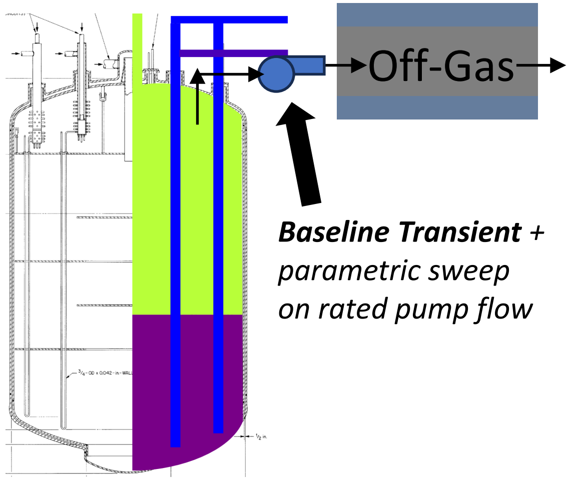
Sensitivity Cases: Case 2

- Parametric sweep on off gas pump flow rate

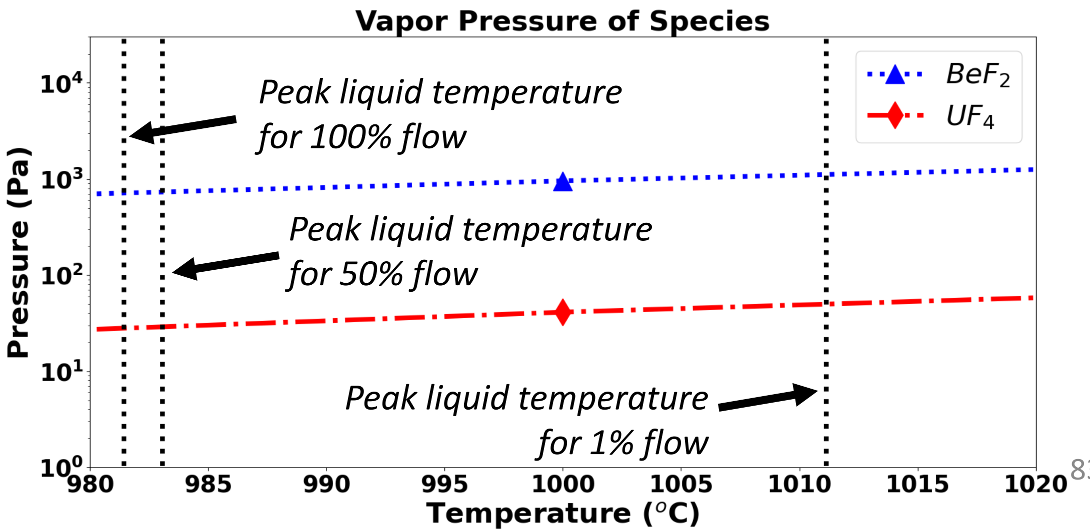






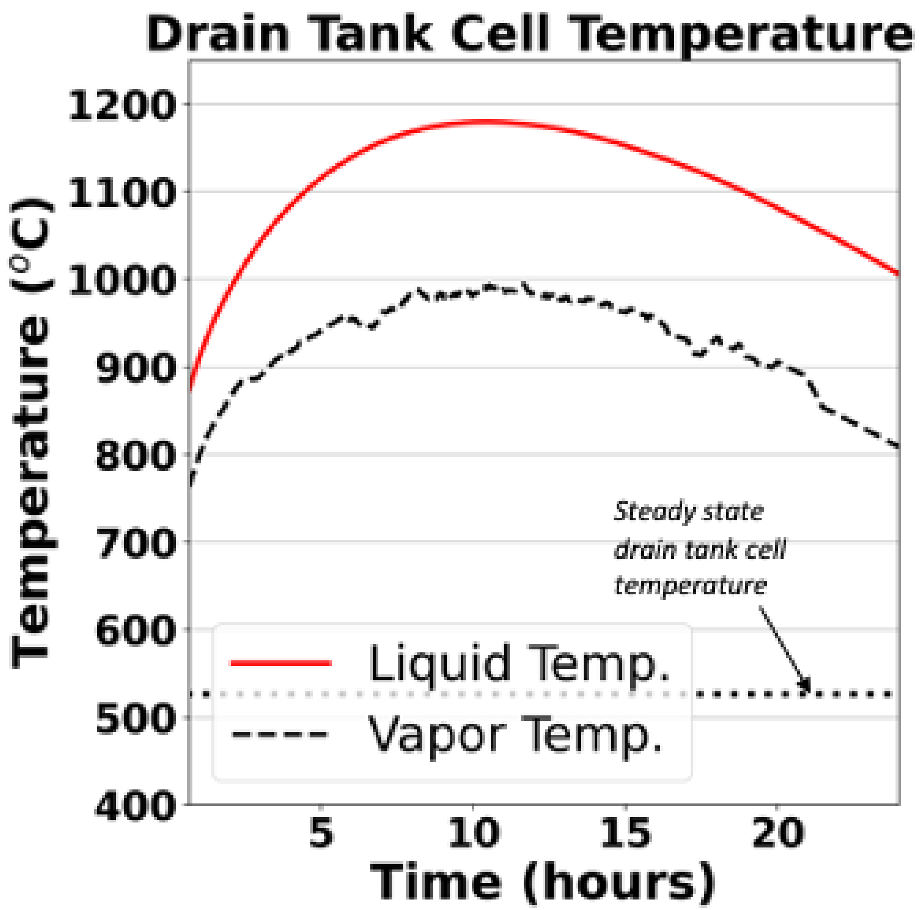


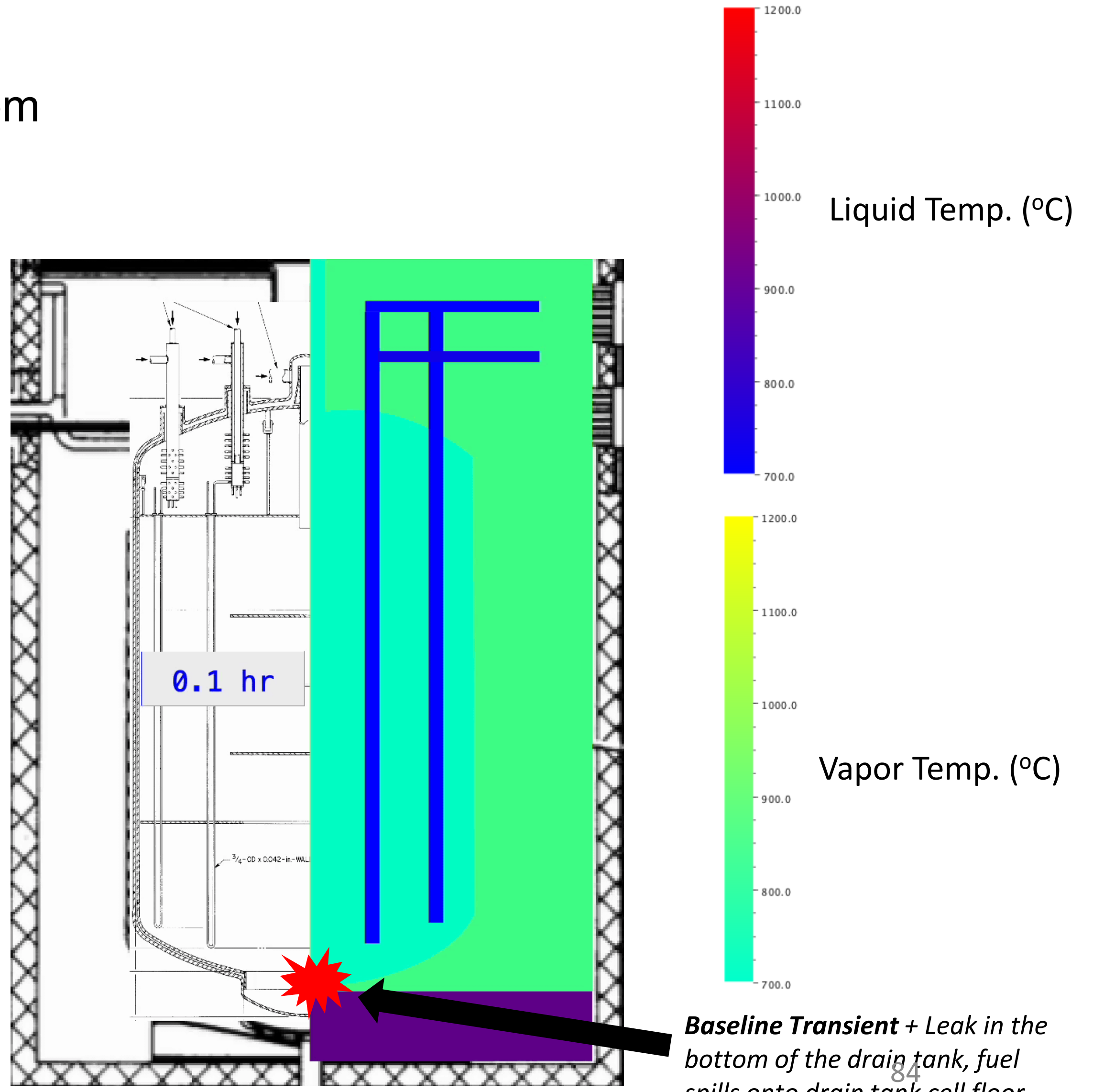
- Similar fraction of total airborne species for all off-gas pump flow rates
- Airborne release of chemical spices largely influenced by liquid temperatures
  - Vaporization relatively invariant **at drain tank temperature range in parametric sweep cases**



Sensitivity Cases: Case 3

- 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

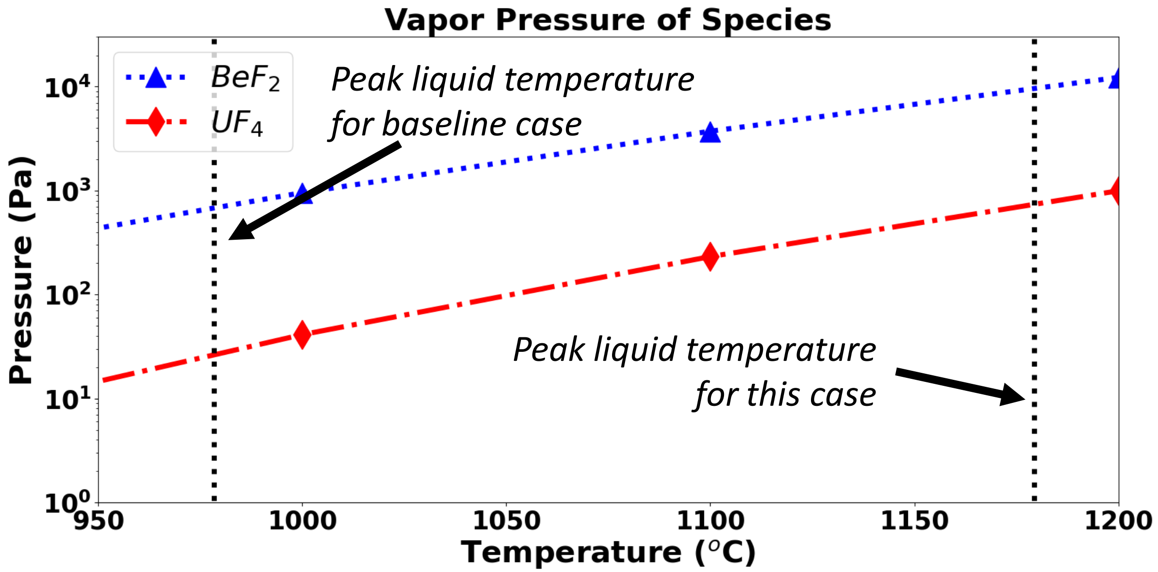


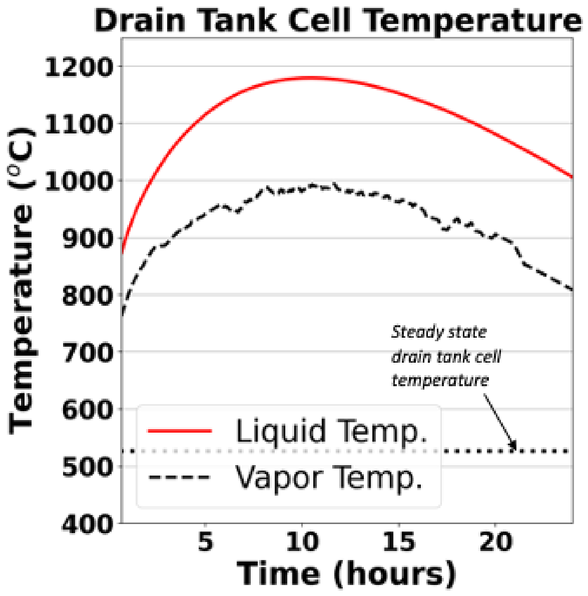


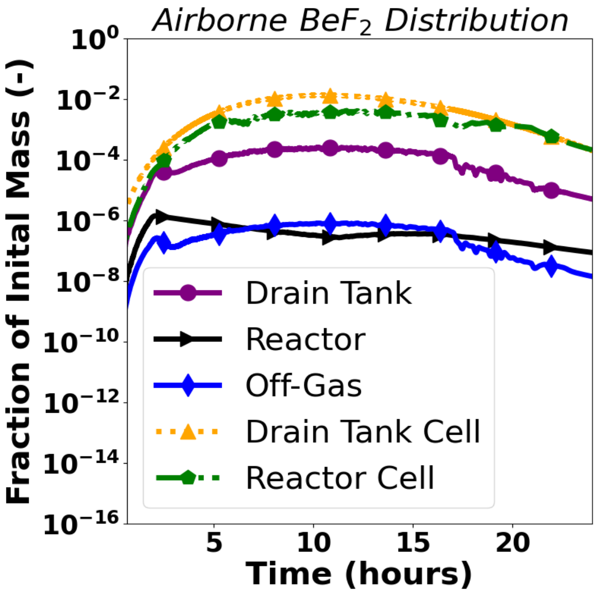
Baseline Transient *+ Leak in the bottom of the drain tank, fuel spills onto drain tank cell floor*

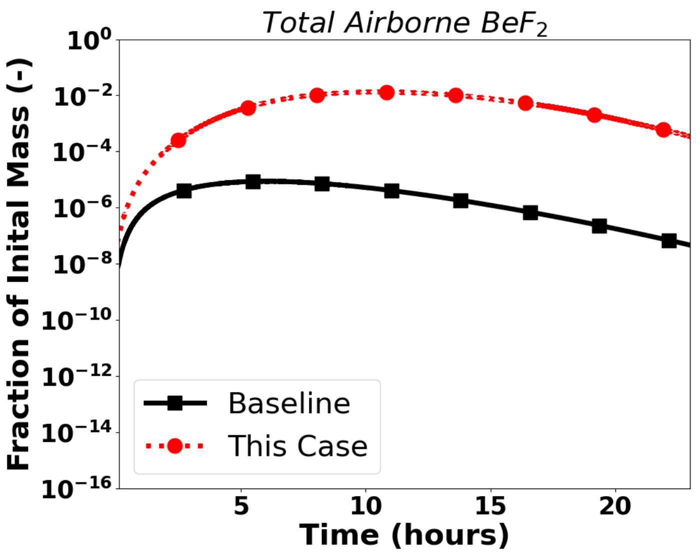
Sensitivity Cases: Case 3

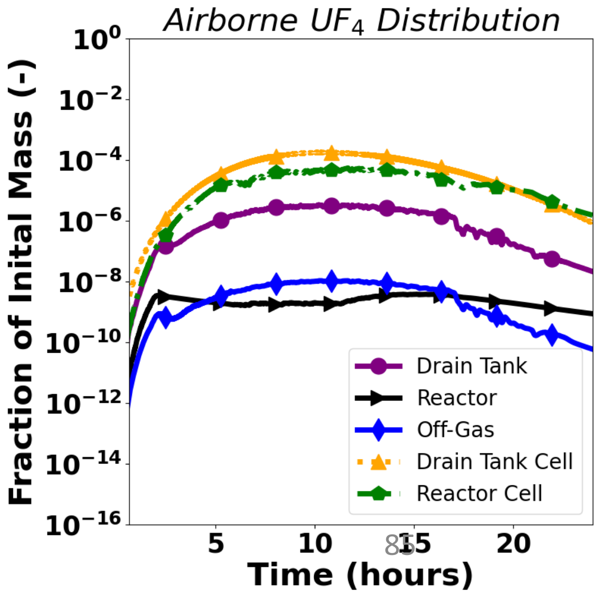
- Higher liquid temperatures due to insufficient cooling, around an order of magnitude higher vapor pressure
- Initially lower atmosphere pressure in drain tank cell than drain tank
- **Much larger fraction of airborne BeF_2 and UF_4 than in baseline case**
  - Significant fraction of airborne species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











MELCOR Summary

MELCOR MSR Fuel Cycle Demo Summary

- New MELCOR MSR capabilities were demonstrated
  - Coupling MSTDB-TC chemistry insights with ORNL neutronic analyses to define fuel composition
  - Application of radionuclide & chemical species transport models
    - Future possibilities for tritium transport (salt transmutations/fusion systems)
  - Demonstration of simultaneous & independent ORIGEN/MELCOR nuclide behavior and transport in multiple regions (drain tank liquid, drain tank airborne, off-gas system)
  - New MSBR model developed for the workshop
- Capabilities for MSR fuel cycle accident scenarios
  - MSR thermal hydraulics
  - Molten fuel salt radionuclide chemistry
  - Fission product release from molten salt fuel
  - Radionuclide mobility transport changes tracked in daughter products
- Future work and data needs
  - Expand fission product release & retention modeling from spills, vaporization, deposition, and transmutation
  - Continue incorporation of data from chemistry databases

Workshop Summary

Closing Remarks

- *Demonstration of NRC's Code Readiness for Reviewing non-LWRs*
  - *HTGR Nuclear Fuel Cycle (February 2023)*
  - *SFR Nuclear Fuel Cycle (September 2023)*
  - *MSR Nuclear Fuel Cycle (July 2024)*

- *Next Steps*
  - *Public Reports*
    - *ML24004A270 - "Non-LWR Fuel Cycle Scenarios for SCALE and MELCOR Modeling Capability Demonstrations"*
    - *ML24129A035 – "SCALE Demonstration for SFR Fuel Cycle Analysis"*

  - *Microreactor Nuclear Fuel Cycle Workshop (2025)*

Backup

MELCOR Application to Fuel Cycle Safety Assessment

MELCOR is used in the DOE complex for facility safety analysis

MELCOR has **general and validated** models for thermal hydraulic behavior of enclosures and hazardous material transport

- Enables modeling of potential for fission products to be released from an enclosure to the environment

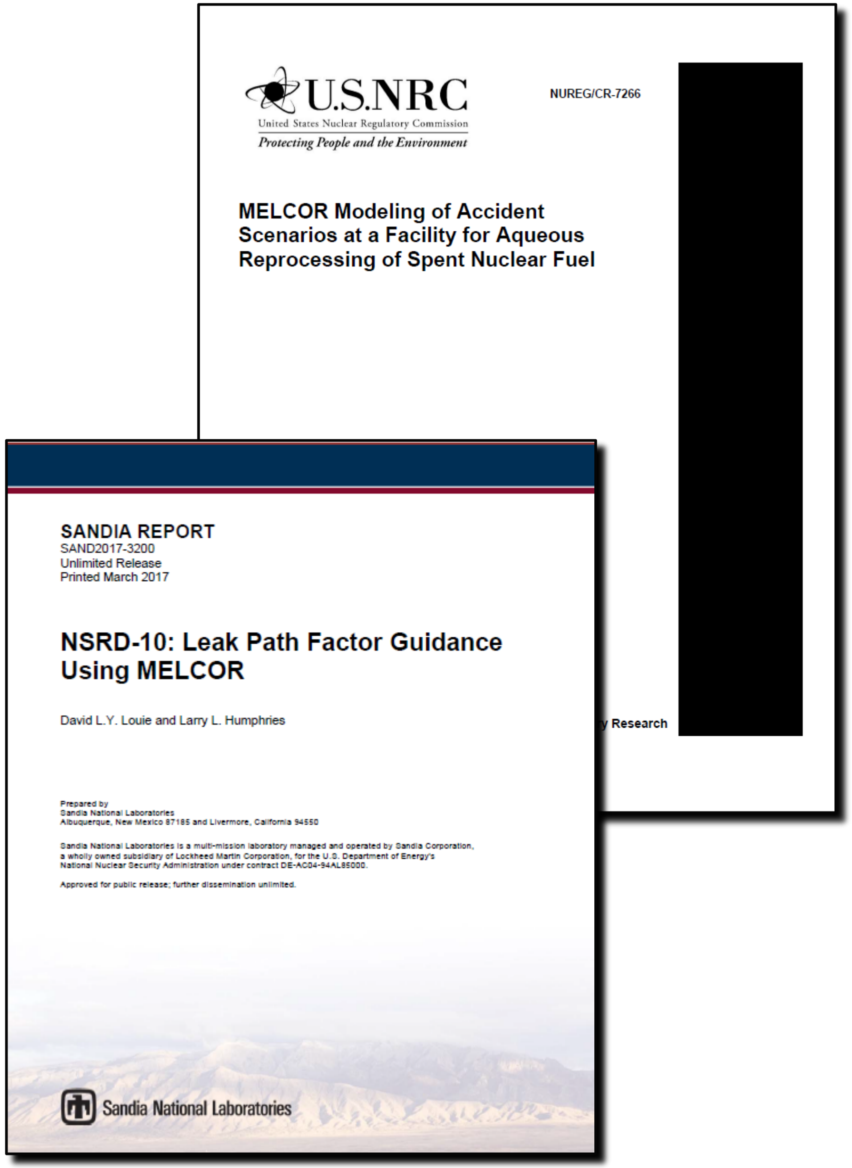
MELCOR has been applied to safety basis development for a broad range of facility accidents that can lead to accident release of hazardous material

- Inadvertent nuclear criticality events
- Explosions
- Broad range of facility fires
- Radioactive material spills and drops

MELCOR enables assessment of a range of conditions that can impact hazardous material release to the environment

- External winds promoting enhanced transport from an enclosure to environment
- Retention of hazardous material in filters
- Removal of hazardous material from enclosure atmospheres by decontamination sprays

Recent NRC research application of MELCOR to demonstration of safety assessment at Barnwell reprocessing facility



U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment
NUREG/CR-7266

MELCOR Modeling of Accident Scenarios at a Facility for Aqueous Reprocessing of Spent Nuclear Fuel

Research

SANDIA REPORT
SAND2017-3200
Unlimited Release
Printed March 2017

NSRD-10: Leak Path Factor Guidance Using MELCOR

David L.Y. Louie and Larry L. Humphries

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Element Grouping

Class Name	Elements in Class		Class Name	Elements in Class
XE	He, Ne, Ar, Kr, Xe, Rn, H, N		**NB**	Nb, Zn, Cd, Se, Te
CS	Li, Na, K, Rb, Cs, Fr, Cu		**CE**	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
BA	~~Be,~~ Mg, Ca, Sr, Ba, Ra, Es		**LA**	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
I2	~~F,~~ Cl, Br, I, At		**~~UO2~~ UF**	U
S	S, Po		**CD**	Hg, Ga, In
RE	Re, Os, Ir, Pt, Au, Ni		**AG**	Pb, Tl, Bi
V	V, Cr, Fe, Co, M, Ta, W		**BO2**	B, Si, P
MO	Mo, Tc, Ru, Rh, Pd, Ag, Ge, As, Sn, Sb		**BEF**	Be, F

List of Acronyms

AC - Actinides

BOC – Beginning of Cycle

CE – Continuous Energy

Ci – Curie

CSAS – Criticality Safety Analysis Sequences

EFPY – Effective Full Power Years

ENDF – Evaluated Nuclear Data File

EOC – End of Cycle

EOS – Equation of State

FHR – Fluoride Salt Cooled High Temperature Reactor

FP – Fission Products

HALEU – High Assay Low Enriched Uranium

HPR – Heat Pipe Reactor

HTGR – High Temperature Gas Cooled Reactor

IAP – Implementation Action Plan

IPS – Iron Pipe Size

LT – Light Elements

LWR – Light Water Reactor

MAVRIC – Monaco with Automated Variance Reduction using Importance Calculations

MeV – Mega Electronvolt

MG - Multigroup

MSBR – Molten Salt Breeder Reactor

MSR – Molten Salt Reactor

MSRE – Molten Salt Reactor Experiment

MSTDB – Molten Salt Thermal Properties Database

MTIHM – Metric Ton of Initial Heavy Metal

MWth – Megawatt Thermal

OGS – Off Gas System

Pa – Pascal

pcm – per cent mille

PWR – Pressurized Water Reactor

SFR – Sodium Fast Reactor

Sv – Sievert

TRISO – Tri-structural Isotropic

UCB – University of California Berkely