SAND2022-12146 PE

SCALE/MELCOR Non-LWR Source Term Demonstration Project – Molten Salt Reactor (MSR)

September 13, 2022

U.S.NRC

Sandia National Laboratories

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. SAND20XX-XXXX P

U.S. DEPARTMENT OF ENERGY

NNSA

Outline

NRC strategy for non-LWR source term analysis

Project scope

Overview of Molten Salt Reactor (MSR)

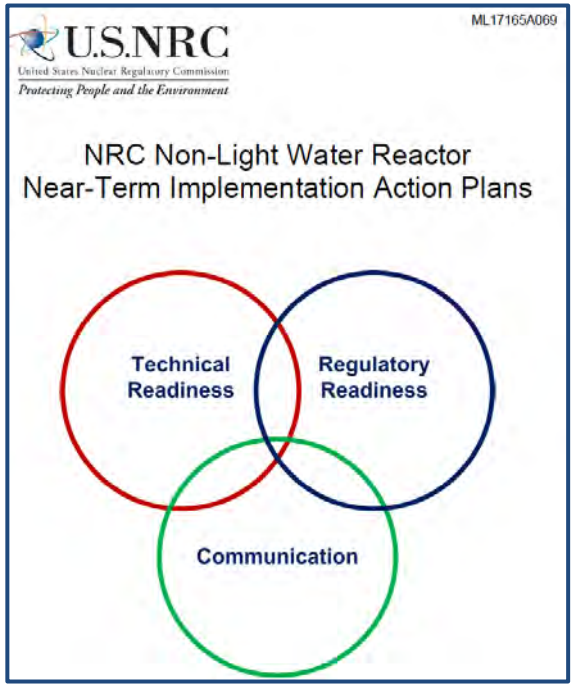
MSR reactor fission product inventory/decay heat methods & results

MELCOR molten salt models

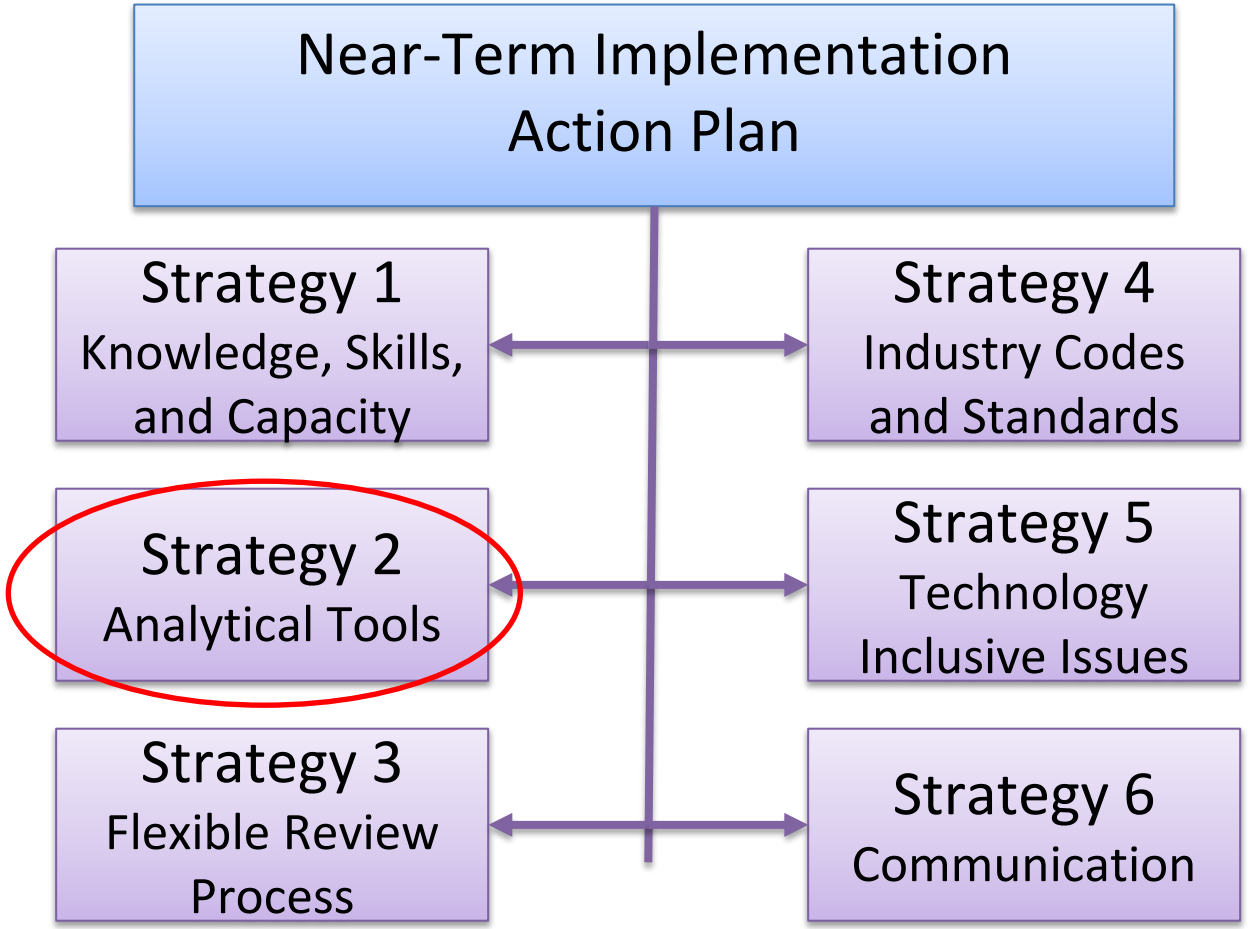
MSR plant model and source term analysis

Summary

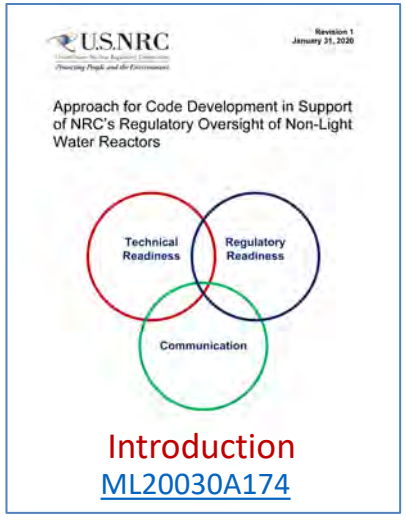
Integrated Action Plan (IAP) for Advanced Reactors



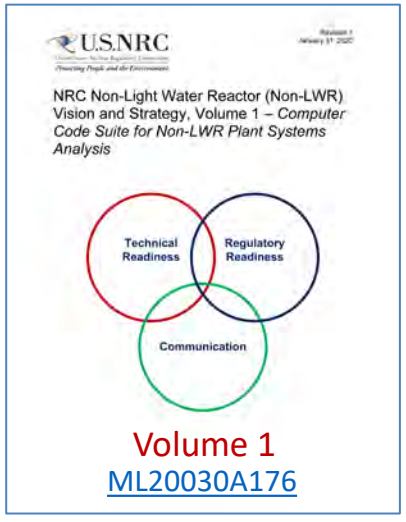
ML17165A069



IAP Strategy 2 Volumes



Introduction
ML20030A174

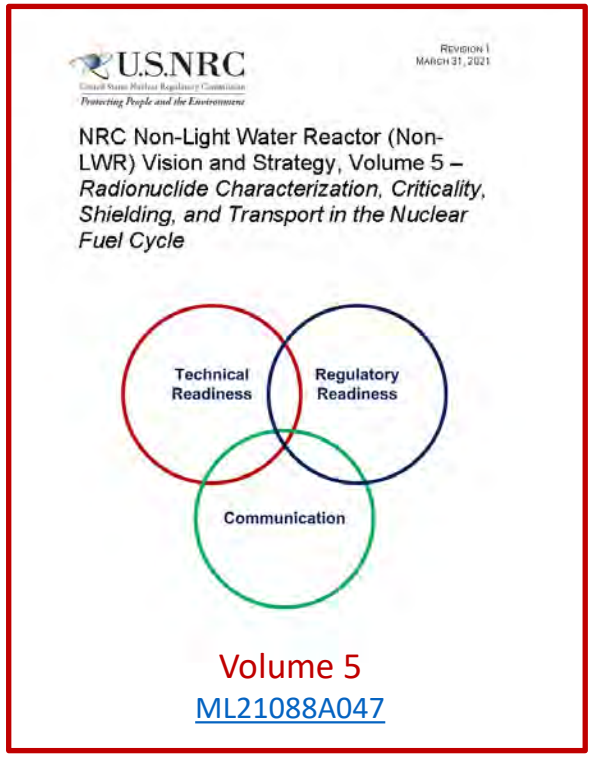


Volume 1
ML20030A176

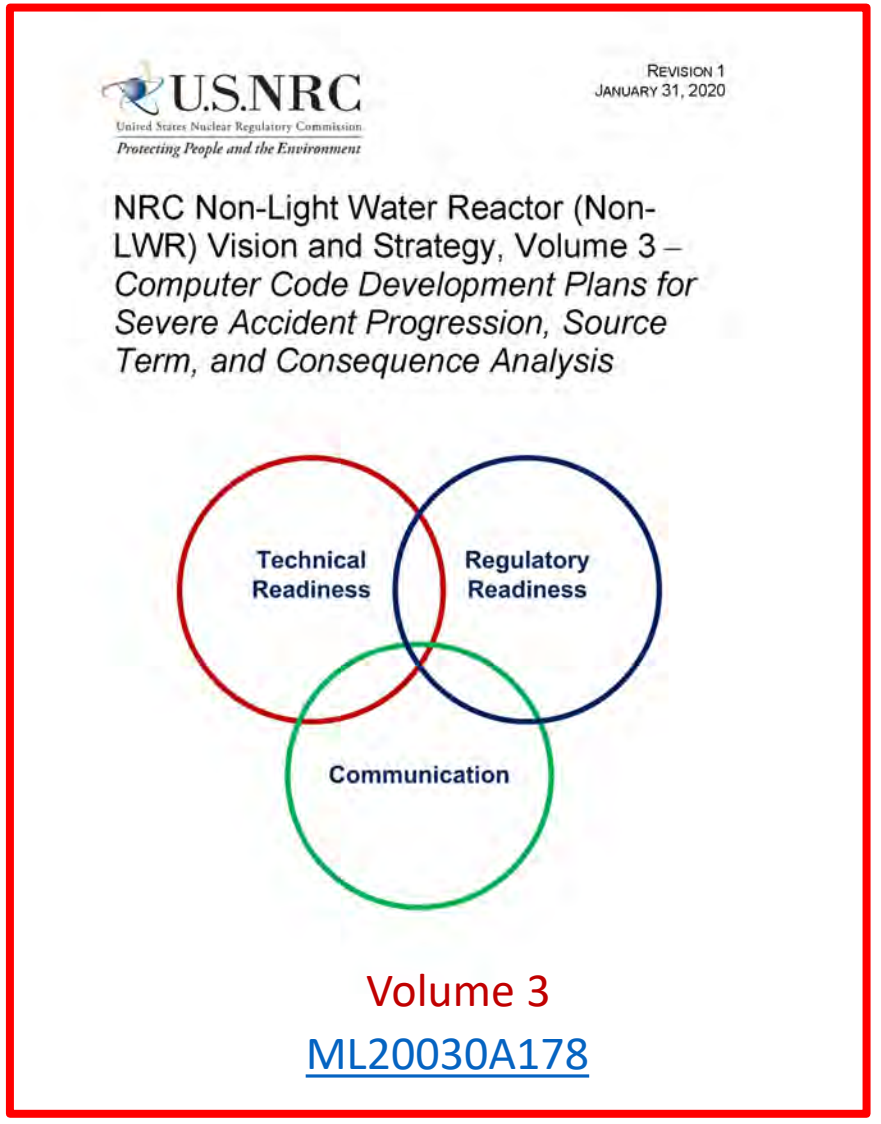
Volume 2
ML20030A177

Volume 4
ML21085A484

These Volumes outline the specific analytical tools to enable independent analysis of non-LWRs, "gaps" in code capabilities and data, V&V needs and code development tasks.



Volume 5
ML21088A047



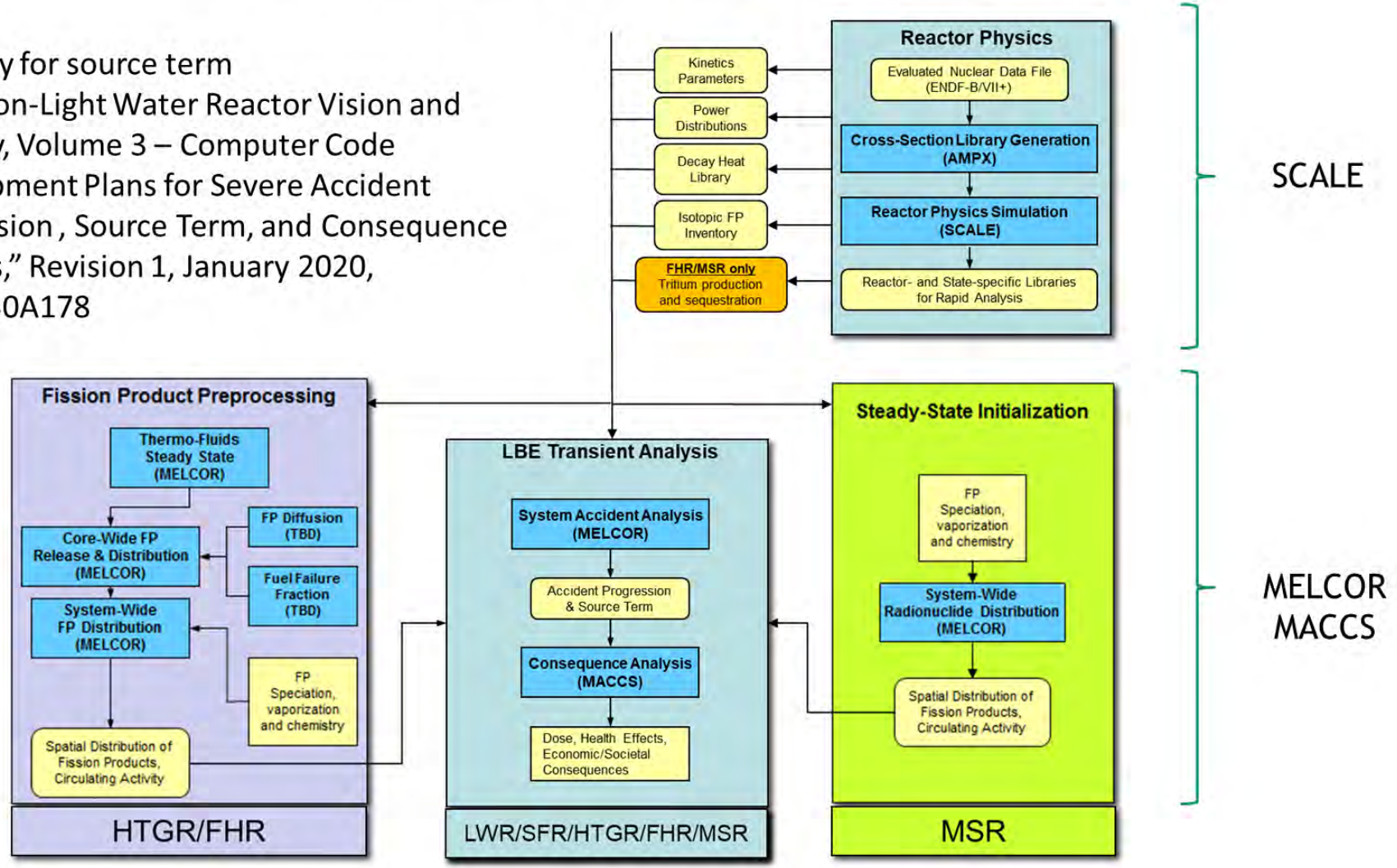
Volume 3
ML20030A178

NRC strategy for non-LWR analysis (Volume 3)

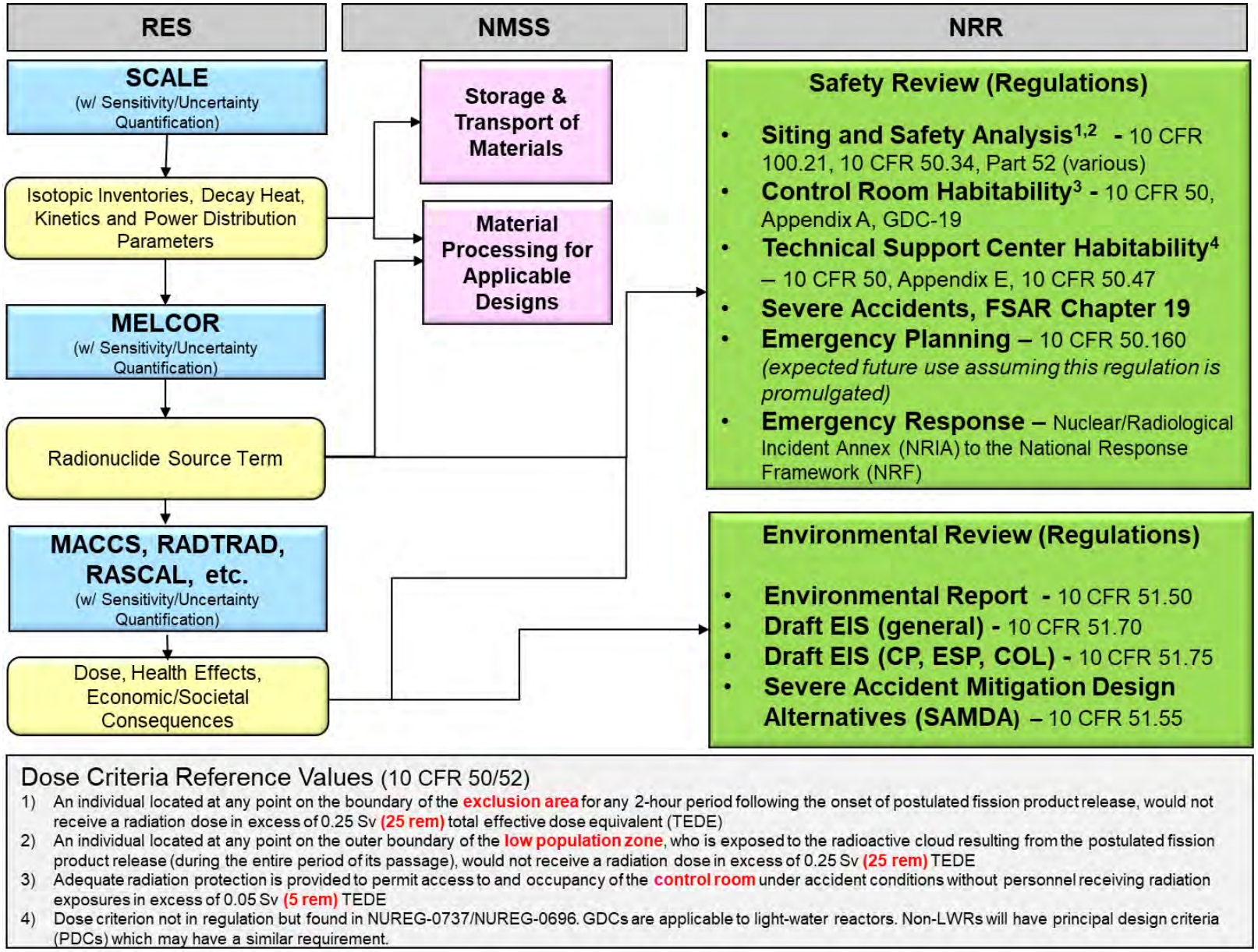
Evaluation Model and Suite of Codes

Code strategy for source term

"NRC Non-Light Water Reactor Vision and Strategy, Volume 3 – Computer Code Development Plans for Severe Accident Progression , Source Term, and Consequence Analysis," Revision 1, January 2020, ML20030A178



Role of NRC severe accident codes



Dose Criteria Reference Values (10 CFR 50/52)

1) An individual located at any point on the boundary of the **exclusion area** for any 2-hour period following the onset of postulated fission product release, would not receive a radiation dose in excess of 0.25 Sv **(25 rem)** total effective dose equivalent (TEDE)
2) An individual located at any point on the outer boundary of the **low population zone**, who is exposed to the radioactive cloud resulting from the postulated fission product release (during the entire period of its passage), would not receive a radiation dose in excess of 0.25 Sv **(25 rem)** TEDE
3) Adequate radiation protection is provided to permit access to and occupancy of the **control room** under accident conditions without personnel receiving radiation exposures in excess of 0.05 Sv **(5 rem)** TEDE
4) Dose criterion not in regulation but found in NUREG-0737/NUREG-0696. GDCs are applicable to light-water reactors. Non-LWRs will have principal design criteria (PDCs) which may have a similar requirement.

Project Scope

U.S.NRC

OAK RIDGE National Laboratory

Sandia National Laboratories

Project objectives

Understand severe accident behavior

- Provide insights for regulatory guidance

Facilitate dialogue on staff's approach for source term

Demonstrate use of SCALE and MELCOR

- Identify accident characteristics and uncertainties affecting source term
- Develop publicly available input models for representative designs

Project scope

Full-plant models and sample calculations for representative non-LWRs

2021

- Heat pipe reactor – INL Design A
- Pebble-bed gas-cooled reactor – PBMR-400
- Pebble-bed molten-salt-cooled – UCB Mark 1
- Public workshop videos, slides, reports at advanced reactor source term webpage

2022

- Molten-salt-fueled reactor – MSRE – public workshop 9/13/2022
- Sodium-cooled fast reactor – ABTR – public workshop 9/20/2022

2023

- Additional code enhancements and sample calculations

Project approach

1. Build SCALE core model and MELCOR full-plant model
2. Select scenarios that demonstrate code capabilities
3. Perform simulations
    - Use SCALE to model decay heat, core radionuclide inventory, and reactivity feedback
    - Use MELCOR to model accident progression and source term
    - Perform sensitivity cases

Molten Salt Reactor (MSR)

U.S.NRC

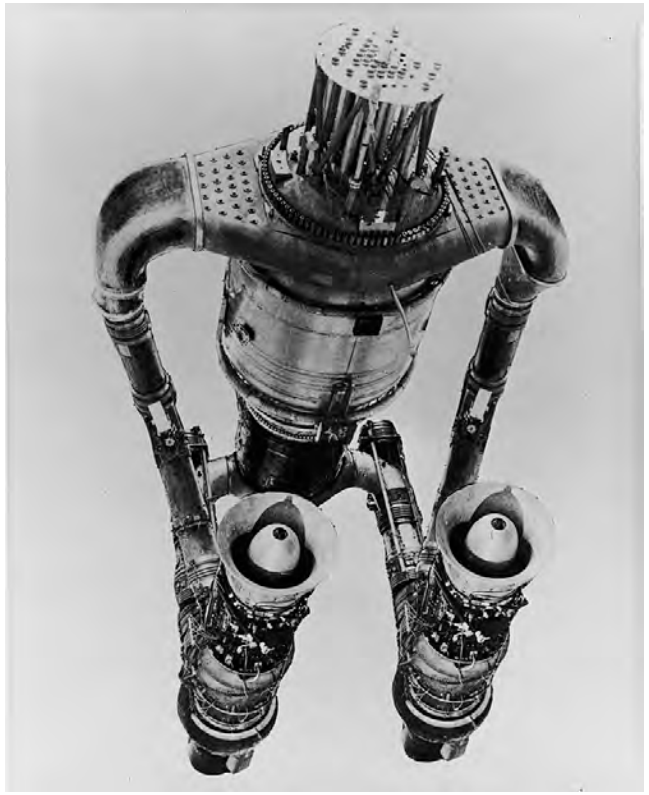
Sandia
National
Laboratories

Molten-salt reactor history (1/2)

Aircraft Nuclear Propulsion Program (ANP) – 1946-1961

- Long-term strategic bomber operation using nuclear power
- ORNL developed the nuclear concept with the Aircraft Reactor Experiment (ARE)
  - Originally sodium cooled, but shifted to molten salt
  - 2.5 MW molten salt-cooled reactor operated for 96-MW-hours in November 1954
- Three Heat Transfer Reactor Experiments at Idaho National Laboratory to demonstrate the jet engine propulsion
- Aircraft Shield Test (AFT) – B-36 with an operating reactor flew 47 times over West Texas and New Mexico to study shielding (i.e., the reactor was operating but not part of the propulsion system)
- Terminated due to inventing ballistic missile and supersonic aviation

The B-36 Aircraft Shield Test
[https://en.wikipedia.org/wiki/Convair_NB-36H#/media/File:NB36H-1.jpg]

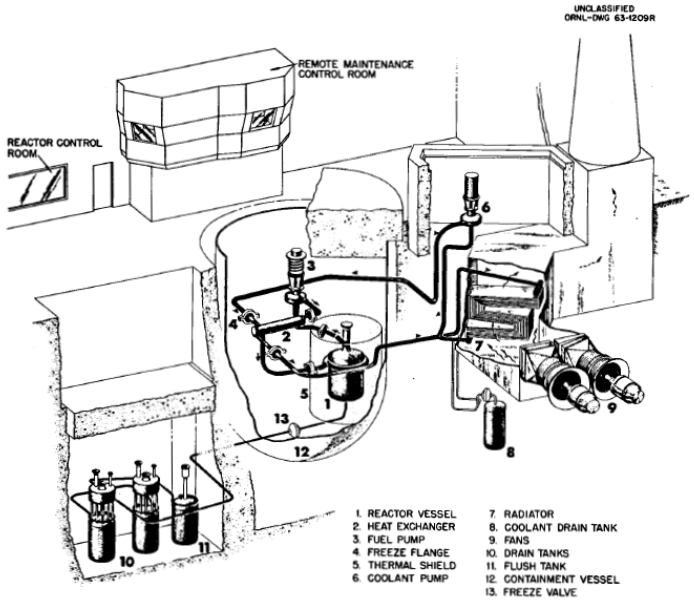


Heat Transfer Reactor Experiment #3
[https://en.wikipedia.org/wiki/Aircraft_Nuclear_Propulsion#/media/File:HTRE-3.jpg]

Molten-salt reactors history (2/2)

ORNL Molten Salt Reactor Experiment (MSRE)

- AEC funded
- Operated from 1965 to 1969
- 10 MW_{th}
- Used for SCALE MELCOR source term demonstration calculations



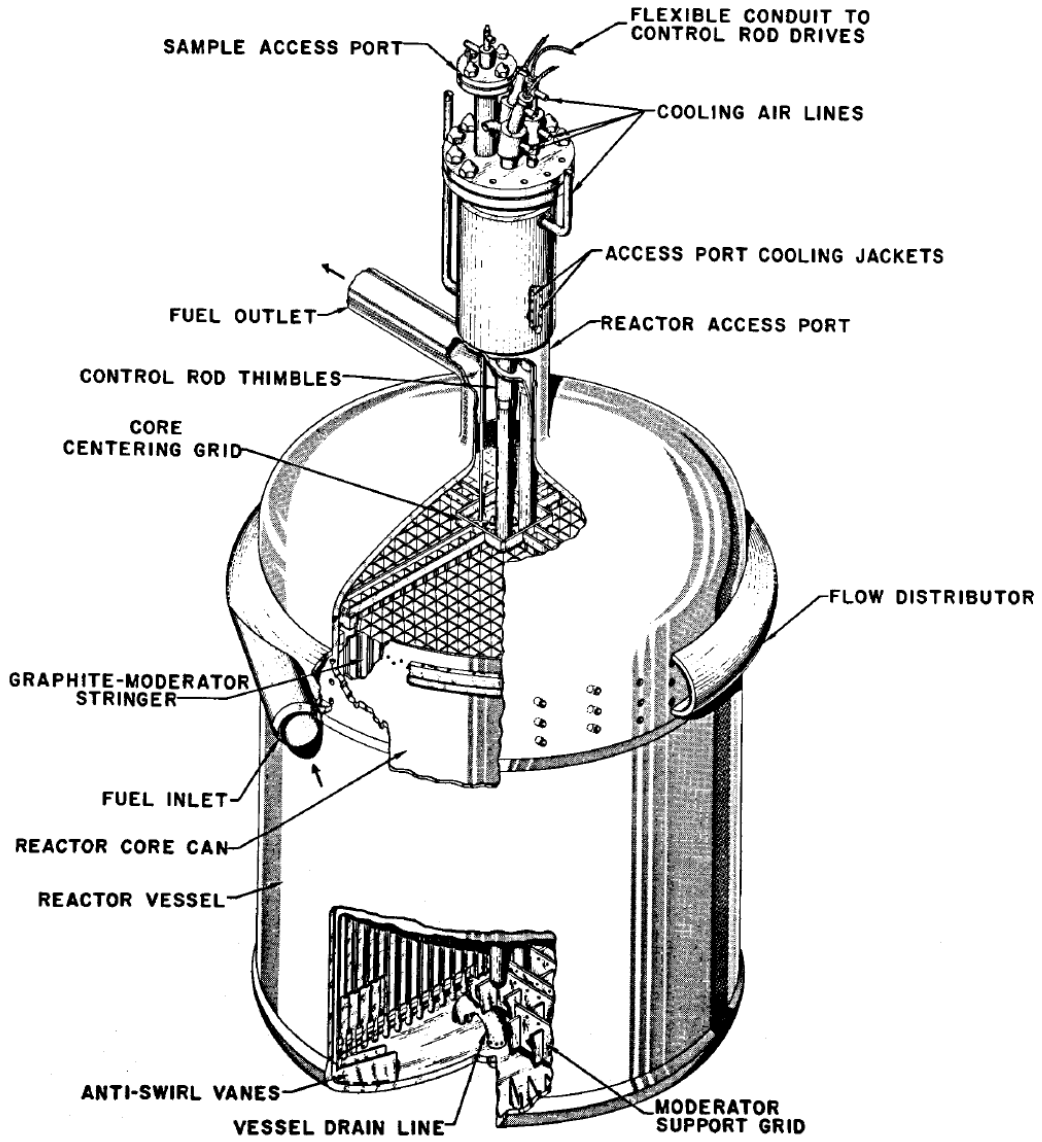
MSRE
[ORNL-TM-0728]

MSRE Graphite Core Structure
[https://en.wikipedia.org/wiki/Molten-Salt_Reactor_Experiment]

MSRE (1/5)

Reactor

- 10 MW_{th}
- Reactor consists of a graphite core structure (see photo on previous slide)
- Fuel dissolved in the molten salt coolant fissions when it passes through the graphite core structure
- Graphite provides moderation
- 0.075 m^3/s (1200 gpm) core flowrate
- 635℃ core inlet
- 668℃ core outlet
- Near atmospheric pressure in the helium above the salt
- Coolant included variations of lithium, beryllium, and zirconium fluoride salts that contain uranium, or uranium and thorium fluorides
- INOR-8 nickel-based alloy vessel



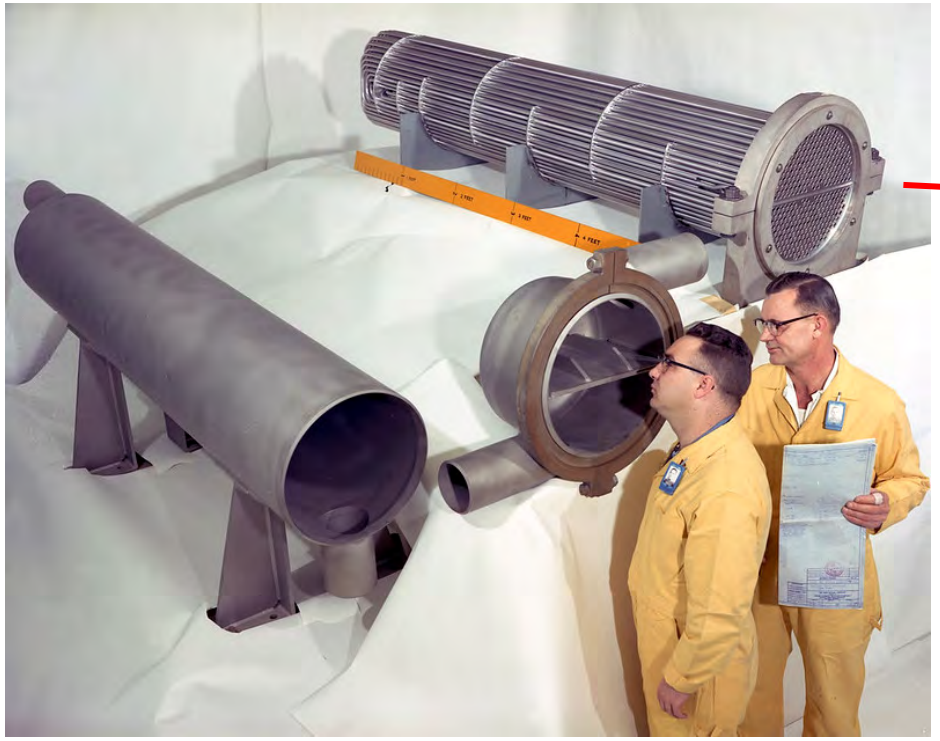
MSRE vessel
[ORNL-TM-0728]

MSRE (2/5)

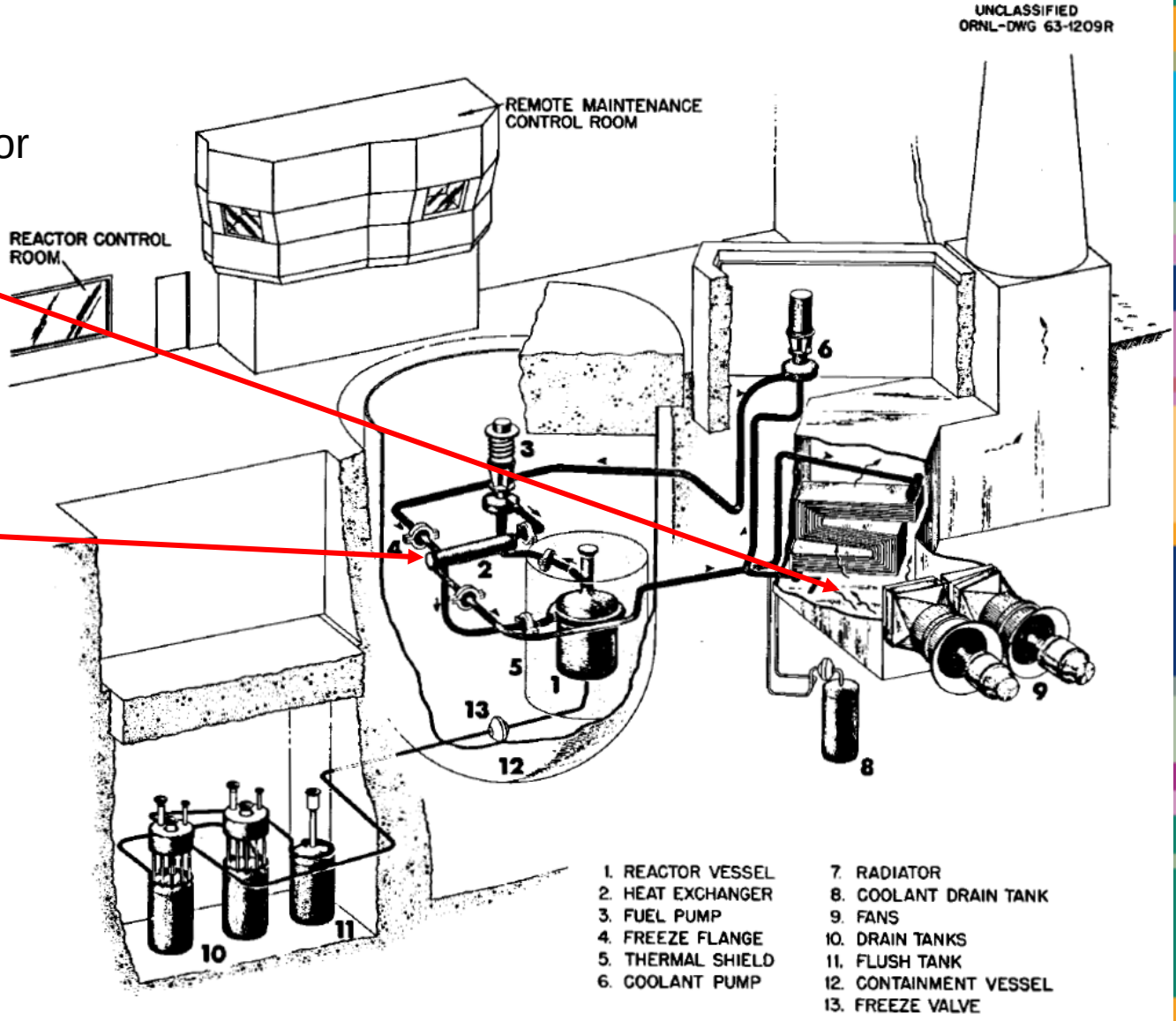
Coolant salt circulation

- Primary loop with pump and heat exchanger
- Intermediate loop with pump and air-cooled radiator
- No fuel in intermediate loop

Air-cooled radiator rejects heat to the plant stack



MSRE primary heat exchanger
[https://www.flickr.com/photos/oakridgelab/albums/72157659472696880/with/21573745744/]

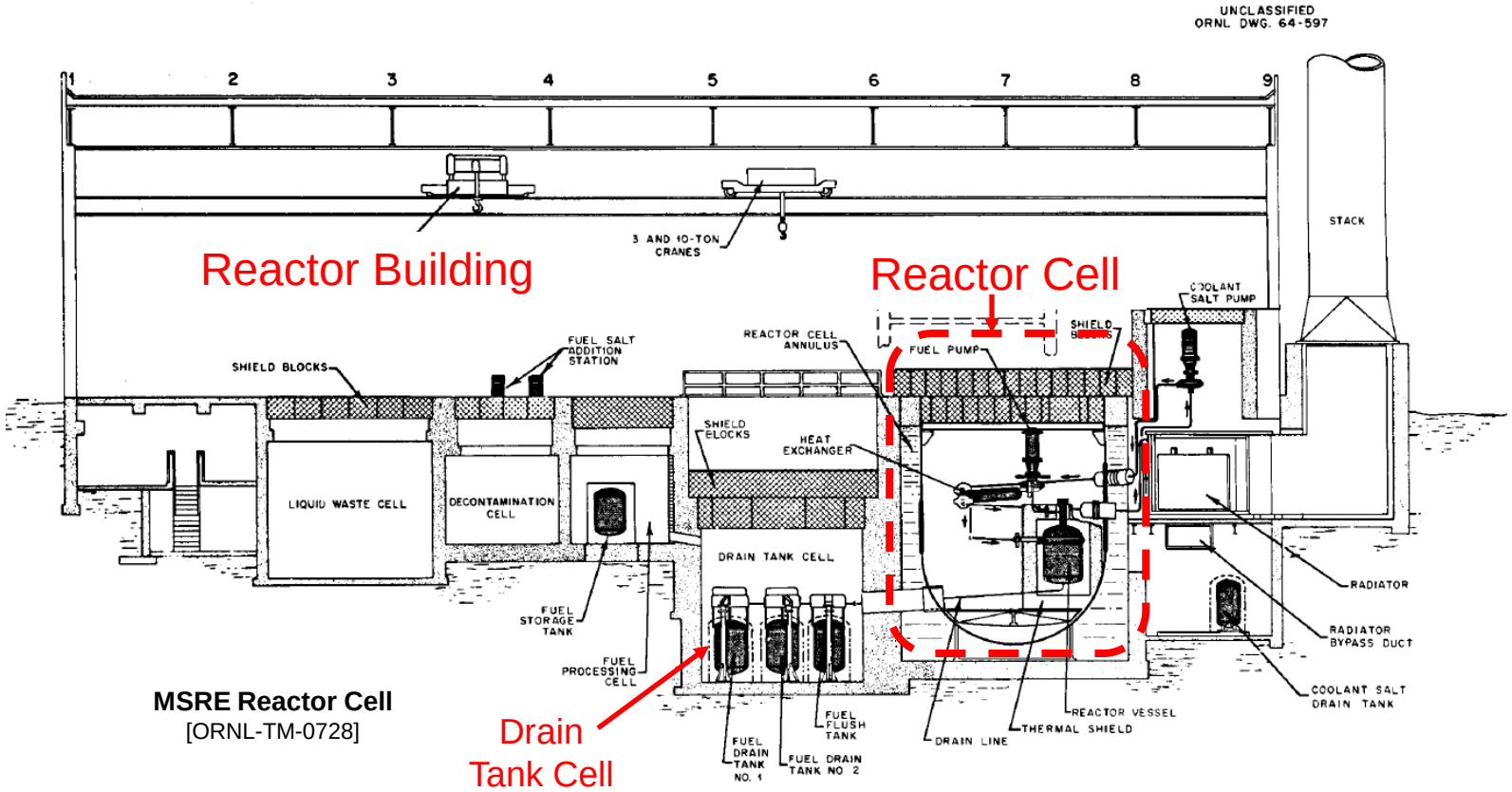


MSRE schematic
[ORNL-TM-0728]

MSRE (3/5)

Reactor Cell acts as containment

- Contains the reactor vessel, the primary circulating fuel loop, and most of the coolant salt loop
- Circulating salt to air-cooled radiators located outside of the reactor cell
- 95% N_2
- 0.875 bar absolute
- 320 m^3
- Leak rate = 0.42 standard liters per hour at 0.875 bar (12.7 psia) (0.23 mm dia.)
- Attached by a tunnel to the drain tank cell

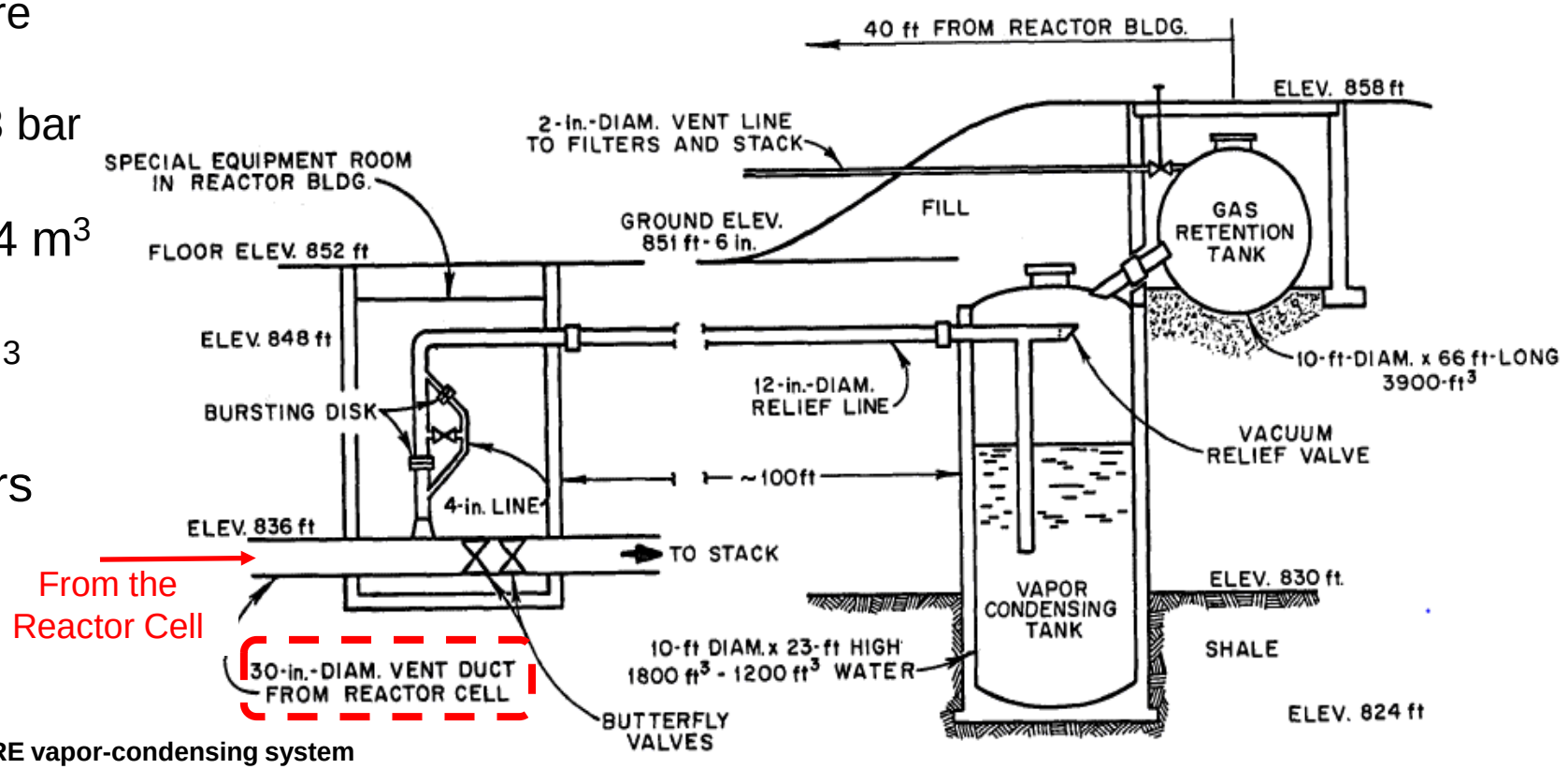


MSRE Reactor Cell
[ORNL-TM-0728]

MSRE (4/5)

Vapor-condensing system

- Connects to the reactor cell via a 30” pipe
- Normally isolated from the stack with 2 rupture disks
  - 30.5 cm (12”) line with 1.38 bar (20 psig) rupture disk
  - 10 cm (4”) line with 1.03 bar (15 psig) rupture disk
- Condensing tank with 34 m^3 (1200 ft^3) of water
- Gas retention tank 93 m^3 (3300 ft^3)
- 5 cm (2”) line to the filters and the stack

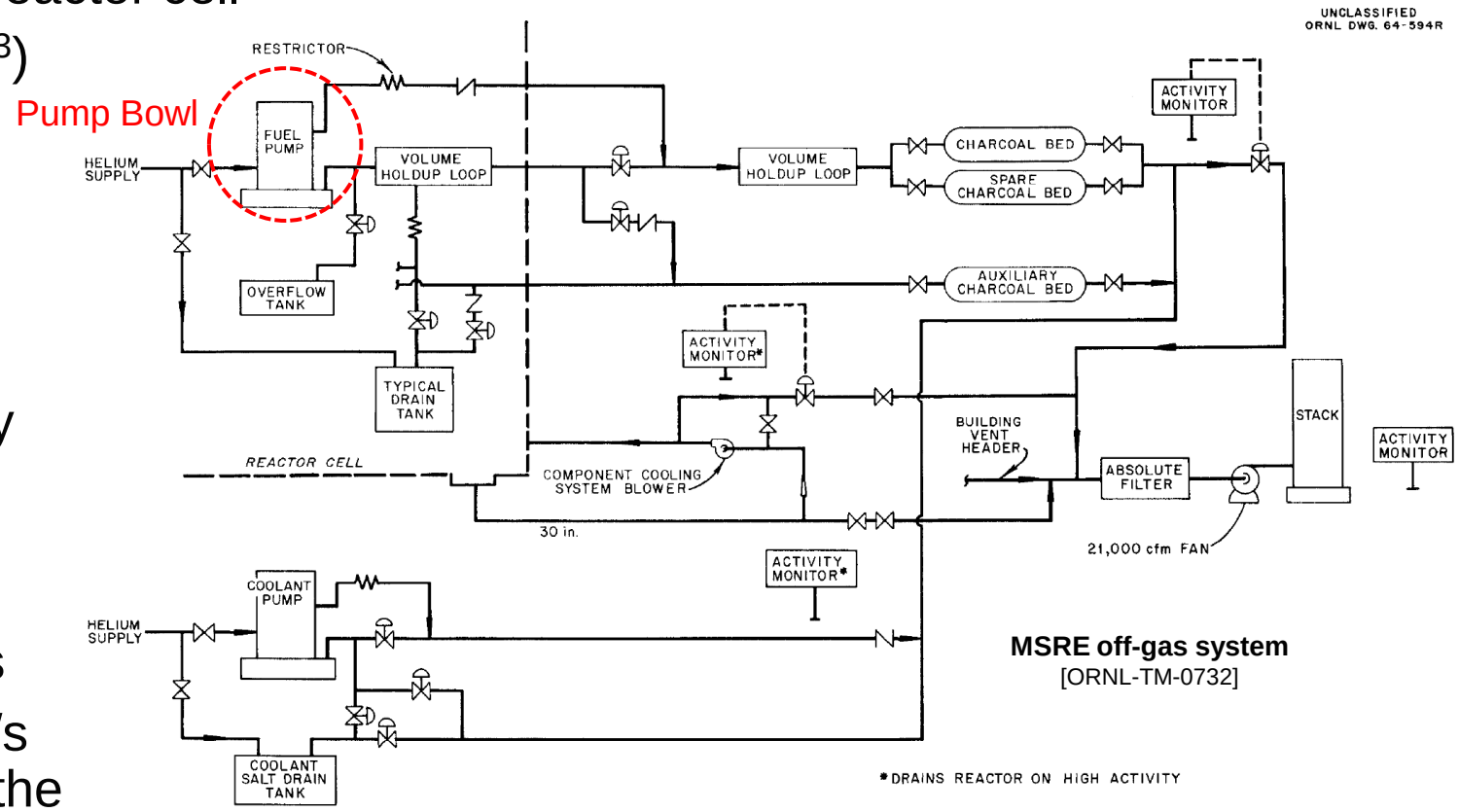


MSRE vapor-condensing system
[ORNL-TM-0728]

MSRE (5/5)

Off-gas filtration system

- Large network that includes 6000 liter/day helium flow through the primary and secondary pump bowls
- Pump bowl helium effluent connects to a series of holdup volumes (large volume & low flow) inside and outside the reactor cell
- 2 filter trains with 0.623 m^3 (22 ft^3) of charcoal
  - One train typically isolated
  - Auxiliary charcoal filter for reactor cell venting
- 3x32 m^2 (3x350 ft^2) fiberglass roughing filters 90-95% efficiency for dust
- 3x2.23 m^2 (3x24 ft^2) HEPA "absolute" filters with 99.7% efficiency for 0.3 micron particles
- Filtered flow merges with 9.9 m^3/s (21,000 cfm) building HVAC out the plant stack for dilution



MSRE off-gas system
[ORNL-TM-0732]

SCALE Molten Salt Reactor Inventory, Decay Heat, Power, and Reactivity Methods and Results

U.S.NRC

Sandia National Laboratories

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. SAND20XX-XXXX P

NRC SCALE/MELCOR Non-LWR Demonstration Project

Objectives:

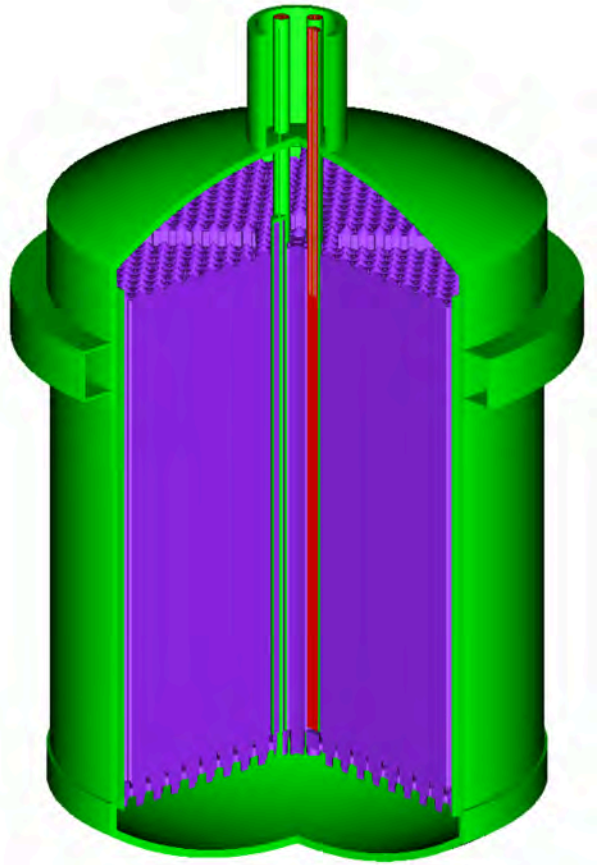
- Develop approach and models for SCALE analysis to obtain:
  - Radionuclide inventory
  - System decay heat
  - Power profiles
  - Reactivity coefficients

Key differences to LWR analysis:

- Continuous circulation of the fuel
- Consideration of both core and loop
- Nuclide removal in loop

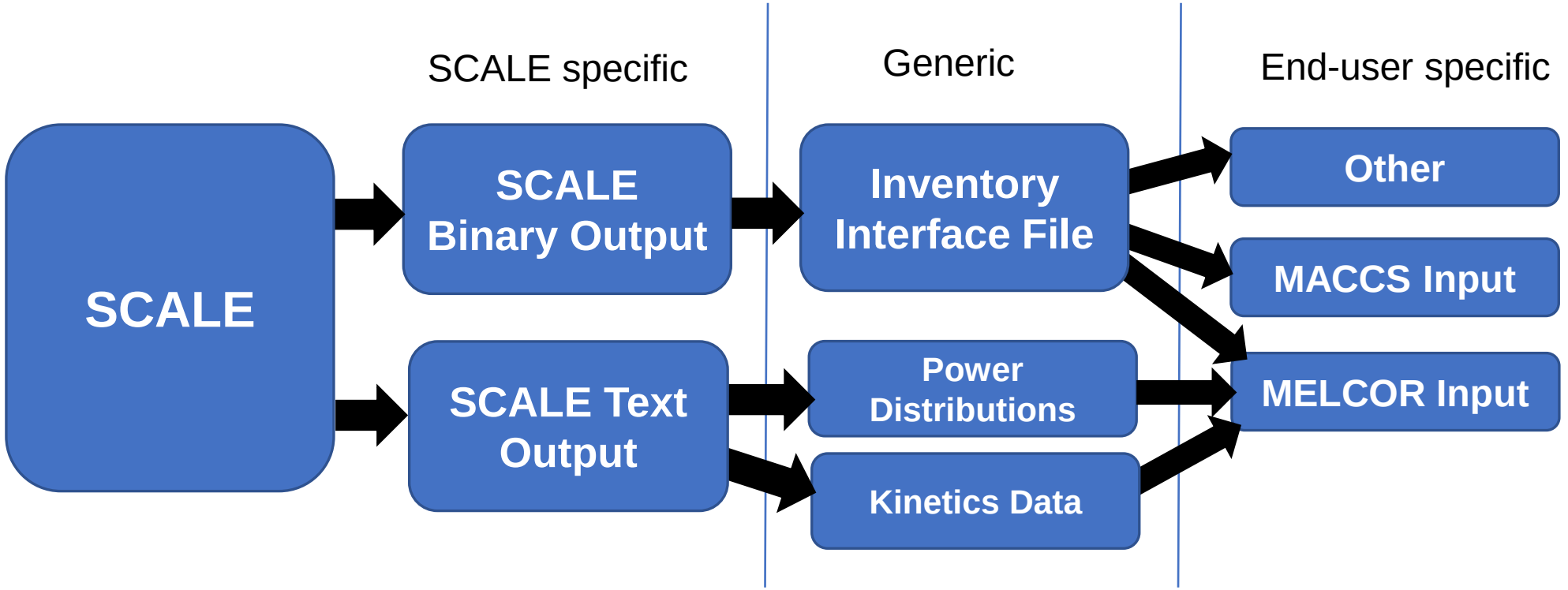
Approach:

- Generate system fuel salt composition considering continuous circulation of the fuel salt and nuclide removal in the loop
- Investigate location-dependent fuel salt inventory in the system
- Evaluate neutronic characteristics at specific point in time



SCALE MSRE core model

Workflow



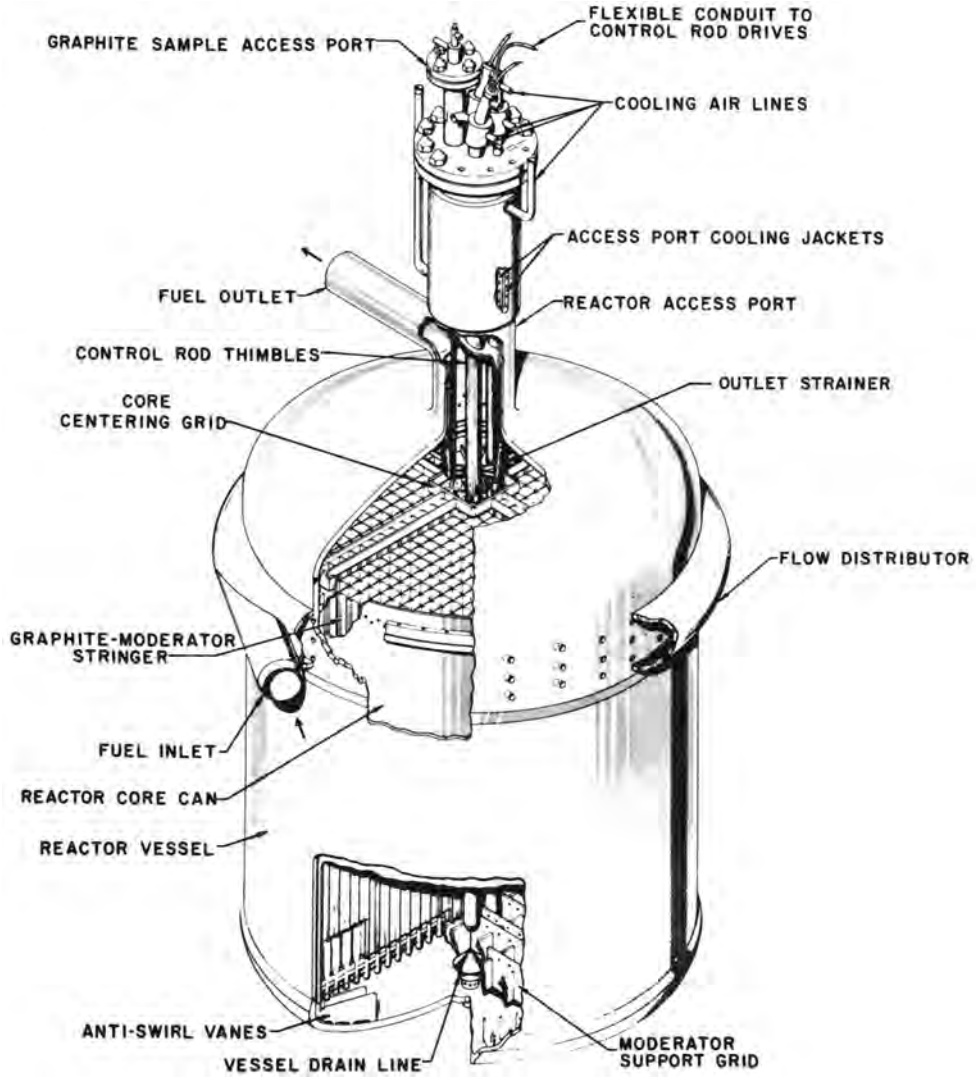
- **SCALE capabilities used:**
  - Codes:
    - ORIGEN for depletion
    - KENO-VI 3D Monte Carlo neutron transport
  - Data: ENDF/B-VII.1 nuclear data library*
  - Sequences:
    - CSAS for criticality/reactivity
    - TRITON for reactor physics & depletion

* The recently published NUREG/CR-7289 "Nuclear Data Assessment for Advanced Reactors" details the impact of the nuclear data library on non-LWR reactor physics calculations.

MSRE Model Description

Description	Value
Power	10 MWth (initial criticality) / 8 MWth (during operation)
Fuel/coolant	LiF-BeF_2-ZrF_2-UF_2
Enrichment	34.5 wt.% ^{235}U
Moderator	Graphite
Structure	Nickel-based alloys
Core volume	0.7 m^3
System volume	2 m^3
Heavy metal loading	0.233 tHM
Loop transit time	25.2 seconds
Nuclide removal	• Noble gases via Off-Gas System (OGS) • Noble metal plate-out at heat exchanger (HX)
Re-fueling	Irregular re-fueling by capsules with HEU fuel salt
Operating time	~375 equivalent full-power days with ^{235}U fuel

Basis for core model development: Zero-power first critical experiment with ^{235}U from the OECD/NEA International Handbook of Reactor Physics Experiments [2]



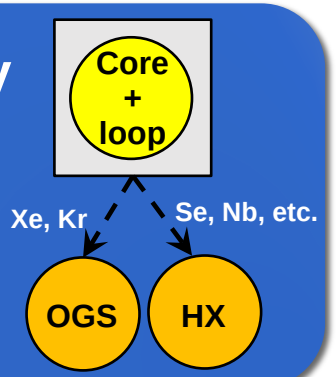
MSRE reactor vessel [1]

[1] R. C. Robertson (1965), "MSRE Design and Operations Report Part I: Description of Reactor Design," ORNL-TM-0728, ORNL.
[2] M. Fratoni, et al. (2020), "Molten Salt Reactor Experiment Benchmark Evaluation," DOE-UCB-8542, 16-10240, UC Berkeley, doi:10. 2172/1617123

SCALE analysis approach

Time-dependent inventory

- Considers core + loop + off-gas + plating-out
- Predicts system-average inventory over time

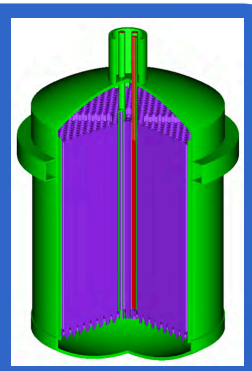


System-average inventory at point in time

System-average inventory at point in time

Core power/flux distribution

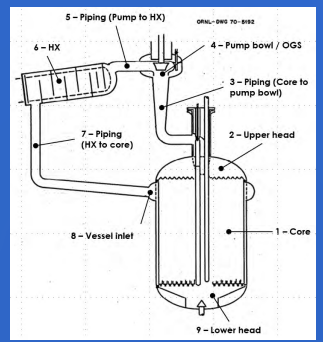
- Predicts neutron flux and power profiles at point in time



Power/flux profile

Location-dependent inventory in loop

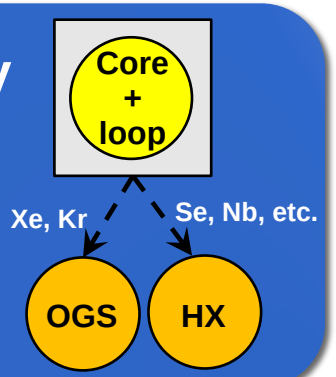
- Considers power profile and off-gas
- Predicts inventory in each region of the loop



SCALE analysis approach

Time-dependent inventory

- Considers core + loop + off-gas + plating-out
- Predicts system-average inventory over time



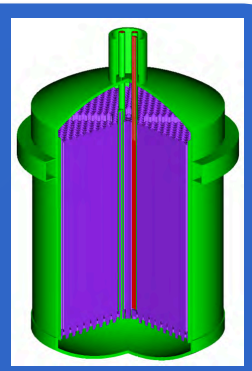
System-average inventory at point in time

System-average inventory at point in time

Sensitivity study: Region-dependent nuclide inventory

Core power/flux distribution

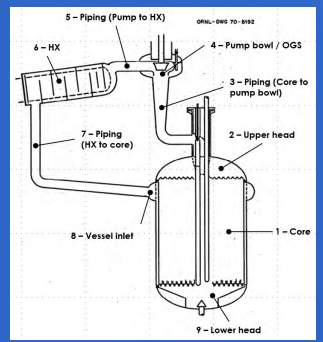
- Predicts neutron flux and power profiles at point in time



Power/flux profile

Location-dependent inventory in loop

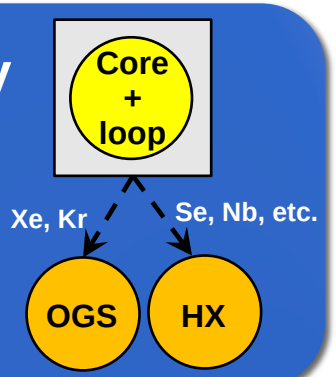
- Considers power profile and off-gas
- Predicts inventory in each region of the loop



SCALE analysis approach

Time-dependent inventory

- Considers core + loop + off-gas + plating-out
- Predicts system-average inventory over time



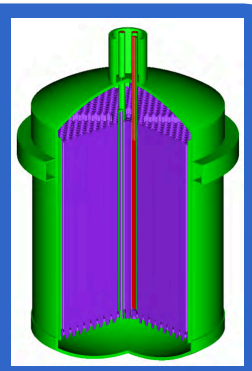
System-average inventory at point in time

Consistency assessment on removal rates

System-average inventory at point in time

Core power/flux distribution

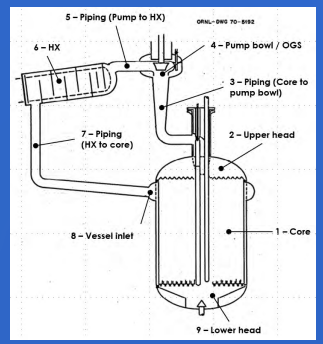
- Predicts neutron flux and power profiles at point in time



Power/flux profile

Location-dependent inventory in loop

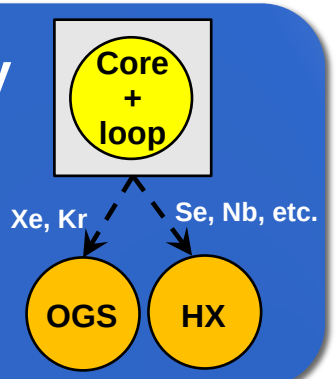
- Considers power profile and off-gas
- Predicts inventory in each region of the loop



SCALE analysis approach

Time-dependent inventory

- Considers core + loop + off-gas + plating-out
- Predicts system-average inventory over time



System-average + OGS inventory and decay heat, and removal rates for MELCOR

Region-dependent inventory and decay heat for MELCOR

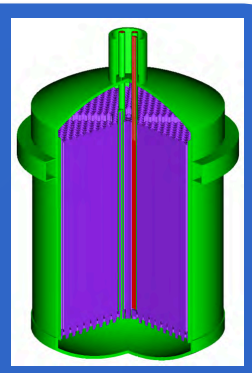
Power profiles and temperature-dependent reactivity coefficients

System-average inventory at point in time

System-average inventory at point in time

Core power/flux distribution

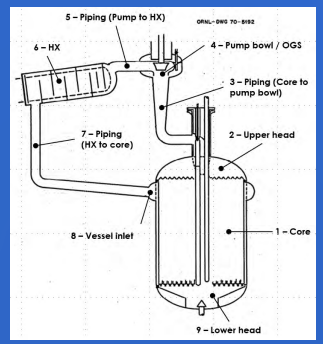
- Predicts neutron flux and power profiles at point in time



Power/flux profile

Location-dependent inventory in loop

- Considers power profile and off-gas
- Predicts inventory in each region of the loop



SCALE MSRE full core model

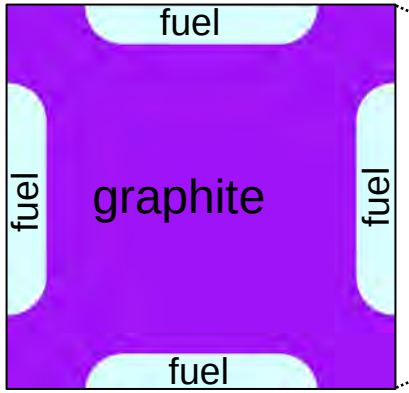
U.S.NRC

Sandia
National
Laboratories

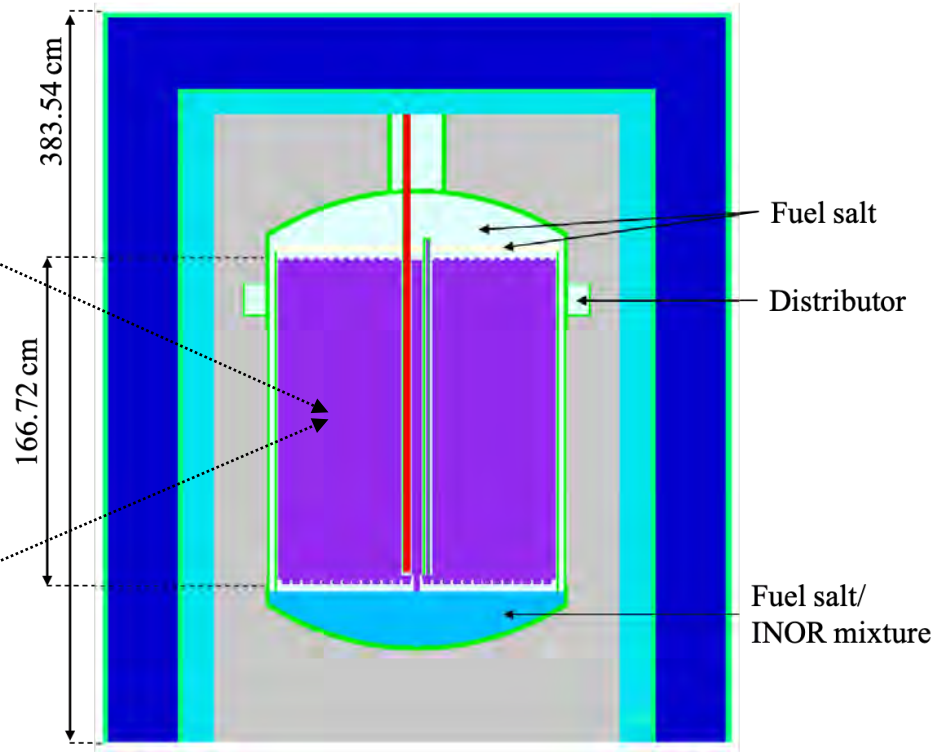
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND20XX-XXXX P

MSRE full core model

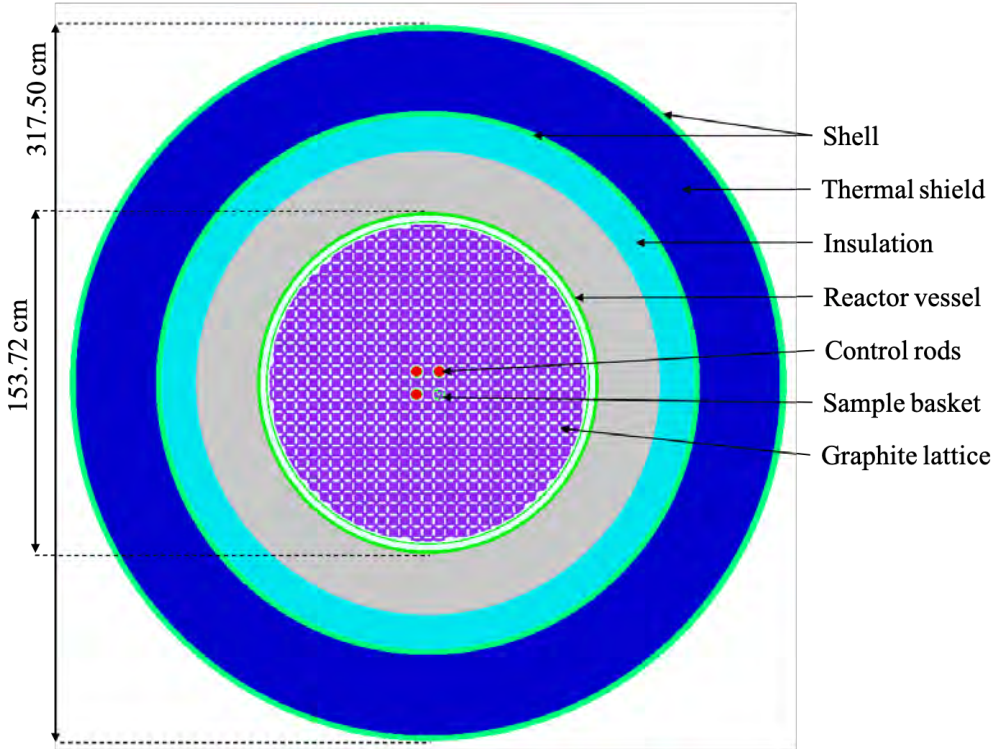
TRITON-KENO model based on IRPhEP benchmark specifications



Cross section of graphite stringer



YZ-cut through SCALE 3D model



XY-cut through SCALE 3D model

Time-dependent inventory

U.S.NRC

OAK RIDGE National Laboratory

Sandia National Laboratories

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. SAND20XX-XXXX P

U.S. DEPARTMENT OF ENERGY

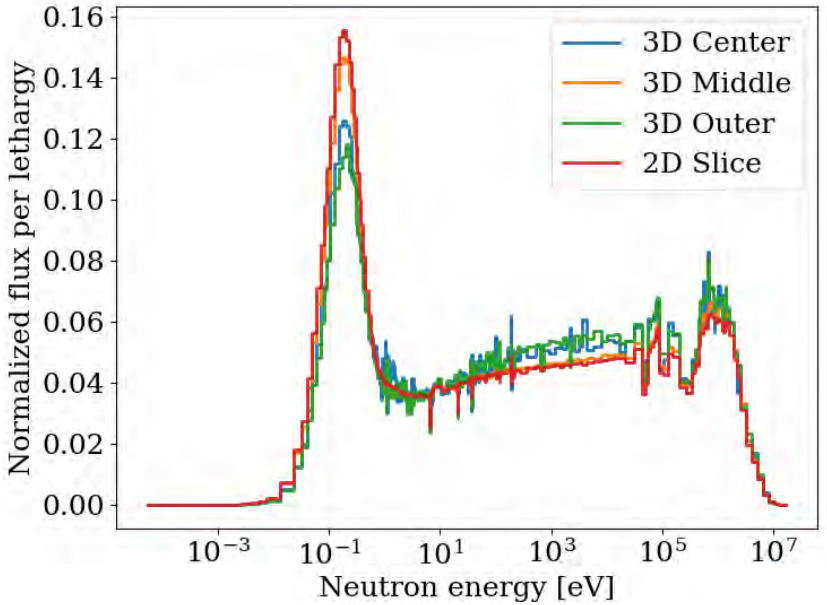
NNSA

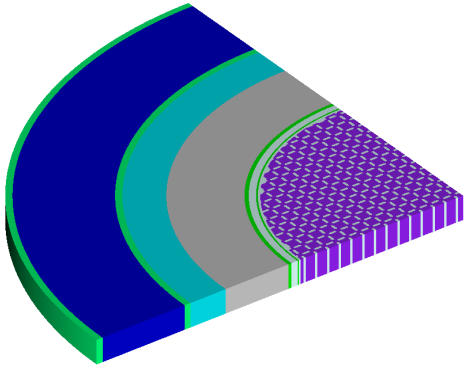
Time-dependent inventory – model development

Goal: Generate system-average (fuel salt in core+loop) nuclide inventory at end of operation

Model: TRITON-KENO core slice model

- Representative spectral conditions through radial leakage and representative moderator-to-fuel ratio, while allowing shorter runtimes compared to full core
- Depletion up to 375 days, the total operation time of MSRE with ^{235}U fuel
- Representation of system (core+loop) through adjusted power level:
  - Core power 8 MWth, total mass of 0.218 tHM in the system
  - Specific power of 36.697 MW/tHM
- Consideration of nuclide removal through “TRITON-MSR” [1,2] (next slide)





SCALE “2D” slice model

[1] B. R. Betzler, al., “Molten salt reactor fuel depletion tools in SCALE,” Proc. Global/Top Fuel, Seattle, WA, September 22-27, 2019.
[2] P. J. V. Valdez, et al., “Modeling Molten Salt Reactor Fission Product Removal with SCALE,” ORNL/TM-2019/1418, 2020.

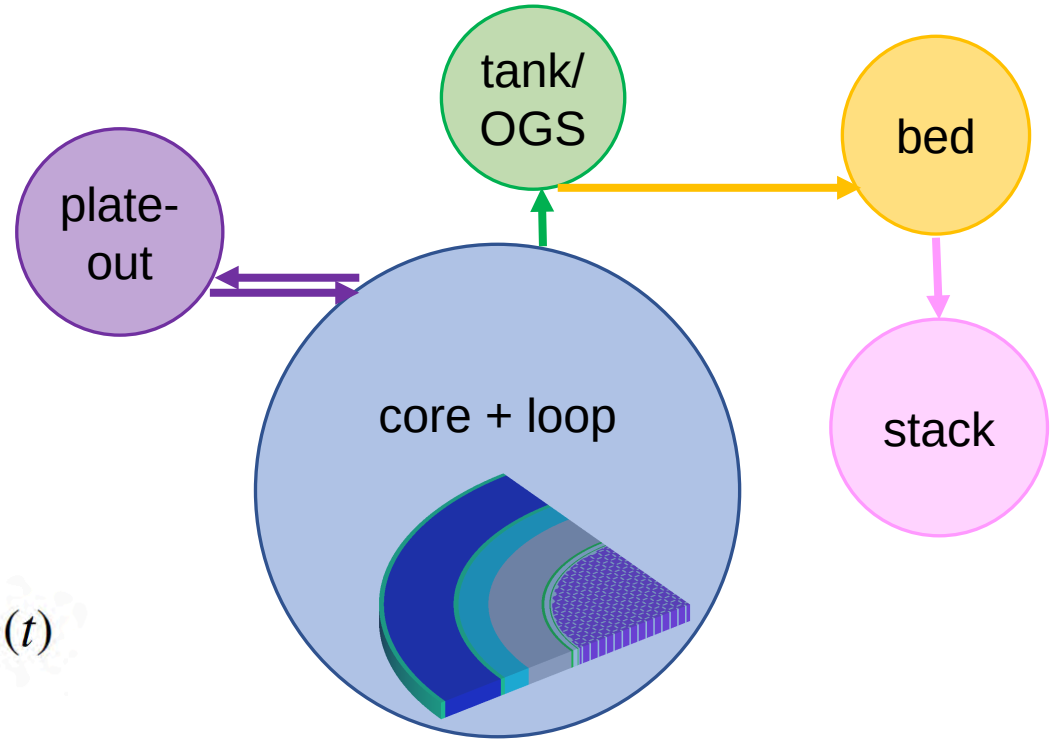
Time-dependent inventory – nuclide removal

Nuclide removal via “TRITON-MSR”

- Time-dependent removal of nuclides from one mixture into another
- User-specified removal constant $\lambda_{i,rem}$ as used by ORIGEN to solve ODE:

$$\frac{dN_i}{dt} = \sum_{j \neq i} (l_{ij}\lambda_j + f_{ij}\sigma_j\Phi)N_j(t) - (\lambda_i + \lambda_{i,rem} + \sigma_i\Phi)N_i(t) + S_i(t)$$

Production of nuclide i from decay and/or irradiation of nuclide j – *Loss rate of nuclide i due to decay, irradiation, or other means (flow)* + *Source of nuclide i*



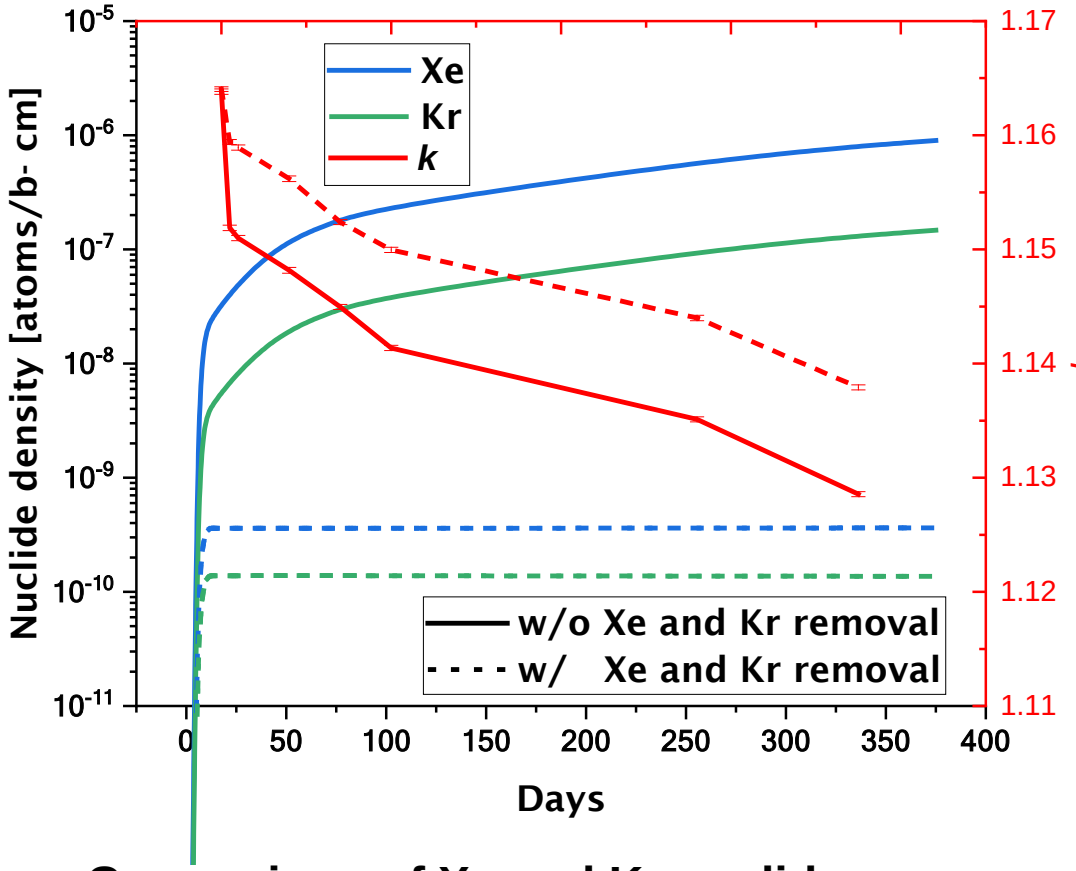
Time-dependent inventory – nuclide removal

- Noble gas removal in the off-gas system:
  - Main experimental basis is the xenon poison fraction (ratio of absorption by ^{135}Xe to absorption by ^{235}U), reported as 0.3-0.4%
  - Noble gas removal fraction was set at 0.03 to match xenon poison fraction
- Noble metal plating-out at the heat exchanger:
  - After operation, plated-out noble metals found, with 40% of noble metals plated out in heat exchanger, 50% on all other surfaces in the loop
  - Noble metal plate-out removal rate determined from region-wise removal rates, as determined from mass transfer rate, surface area, and fuel salt volume
  - Total removal rate calculated as sum of component-wise removal rates

Time-dependent inventory

- Depletion at low power level of 8 MWth, with flux level 1.88 · 10^{13} n/cm^2-s
- No re-fueling in this depletion calculation
- At 375 days:
  - 5.627% ^{235}U consumed,
  - 0.455% ^{238}U consumed,
  - 13.76 GWd/tHM burnup achieved

	Amount removed after 375 days
Noble gas (Xe + Kr)	0.170 kg / 30.6 L
Insoluble metals (Mo + Tc + Ru + Rh + Pd + Ag + Sb)	0.611 kg
Sometimes soluble metals (Se + Nb + Te)	0.057 kg

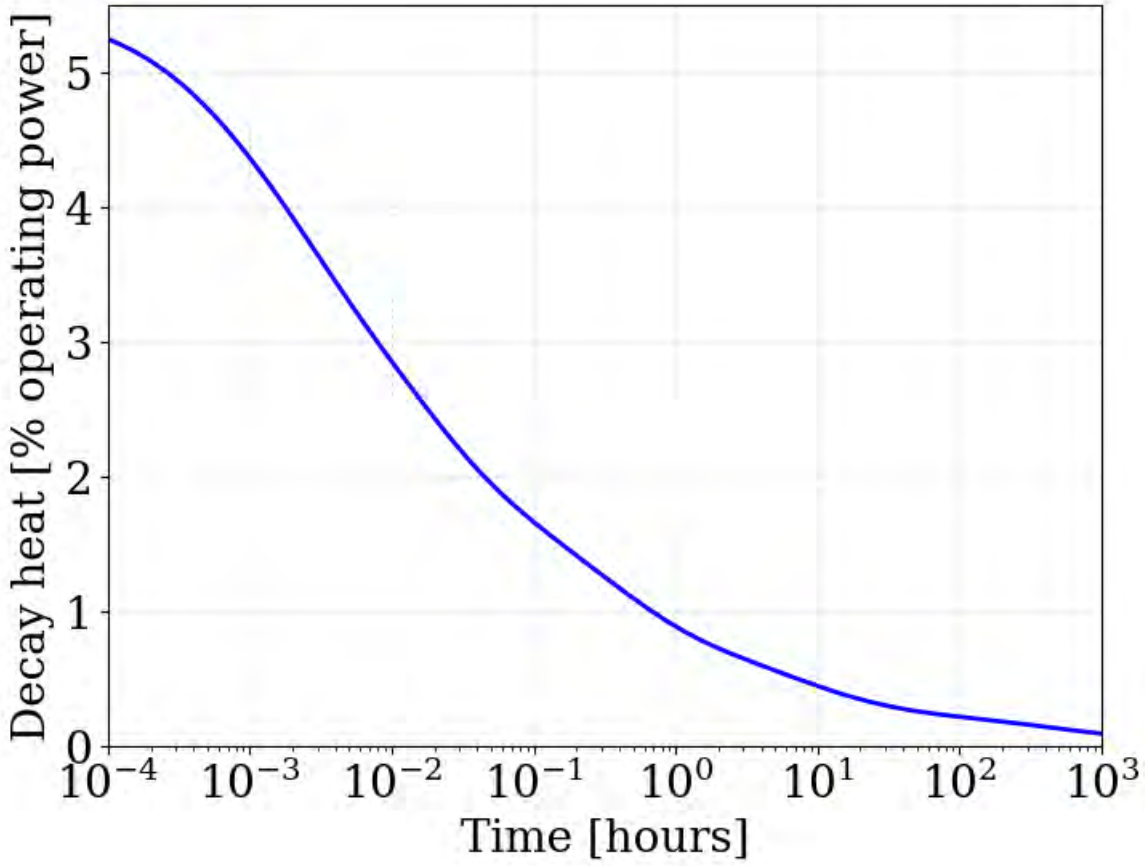


Comparison of Xe and Kr nuclide densities with and without Xe/Kr removal

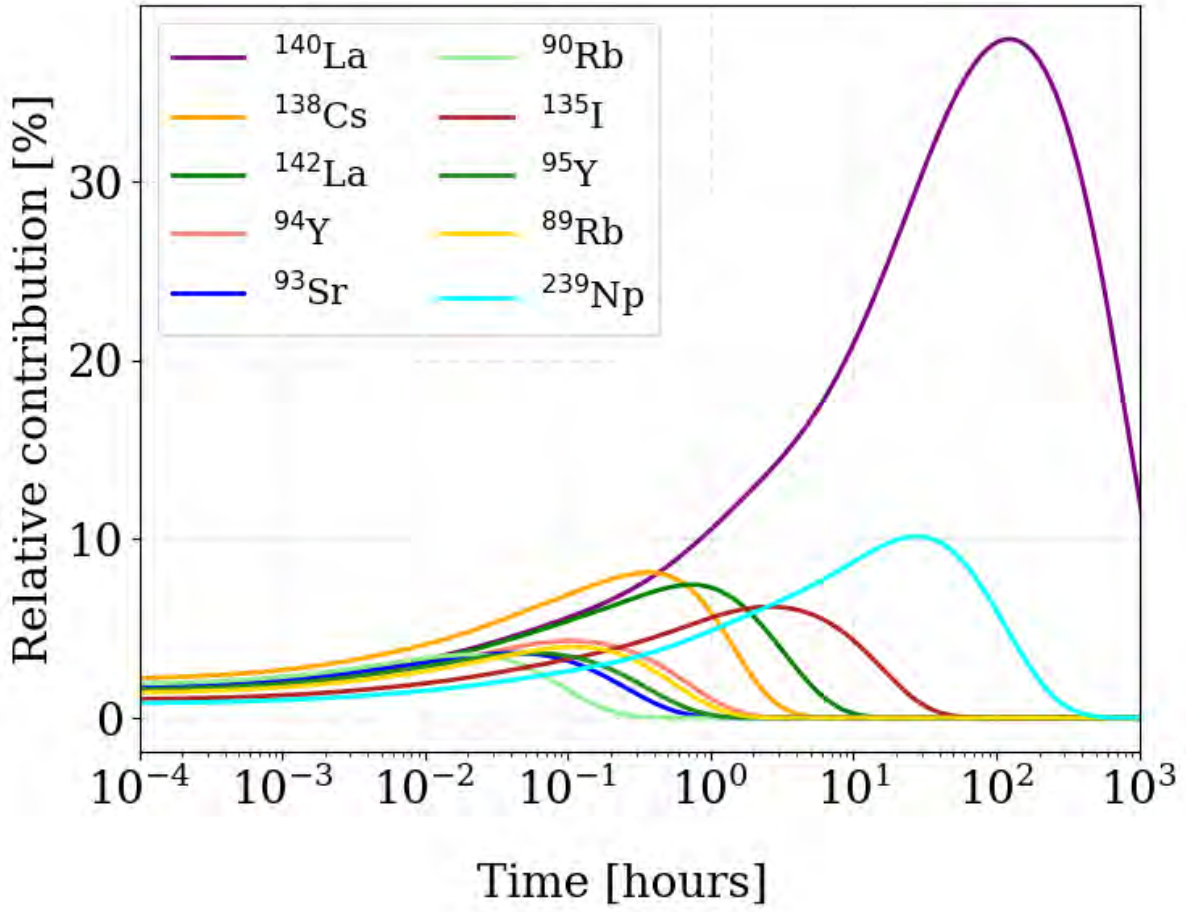
Decay heat after shutdown at 375 days

U.S.NRC
OAK RIDGE National Laboratory
Sandia National Laboratories

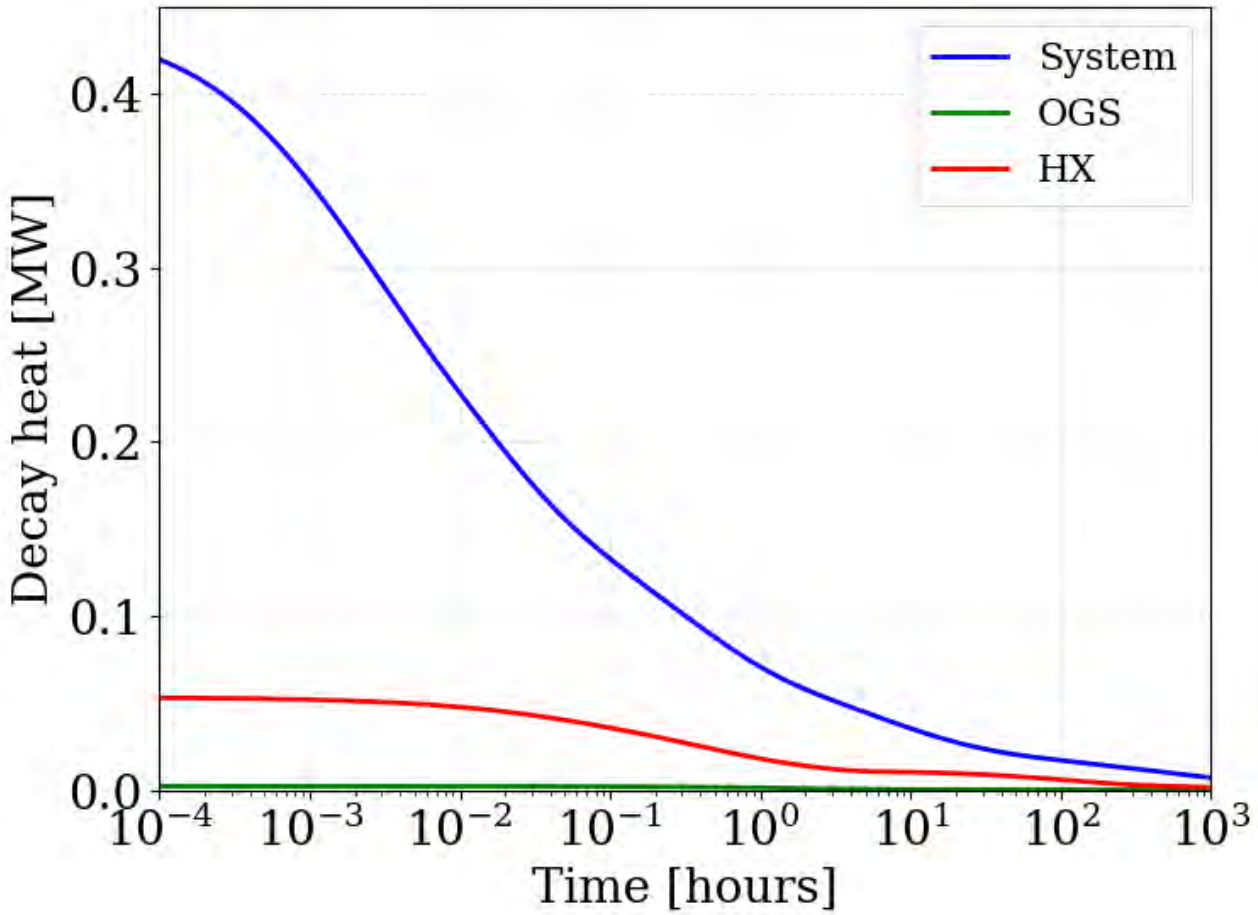
System decay heat [% operating power]

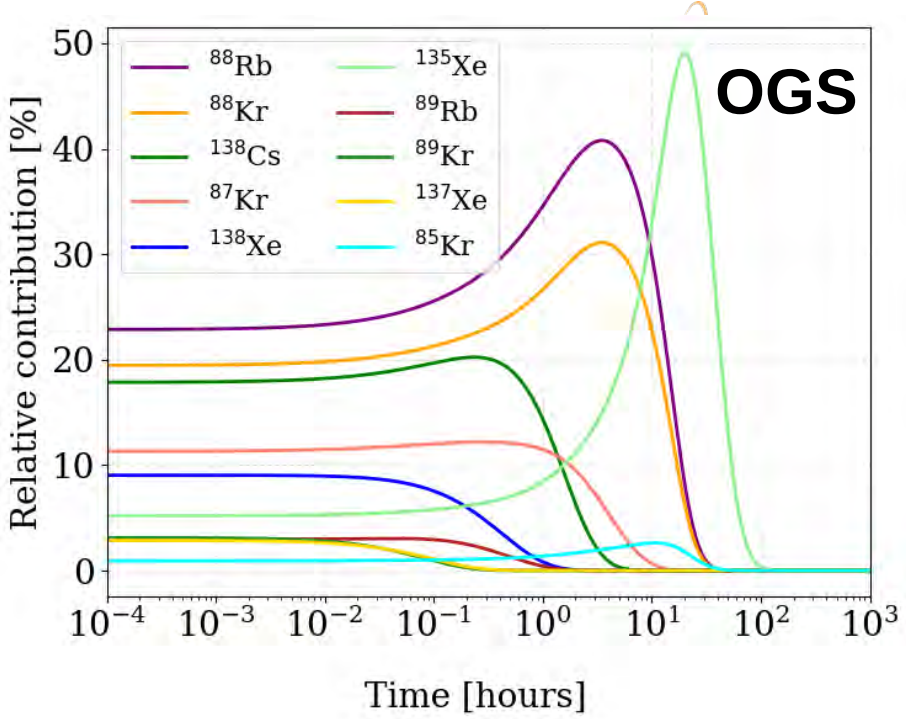


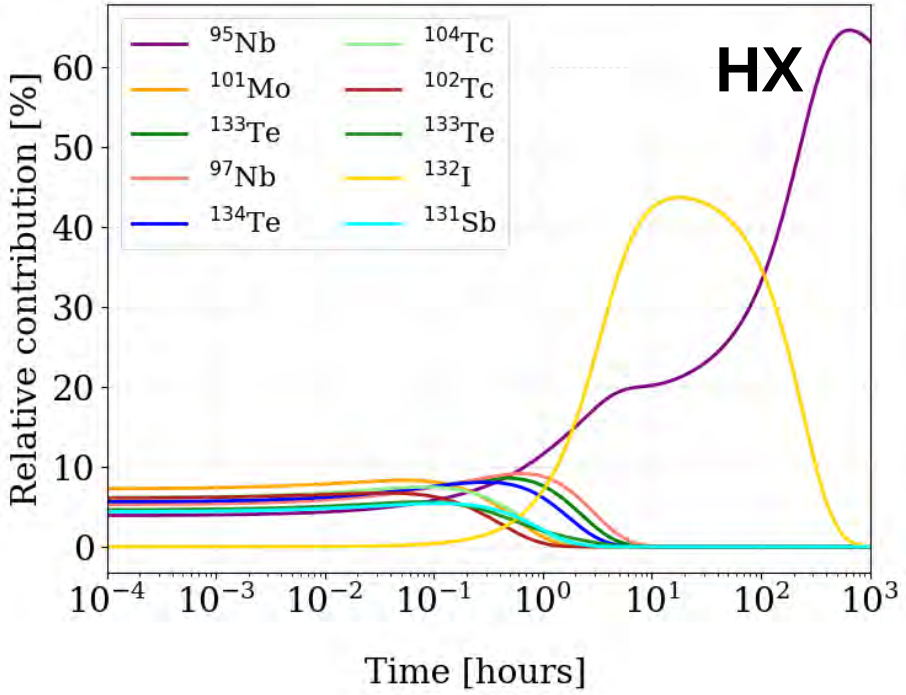
Top contributors



Decay heat after shutdown at 375 days



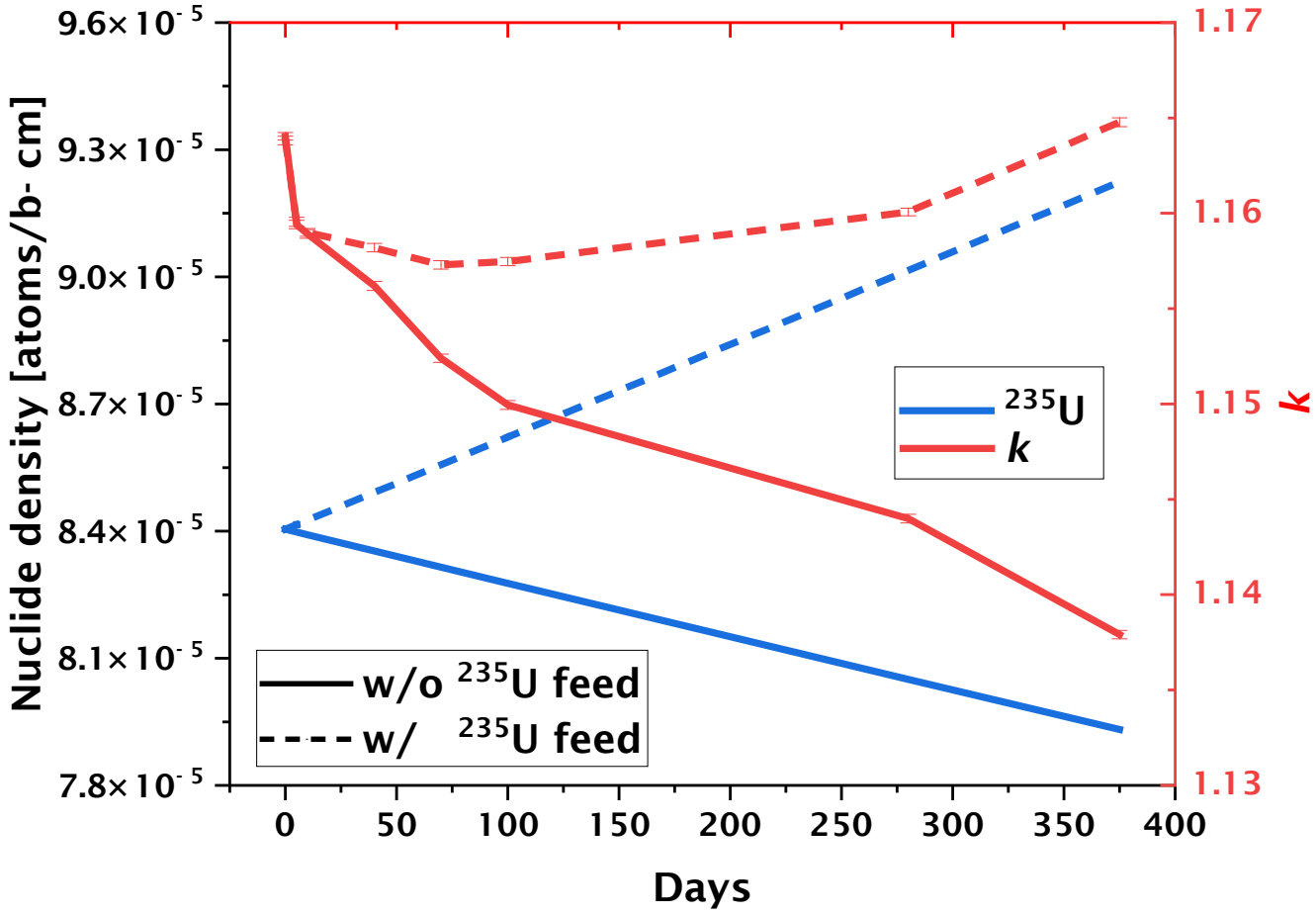




MSRE operating power: 8 MWth

Demonstration of continuous feed / refueling

- Side calculation with ^{235}U feed through TRITON-MSR
- Continuous feed rate of 1.49×10^{-3} g/s to yield approximately constant eigenvalue
- Increasing ^{235}U fuel concentration compensates for fission product buildup
- Consider low burnup, and hardly any ^{239}Pu buildup



Comparison of ^{235}U nuclide densities and eigenvalue with and without ^{235}U feed

Core power/flux distribution

U.S.NRC

OAK RIDGE National Laboratory

Sandia National Laboratories

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. SAND20XX-XXXX P

U.S. DEPARTMENT OF ENERGY

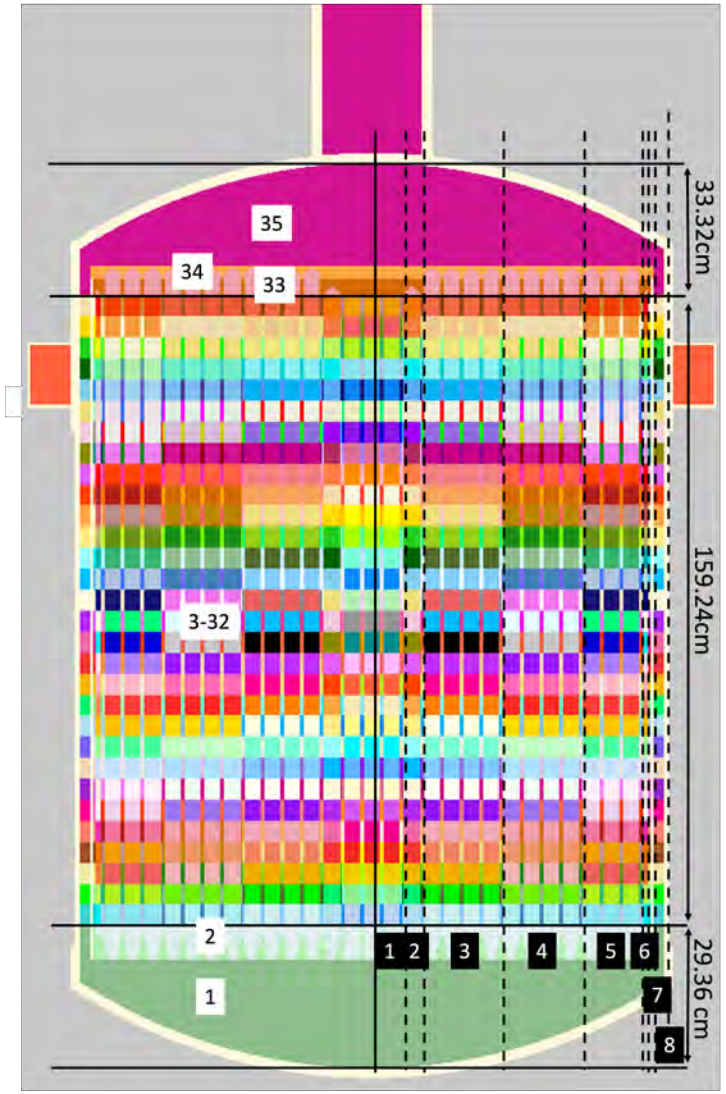
NNSA National Nuclear Security Administration

Core power/flux distribution – model development

Used TRITON-KENO 3D full core model based on IRPhEP benchmark specifications as basis

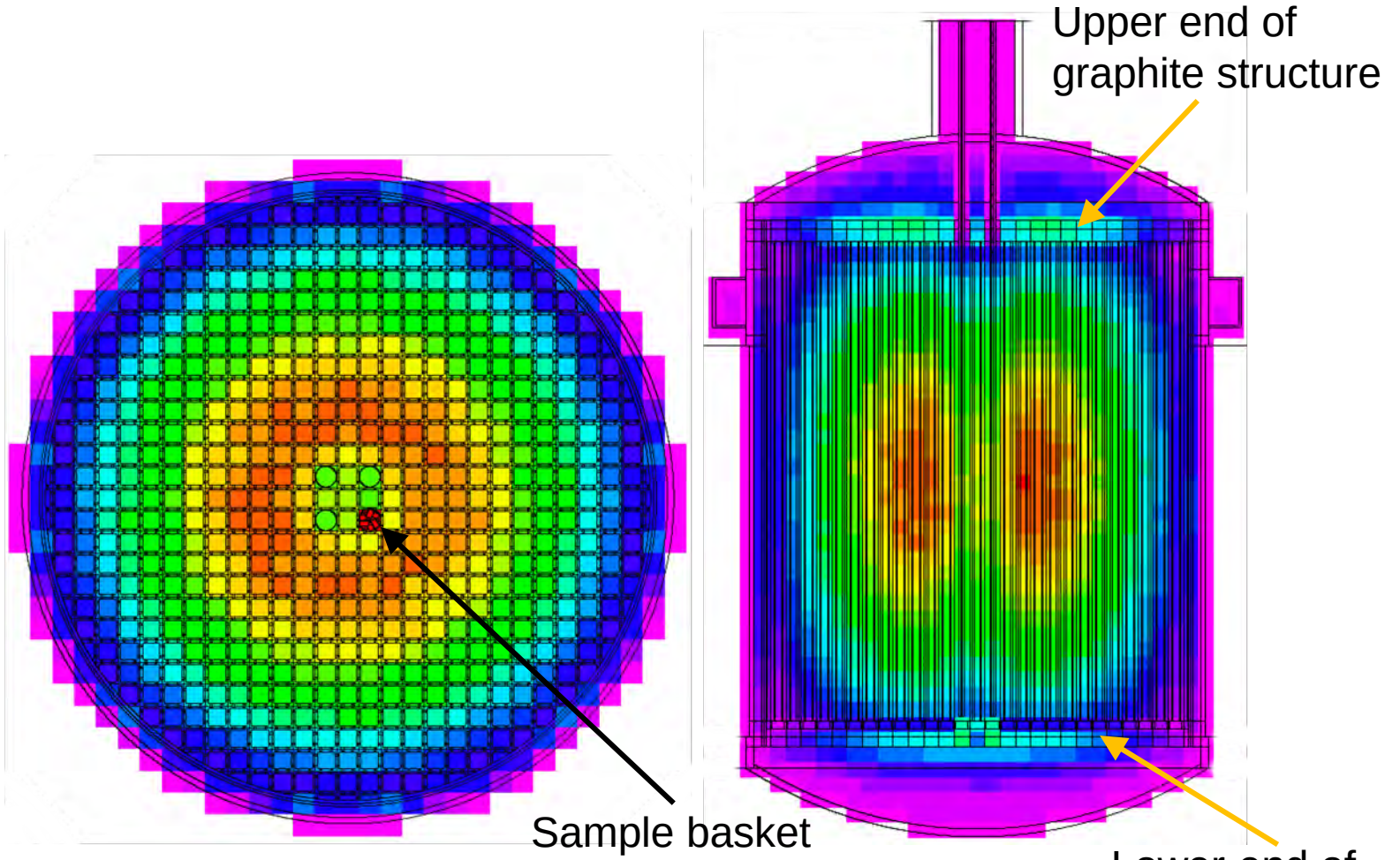
Analyzed 3D flux profiles and 3D fission rate via mesh tally capability informed discretization of core region

Discretized model uses 34 axial and 8 radial zones

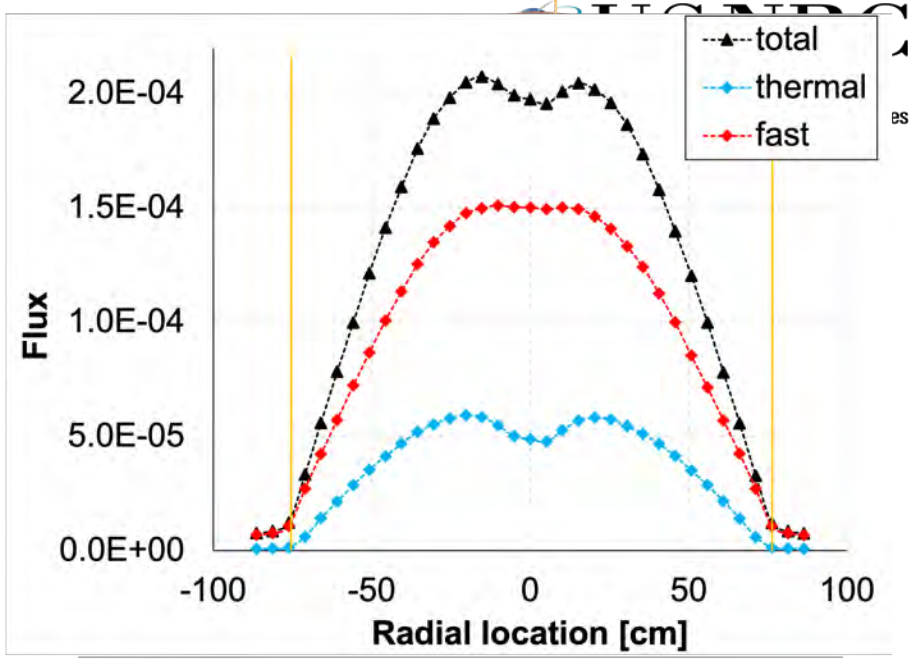


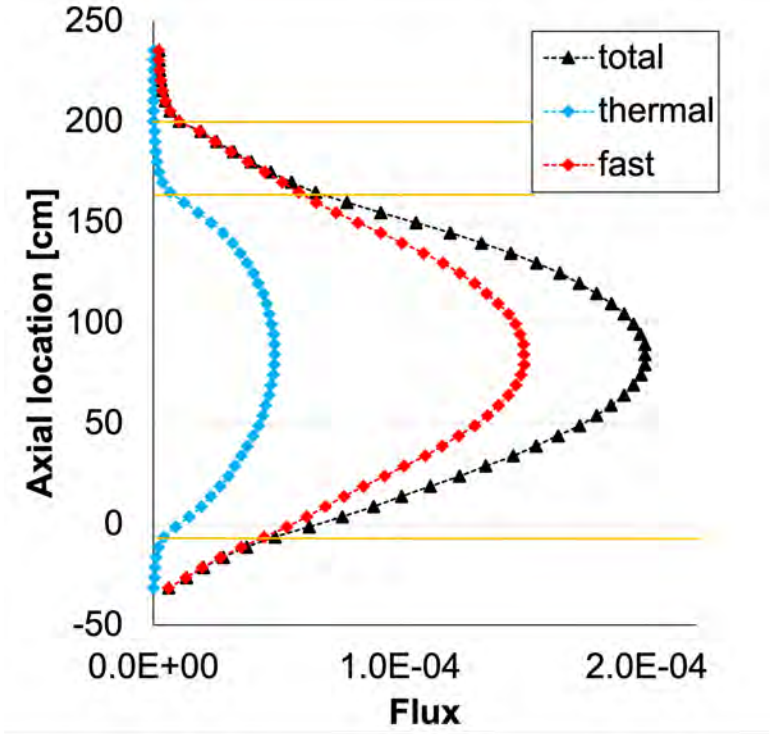
Discretized model

Core power/flux distribution – fission rate and flux

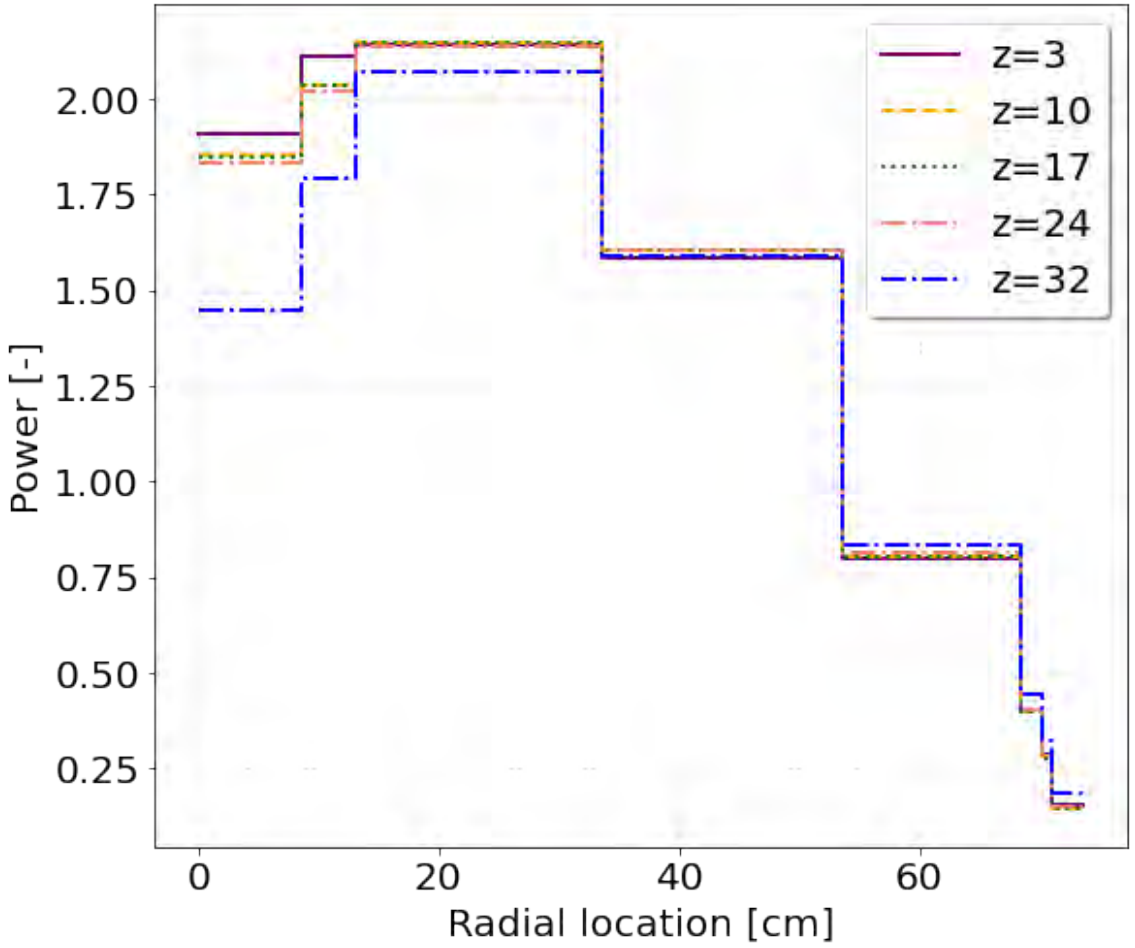


Fission rate distributions





Core power/flux distribution – power

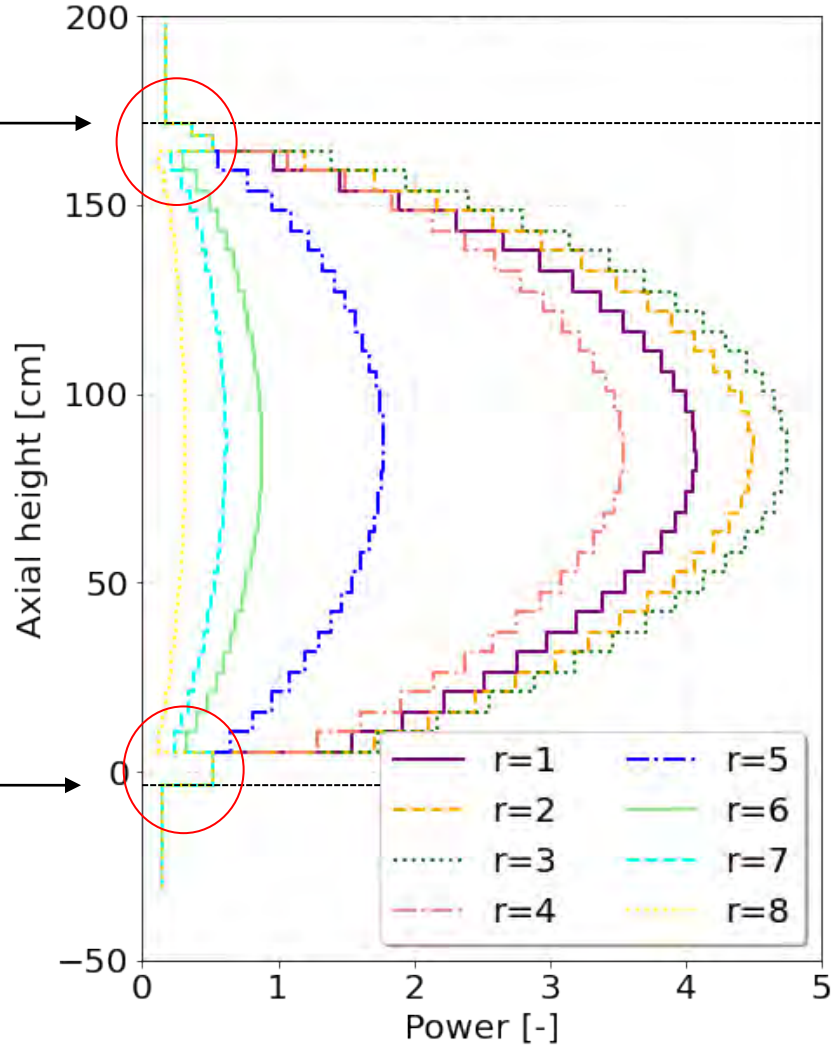


Normalized radial power

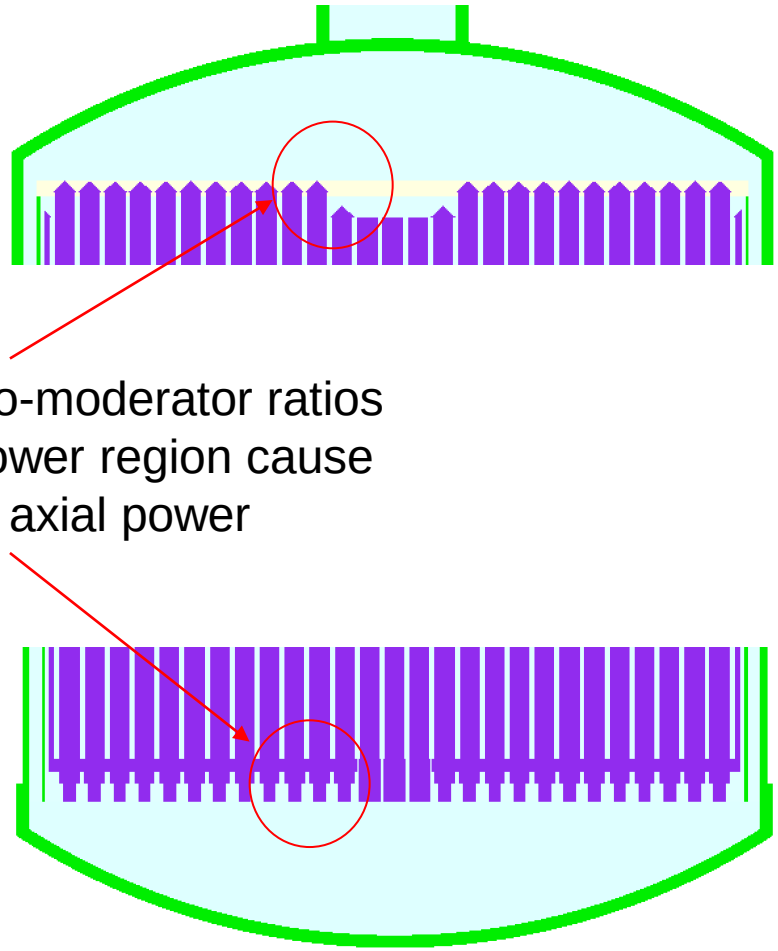
Core power/flux distribution – power

Top of graphite stringers

Bottom of graphite stringers



Normalized axial power

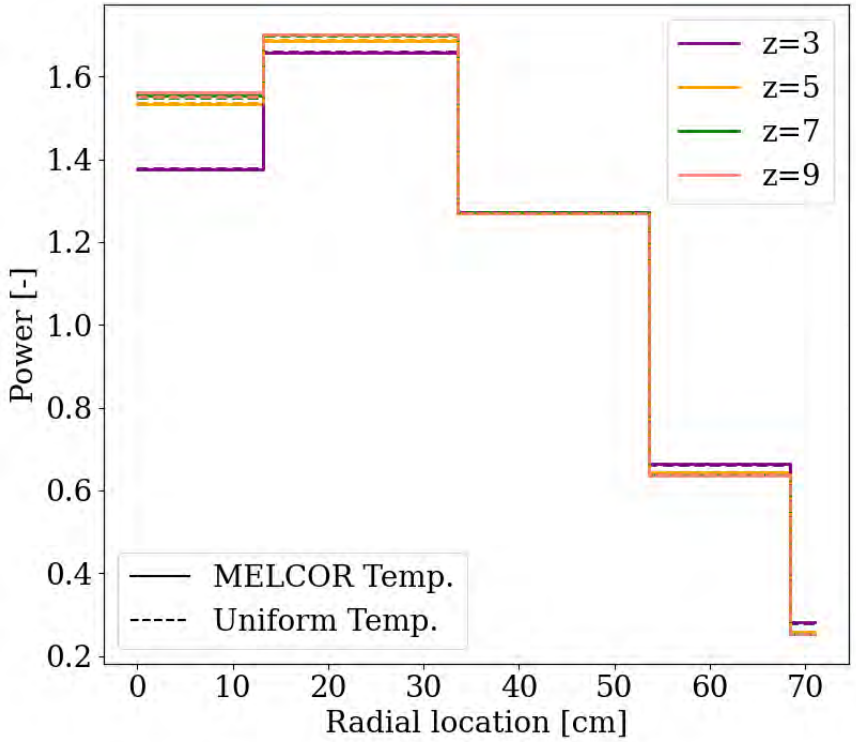


Different fuel-to-moderator ratios in upper and lower region cause small peaks in axial power

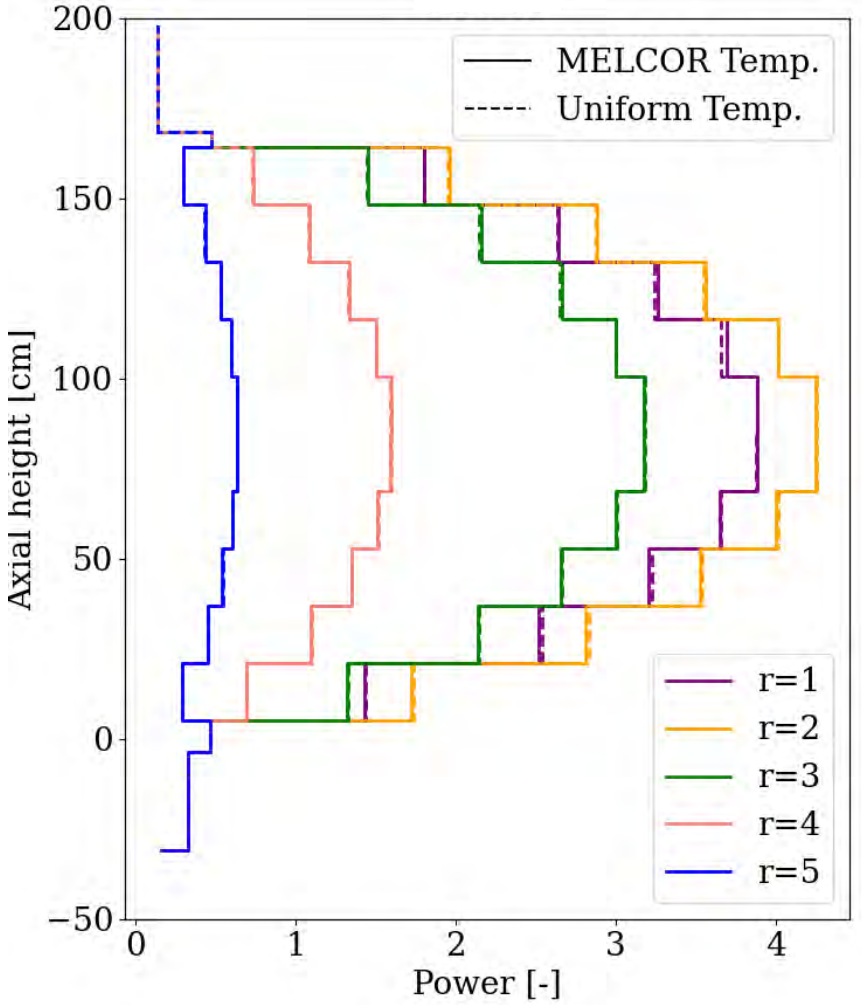
Core power/flux distribution – power

Impact of temperature distribution on the power profile

- Nominal case: 911 K in the fuel salt and graphite structure
- Temperature distribution from MELCOR: 910.5 –937.7 K for the fuel salt, 912.3–937.7 K for the graphite structure



Normalized radial power profile



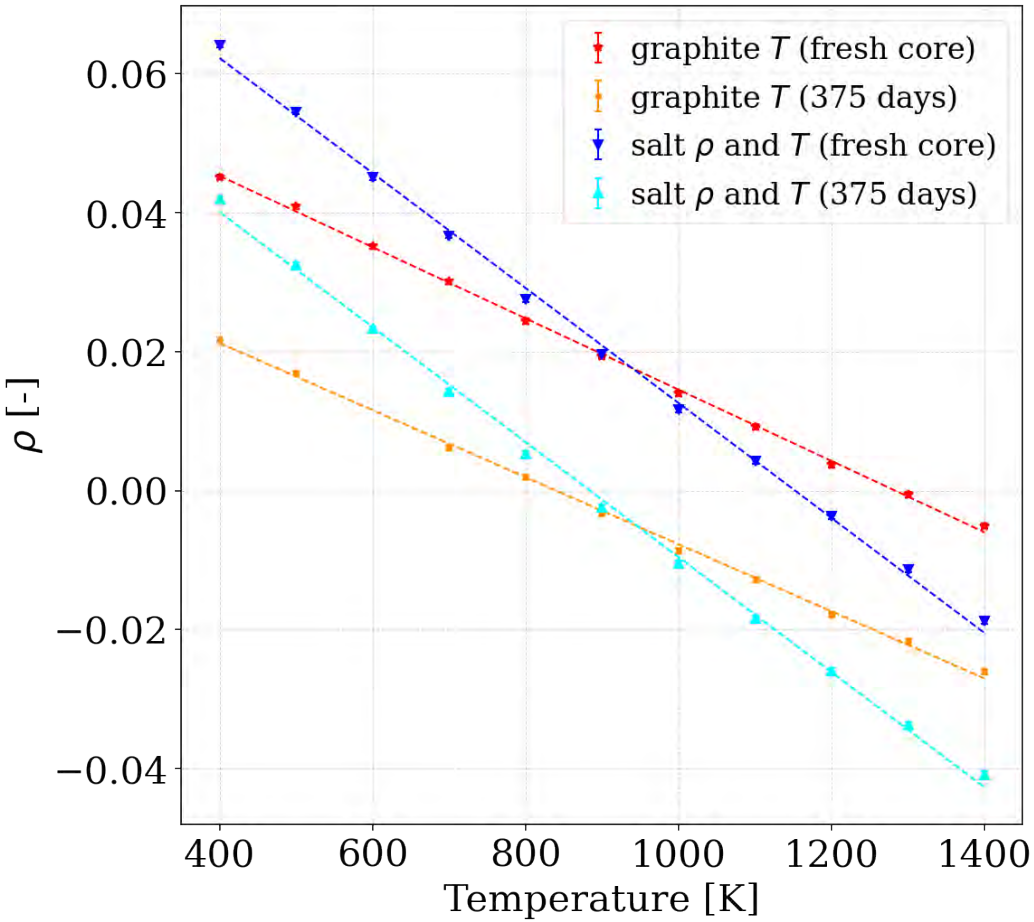
Normalized axial power profile

Core power/flux distribution – reactivity coefficients

Determined reactivity coefficients by temperature/density perturbation:

- Calculated reactivity at multiple temperature/density points
- Fitted reactivity
- Determined reactivity coefficient as derivative of fitted curve

Component	Fresh core	375 days
β_{eff} [pcm]	704 ± 14	697 ± 22
Graphite temperature reactivity coefficient [pcm/K]	-5.13 ± 0.05	-4.83 ± 0.07
Fuel salt temperature *and density* reactivity coefficient [pcm/K]	-8.27 ± 0.12	-8.28 ± 0.12



Location-dependent inventory in loop

U.S.NRC

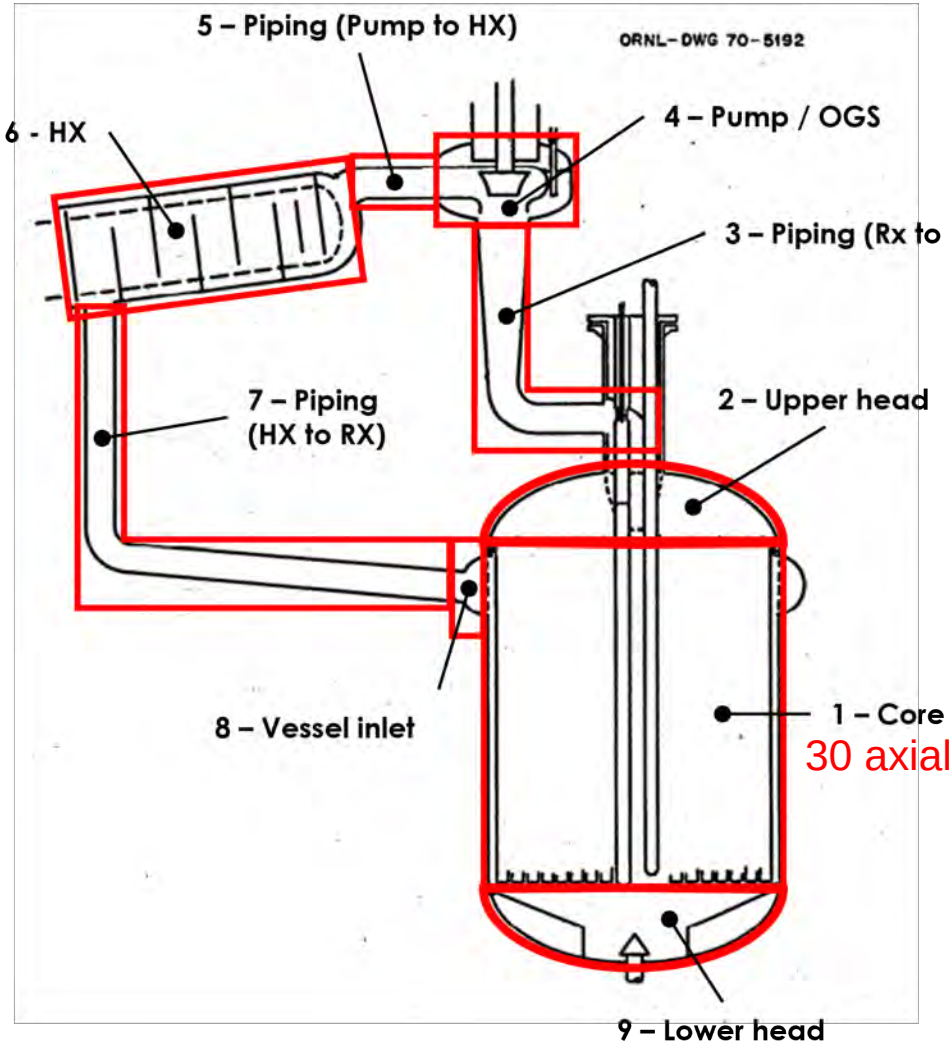
Sandia National Laboratories

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. SAND20XX-XXXX P

Location dependent inventory – model development

Developed ORIGEN model to predict nuclide inventory **in each region** of the loop at ~375 days

- Divided MSRE system into 9 general regions, with the core region subdivided into 30 axial zones
- Used fuel salt composition from 2D TRITON-MSR calculation at 375 days as the start
- Developed chain of ORIGEN inputs that use residence time and flux of the fuel salt in each region and removes noble gases (Kr, Xe) in off-gas system
- 1 ORIGEN input corresponds to the salt traveling 1 time through the whole loop



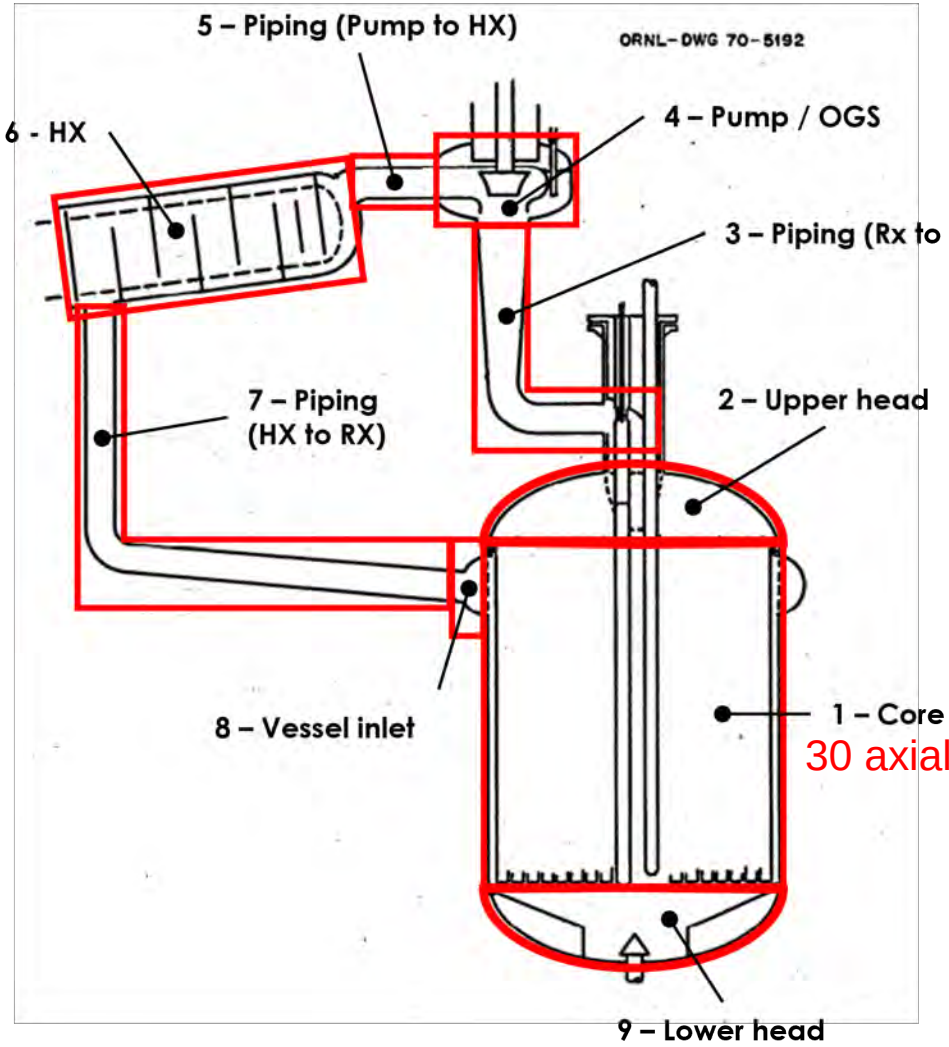
Regions in MSRE system for ORIGEN model

Location dependent inventory – model development

As fuel salt travels the loop

- Long-lived* nuclides will slowly accumulate/be removed
- Short-lived* nuclides will oscillate around an equilibrium
- Equilibrium established after a few loops (resulting in inventory at just a few minutes after 375 days)

*relative to the loop transit time (~25 s for MSRE)

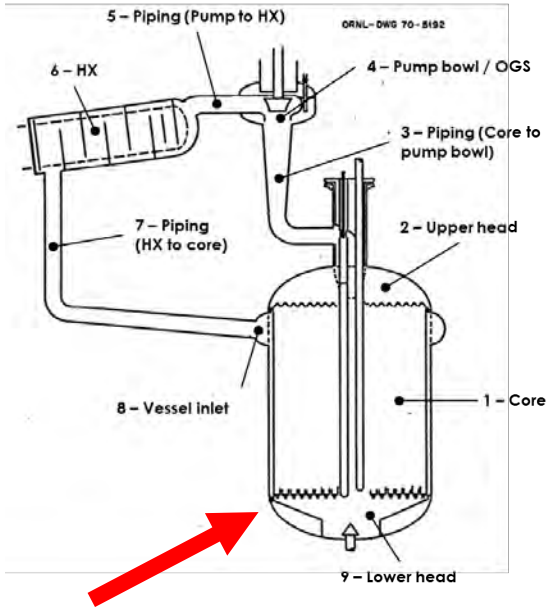


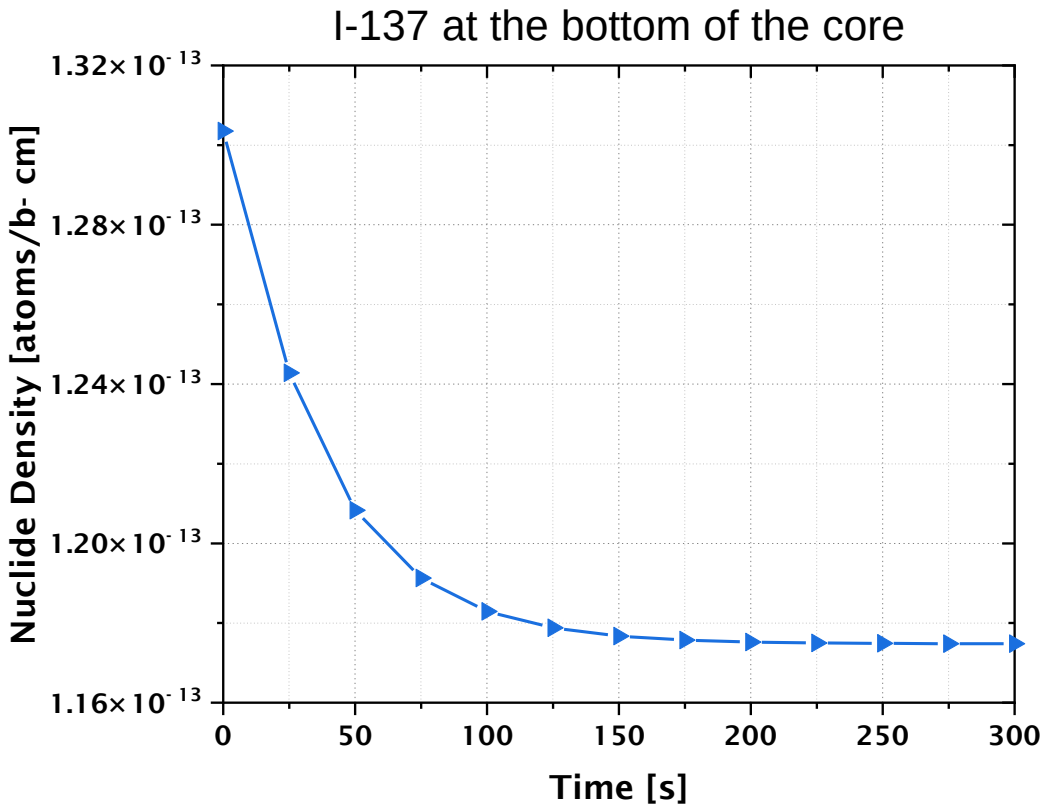
Regions in MSRE system for ORIGEN model

Location dependent inventory analysis example

- Observed constant densities of long-lived nuclides for several loops
- Observed convergence of short-lived nuclides after ~6 loops

Example: Short-lived nuclide (I-137, $t_{1/2}$=24.5s) **as a function of <u>time</u>** at the bottom of the core

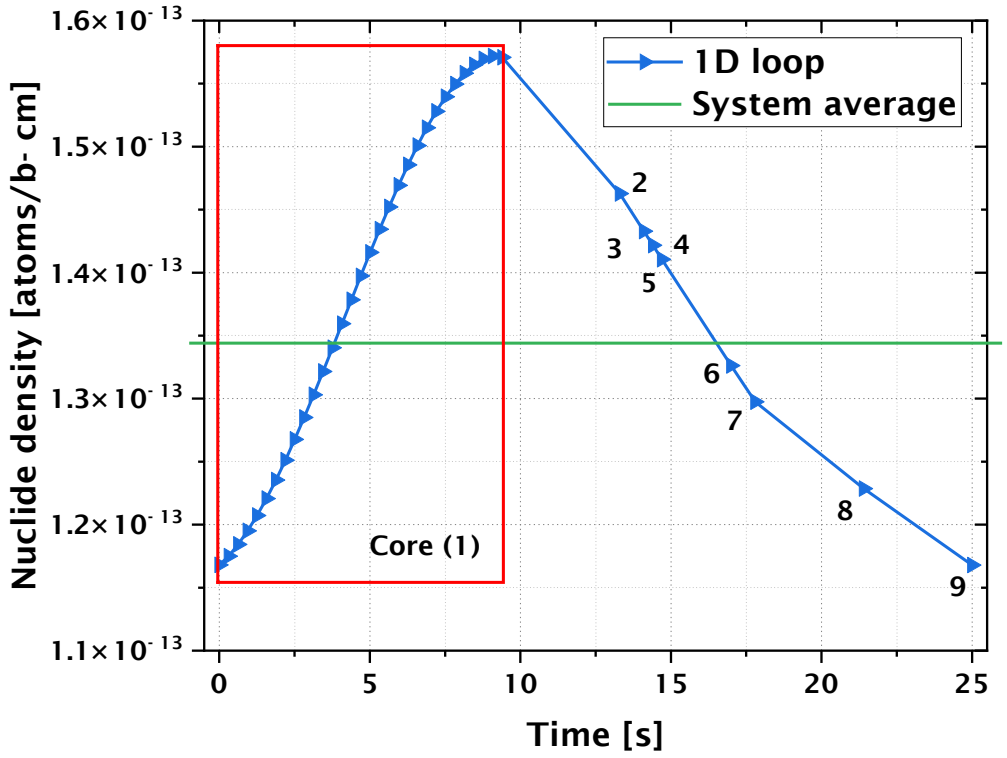




Location dependent inventory analysis example

- Compared short-lived nuclide densities between different regions
- Found that inventory/decay heat does not significantly differ between regions when summed up into element classes due to short loop transit time in MSRE

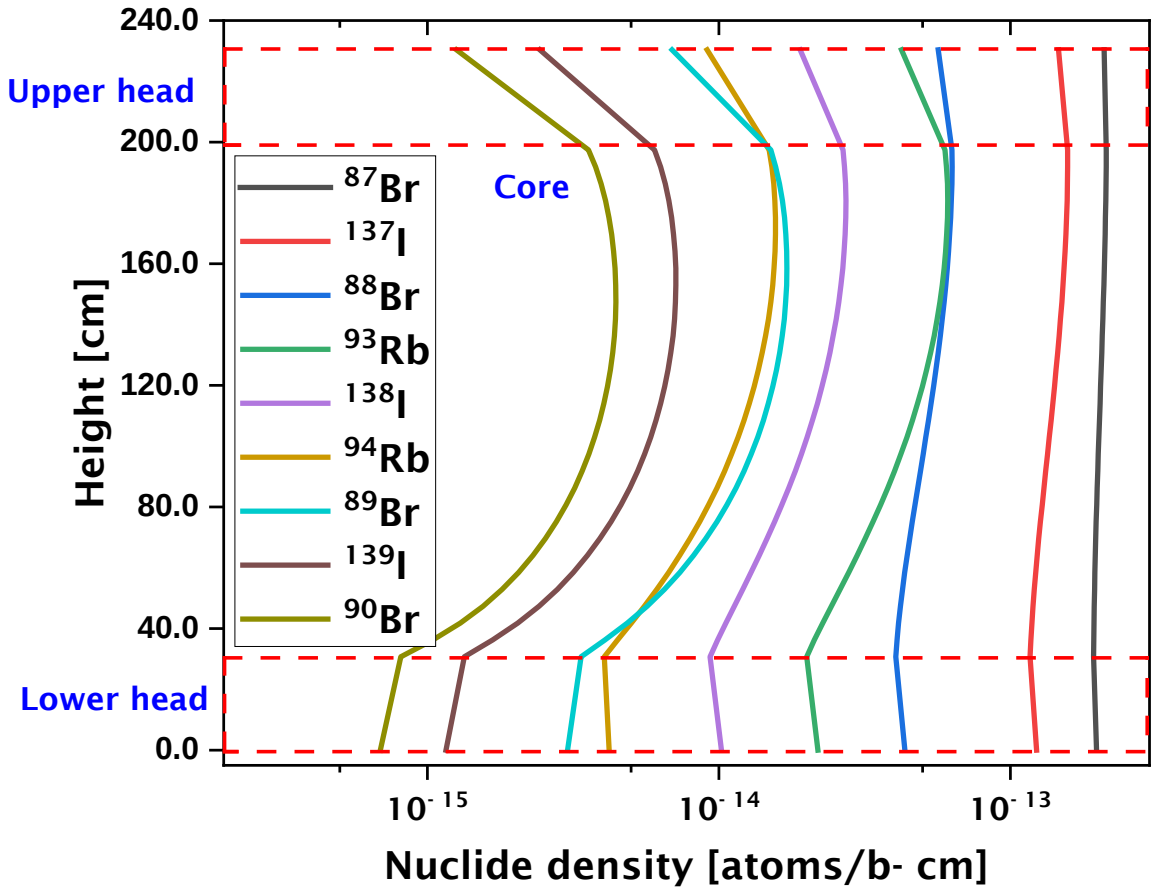
Example: Short-lived nuclide (I-137, $t_{1/2}$=24.5s) **as a function of <u>location</u>** in the loop



1. Core
2. Upper head
3. Piping to Pump
4. Pump/OGS
5. Piping to HX
6. HX
7. Piping to RX
8. Inlet
9. Lower head

Delayed neutron precursor drift

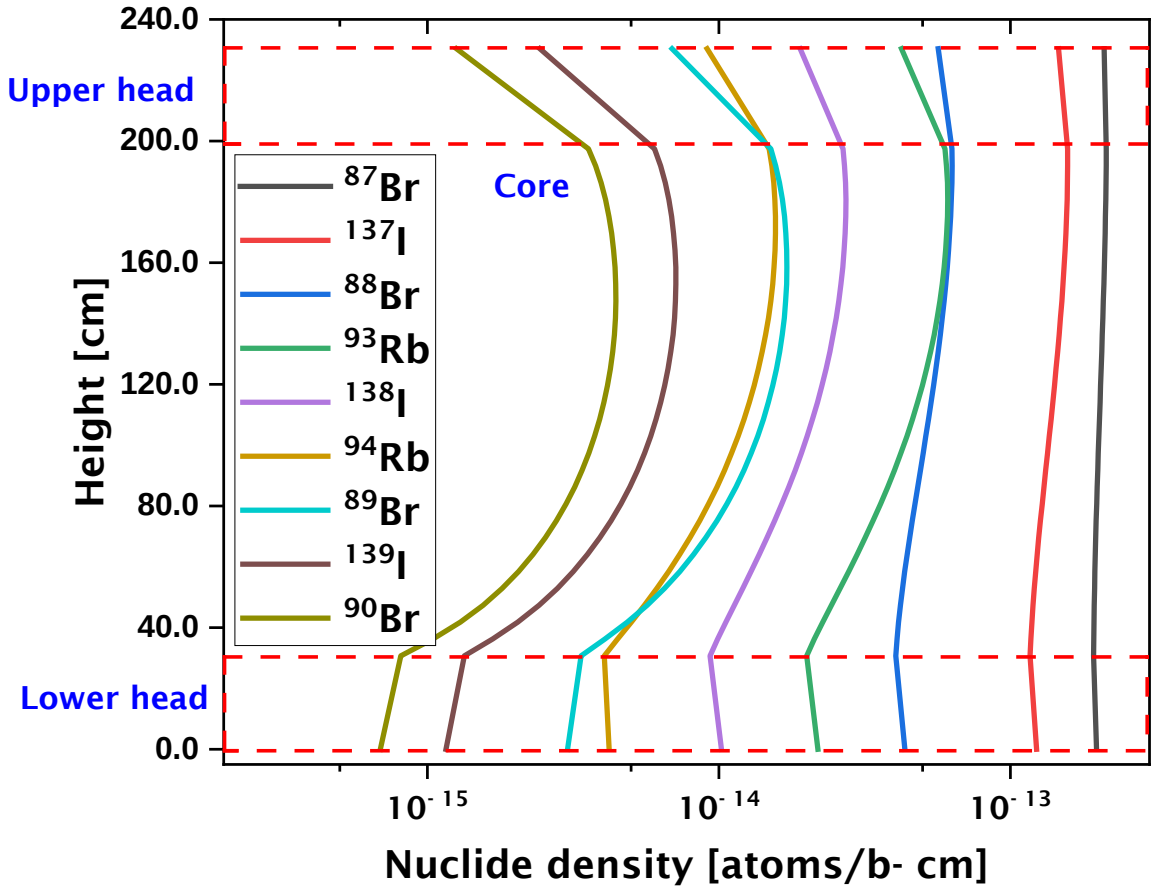
- Delayed neutrons are important for reactivity control
- Fission products that emit delayed neutrons are called “delayed neutron precursors” (DNP)
- In flowing fuel systems, delayed neutrons may be born outside of the core, commonly called DNP “drift”
- For example
  - MSRE β_{eff} ~ 700 pcm without drift
  - β_{eff} decreases as flow speed (drift) increases
- A DNP drift model has not yet been incorporated in this work
- Sensitivity studies show using detailed axial-dependent nuclide density versus system-average has negligible effect on the core power shape



Selected delayed neutron precursors calculated by ORIGEN

Delayed neutron precursor drift (cont.)

- DNP drift is most relevant for transient calculations
- Two approaches will be pursued
  - MELCOR DNP drift model based on standard 6-group delayed neutron precursors
  - New higher-fidelity model in MELCOR based on explicit delayed neutron precursor nuclides, as available through ORIGEN



Selected delayed neutron precursors calculated by ORIGEN

Summary of SCALE methods and results

U.S.NRC

Sandia National Laboratories

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. SAND20XX-XXXX P

SCALE MSR Summary

SCALE's capabilities were demonstrated:

- 3D modeling with TRITON-KENO for time snapshots of power profiles and reactivity coefficients
- TRITON-MSR for time-dependent system-average inventory considering noble gas and noble metal removal through off-gas system and plating out, respectively
- ORIGEN for region-dependent inventory considering noble gas removal

Planned enhancements:

- TRITON-MSR with continuous feed
- Tracking of removed nuclides in ORIGEN
- ORIGAMI for MSRs
- Integration of ORIGEN into MELCOR

MELCOR Molten Salt Reactor Models

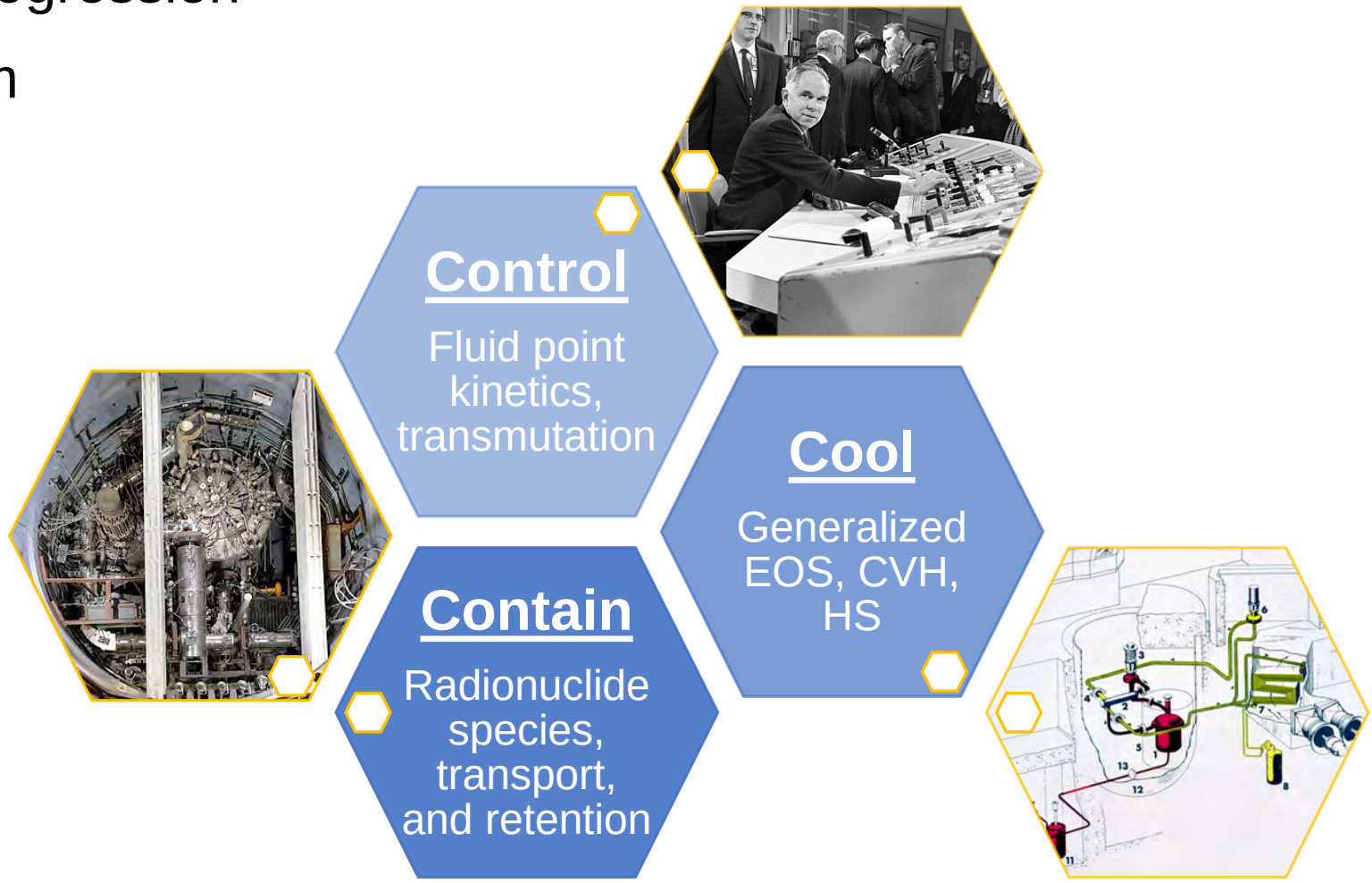
U.S.NRC

Sandia
National
Laboratories

Molten Salt Reactor Modeling

Molten Salt Reactor modeling in MELCOR

- Accident progression
- Source term



Modeling MSR Accidents with MELCOR – *Hydrodynamics and Heat Transport*

MELCOR remains a general purpose, multi-physics code to model integral plant response under accident conditions

- Serves as an effective foundation to support NRC readiness to license advanced nuclear energy technologies

Fluid fuel thermal hydraulics

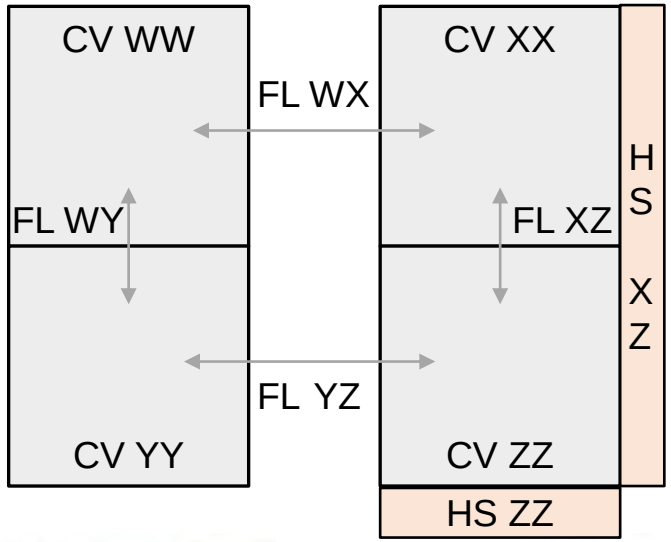
- Leverage existing thermal hydraulics modeling in MELCOR
- Utilize fundamental *two-phase* thermal hydraulic equations
- Introduce new thermo-physical properties and phase diagram of fluid specific to FLiBe
  - Generalized EOS – Equations of state for multiple working fluids are presently available in MELCOR including water, sodium, and FLiBe

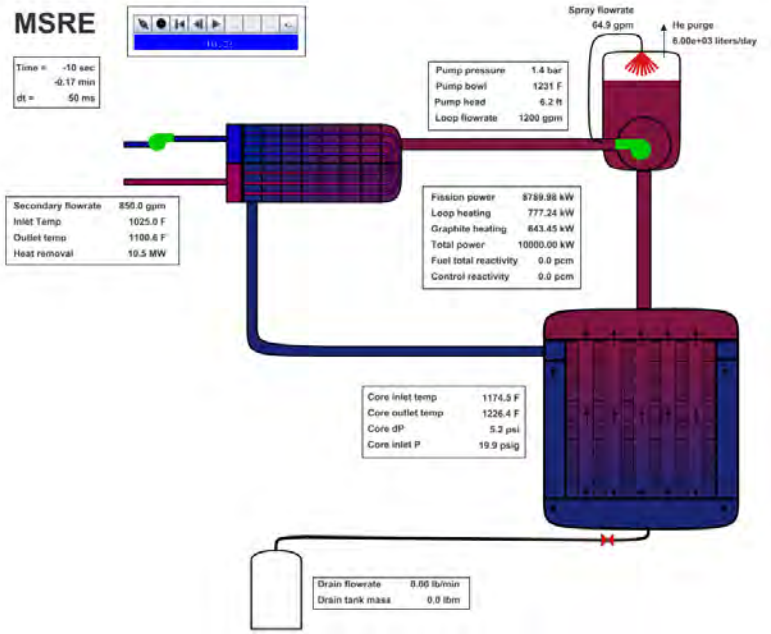
Thermal hydraulics – CVH/FL Model Packages

- Control Volume Hydrodynamics (CVH) package defines control volumes (CV)
- Flow path modeling 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
- CVH package manages convective heat losses





Modeling MSR Accidents with MELCOR – *Reactivity Control*

Fluid fuel point kinetics enables simplified, but appropriate treatment of neutronic transients

Fuel point kinetics – derived from standard point kinetic equations and solved similarly

Range of feedback models available for flexible modeling of transients

- **User-specified external input**
- Other implementations in the code (e.g., Doppler, fuel and moderator density) generally not used for MSR applications because they were derived for other types of reactor cores
- Flow reactivity feedback effects integrated into the equation set

Control volume fluid core with power distribution

- Neutronics model provides power in core-region, distribution of precursor radionuclides in the core and around the loop
- Radionuclides advected with the flowing salt contribute to decay heat in different regions of the reactor

Fission product transmutation enhancement

- Coupling with SCALE/Oak Ridge Isotope GENerator (ORIGEN) ongoing

Modeling MSR Accidents with MELCOR – *Fission Product Transport and Release*

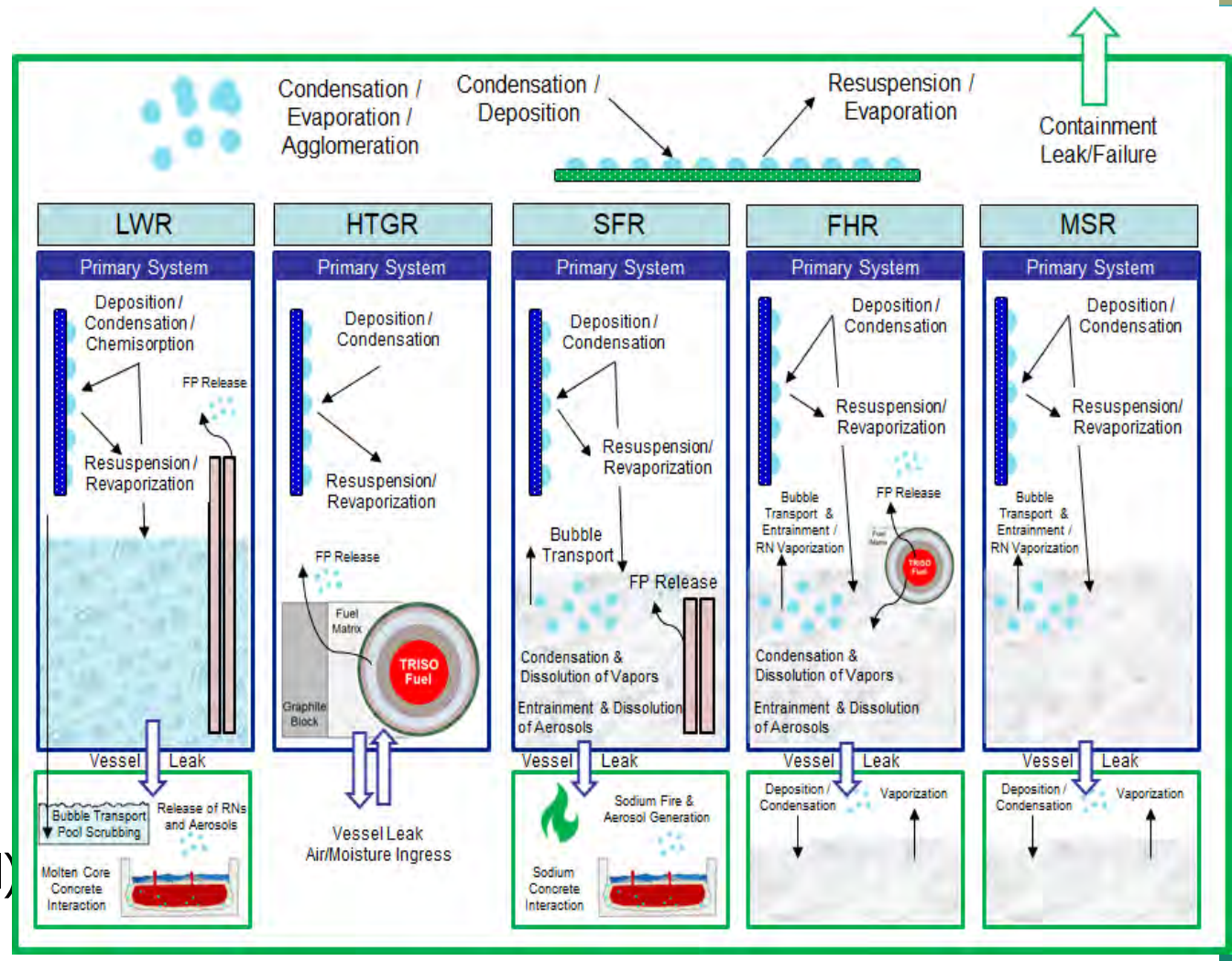
Molten salt serves as a potential means of fission product retention

Generalized Radionuclide Species

- Users can redefine/add RN classes
  - RN classes exhibit similar transport and retention behavior
  - Approach taken for molten salt systems - unique fission product chemistry relative to water-moderated systems
  - See Slide 75 for example grouping chosen for MSRs

Fluid fuel radionuclide transport

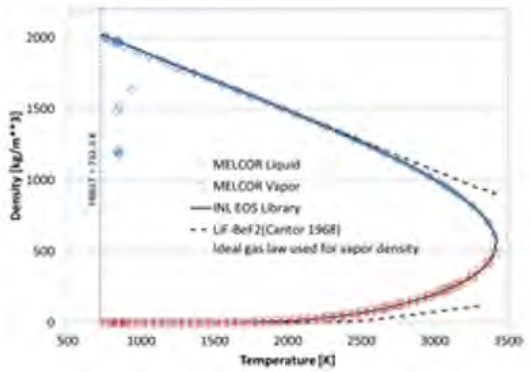
- Generalized Radionuclide Transport and Retention (GRTR) modeling framework
- Molten salt chemistry and physics pertaining to radionuclide transport
- GRTR for MSRs but generalized and applicable to other systems (e.g., liquid metal)

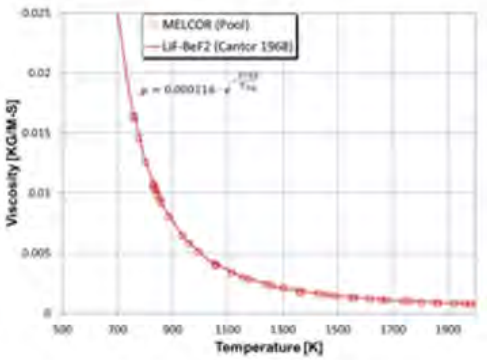


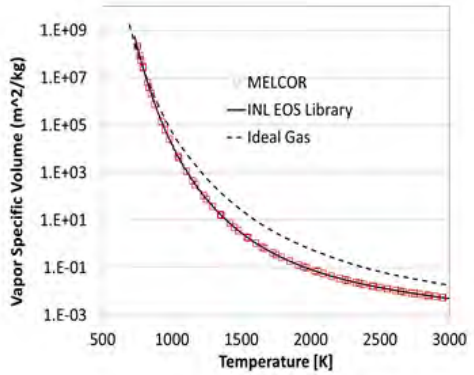
FLiBe Equation of State

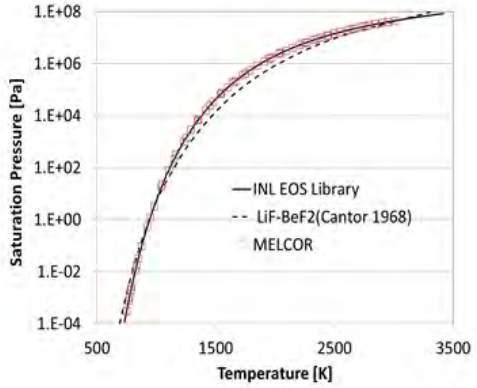
Generic working fluid EOS capability facilitates FLiBe as hydrodynamic material

- MELCOR employs fluid property files – INL fusion safety program
- Chen's soft sphere model used for FLiBe (INL/EXT-17-44148)
- Property database from ORNL data (ORNL-TM-2316)
- Verified MELCOR EOS library and properties for FLiBe









Initial validation activity against ORNL MSRE

FLiBe Equation of State – Implications of Salt Freezing

Freezing of molten salt an important consideration for a range of accident conditions

- Address fluids that freeze in an accident such as a salt spill
- Freezing in cooling systems (e.g., DRACS)

Adding capabilities to explicitly treat freezing of fluids

- Currently an approximation is used to handle conditions where fluids reach temperatures at or below their freezing point
- Generalized capability for other fluids (e.g., sodium)

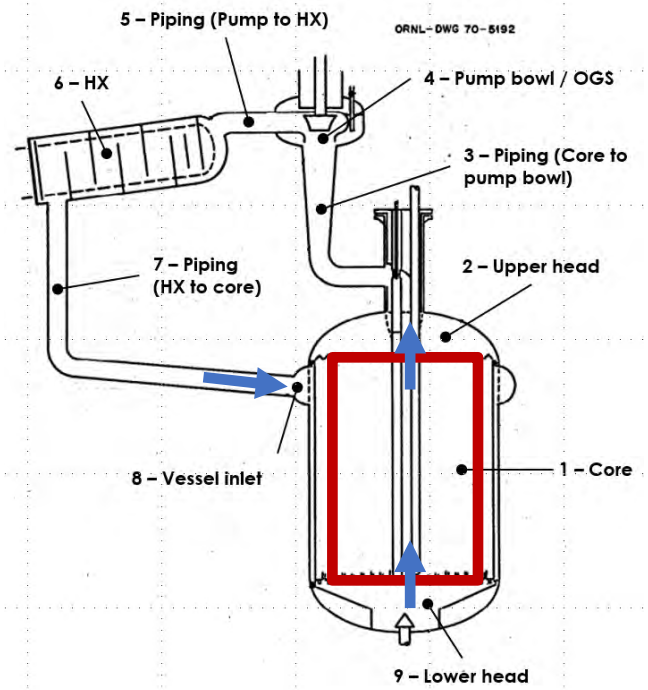
Fluid Core and Power Distribution

Fluid fuel core defined within the graphite stringers

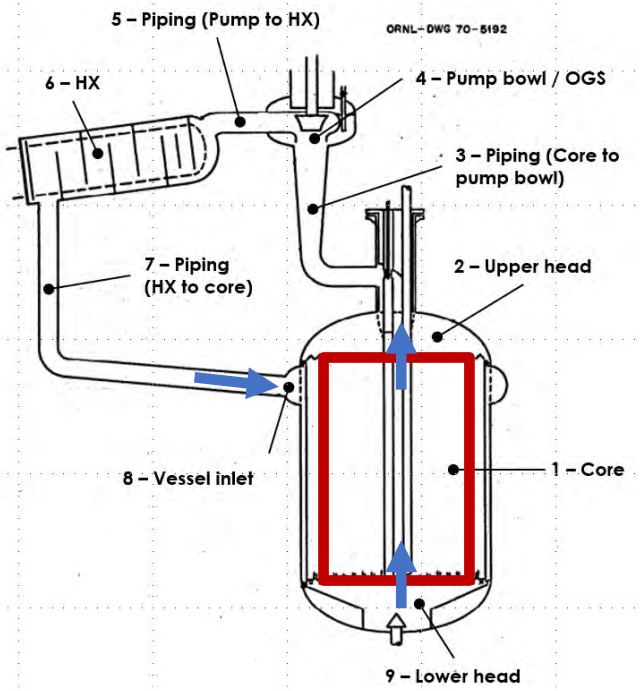
- The fluid volume within the graphite stringers comprise the active “Core”
- “Loop” volumes comprise a portion of the primary fuel flow loop OUTSIDE the active core
- Allows specification of the axial and radial power distribution from SCALE
  - Feedbacks and power governed by flowing fluid fuel point reactor kinetics model

Fission power generation in “core” and “loop” control volumes

- Fission power and feedbacks are calculated for the “core” volumes
- No fission power energy generation in “loop” volumes
- Decay heat (due to radionuclide class mass carried in pool) for both volume types
- Graphite heating due to neutron absorption
- Provisions for shutdown in a spill accident



Fluid Fuel Neutronic Transients – Modified Point Kinetics



Fission inside **core**

- Neutrons generated and moderated
- **DNPs** generated

DNPs that do not decay in core-region flow into loop

- Decay in loop or advect back into core-region

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

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

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

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

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

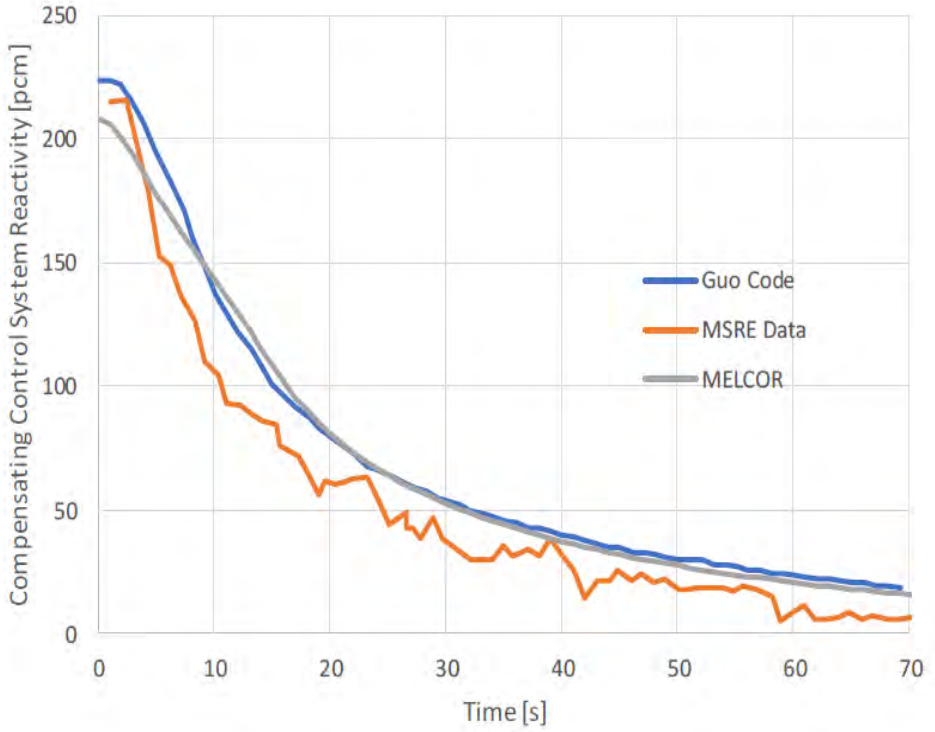
** **DNP** = Delayed Neutron Precursor

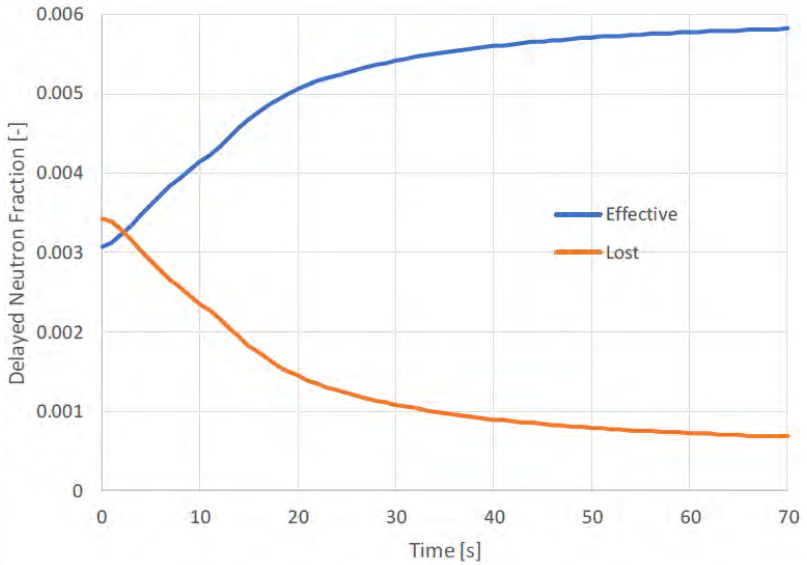
Fluid Fuel Point Kinetics – Initial Validation

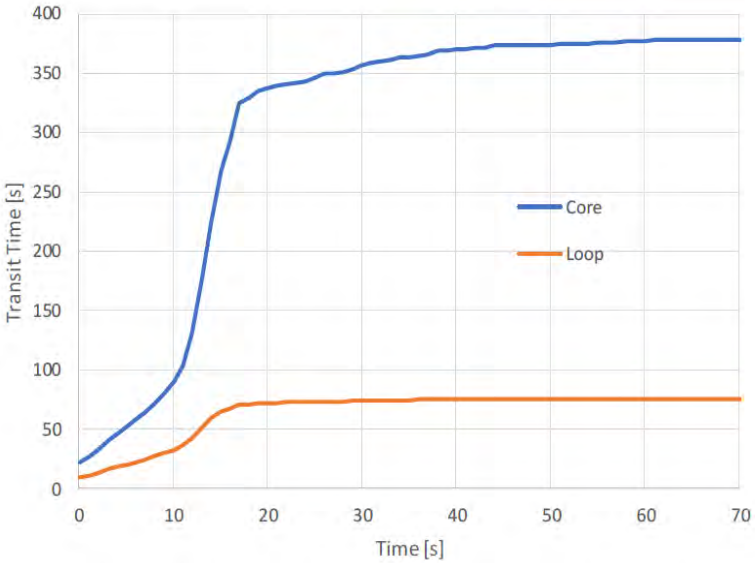
MELCOR non-LWR validation is leveraging available data

- Validation basis will continually expand with evolution of tests and deployments

Initial validation has been performed against zero-power MSRE pump flow coast-down test







GRTR – Generalized Radionuclide Transport and Retention

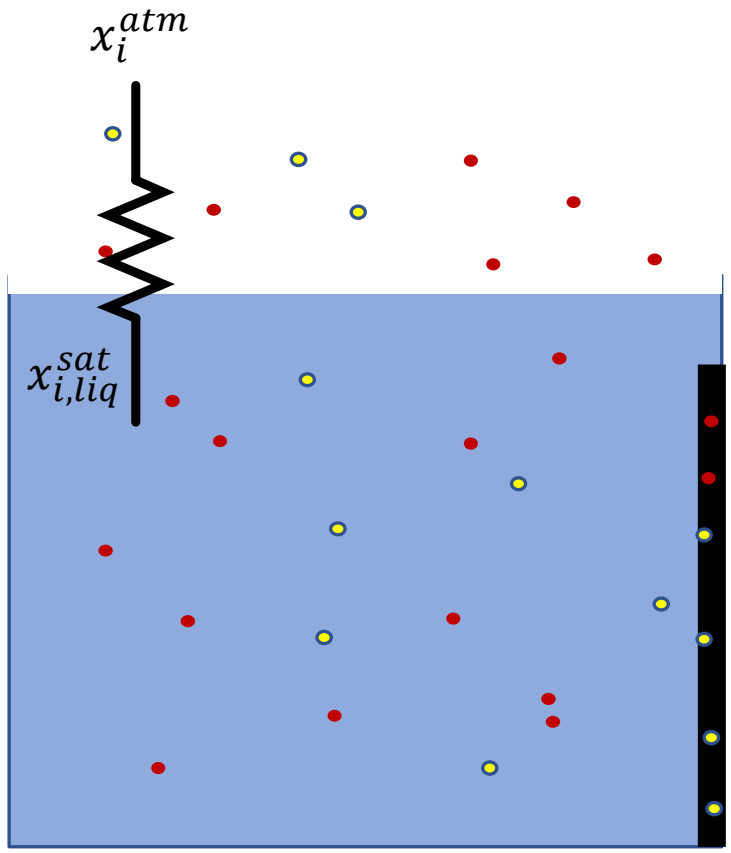
Track where fission products are and how much is released from liquid to atmosphere

Characterizes evolution of fission products between different physico-chemical forms

- Fission product evolution from a liquid pool to an atmosphere
  - Influenced by solubility and vapor pressure
- Insoluble fission product deposition on structures

GRTR mass transport modeling characterizes

- Concentration of radionuclide forms
- Concentration gradients between radionuclide forms
- Resistance to mass transfer between radionuclide forms using standard correlation-based interfacial mass transport theory



GRTR and Integral MELCOR Simulations

Inputs to GRTR Model

- Radionuclide mass in (or released to) liquid pool
- Chemical speciation
- Pressure in hydrodynamic volume
- Temperature in *regions* of hydrodynamic volume (e.g., liquid and atmosphere)
- Advective flows of liquid and atmosphere between hydrodynamic volumes

GRTR Physico-Chemical Transport Dynamics

- Soluble radionuclide form mass
- Colloidal radionuclide form mass
- Deposited radionuclide form mass
- Gaseous radionuclide mass

Advective and Fission/Transmutation Dynamics

- Advection of radionuclides in liquid pool or atmosphere
- Decay of radionuclides in hydrodynamic control volume ***Coupling with ORIGEN***

For Each Timestep

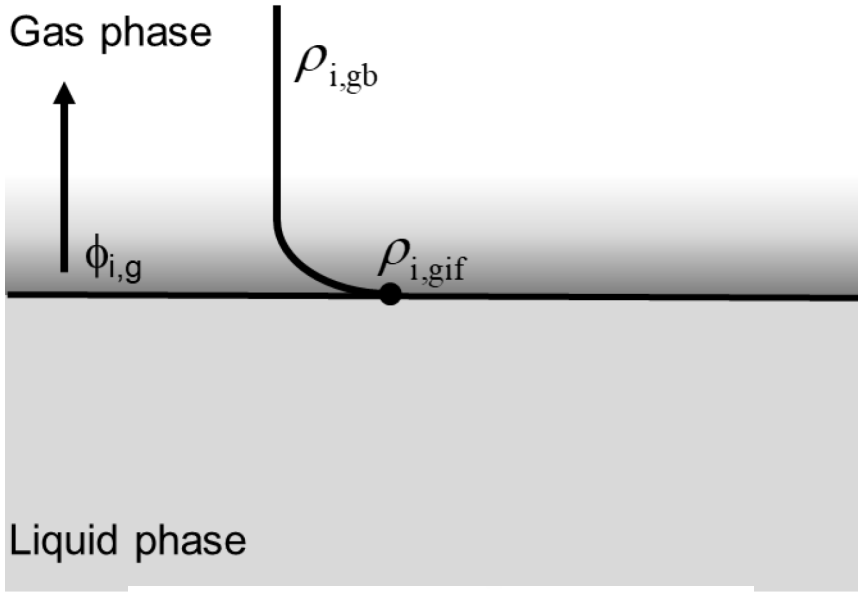
GRTR – Range of Mass Transport Processes

Evolution of fission products from molten salts primarily focused on vaporization

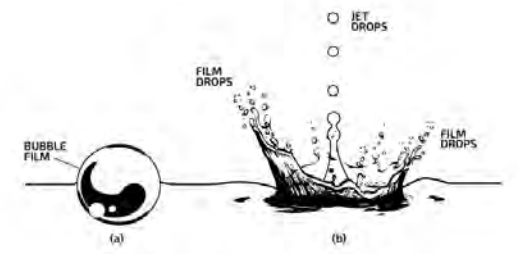
- Provides ability to perform best estimate evaluations of release from molten salts
- Demonstration calculations have focused on direct comparison to MSRE for the maximum hypothetical accident
- Exercise of model will be performed next year

Mass transfer interfaces

- Liquid-gas atmosphere interfaces
- Liquid-solid structure interfaces
- Gas atmosphere-solid structure interfaces
- Model allows new interfaces to be defined

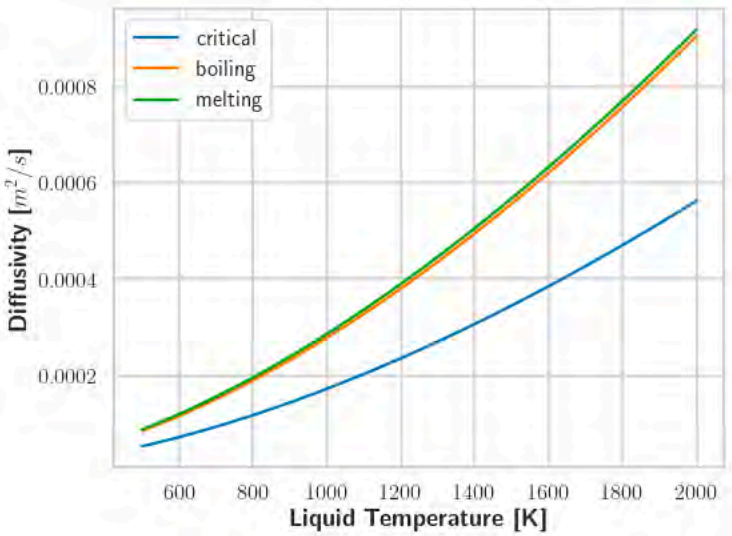


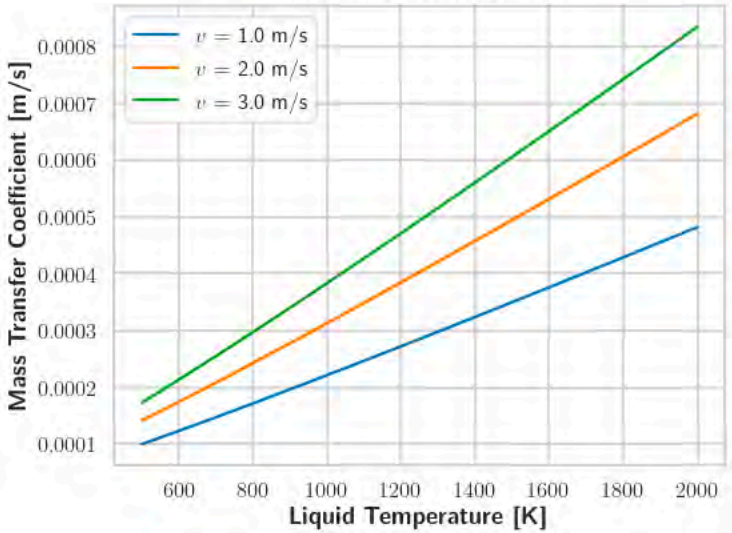
Sparging gas flows (i.e., helium gas injection) will result in fission products entrained in the gas bubble formed by injection

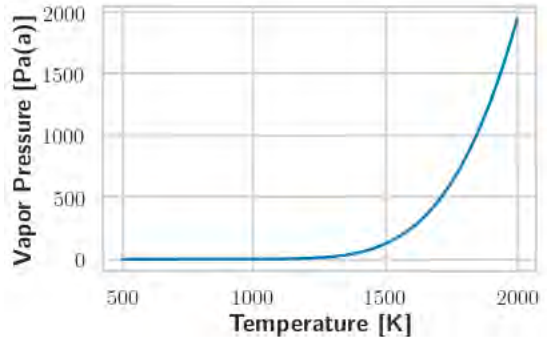


Jet breakup when contaminated fluids are released into a gas atmosphere (e.g., due to a pipe break)

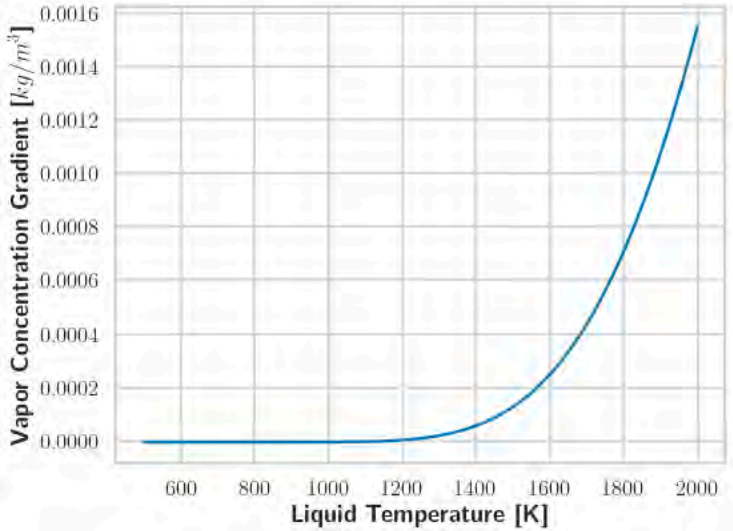
Illustrating Components of Vaporization Mass Transfer



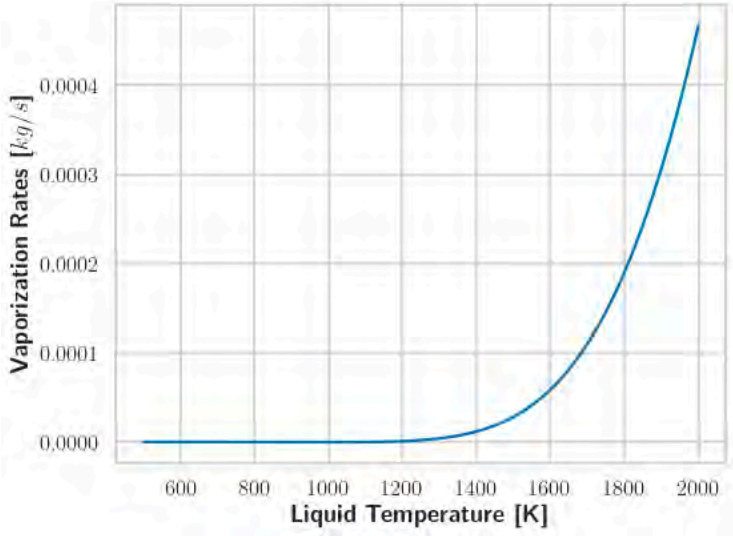




Example CsF vapor pressure – subject to change as thermochemistry evolves



$$\dot{m}_{vap} = h_m A_{int}\left(x_{liq}^{sat} - x_{atm}\right)$$



Mass transfer coefficient captures effectiveness of species diffusion into atmosphere from liquid-gas interface as well as convective flows carrying vapor away from interface

Evolution of GRTR Modeling

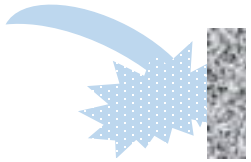
Focus of modeling efforts evolving based on insights from current demonstration calculations

For salt spills, MELCOR GRTR model predicts very small vaporization releases of CsF, CsOH and CsI from salt

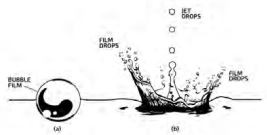
- Relatively low temperature molten salt temperature leads to a very low vaporization (<<10^{-6})
- Contribution of the vaporization term in a spill scenario is negligible

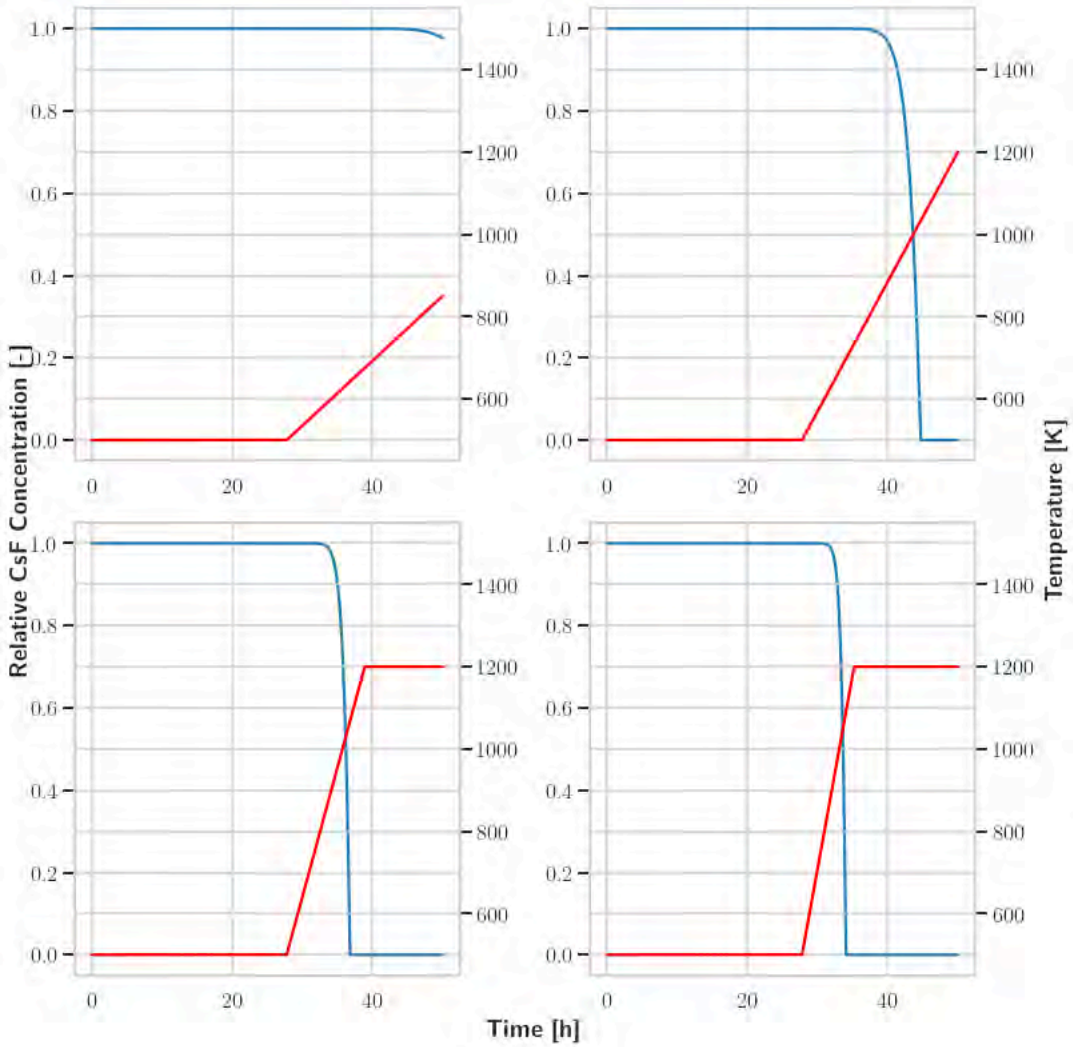
Ongoing model development utilizes flexibility to explore different ways to characterize other release mechanisms

- Jet breakup and splashing models



- Aerosol release from bubble bursting





Molten Salt Reactor Plant Model and Source Term Analysis

U.S.NRC

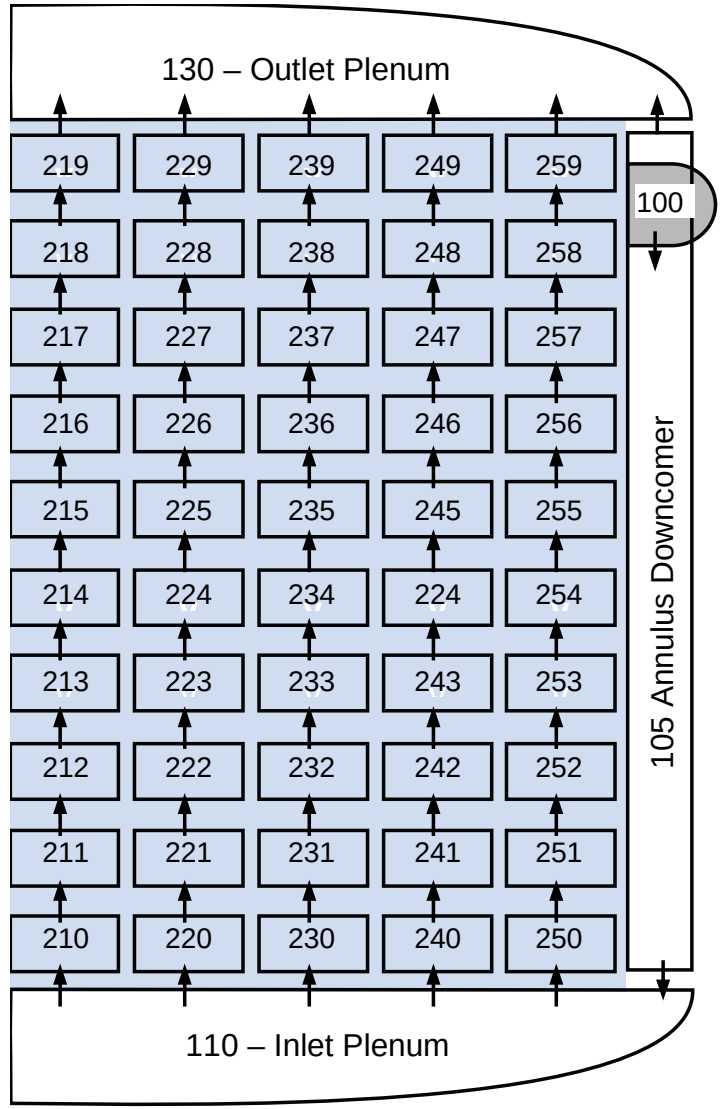
OAK RIDGE National Laboratory

Sandia National Laboratories

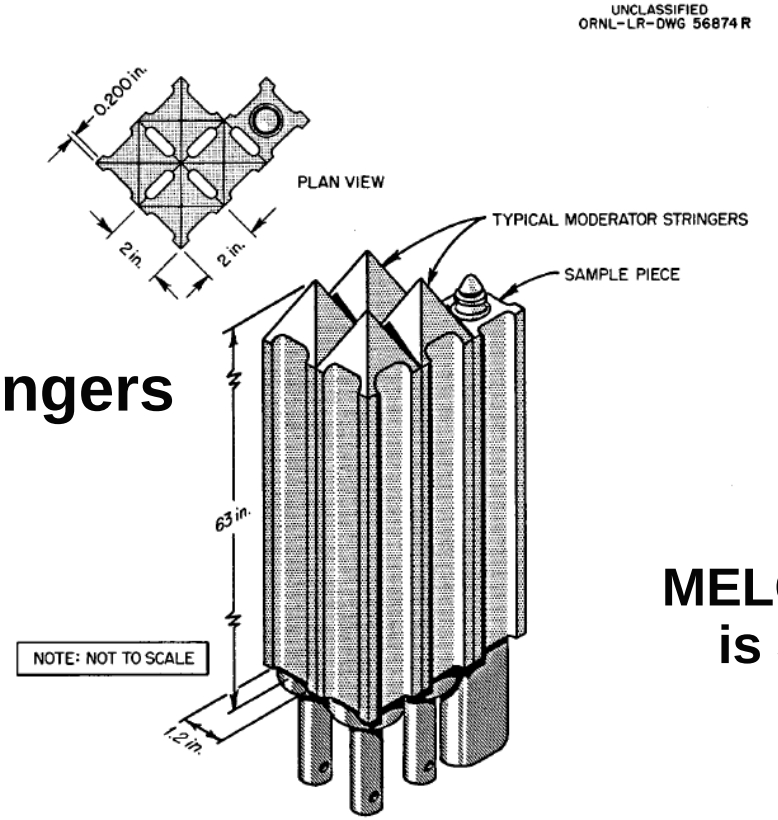
MELCOR nodalization - core and reactor vessel

Vessel nodalization

- Assumes azimuthal symmetry
- The graphite core structure is subdivided into 10 axial levels and 5 radial rings
  - Next slide shows mapping from SCALE
- Molten fuel salt enters through an annular distributor (cv-100) that directs the flow into the annular downcomer (cv-105) and the core inlet plenum (cv-110)
- The core is formed by graphite stringers that include flow channels
- The molten fuel salt flows through the stringers (CV-210 through CV-259), where the fuel fissions

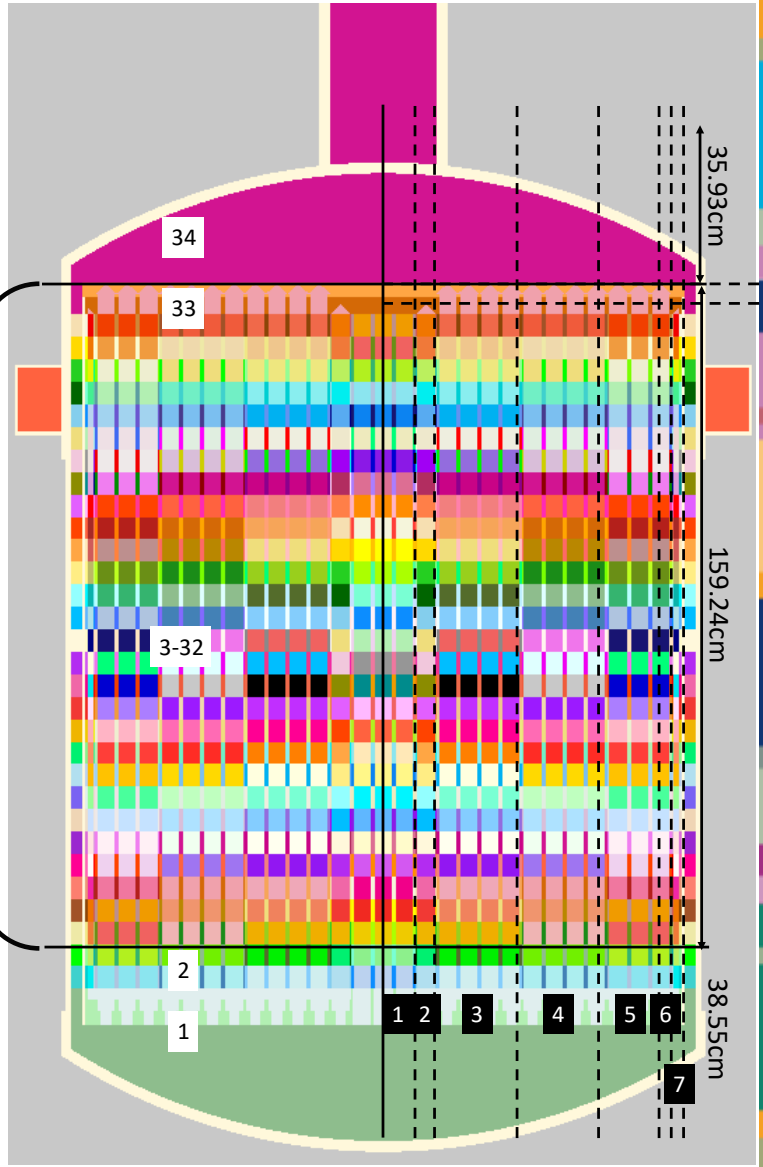


MELCOR core region mapping to SCALE



600 stringers

MELCOR axial mapping is 3 SCALE levels per 1 MELCOR level



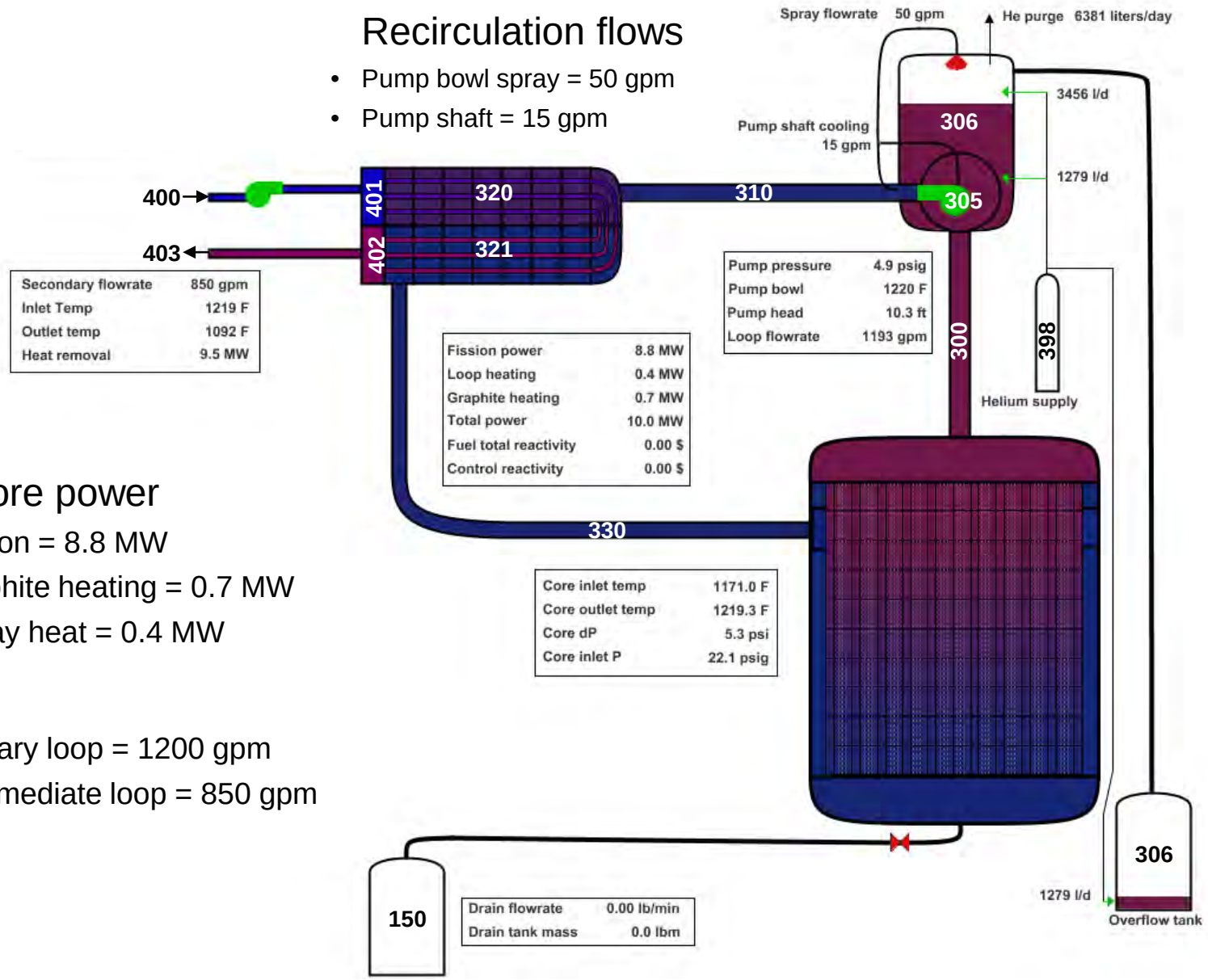
MELCOR radial mapping to SCALE

ORNL Radial Zone (r)	1 & 2	3	4	5	6 & 7
MELCOR Radial Zone (r)	1	2	3	4	5
Percent	3.5%	19.3%	35.3%	36.7%	5.2%

MELCOR nodalization - primary recirculation loop

Recirculation flows

- Pump bowl spray = 50 gpm
- Pump shaft = 15 gpm



Total core power

- Fission = 8.8 MW
- Graphite heating = 0.7 MW
- Decay heat = 0.4 MW

Flows

- Primary loop = 1200 gpm
- Intermediate loop = 850 gpm

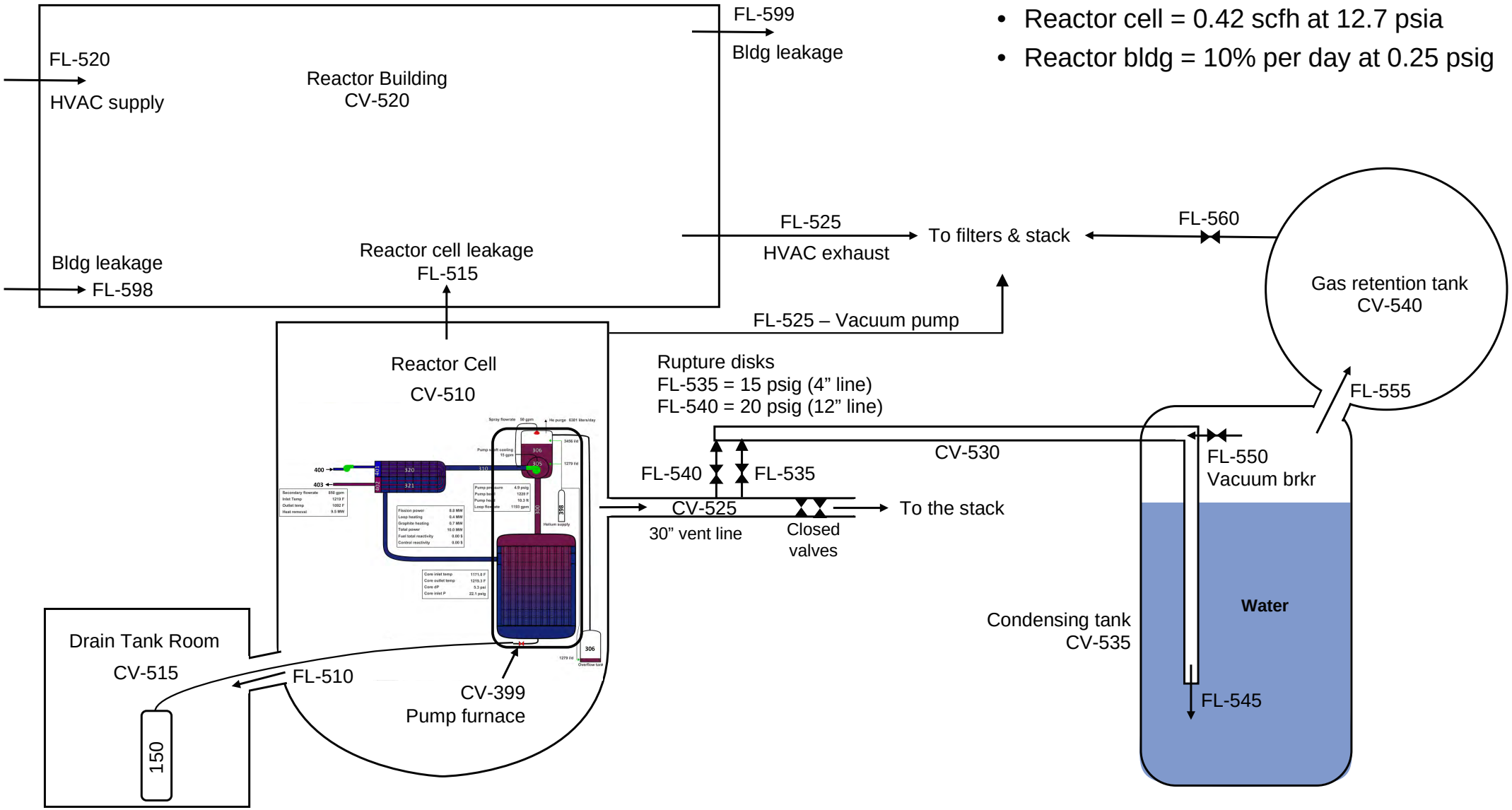
Helium off-gas flows

- Pump shaft = 1279 l/d
- Pump bowl = 3456 l/d
- Overflow tank = 1279 l/d

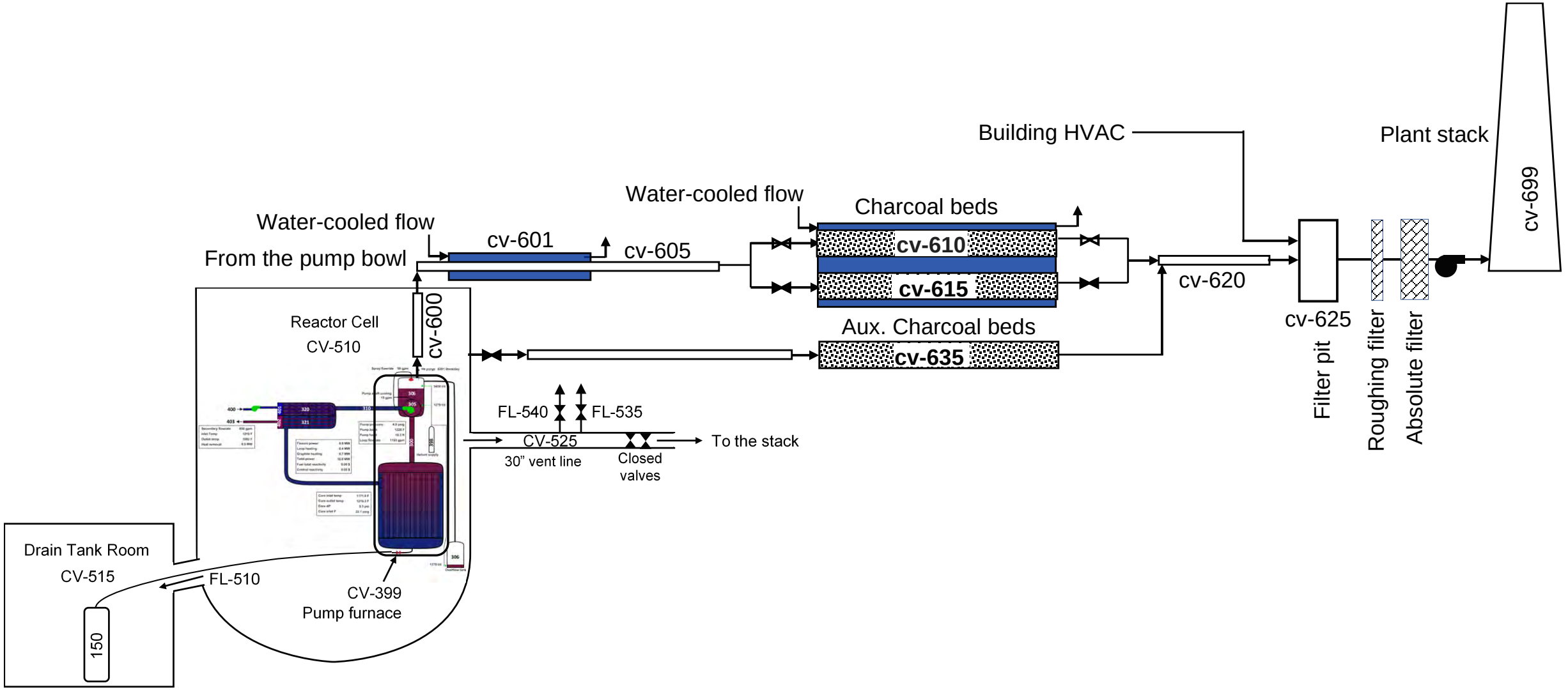
MELCOR nodalization – reactor cell, condensing tank, and reactor building

Leakages

- Reactor cell = 0.42 scfh at 12.7 psia
- Reactor bldg = 10% per day at 0.25 psig



MELCOR nodalization - offgas system



MELCOR model inputs (1/2)

Equilibrium inventory and decay heat by region from SCALE

Radial and axial power profiles from SCALE

Reactivity and Xe feedbacks from SCALE

Radionuclide distribution from SCALE

Collaborative redefinition of radionuclide classes with ORNL

- Re-grouping from LWR definition based on solubility estimations from MSRE empirical experience and suggestions by Britt (ORNL)
- Noble metals isolated into two groups (next slide)

Antoine coefficient estimates for few species (Cs, CsF)

- Cesium and cesium fluoride estimated using MSTDB-TC

[Phillip Britt, Future Research Directions, DOE-NE Molten Salt Chemistry Workshop, April 10-12, 2017, ORNL]

MELCOR model inputs (2/2)

MELCOR Elemental Grouping

Xe : He, Ne, Ar, Kr, Xe, Rn, H, N

Cs : Li, Na, K, Rb, Cs, Fr, Cu

Ba : Be, Mg, Ca, Sr, Ba, Ra, Es

I : F, Cl, Br, I, At

S : S, Po

Re : Re, Os, Ir, Pt, Au, Ni

V : V, Cr, Fe, Co, M, Ta, W

Mo : Mo, Tc, Ru, Rh, Pd, Ag, Ge, As, Sn, Sb

Nb : Nb, Zn, Cd, Se, Te

Ce : Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C

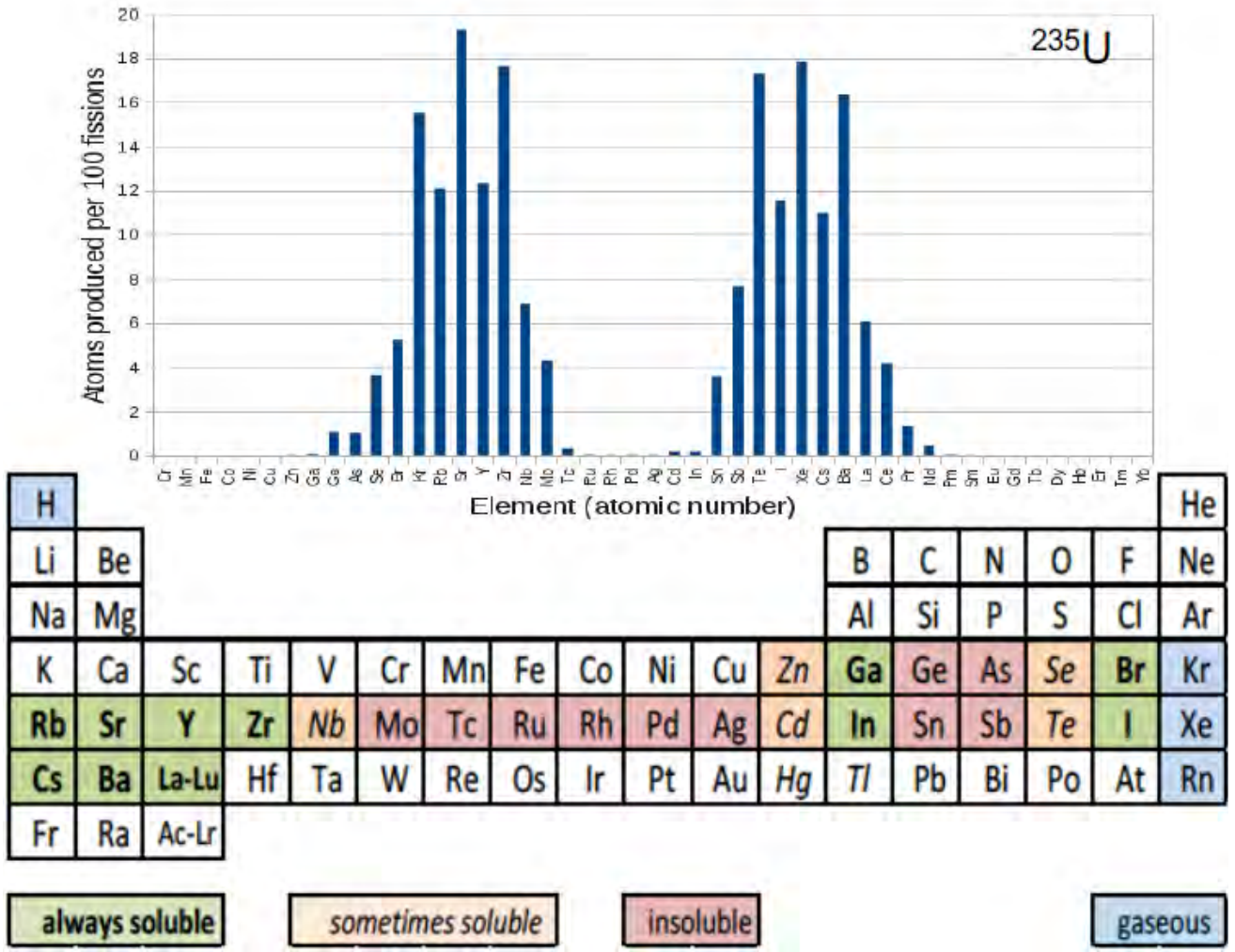
La : Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf

U : U

Cd : Hg, Ga, In

Ag : Pb, Tl, Bi

B : B, Si, P



Mo class assumed to be insoluble

[Phillip Britt, Future Research Directions, DOE-NE Molten Salt Chemistry Workshop, April 10-12, 2017, ORNL]

Scenario

Spill of molten salt into the reactor cell (containment)

- Full reactor spill – maximum credible accident in the MSRE safety analysis
  - Spill onto the floor without coincident water leak (MCA1-MCA5)
  - Spill with coincident water leak (MCA6-MCA9)

Exploratory radionuclide source term due to limited information from the molten salt thermophysical databases

- ORNL-TM-0732 MSRE safety analysis source term
  - Integral calculation with aerosol physics
- GRTR vaporization model without splashing
  - Cs, CsI, and Xe releases

Sensitivities

- HVAC operating or off
- Auxiliary filter operation
- Aerosol size

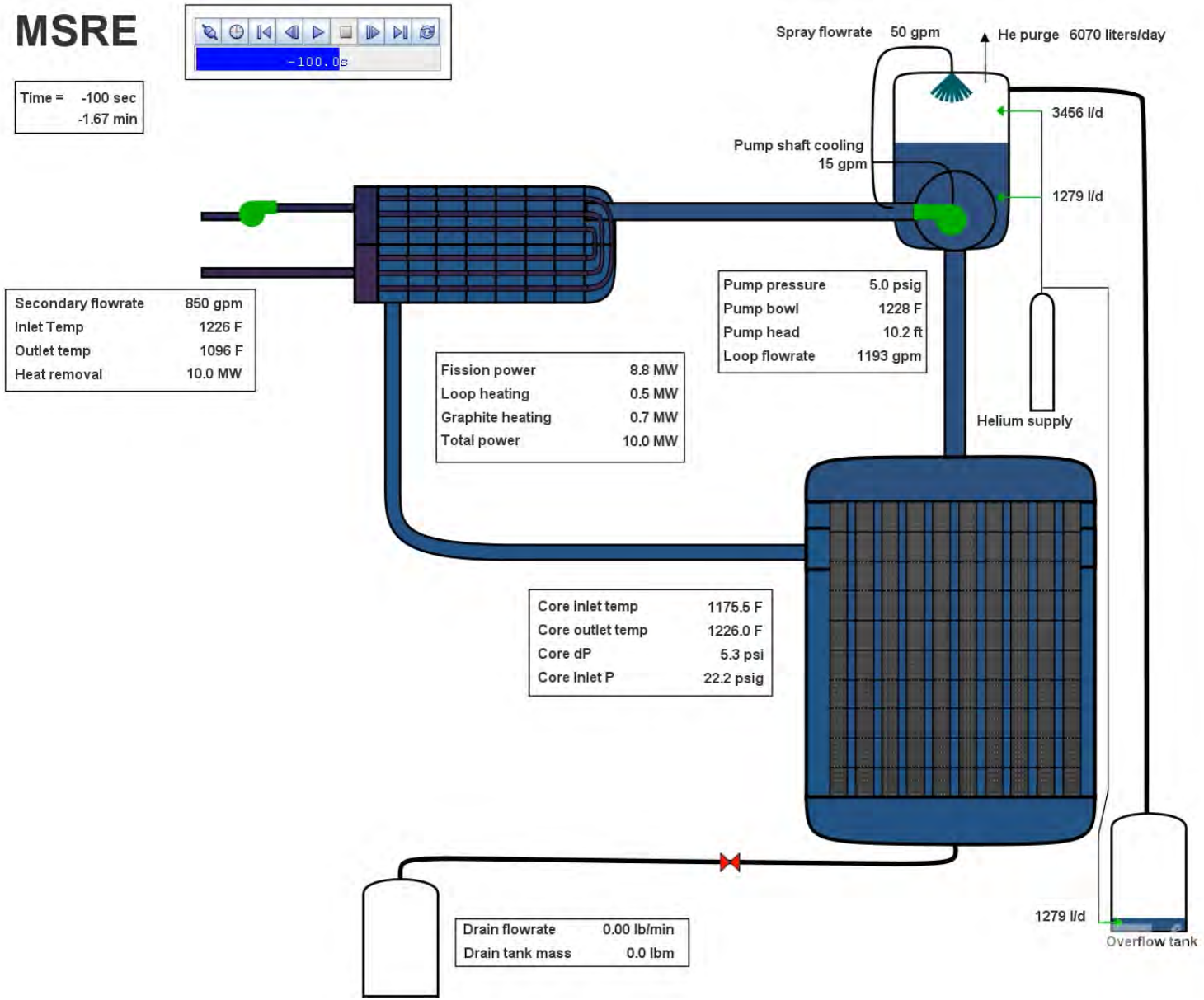
Salt spill cases

Walk-through MCA1 (base case)

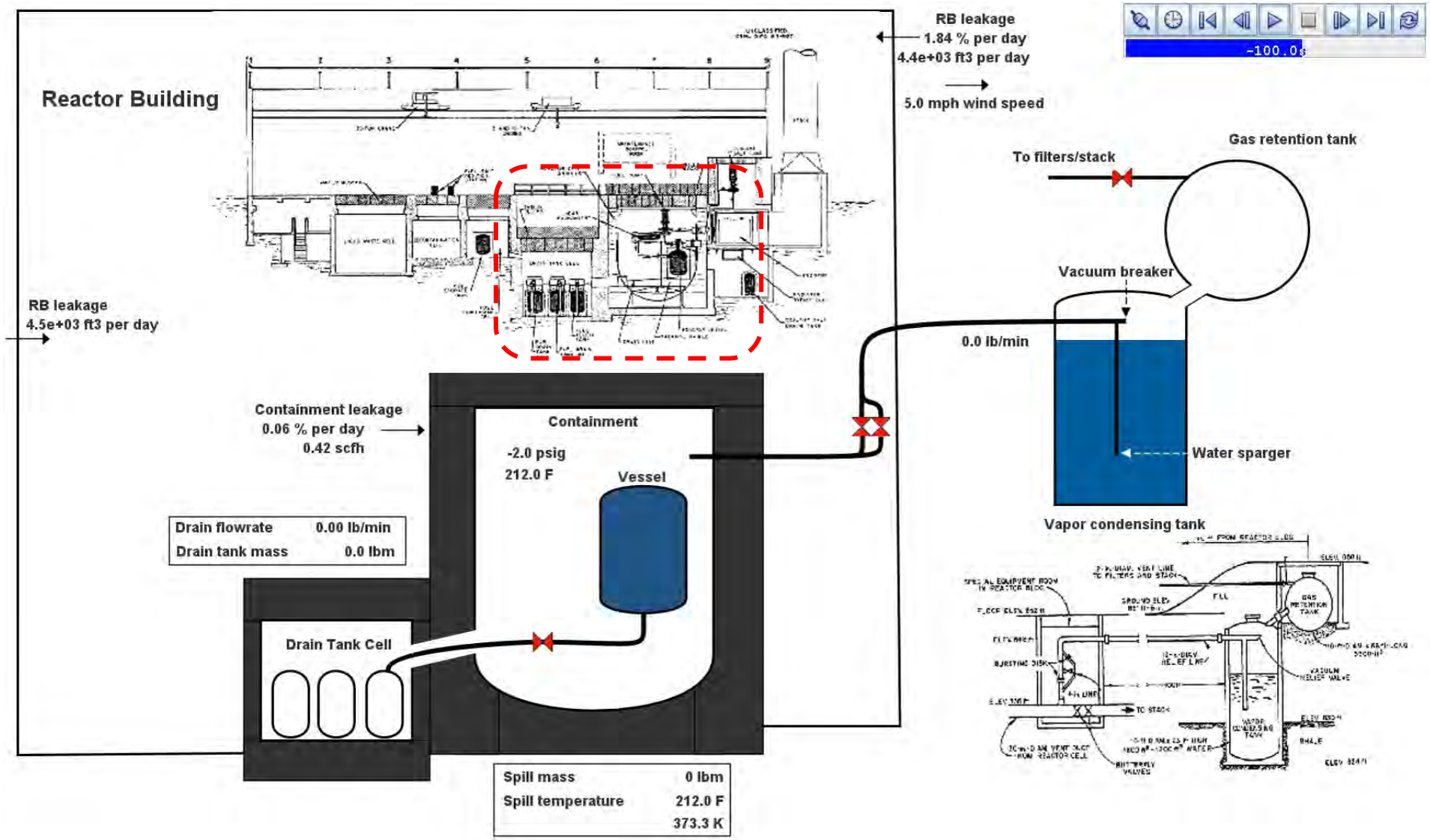
- Spill creates aerosols with 1 μm mass median diameter (MMD) with a 1.5 geometric standard deviation (GSD)
- The HVAC remains running and ventilating the reactor building
- The auxiliary filters are not used to filter the reactor cell
- There is no coincident water spill onto the molten salt

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No
MCA6	1 μm	Yes	No	Yes
MCA7	1 μm	Yes	Yes	Yes
MCA8	1 μm	No	Yes	Yes
MCA9	1 μm	No	No	Yes

MCA1 salt spill base case – Primary System Response

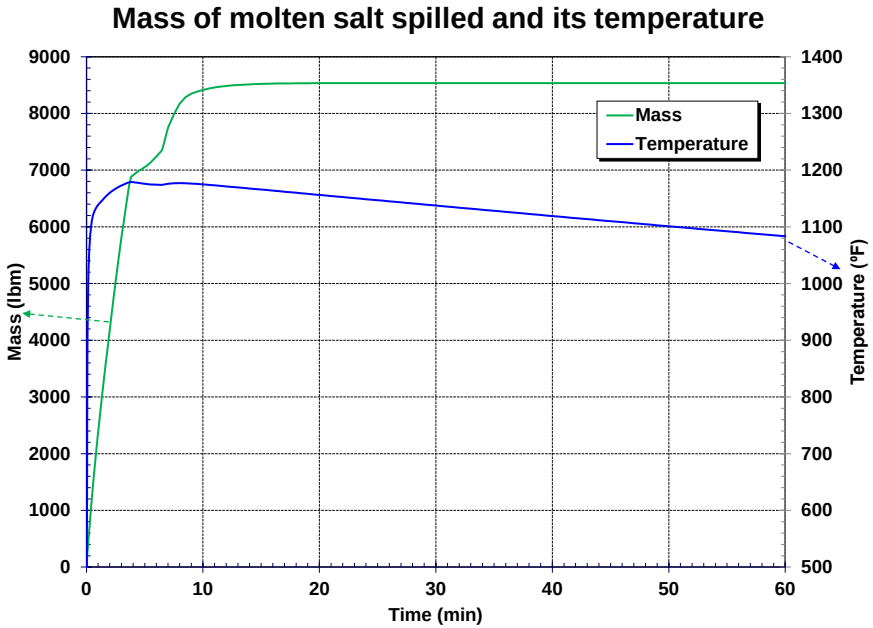


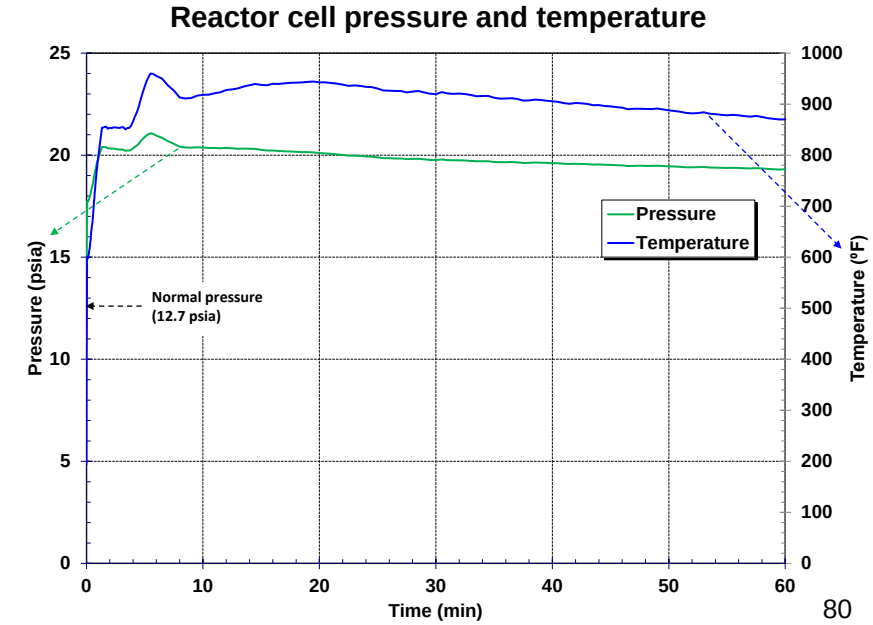
MCA1 salt spill base case – Reactor Cell Response



MCA1 reactor cell thermal-hydraulic response

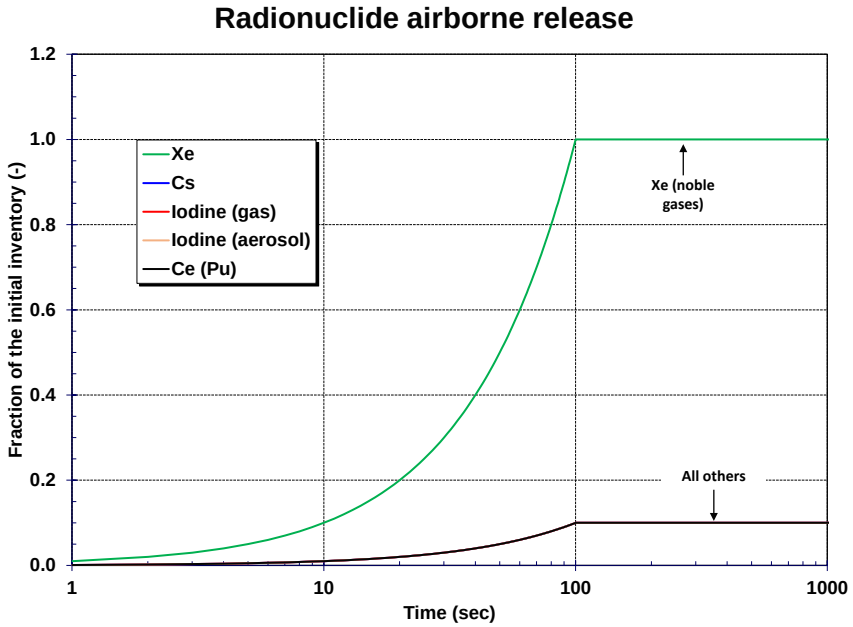
- The primary loop salt inventory spills to the reactor cell in 10 minutes
  - Temperature of the molten salt is relatively constant with a slow cooling trend
- There is an immediate pressurization of the gas space from subatmospheric to ~20 psia
  - Heating due to hot molten salt (~1100ºF)
  - Heating due to the released radionuclides
- Reactor cell gas temperature initially rises to over 900ºF and then slowly cools

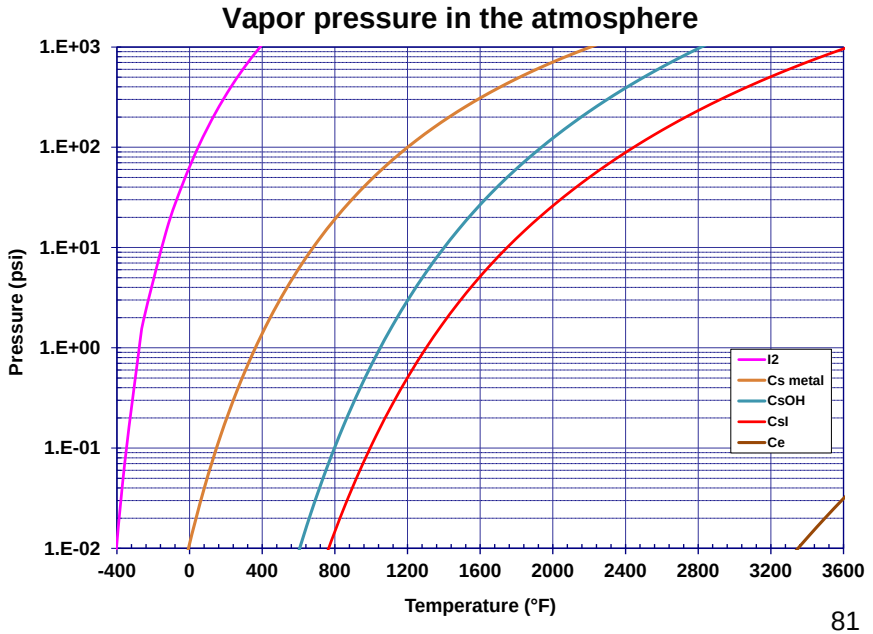




MCA1 reactor cell radionuclide releases

- Airborne release assumptions [ORNL-TM-0732]
  - 100% of the noble gases
  - 10% of the iodine
  - 10% of all other volatile and non-volatile radionuclides
  - MCA from MSRE safety analysis
- Radionuclides phase (aerosol or gas) depends on temperature and chemical form
  - Preliminary analysis used LWR view of chemical forms
    - Some gaseous iodine (5%)
    - Cesium and iodine combine (CsI)
  - MELCOR allows exploration of various chemical forms for the MSR





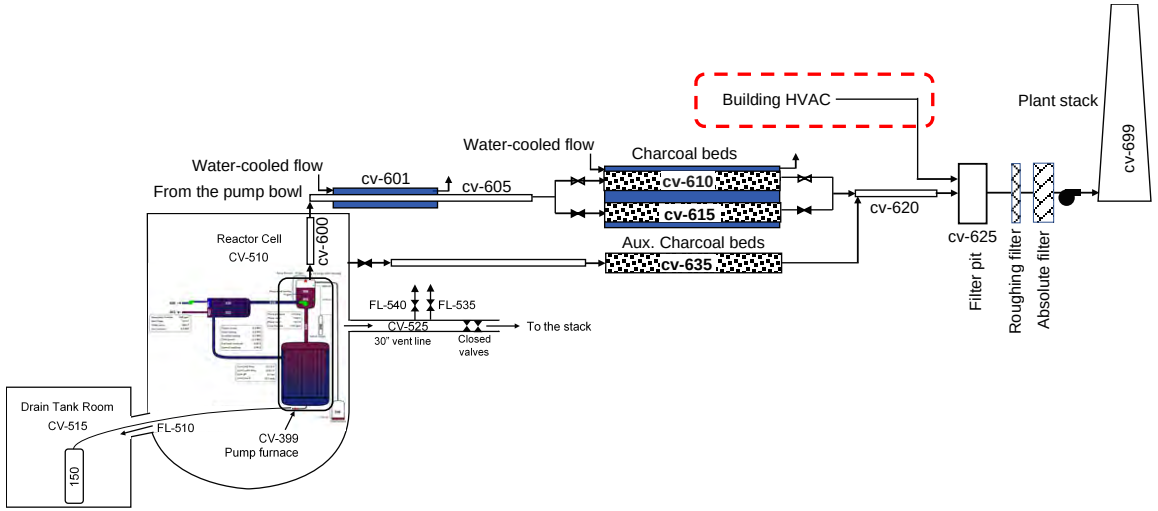
MCA1 gaseous radionuclide distributions

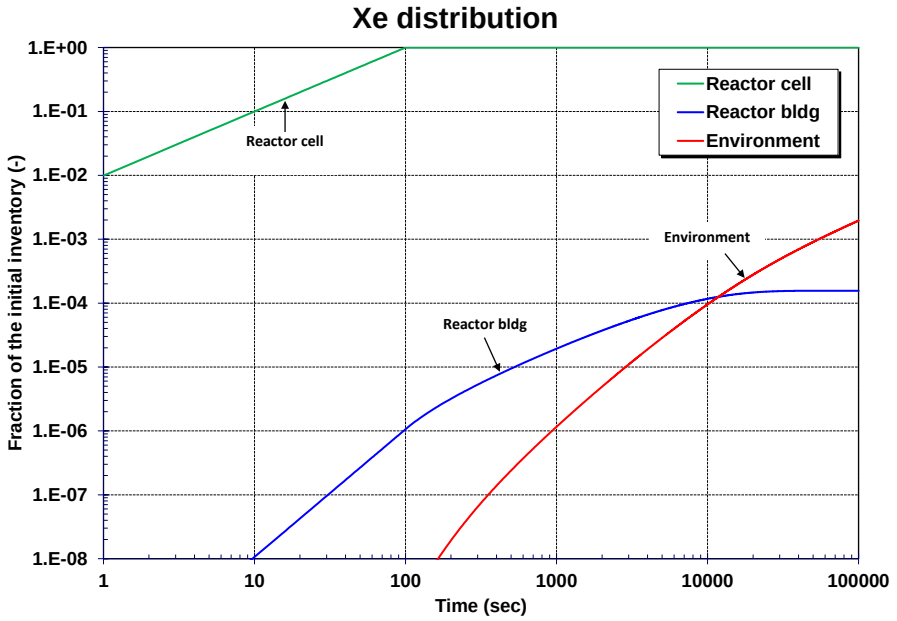
Gaseous releases (xenon and iodine gas) respond similarly

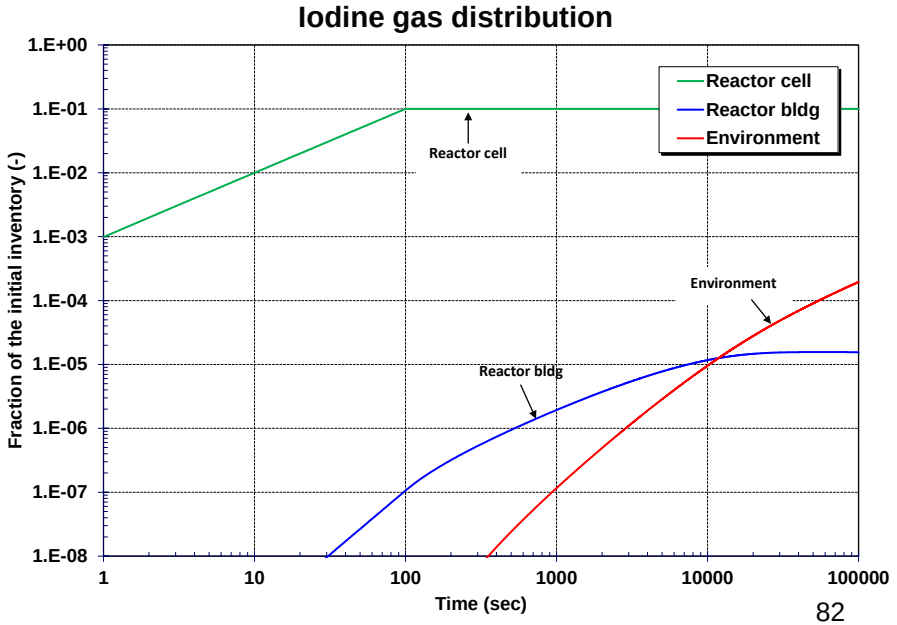
- Most of the gases retained in the reactor cell
- Reactor cell slowly leaks to the reactor building

The reactor building HVAC is operating in MCA1, which exhausts gases from the reactor building through the absolute filters to the plant stack

- 0.2% of the xenon reaches the environment
- 0.02% of the gaseous iodine reaches the environment



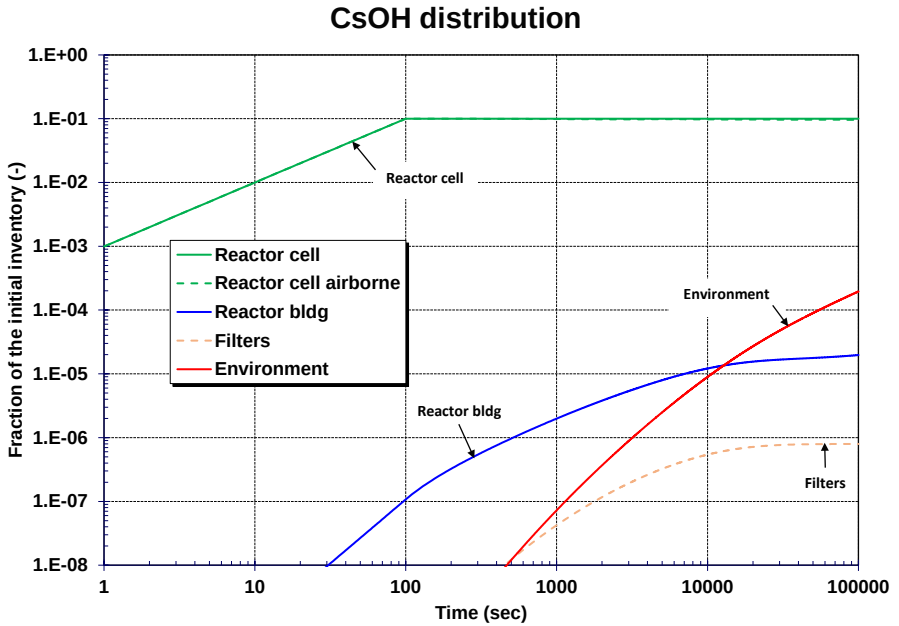


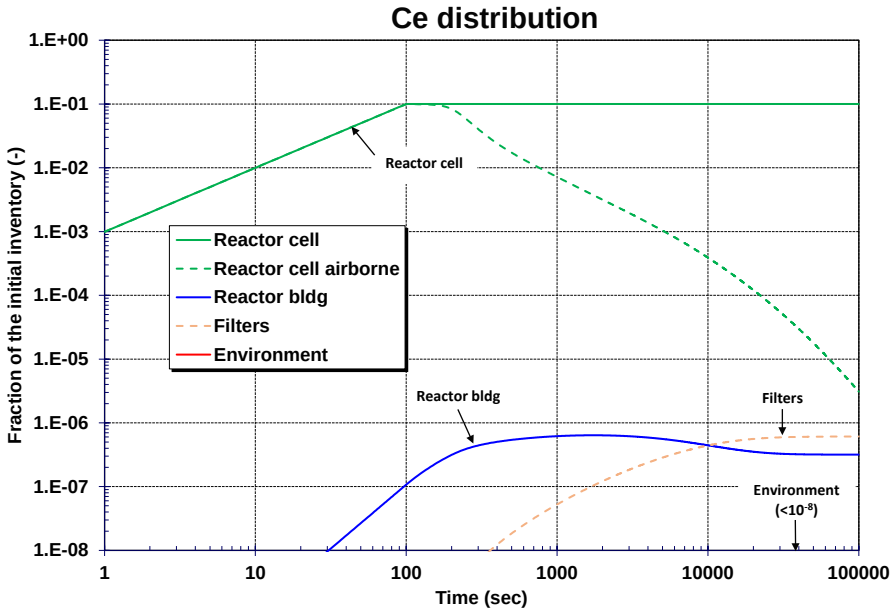


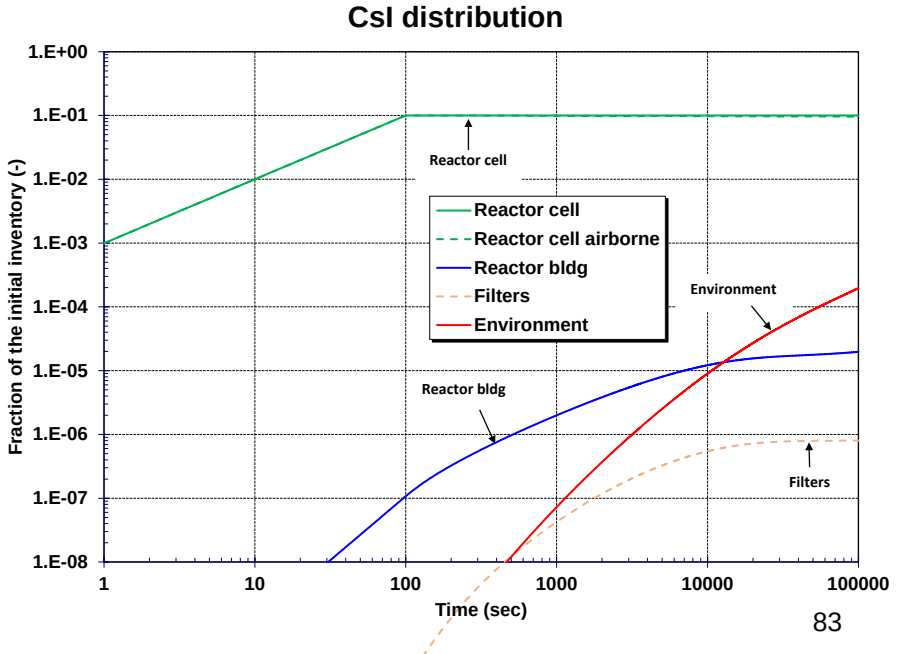
MCA1 aerosol radionuclide distributions

Release fractions of radionuclides that form aerosols in the reactor building

- CsOH and CsI illustrate radionuclide chemical forms that are primarily vapor in the reactor cell with limited settling but aerosols after leakage to the reactor building
- Ce distribution is typical of less volatile radionuclides that settle over time in the reactor cell and are captured by the absolute filters







Salt spill with water base case

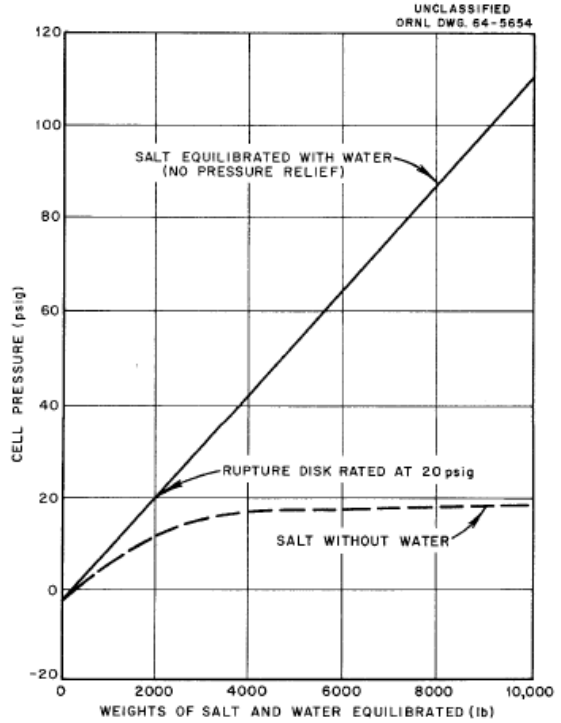
Walk-through MCA6

- Spill creates aerosols with 1 μm mass median diameter (MMD) with a 1.5 geometric standard deviation (GSD)
- The HVAC remains running and ventilating the reactor building
- The auxiliary filters are not used to filter the reactor cell
- Water spill onto the molten salt

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No
MCA6	1 μm	Yes	No	Yes
MCA7	1 μm	Yes	Yes	Yes
MCA8	1 μm	No	Yes	Yes
MCA9	1 μm	No	No	Yes

"Equilibration of all the fuel salt with the cell atmosphere and just enough water to form the maximum amount of saturated steam would result in the maximum pressure in the secondary container. With no relief device, pressures as high as 110 psig could result."

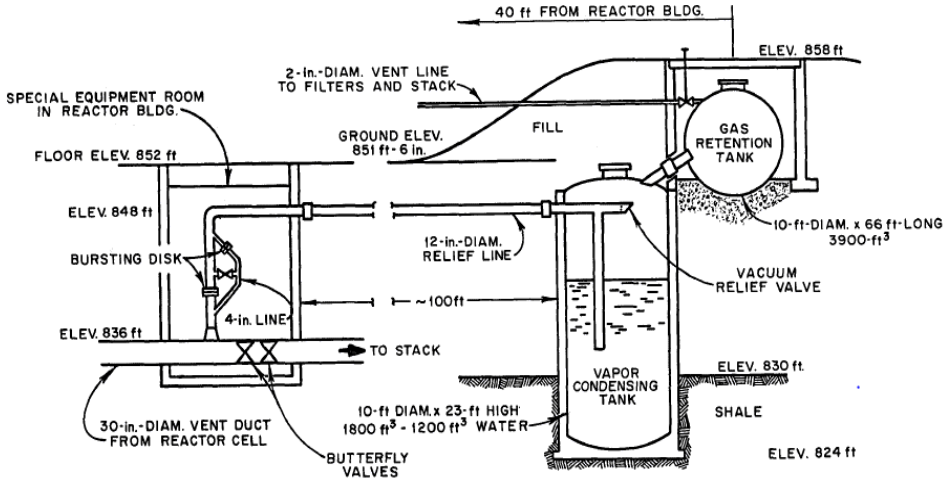
[ORNL-TM-0732]



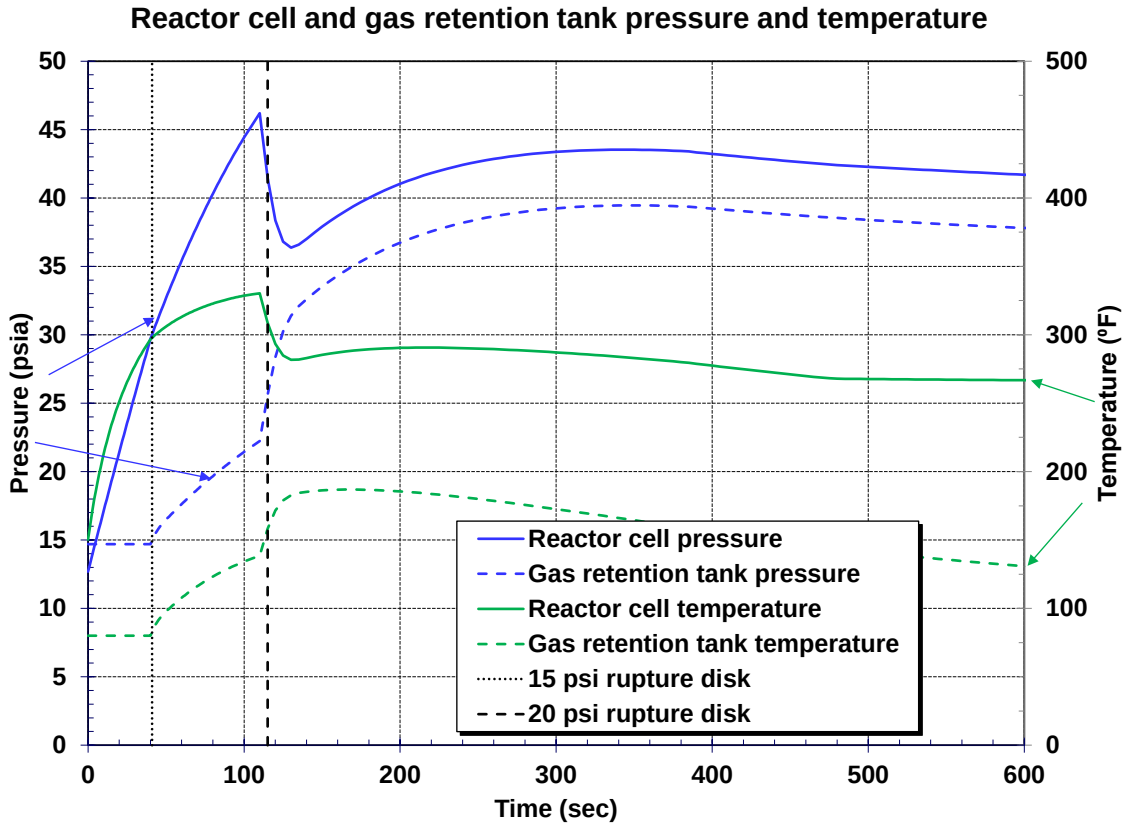
[ORNL-TM-0732]

MCA6 reactor cell thermal-hydraulic response

- Molten salt is assumed to mix with coincidentally spilled water
  - Rapid pressurization of the reactor cell as it fills with steam
- Reactor cell pressure rises to 46 psia
  - 15 psi rupture disk opens at 41 sec
  - 20 psi rupture disk opens at 115 sec
- Reactor cell temperature initially rises to 330ºF but falls after the 20 psi rupture disk opens



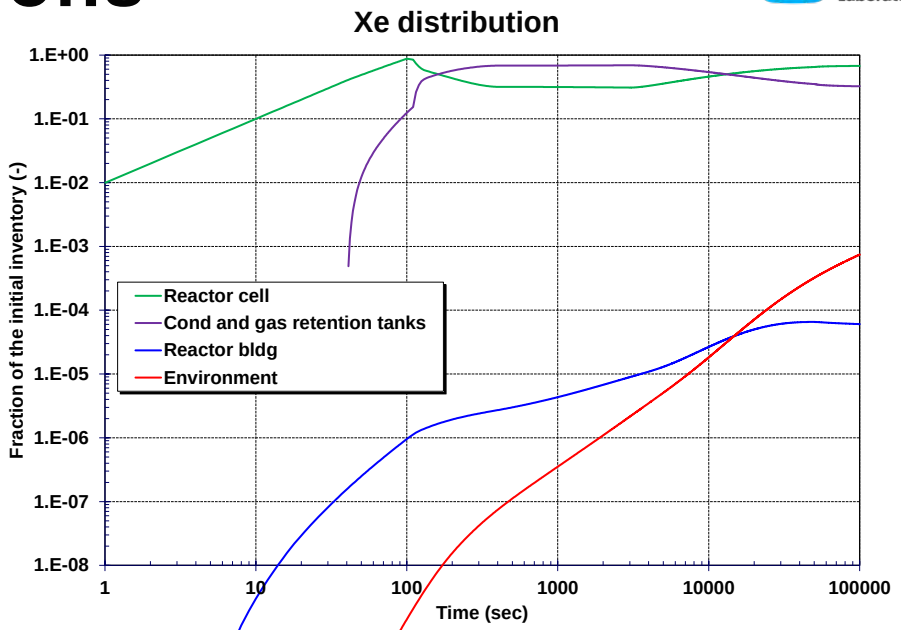
MSRE vapor-condensing system
[ORNL-TM-0728]

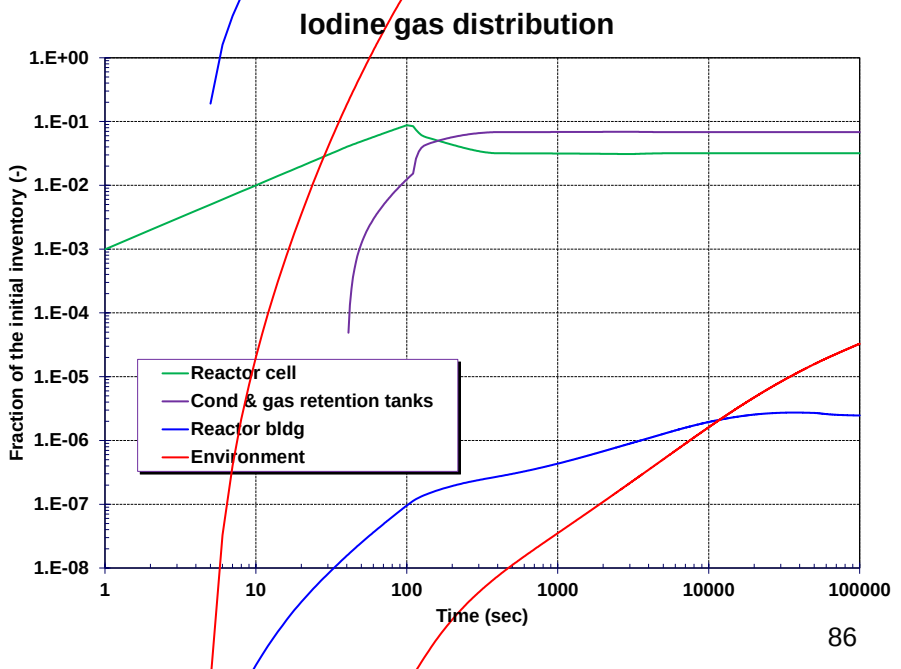


MCA6 gaseous radionuclide distributions

Same MCA airborne releases into reactor cell

- Release assumptions
  - 100% of the noble gases
  - 10% of the iodine
  - 10% of all other volatile and non-volatile radionuclides
- Strong flows to the condensing and gas retention tanks capture most of the radionuclides released from the spilled salt
  - Condensing tank retains most of the aerosols and the gas retention tank captures any radionuclides that pass through the pool
  - All noble gases and most of the gaseous iodine passes through the condensing pool



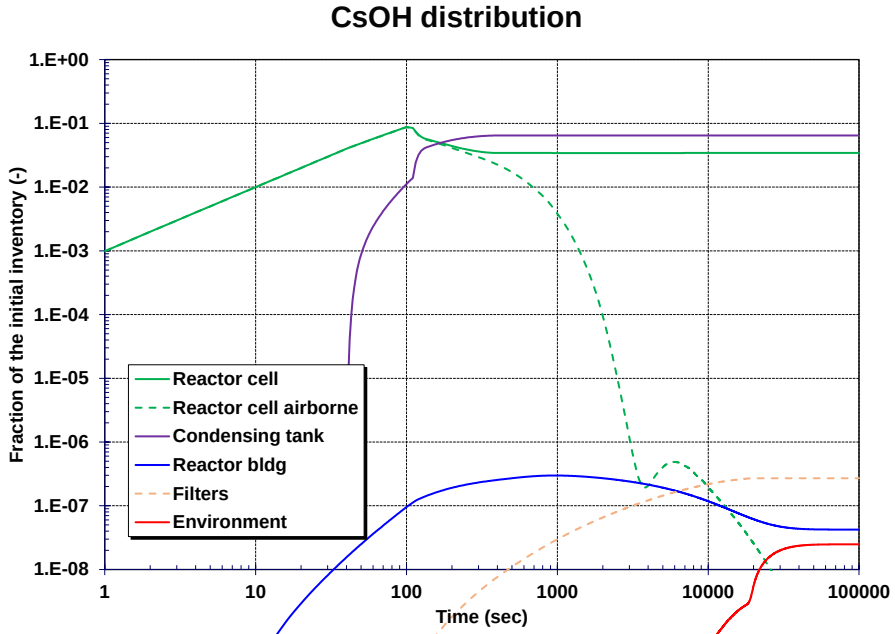


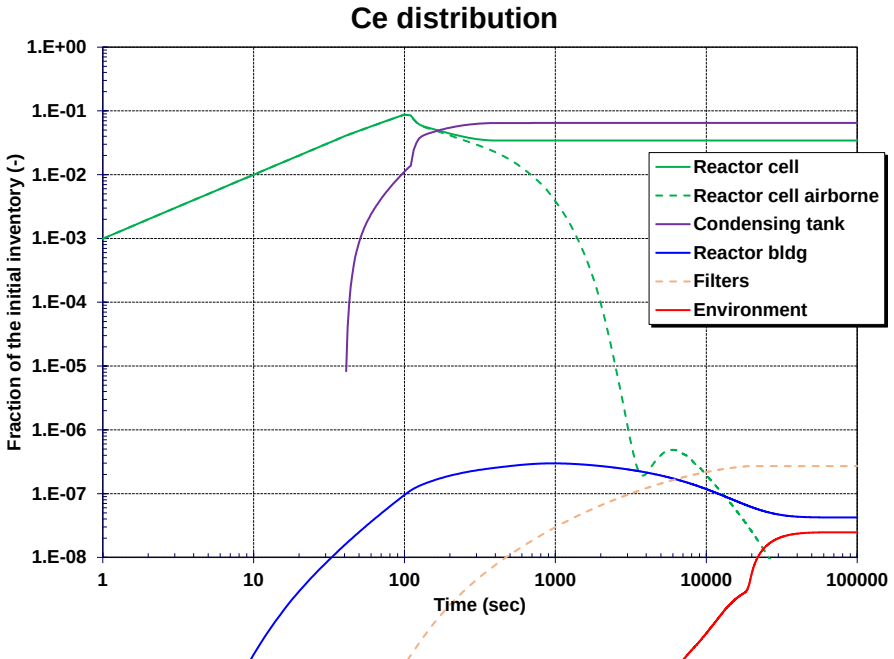
MCA6 aerosol radionuclide distributions

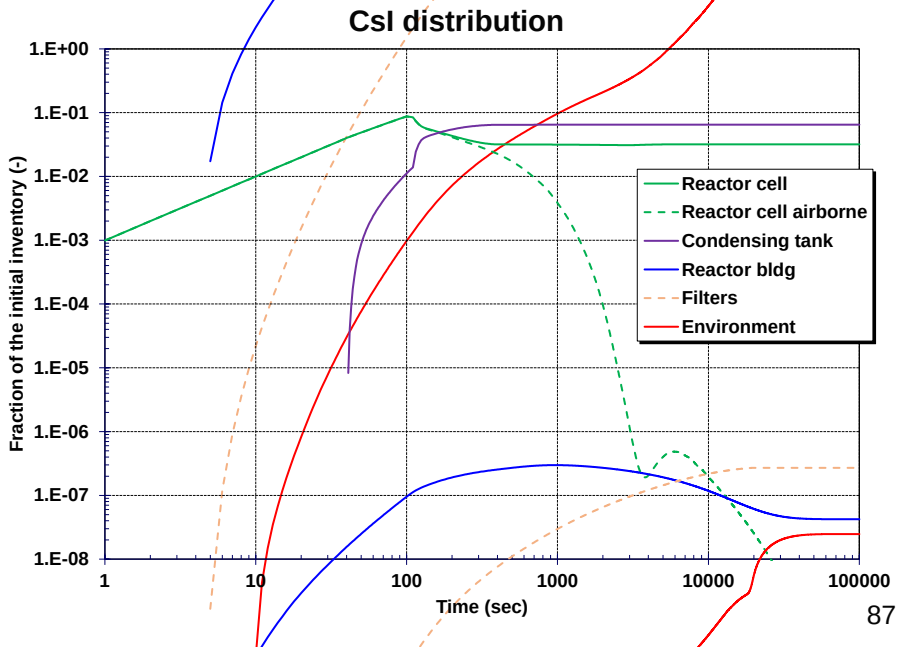
Most of the aerosol releases are retained in the condensing tank

- CsOH and CsI form aerosols in a water spill accident and behave similarly to the cerium aerosols

The large steam source contributes to aerosol agglomeration and more rapid settling in the reactor cell than the dry case





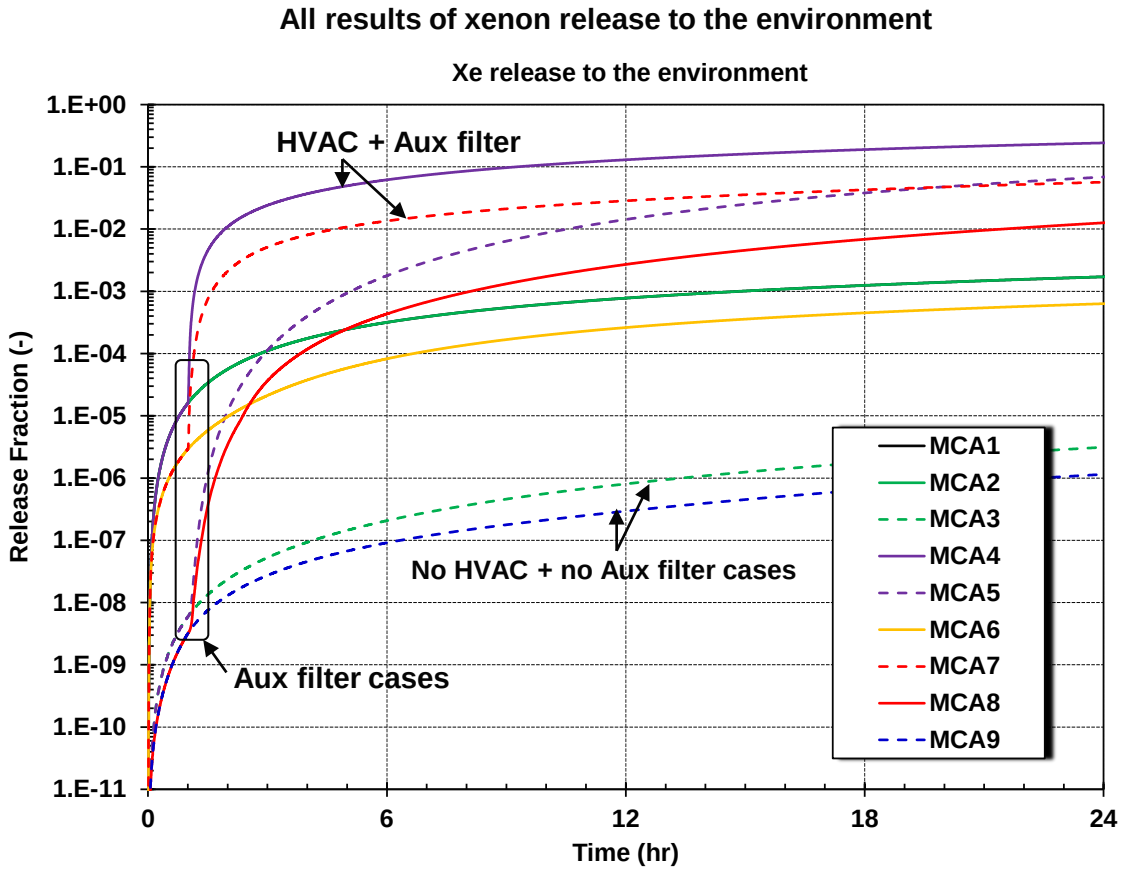


Overall insights (1/4)

The xenon release to the environment spanned many orders of magnitude depending on scenario assumptions

- Lowest releases with no HVAC and no Aux filter flow
- Auxiliary filter operation increases the release of xenon to the environment while it provides filtering of airborne aerosols

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No
MCA6	1 μm	Yes	No	Yes
MCA7	1 μm	Yes	Yes	Yes
MCA8	1 μm	No	Yes	Yes
MCA9	1 μm	No	No	Yes

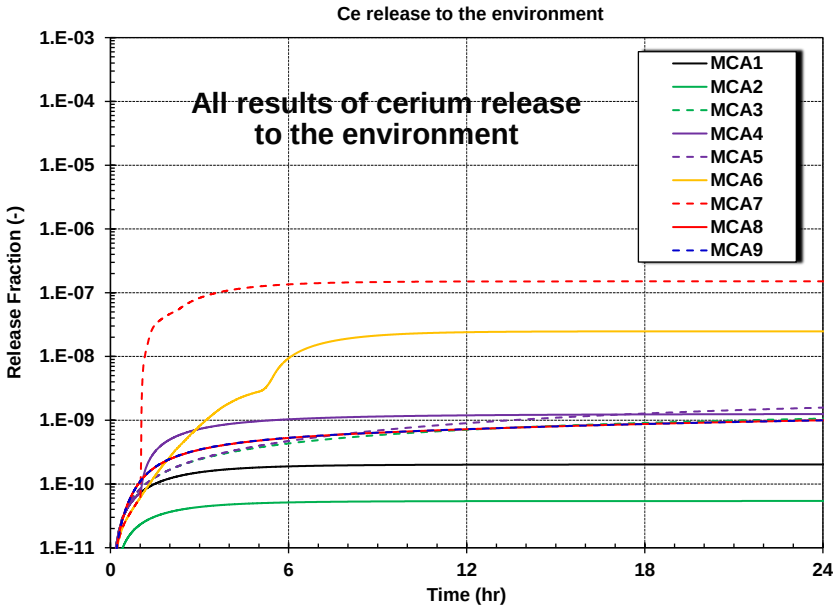


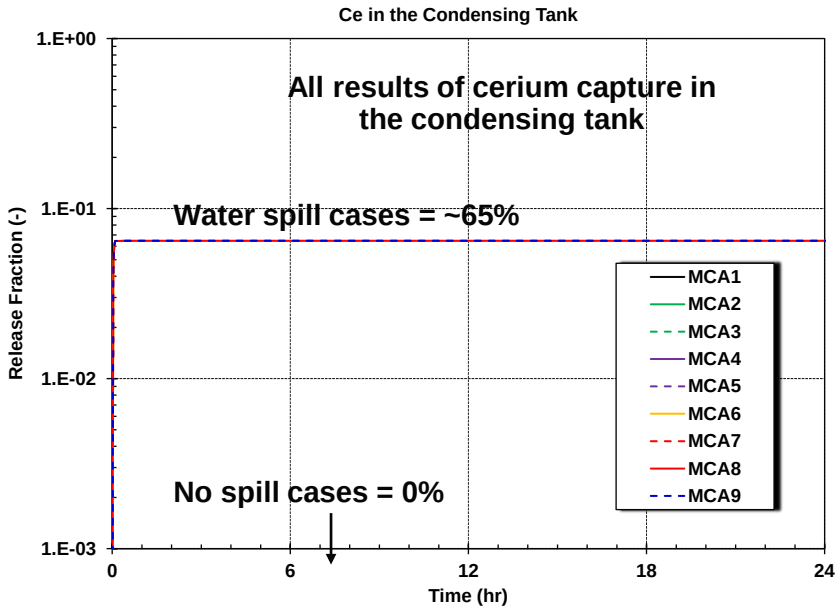
Note: Results assume no xenon retention in the charcoal filters.

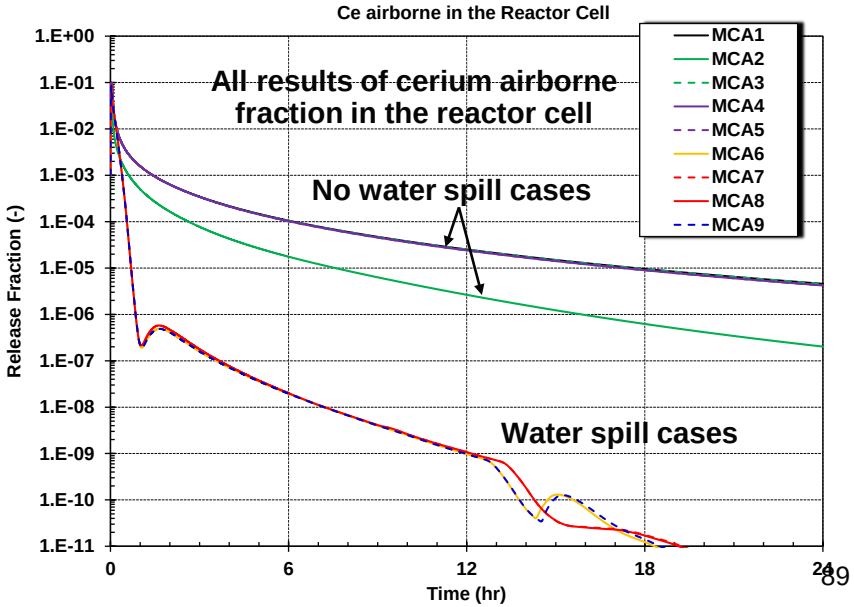
Overall insights (2/4)

The aerosol releases to the environment were small due to:

- Gravitational settling
  - in the reactor cell (all cases),
  - the reactor building, filter pit, and stack (without HVAC flow)
- Capture in the filter
- Capture in the condensing tank in the water spill cases





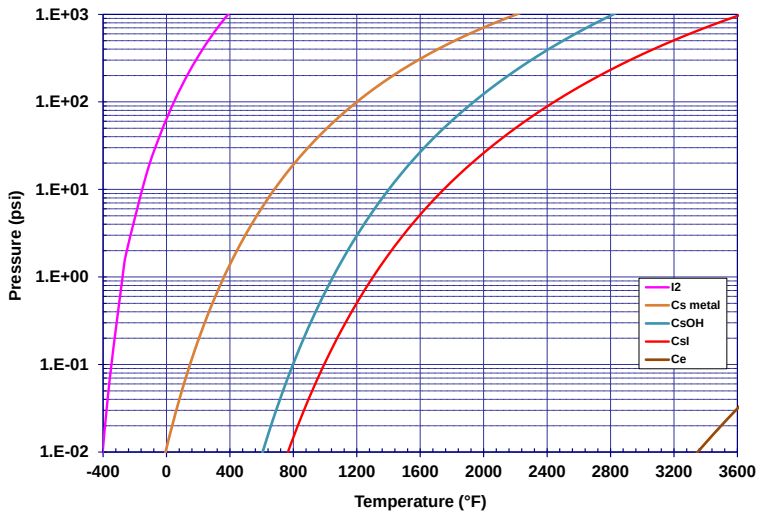


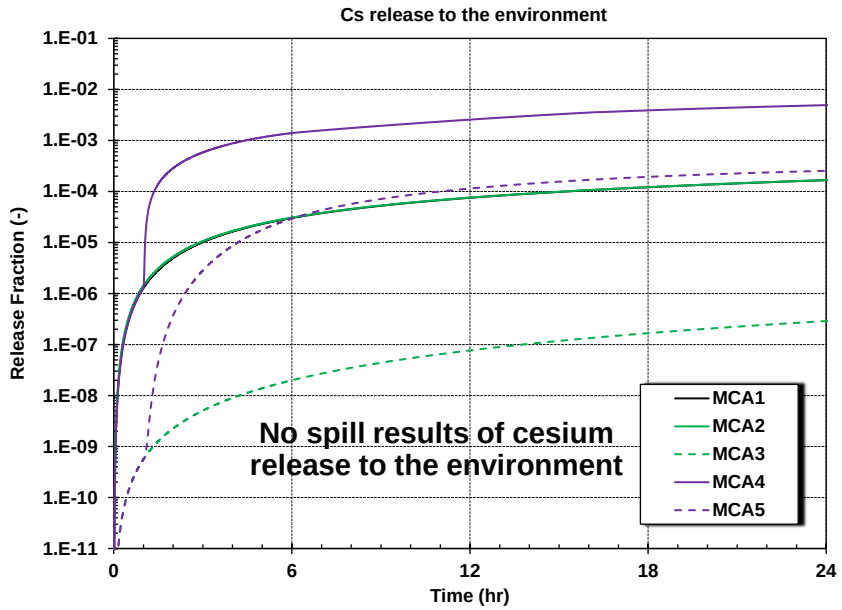
Overall insights (3/4)

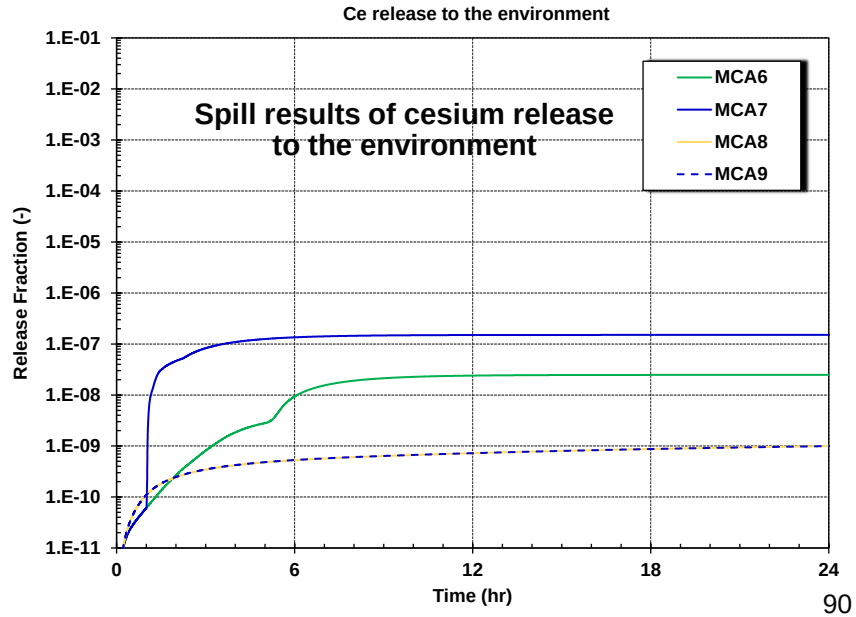
Due to the high temperatures in the reactor cell in the cases without a water spill (~900ºF), the two chemical compounds of cesium were primary in a vapor form

- Any released CsI and CsOH subsequently condensed in the reactor building and the offgas system to form aerosols
- CsOH and CsI remained airborne in the reactor cell versus cerium, which was always an aerosol

This led to higher cesium environmental releases than radionuclides that were aerosols in the reactor cell (e.g., cerium)



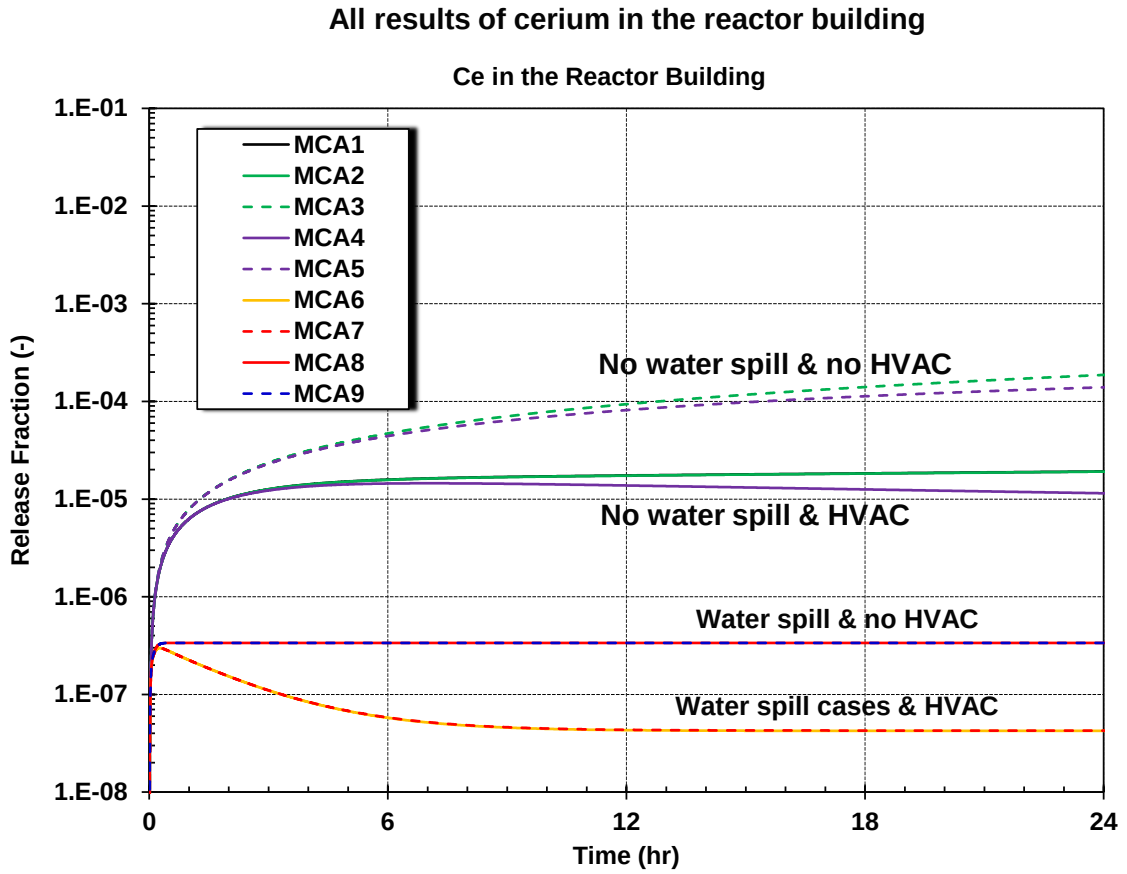




Overall insights (4/4)

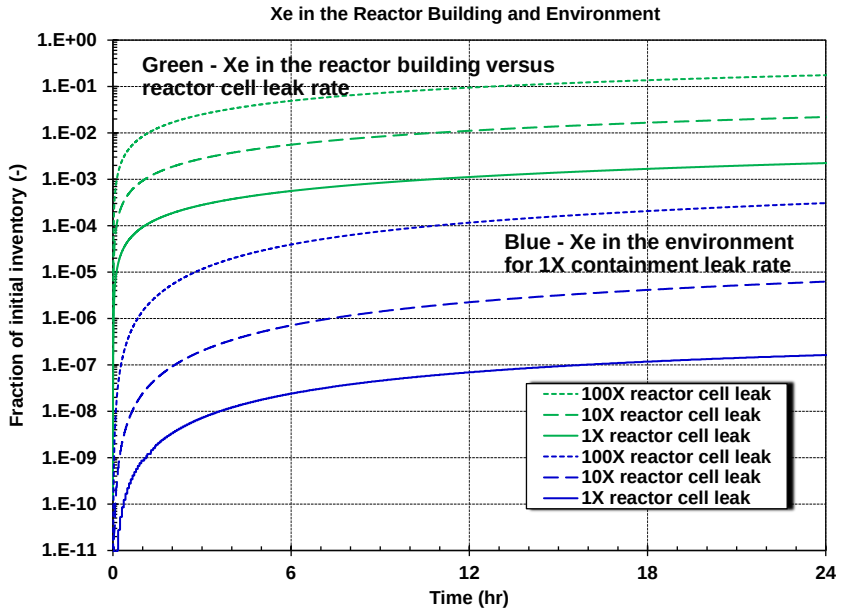
The aerosol mass in the reactor building also spanned many orders of magnitude depending on scenario assumptions

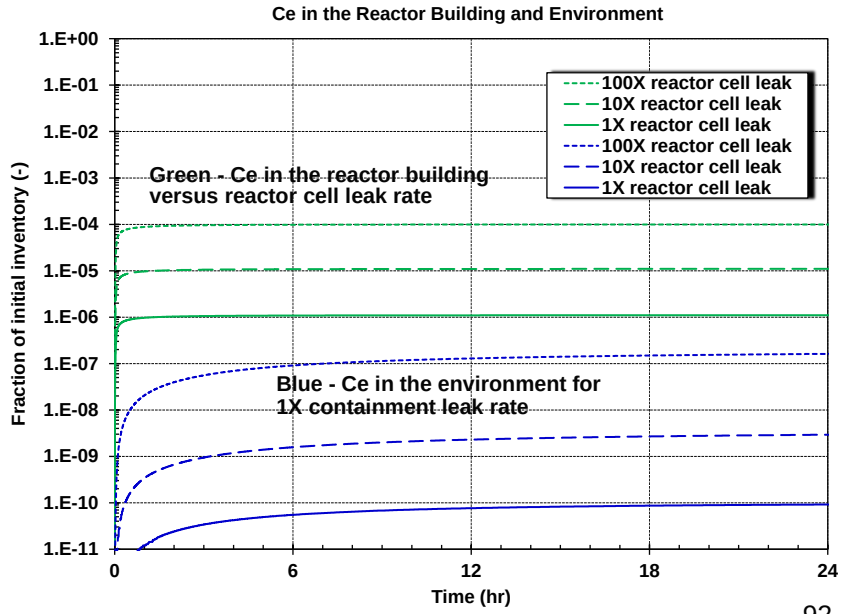
- Lowest amounts occurred when aerosols were captured in the condensing tank and any leaked aerosols were filtered via the reactor building HVAC flow
- The highest amounts occurred when there was no water spill and no HVAC
- Aerosols leaked into the reactor building without HVAC operation primarily settled (flat line)
  - Led to a small amount of leakage to the environment
- Finally, the HVAC swept long-term releases into the reactor building in the no spill cases



Sensitivity to increased reactor cell leakage

- Green line shows impact of reactor cell leakage to the reactor building for the MCA3 scenario
  - Gaseous Xe leak to the reactor building continues while the Ce aerosol leakage stops early due to aerosol settling
- Blue line shows impact of reactor cell leakage on environmental releases for the MCA3 scenario
  - The leakage to the reactor cell has an approximately linear impact on the reactor cell leak rate versus a slightly larger than linear effect on the environment leakage
- The impacts are expected to be smaller with HVAC operation





Cases without a water spill

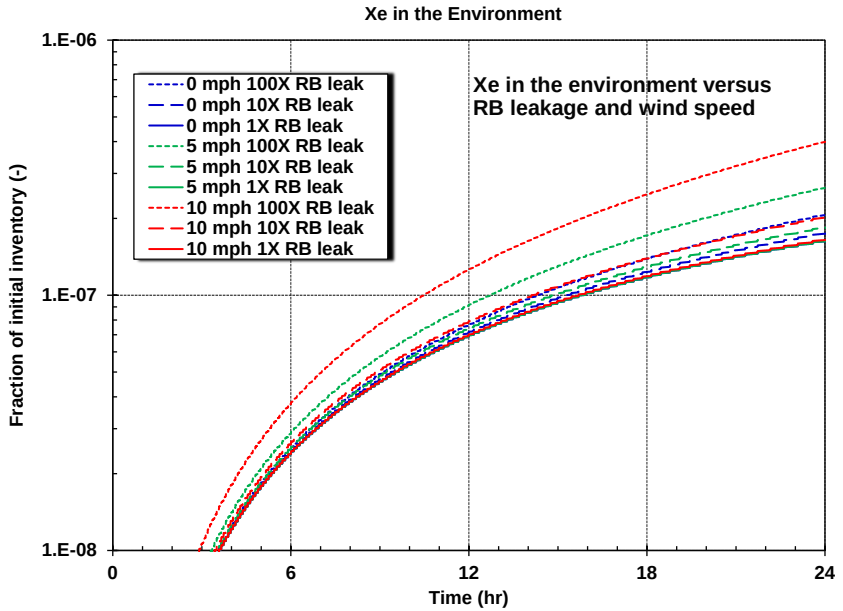
Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No

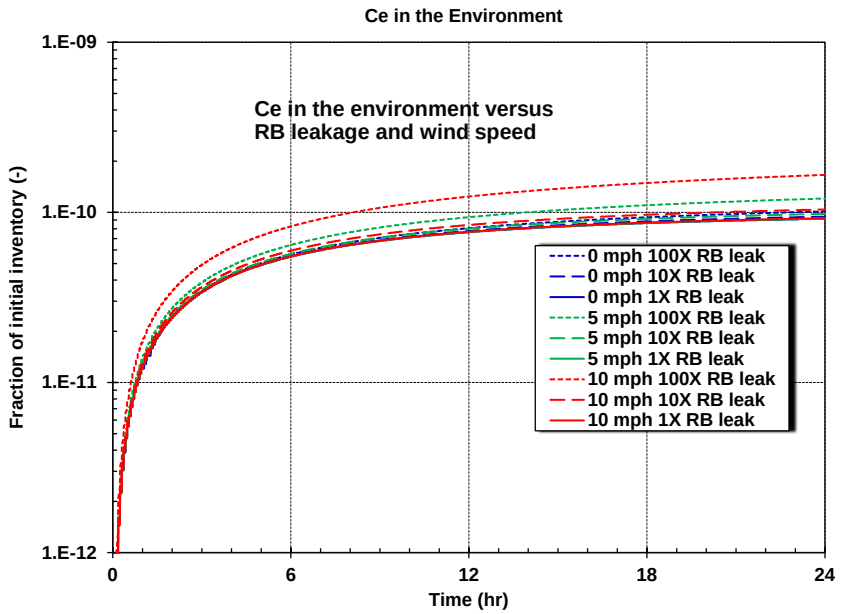
Sensitivity to increased reactor building leakage

- The reactor building surrounds the reactor cell and provides the final barrier for leakage when the filters are not operating
- Impact of reactor building leakage as a function of wind speed shows a very small impact on the release to the environment for the MCA3 scenario
  - Similar to increased building leakage, a higher wind speed increases the building infiltration and exfiltration rate
  - The impact is slightly larger for gas leakage (i.e., aerosols also settle)
- The nominal (1X) building leakage is very low
  - Only 10% per day at 0.25 psig, 0.002 in^2
  - The very large building (480,000 ft^3) has no appreciable pressurization (i.e., <<0.25 psig)

Cases without a water spill

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No





Summary

U.S.NRC

Sandia
National
Laboratories

Conclusions

- Demonstrated use of SCALE and MELCOR for MSRE safety analysis
- Simulated the entire accident starting with the initiating event
  - system thermal hydraulic response
  - fuel heat-up
  - heat transfer through the reactor to the surroundings
  - radiological release
- Evaluated effectiveness of passive mitigation features

Background Slides

U.S.NRC

OAK RIDGE National Laboratory

Sandia National Laboratories

Further SCALE analysis details

U.S.NRC

OAK RIDGE National Laboratory

Sandia National Laboratories

Time-dependent inventory – nuclide removal

Nuclide removal from fuel salt in core+loop:

- Plating-out of noble metals (Se, Nb, Mo, Tc, Ru, etc.) at heat exchanger
- Removal of halogens (I, Br) from plated-out material
- Removal of noble gases from plated-out materials
- Removal of noble gases (Xe, Kr) from fuel into off-gas system
- Removal of gas into charcoal bed
- Removal of gas into stack

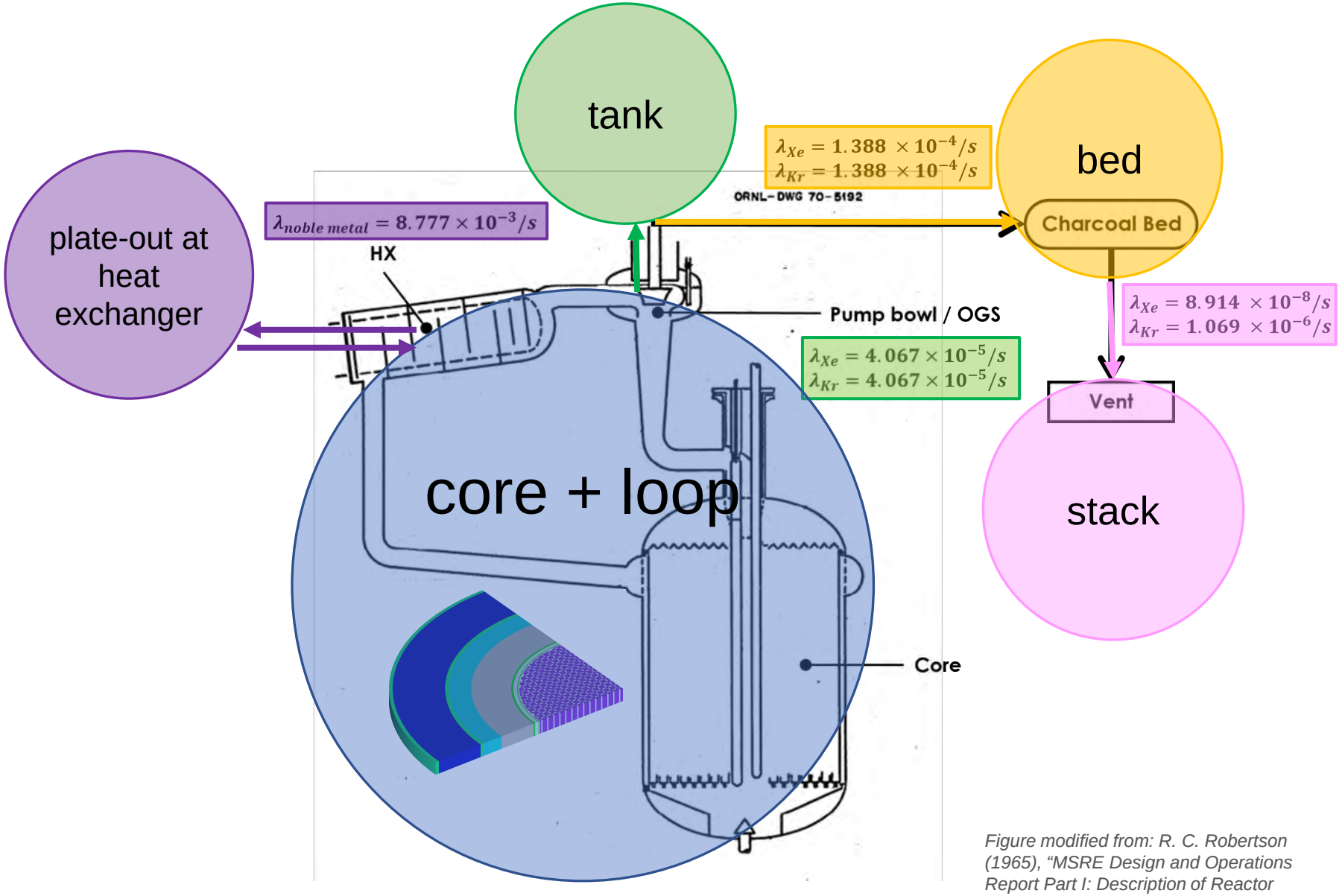
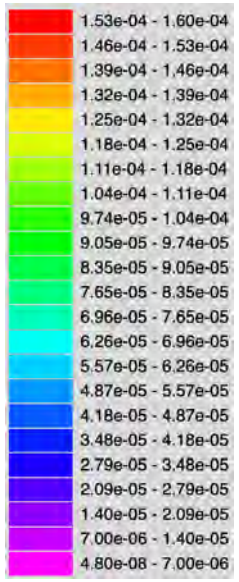
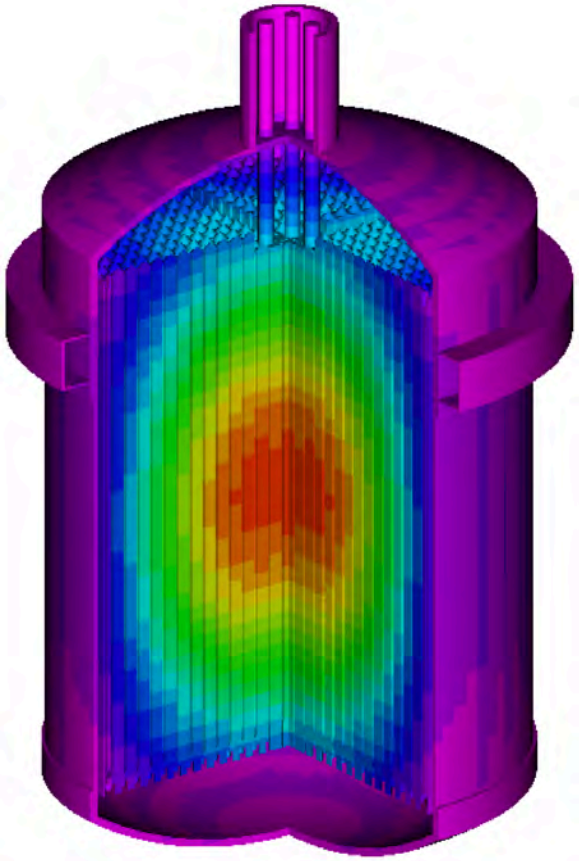


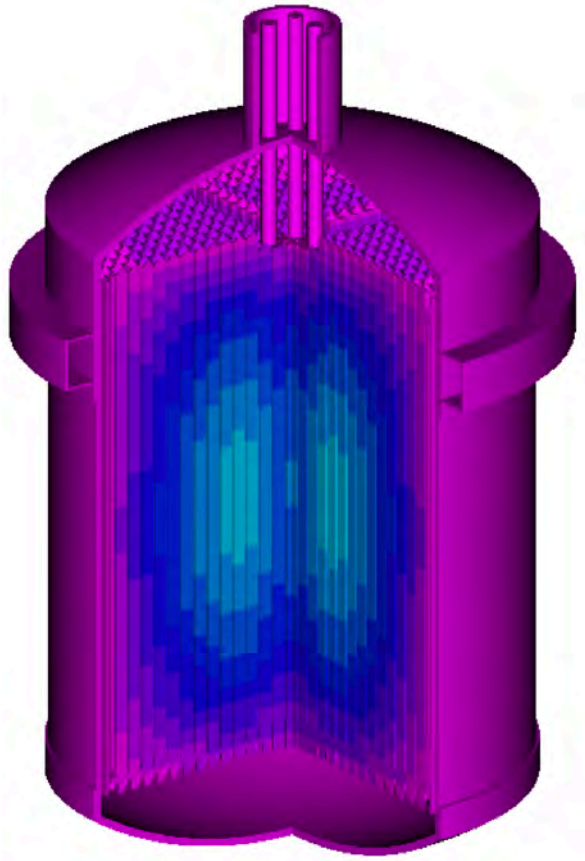
Figure modified from: R. C. Robertson (1965), "MSRE Design and Operations Report Part I: Description of Reactor Design," ORNL-TM-0728, ORNL.

Core power/flux distribution – flux

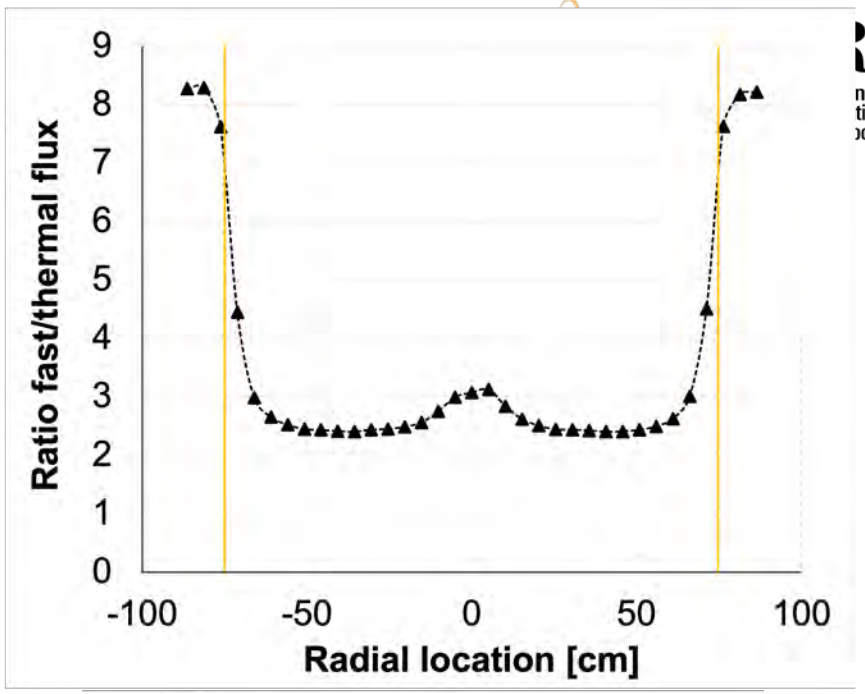


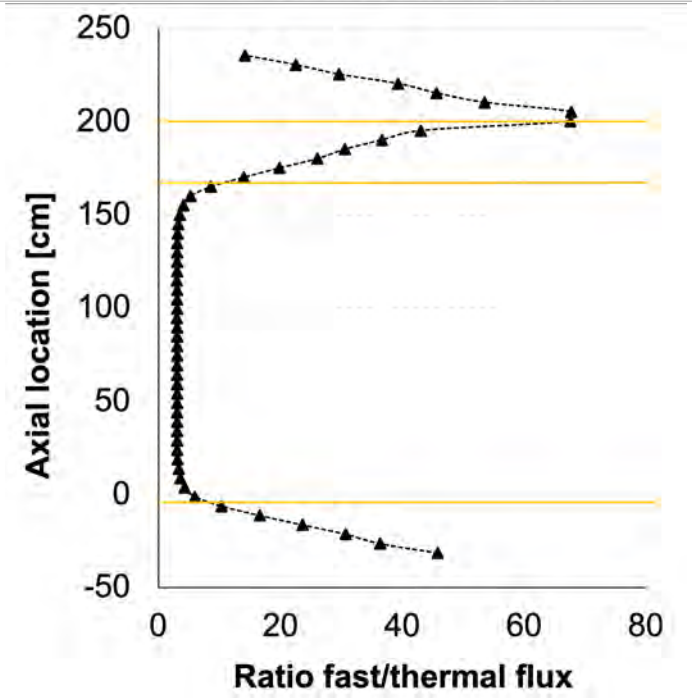


Thermal flux
(< 0.625 eV)



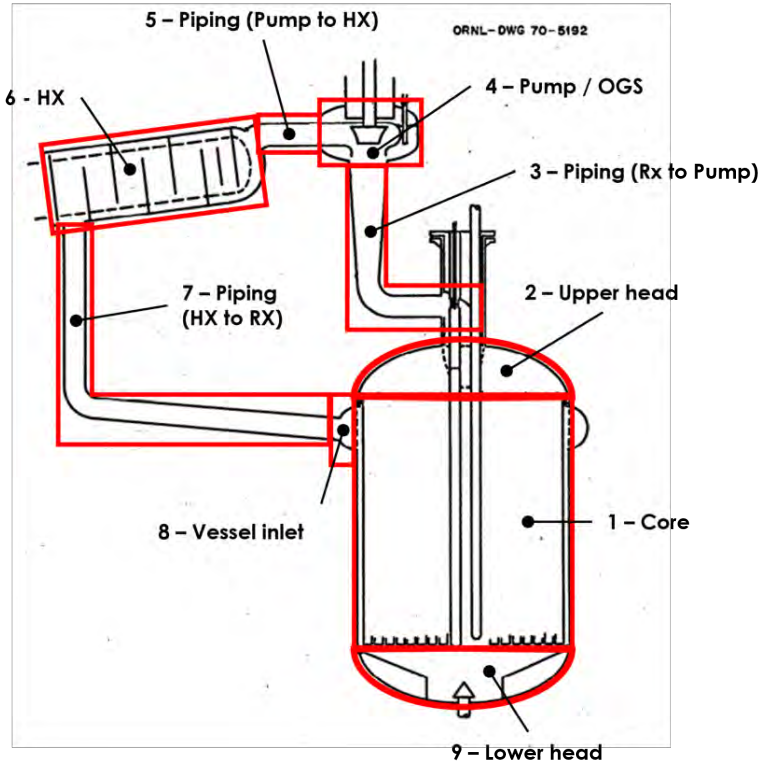
Fast flux
(> 0.625 eV)





Region-wise data

Region	Description	Volume (m^3)	Residence Time (s)	^{235}U Mass (kg)
1	Core	0.708	9.4	77
2	Upper Plenum	0.297	3.9	32
3	Reactor to Pump	0.059	0.8	6
4	Pump	0.116	0.3	13
5	Pump to Heat Exchanger	0.023	0.3	2
6	Heat Exchanger	0.173	2.3	19
7	Heat Exchanger to Inlet	0.062	0.8	7
8	Inlet	0.275	3.6	30
9	Lower Plenum	0.283	3.8	31
	System Total	**1.996**	**25.2**	**218**

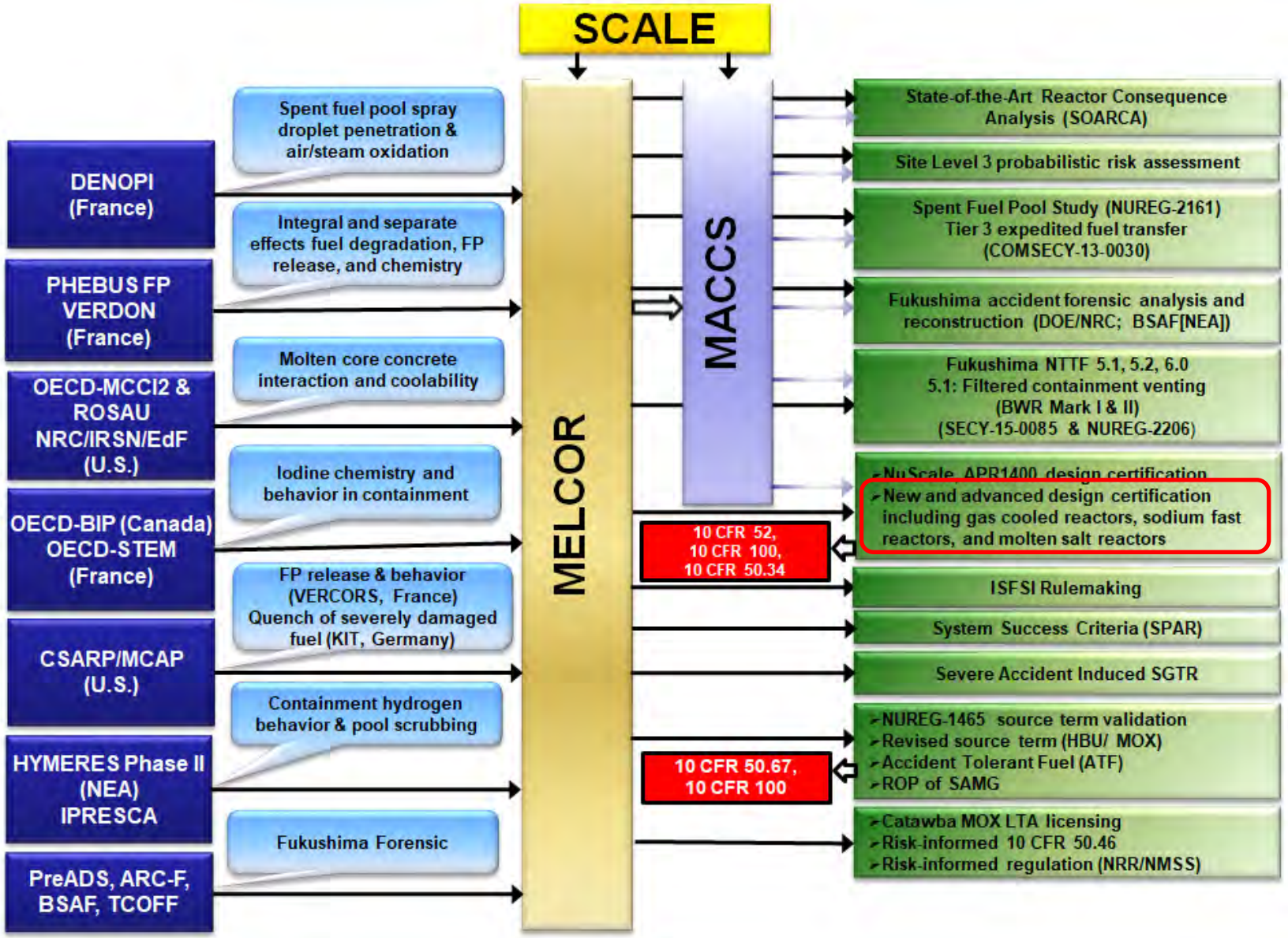


MELCOR for Accident Progression and Source Term Analysis

U.S.NRC

Sandia
National
Laboratories

MELCOR Development for Regulatory Applications



What Is It?
MELCOR is an engineering-level code that simulates the response of the reactor core, primary coolant system, containment, and surrounding buildings to a severe accident.

Who Uses It?
MELCOR is used by domestic universities and national laboratories, and international organizations in around 30 countries. It is distributed as part of NRC's Cooperative Severe Accident Research Program (CSARP).

How Is It Used?
MELCOR is used to support severe accident and source term activities at NRC, including the development of regulatory source terms for LWRs, analysis of success criteria for probabilistic risk assessment models, site risk studies, and forensic analysis of the Fukushima accident.

How Has It Been Assessed?
MELCOR has been validated against numerous international standard problems, benchmarks, separate effects (e.g., VERCORS) and integral experiments (e.g., Phebus FPT), and reactor accidents (e.g., TMI-2, Fukushima).

Source Term Development Process

Experimental Basis

PIRT process

Oxidation/Gas Generation

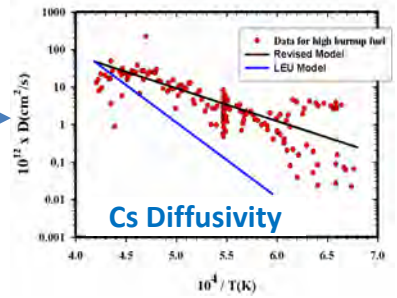
Melt Progression

Fission Product Release

Fission Product Transport

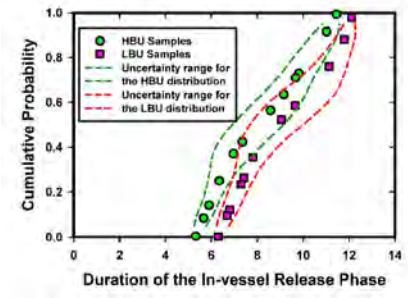
MELCOR

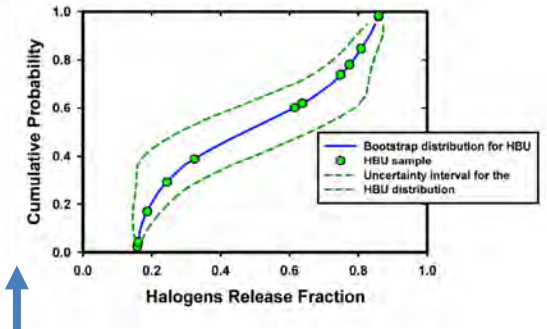
Cesium release from high burnup fuel
Comparison to results of VERCORS Test



Accident Analysis

Scenario # 1	Scenario # 2
.....	.....
Scenario # n-1	Scenario # n

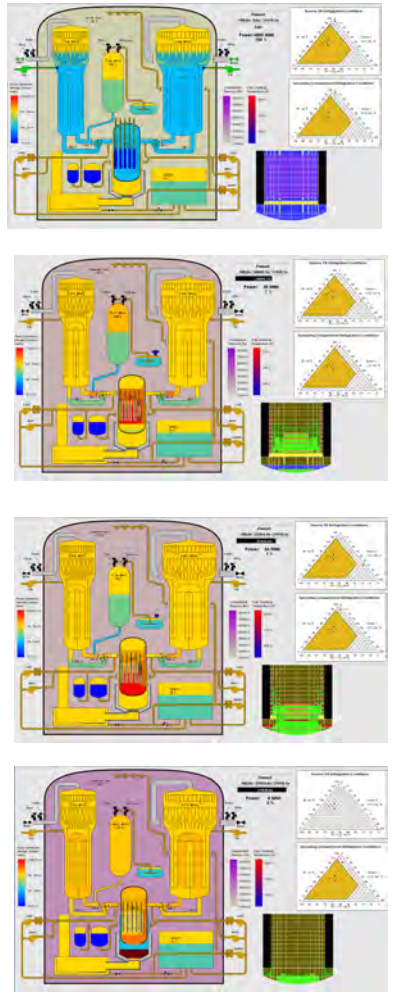




Synthesize timings and release fractions

Design Basis Source Term

Fission Product class	Gap 0.5 hr	In-vessel 1.3 hr	Ex-vessel 2 hr	Late 10 hr
Noble Gases	5%	95%	~0	~0
Iodine, bromine	5%	35%	25%	1%
Cesium	5%	25%	35%	1%
Tellurium	~0	5%	25%	0.5%
Ba, Sr	~0	2%	10%	~0
Ru, Mo, Pd, etc.	~0	0.25%	0.25%	~0
Lanthanides	~0	0.02%	0.5%	~0
Cerium group	~0	0.05%	0.5%	~0



SCALE/MELCOR/MACCS

U.S.NRC
OAK RIDGE National Laboratory
Sandia National Laboratories

SCALE — Neutronics

- Criticality
- Shielding
- Radionuclide inventory
- Burnup credit
- Decay heat

MELCOR — Integrated Severe Accident Progression

- Hydrodynamics for range of working fluids
- Accident response of plant structures, systems and components
- Fission product transport

MACCS — Radiological Consequences

- Near- and far-field atmospheric transport and deposition
- Assessment of health and economic impacts

Nuclear Reactor System Applications

Safety/Risk Assessment

- Technology-neutral
  - Experimental
  - Naval
  - Advanced LWRs
  - Advanced Non-LWRs
- Accident forensics (Fukushima, TMI)
- Probabilistic risk assessment

Regulatory

- License amendments
- Risk-informed regulation
- Design certification (e.g., NuScale)
- Vulnerability studies
- Emergency preparedness
- Emergency Planning Zone Analysis

Design/Operational Support

- Design analysis scoping calculations
- Training simulators

Non-Reactor Applications

Fusion

- Neutron beam injectors
- Li loop LOFA transient analysis
- ITER cryostat modeling
- He-cooled pebble test blanket (H^3)

Spent Fuel

- Risk studies
- Multi-unit accidents
- Dry storage
- Spent fuel transport/package applications

Facility Safety

- Leak path factor calculations
- DOE safety toolbox codes
- DOE nuclear facilities (Pantex, Hanford, Los Alamos, Savannah River Site)

MELCOR Attributes

Foundations of MELCOR Development

Fully integrated, engineering-level code

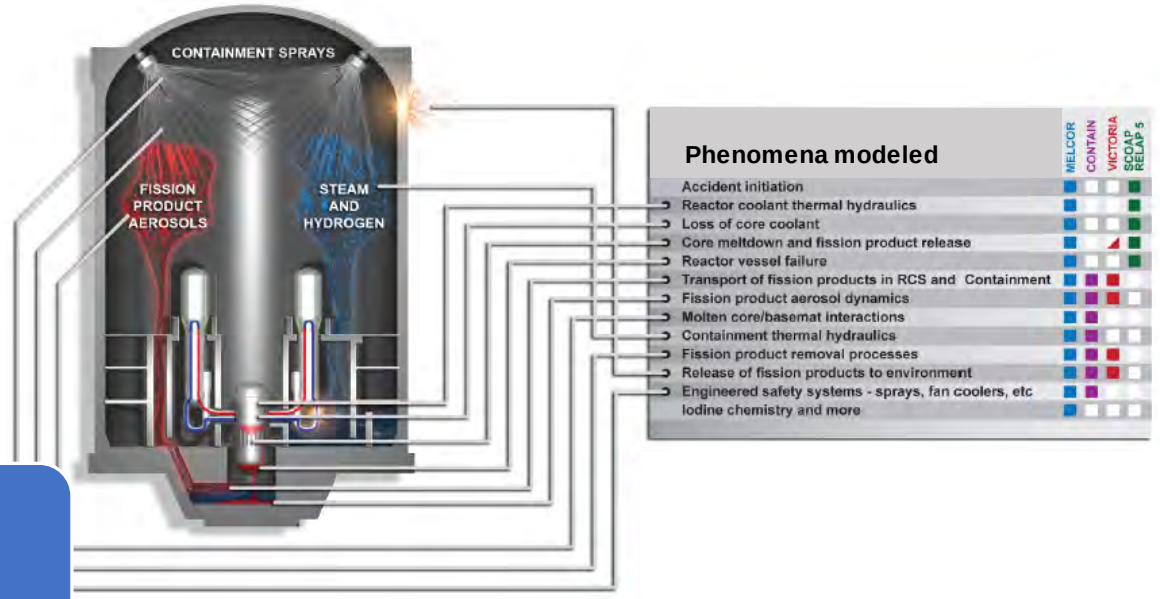
- Thermal-hydraulic response of reactor coolant system, reactor cavity, rector enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

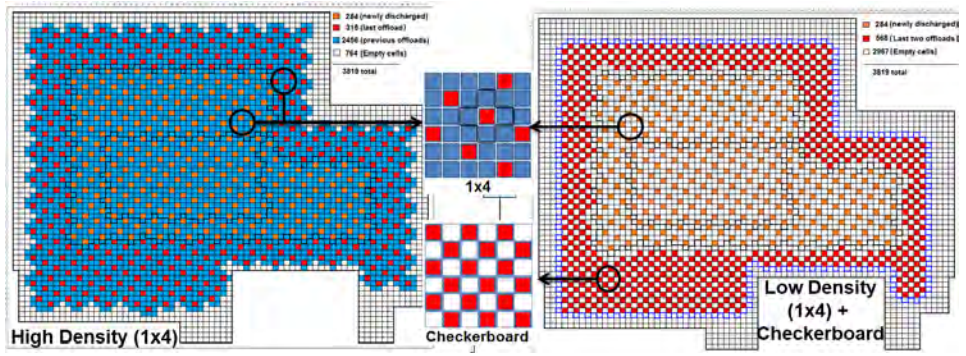
Level of physics modeling consistent with

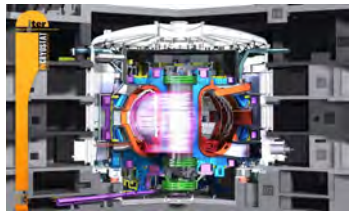
- State-of-knowledge
- Necessity to capture global plant response
- Reduced-order and correlation-based modeling often most valuable to link plant physical conditions to evolution of severe accident and fission product release/transport

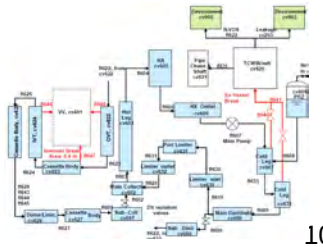
Traditional application

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









MELCOR Attributes
MELCOR Pedigree

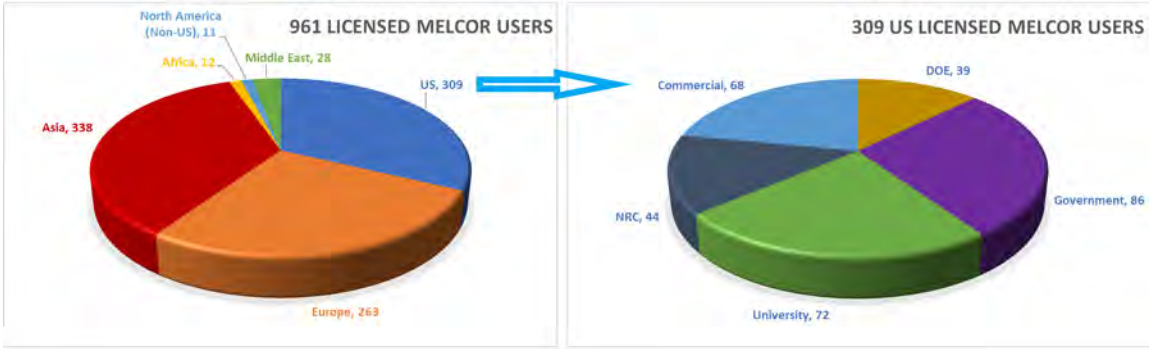
Validated physical models

- International Standard Problems, benchmarks, experiments, and reactor accidents
- Beyond design basis validation will always be limited by model uncertainty that arises when extrapolated to reactor-scale

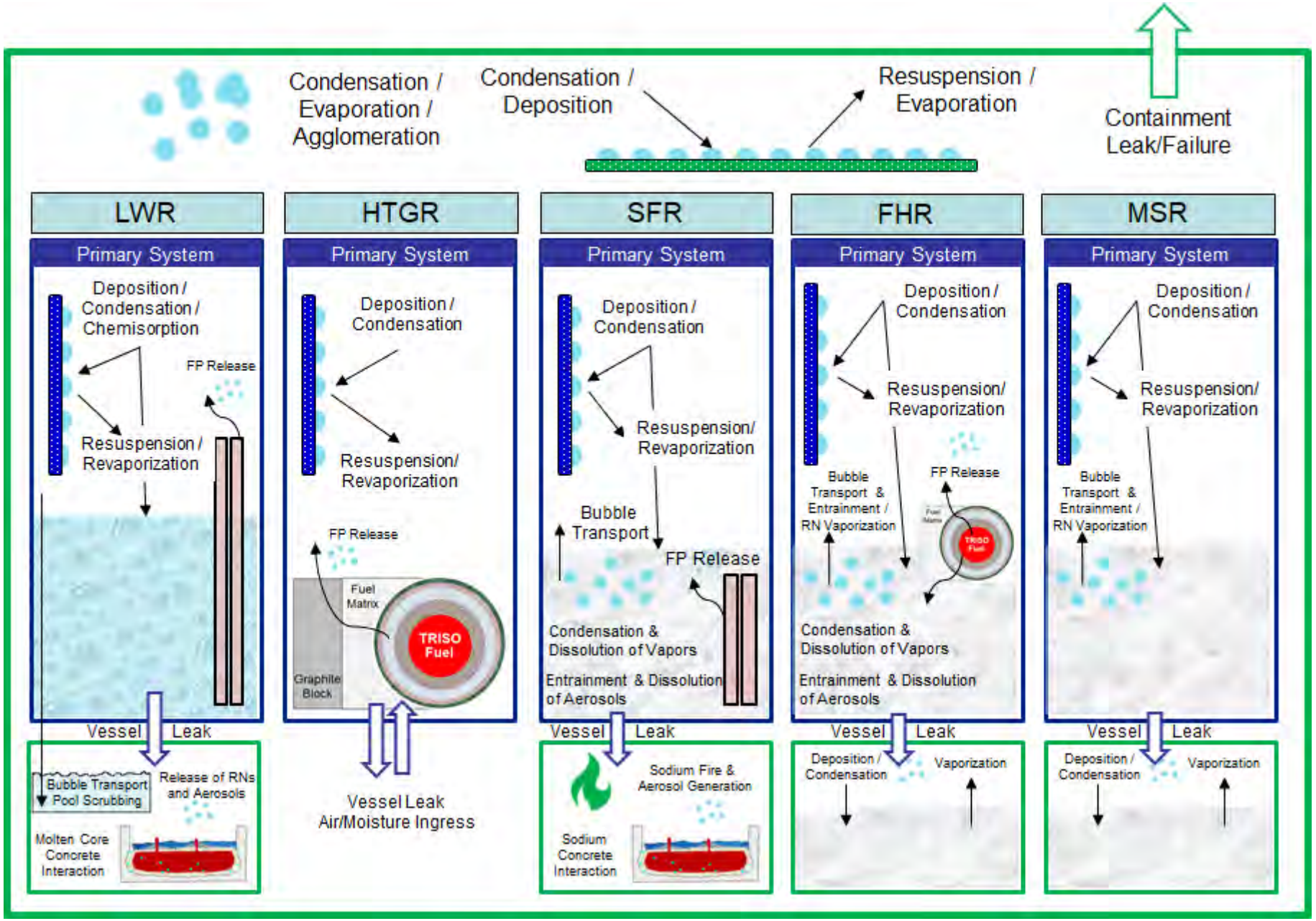
Cooperative Severe Accident Research Program (CSARP) is an NRC-sponsored international, collaborative community supporting the validation of MELCOR

International LWR fleet relies on safety assessments performed with the MELCOR code

International Collaboration
Cooperative Severe Accident Research Program (CSARP) – June/U.S.A
MELCOR Code Assessment Program (MCAP) – June/U.S.A
European MELCOR User Group (EMUG) Meeting – Spring/Europe
Asian MELCOR User Group (AMUG) Meeting – Fall/Asia



Common Phenomenology



MELCOR Modeling Approach

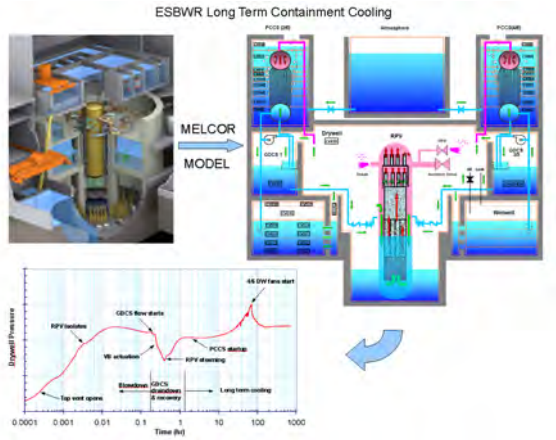
Modeling is mechanistic consistent with level of knowledge of phenomena supported by experiments

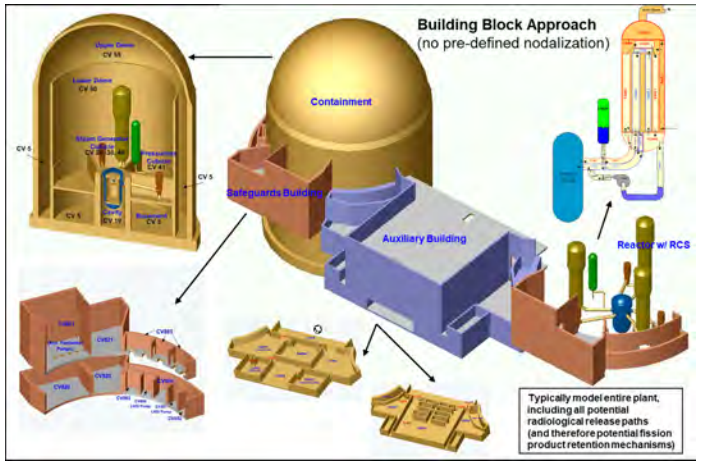
Parametric models enable uncertainties to be characterized

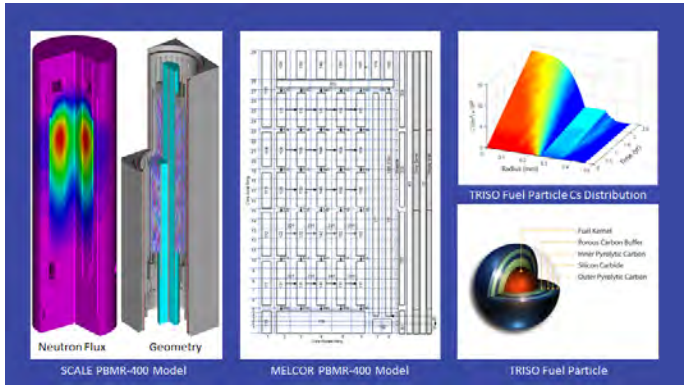
- Majority of modeling parameters can be varied
- Properties of materials, correlation coefficients, numerical controls/tolerances, etc.

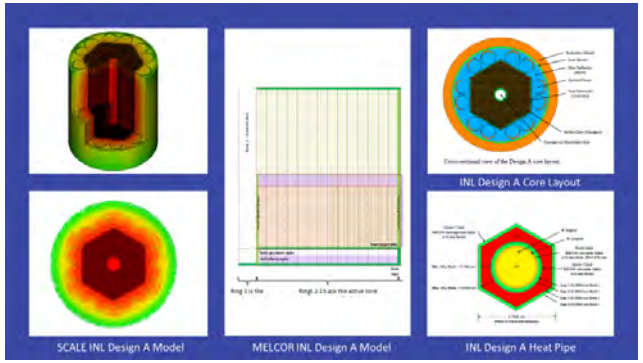
Code models are general and flexible

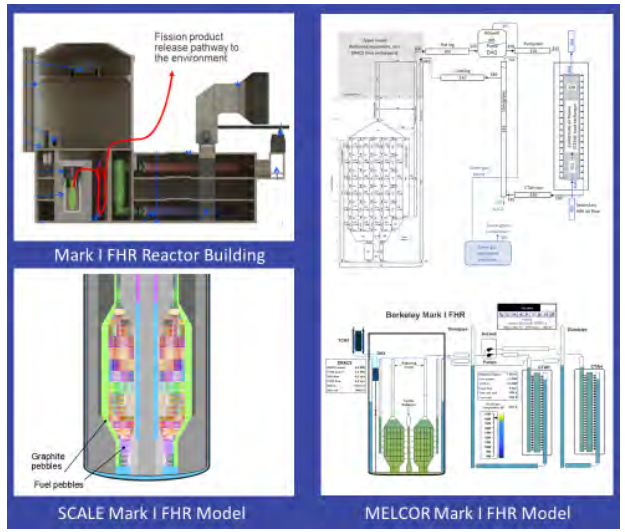
- Relatively easy to model novel designs
- All-purpose thermal hydraulic and aerosol transport code





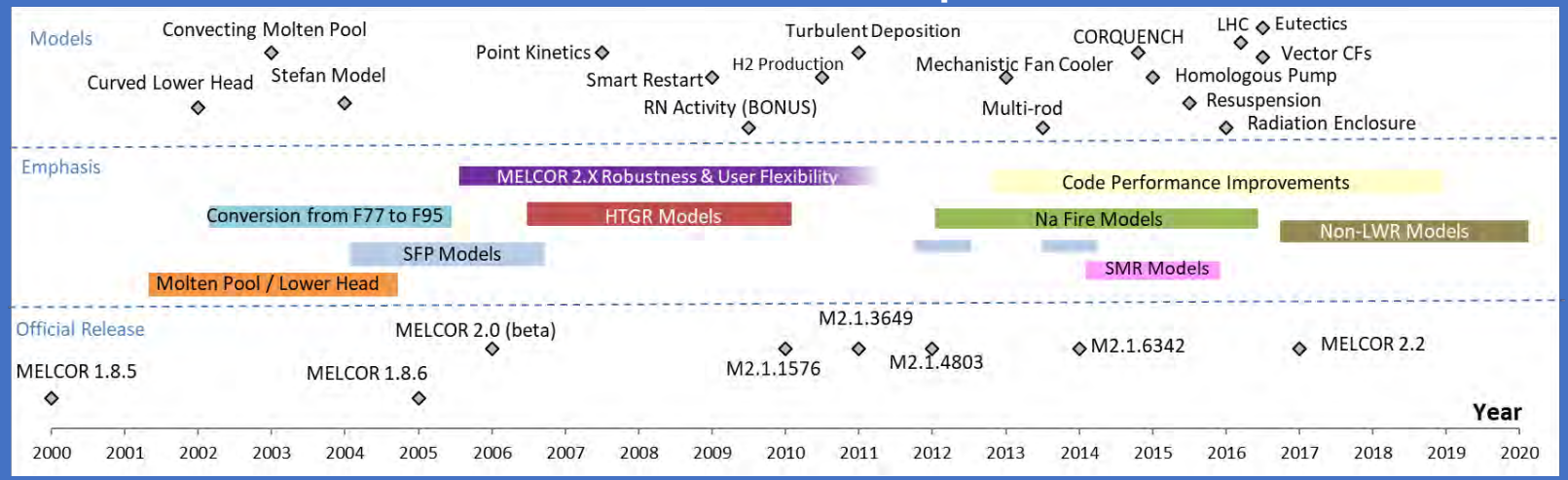






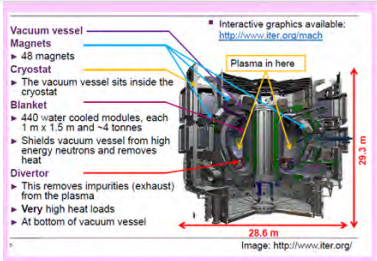
MELCOR State-of-the-Art

MELCOR Code Development



M2x Official Code Releases

Version	Date
2.2.18180	December 2020
2.2.14959	October 2019
2.2.11932	November 2018
2.2.9541	February 2017
2.1.6342	October 2014
2.1.4803	September 2012
2.1.3649	November 2011
2.1.3096	August 2011
2.1.YT	August 2008
2.0 (beta)	Sept 2006



Fusion

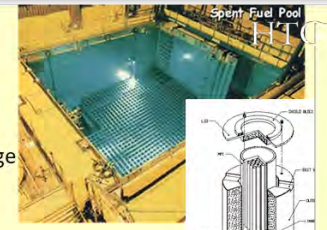
- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

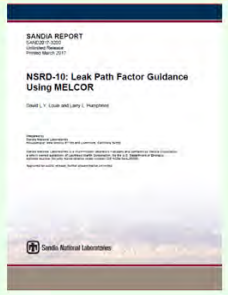
Spent Fuel

Spent fuel pool risk studies

Multi-unit accidents (large area destruction)

Dry Storage



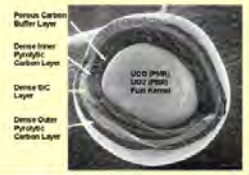


Non-Nuclear Facilities

- Leak Path Factor Calculations (LPF)
  - Release of hazardous materials from facilities, buildings, confined spaces
- DOE Safety Toolbox code
- DOE nuclear facility users
  - Pantex
  - Hanford
  - Los Alamos
  - Savannah River Site

HTGR Reactors

- Helium Properties
- Accelerated steady-state initialization
- Two-sided reflector (RF) component
- Modified Fuel components (PMR/PBR)
- Point kinetics
- Fission product diffusion, transport, and release
- TRISO fuel failure



Sodium Reactors

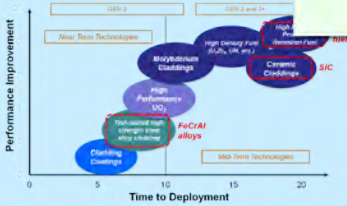
Sodium Properties
- Sodium Equation of State
- Sodium Thermo-mechanical properties

Containment Modeling
- Sodium pool fire model
- Sodium spray fire model
- Atmospheric chemistry model
- Sodium-concrete interaction

Molten Salt Reactors

- Properties for LiF-BeF2 have been added
  - Equation of State
  - Thermal-mechanical properties

Accident Tolerant Fuels



MELCOR Software Quality Assurance – Best Practices

U.S.NRC
OAK RIDGE National Laboratory
Sandia National Laboratories

MELCOR SQA Standards

SNL Corporate procedure IM100.3.5
CMMI-4+
NRC NUREG/BR-0167

Emphasis is on Automation

Affordable solutions
Consistent solutions

MELCOR Wiki

- Archiving information
- Sharing resources (policies, conventions, information, progress) among the development team.

Code Configuration Management (CM)

- 'Subversion'
- TortoiseSVN
- VisualSVN integrates with Visual Studio (IDE)

Reviews

- Code Reviews: Code Collaborator
- Internal SQA reviews

Continuous builds & testing

- DEF application used to launch multiple jobs and collect results
- Regression test report
- More thorough testing for code release
- Target bug fixes and new models for testing

Bug tracking and reporting

- Bugzilla online

Code Validation

- Assessment calculations
- Code cross walks for complex phenomena where data does not exist.

Documentation

- Available on 'Subversion' repository with links from wiki
- Latest PDF with bookmarks automatically generated from word documents under Subversion control
- Links on MELCOR wiki

Project Management

- Jira for tracking progress/issues
- Can be viewable externally by stakeholders

Sharing of information with users

- External web page
- MELCOR workshops
- MELCOR User Groups (EMUG & AMUG)

Case	BUR	CAV	CF	COR	CVH	DCH	FCL	FDI	FL	HS	NCO	PAR	RN	SPR
M-8-1 NoMix			X		X				X	X	X			
M-8-1 SYM			X		X				X	X	X			
Lace7			X		X	X			X	X	X		X	
Lace8			X		X	X			X	X	X		X	
Vanam-M3			X		X				X	X	X		X	
Molten Salt			X	X	X				X	X	X			
PHEBUS-B9			X	X	X				X	X	X			
FPT1			X	X	X	X			X	X	X		X	
LOFT			X	X	X	X			X	X	X			
Test Inew	X	X	X	X	X	X	X	X	X	X	X	X	X	X
SURRY (LBLOCA)	X	X	X	X	X	X	X	X	X	X	X		X	X
Zion (SBO)		X	X	X	X	X	X	X	X	X	X	X	X	X
PeachBottom (SBO)	X	X	X	X	X	X			X	X	X		X	X
Grand Gulf (SBO)	X	X	X	X	X	X		X	X	X	X		X	

Table 1-1: Physics Package Coverage

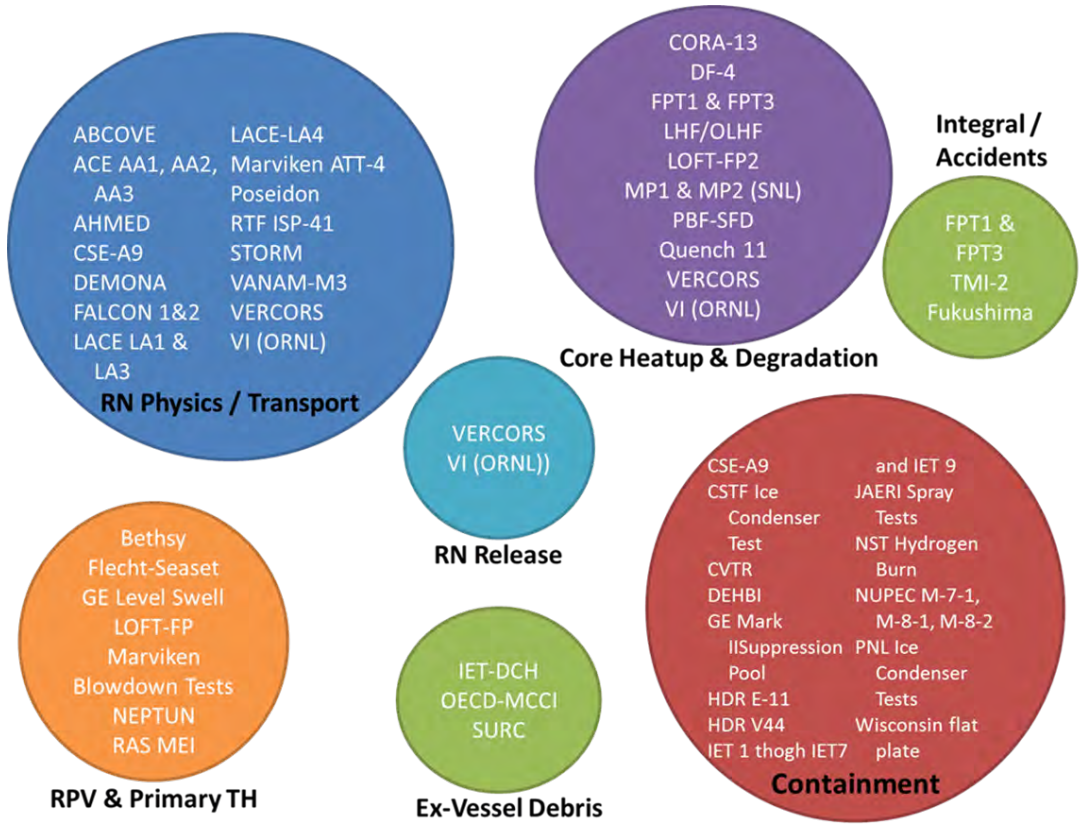
MELCOR Verification & Validation Basis

Volume 1: Primer & User Guide
Volume 2: Reference Manual
Volume 3: MELCOR Assessment Problems
[SAND2015-6693 R]

Analytical Problems

Saturated Liquid Depressurization
Adiabatic Expansion of Hydrogen
Transient Heat Flow in a Semi-Infinite Heat Slab
Cooling of Heat Structures in a Fluid
Radial Heat Conduction in Annular Structures
Establishment of Flow

LWR & non-LWR applications



Specific to non-LWR application

Sample Validation Cases

TRISO Diffusion Release

IAEA CRP-6 Benchmark
Fractional Release

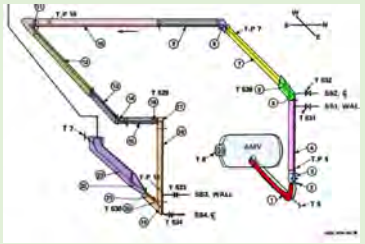
Case	1a	1b	2a	2b	3a	3b
US/INL	0.467	1.0	0.026	0.996	1.32E-4	0.208
US/GA	0.453	0.97	0.006	0.968	7.33E-3	1.00
US/SNL	**0.465**	**1.0**	**0.026**	**0.995**	**1.00E-4**	**0.208**
US/NRC	0.463	1.0	0.026	0.989	1.25E-4	0.207
France	0.472	1.0	0.028	0.995	6.59E-5	0.207
Korea	0.473	1.0	0.029	0.995	4.72E-4	0.210
Germany	0.456	1.0	0.026	0.991	1.15E-3	0.218

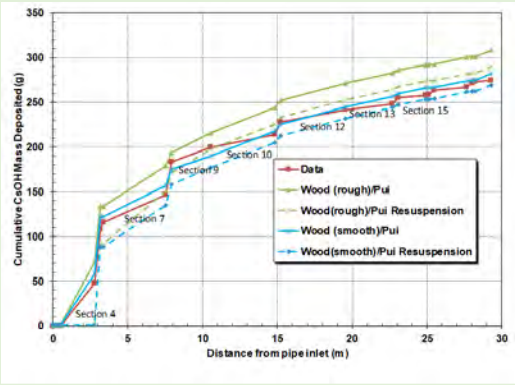
(1a): Bare kernel (1200 °C for 200 hours)
(1b): Bare kernel (1600 °C for 200 hours)
(2a): kernel+buffer+iPyC (1200 °C for 200 hours)
(2b): kernel+buffer+iPyC (1600 °C for 200 hours)
(3a): Intact (1600 °C for 200 hours)
(3b): Intact (1800 °C for 200 hours)

A sensitivity study to examine fission product release from a fuel particle starting with a bare kernel and ending with an irradiated TRISO particle;

Turbulent Deposition

LACE LA1 and LA3 tests experimentally examined the transport and retention of aerosols through pipes with high speed flow



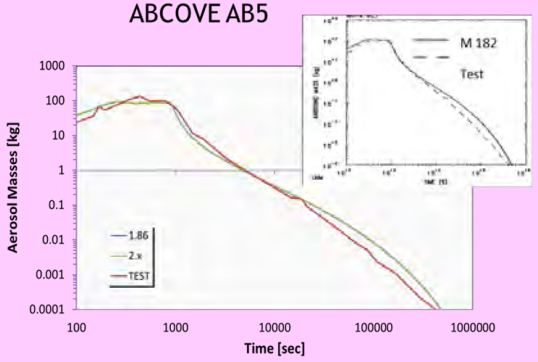


Aerosol Physics

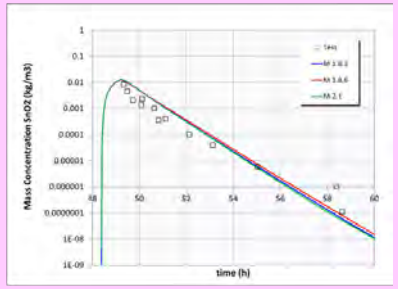
- Agglomeration
- Deposition
- Condensation and Evaporation at surfaces

Validation Cases
- Simple geometry: AHMED, ABCOVE (AB5 & AB6), LACE(LA4),
- Multi-compartment geometry: VANAM (M3), DEMONA(B3)
- Deposition: STORM, LACE(LA1, LA3)

ABCOVE AB5

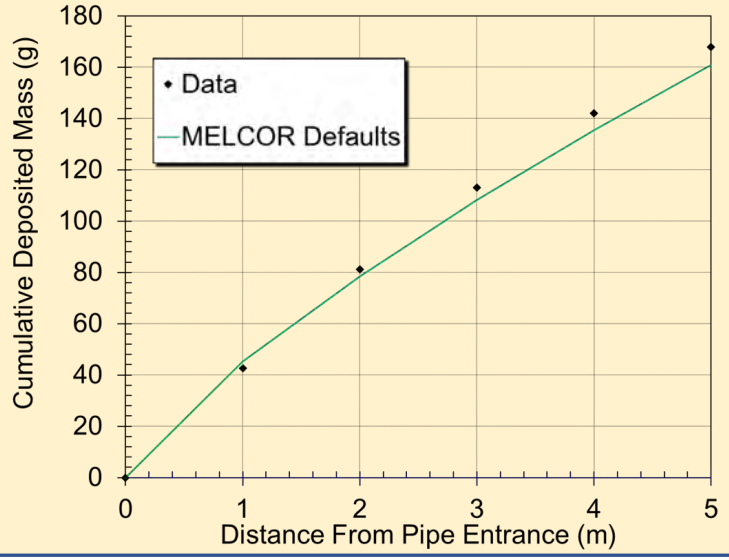


DEMONA-B3



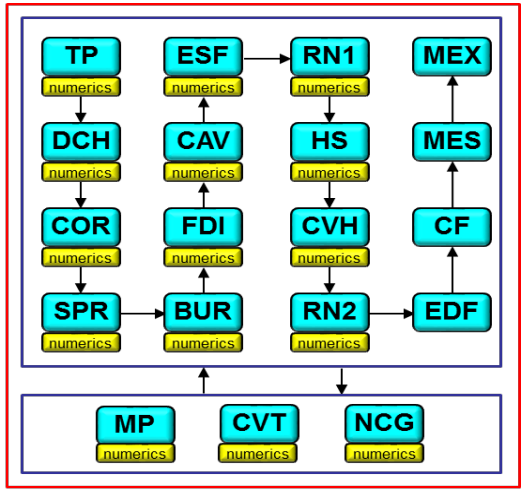
Resuspension

STORM (Simplified Test of Resuspension Mechanism) test facility

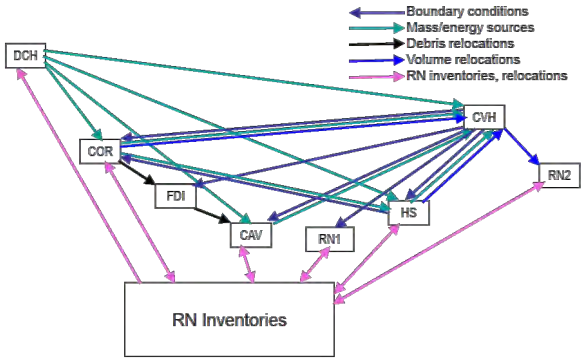


MELCOR Modernization

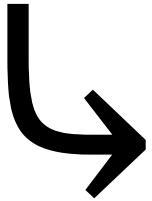
- Generalized numerical solution engine
- Hydrodynamics
- In-vessel damage progression
- Ex-vessel damage progression
- Fission product release and transport

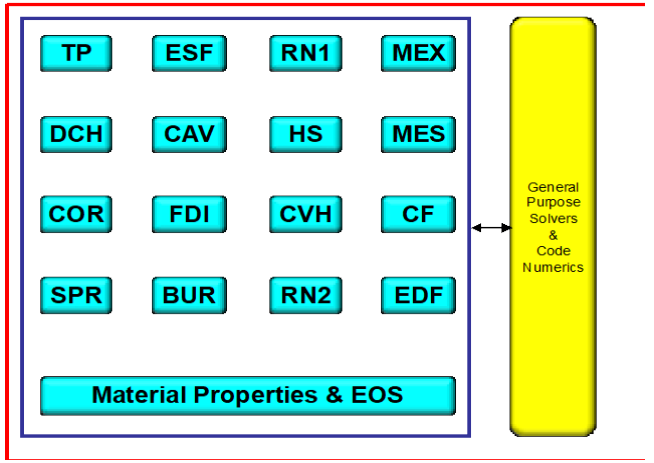


TP = Transfer Process
DCH = Decay Heat
COR = Core
SPR = Containment Spray
BUR = Gas Combustion
FDI = Fuel Dispersal Interaction
CAV = Cavity (MCCI)
ESF = Engineered Safety Features
MP = Material Properties
RN = Radionuclide
HS = Heat Structure
CVH = CV Hydrodynamics
EDF = External Data File
CF = Control Function
MES = Special Messages
MEX = Executive
CVT = CV Thermodynamics
NCG = Non Condensible Gas

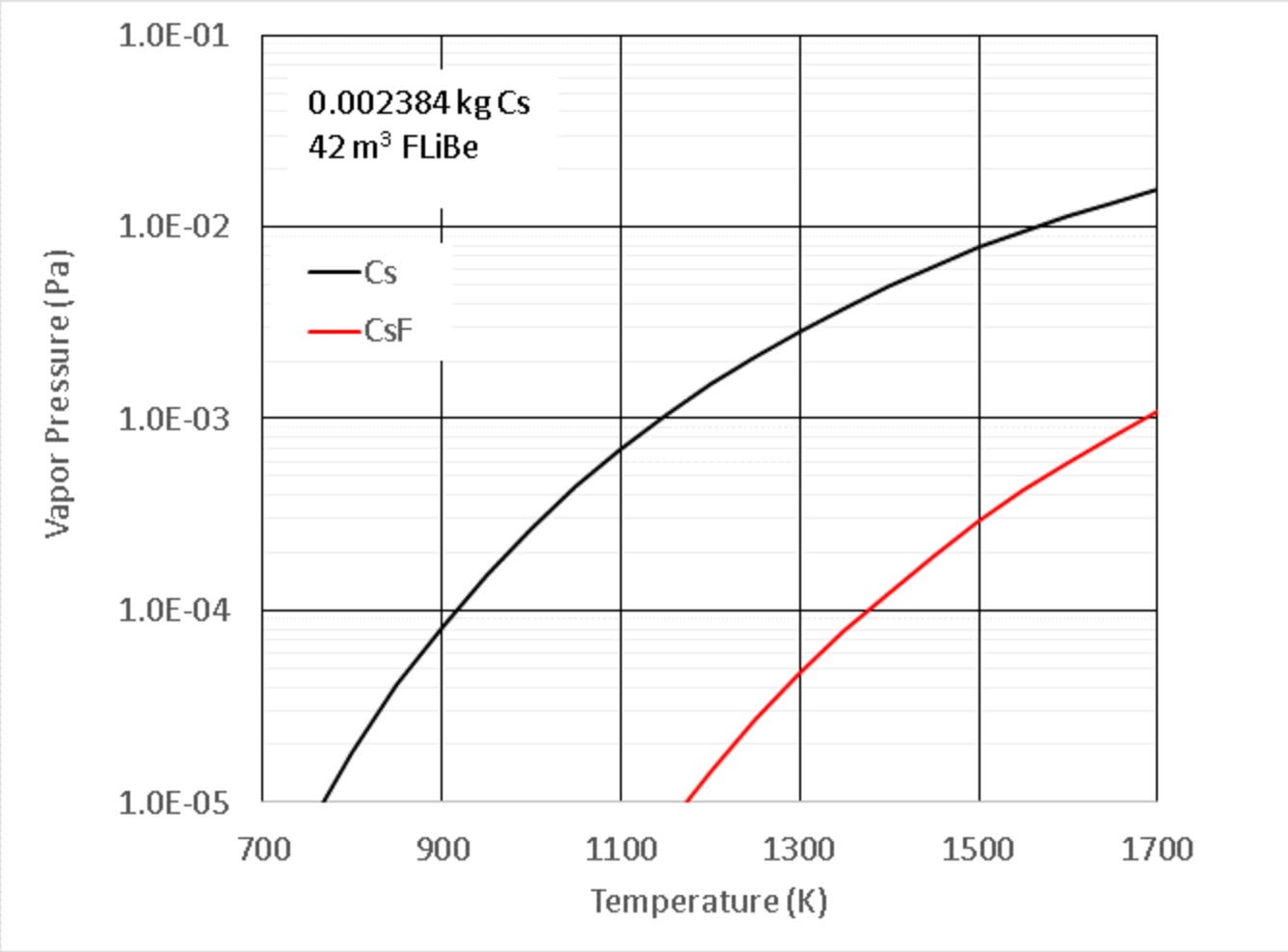


Separate **Physics** & **Numerics**





Cs vapor pressures in GRTR calculations



GRTR – Generalized Radionuclide Transport and Retention

Enhancement to MELCOR radionuclide transport modeling

- Incorporate unique chemistry of fission products in new fluids potentially mitigating release to atmospheres of reactor vessel, off-gas systems, and confinement/containment

Retention in fluids influenced by physico-chemical form of fission products – strong influence of thermochemistry

- Is the fission product compound soluble?
- Is the fission product compound insoluble (i.e., colloidal)?
- Is the fission product compound a gaseous vapor?
- Has the fission product compound deposited on a structural surface?
- Is the fission product located at a liquid-atmosphere interface?
  - Interface between liquid pool and overlying gas atmosphere
  - Interface between liquid and gas bubbles (e.g., generated by sparging helium gas)

Introduce new physico-chemical *forms* that supplement existing MELCOR representation of distinct radionuclide classes

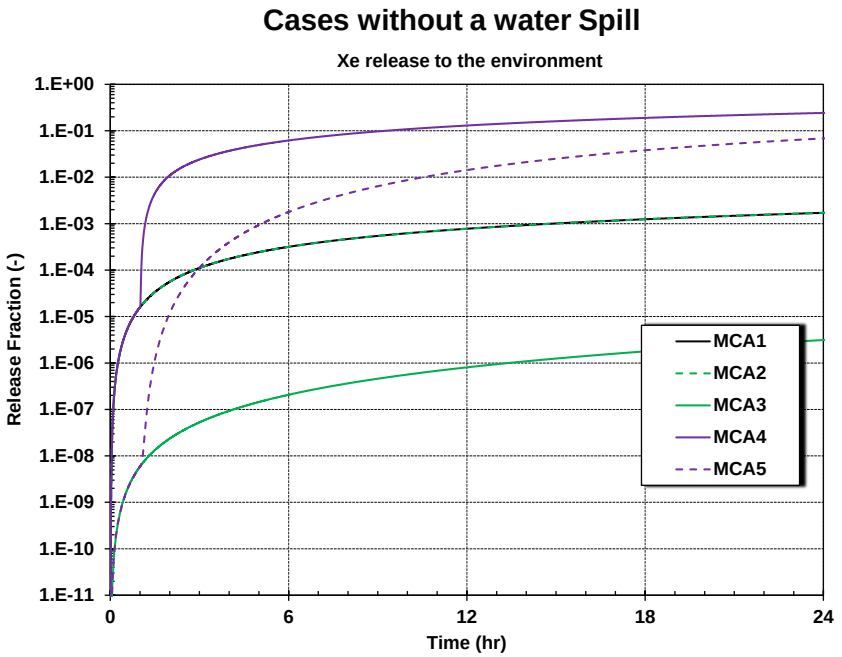
- Soluble fission products
- Insoluble/colloidal fission products
- Deposited fission products
- Gaseous fission products

Each tracked form is identified with either a liquid pool, an atmosphere, or deposited on a structure

Results of the sensitivity studies

Gaseous xenon release to the environment without a water spill

- MCA4 had the highest release due to auxiliary filter venting of the reactor cell after 1-hr and enhanced leakage due the HVAC flow through the reactor building
- MCA3 had the lowest release with no HVAC flow in the reactor building (stack fans) and no auxiliary flow
- MCA1 and MCA2 were identical because xenon is not an aerosol
- MCA5 did not have enhanced releases due to HVAC venting the reactor building leaks but did include the auxiliary filter flow after 1-hr



Cases without a water spill

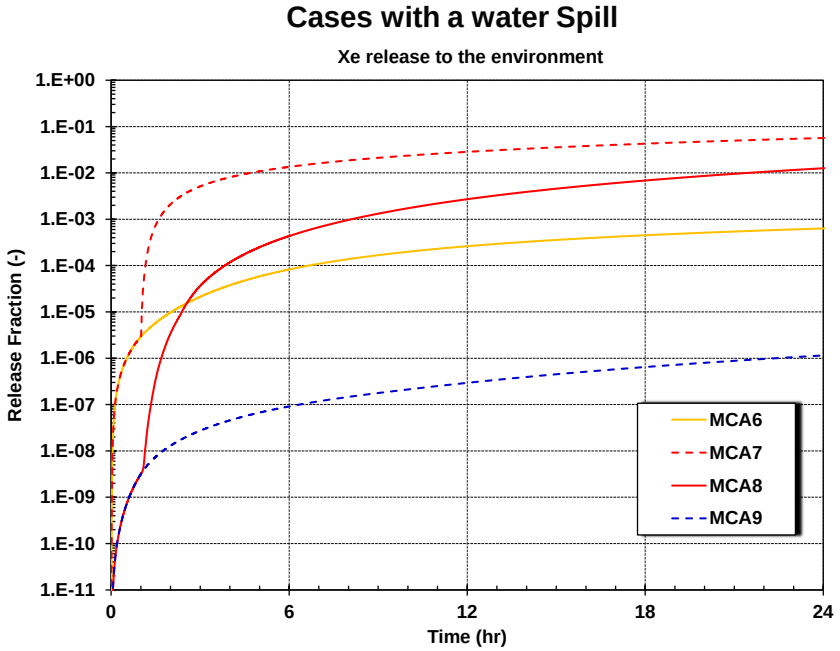
Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No

Note: Results assume no xenon retention in the charcoal filters.

Results of the sensitivity studies

Gaseous xenon release to the environment with a water spill

- MCA7 had the highest release due to auxiliary filter venting of the reactor cell after 1-hr and enhanced leakage due the HVAC flow through the reactor building
- MCA7 had a lower release than the corresponding dry case due to xenon capture in the gas retention tank
- MCA9 had the lowest release due to no HVAC flow in the reactor building (stack fans) and no auxiliary filter flow
- Leaks into the reactor building from MCA6 were vented to the environment due to the HVAC operation
- MCA8 did not have enhanced releases due to HVAC venting any reactor building leaks but did include venting to the environment from the auxiliary filter flow after 1-hr



Cases with a water spill

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA6	1 μm	Yes	No	Yes
MCA7	1 μm	Yes	Yes	Yes
MCA8	1 μm	No	Yes	Yes
MCA9	1 μm	No	No	Yes

Note: Results assume no xenon retention in the charcoal filters.

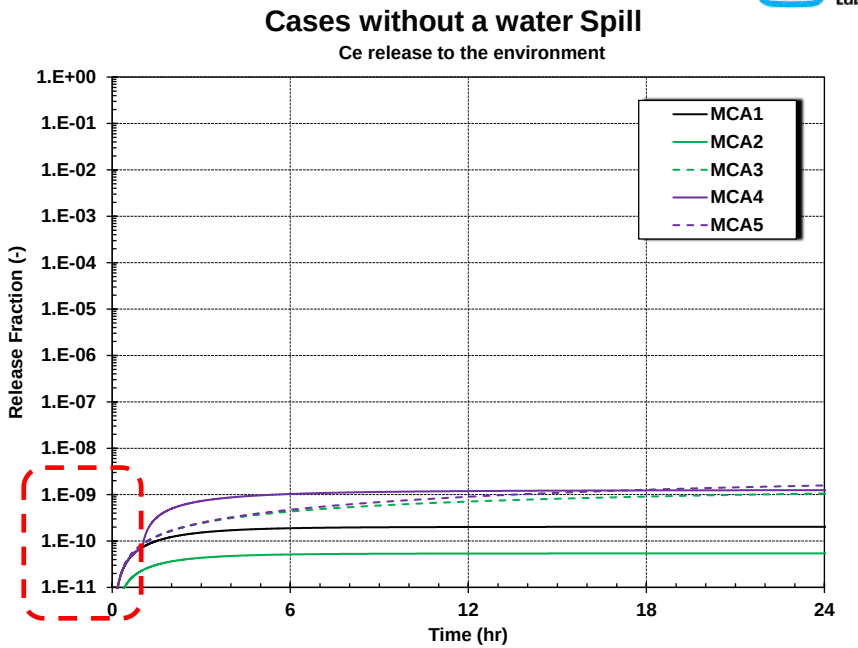
Results of the sensitivity studies

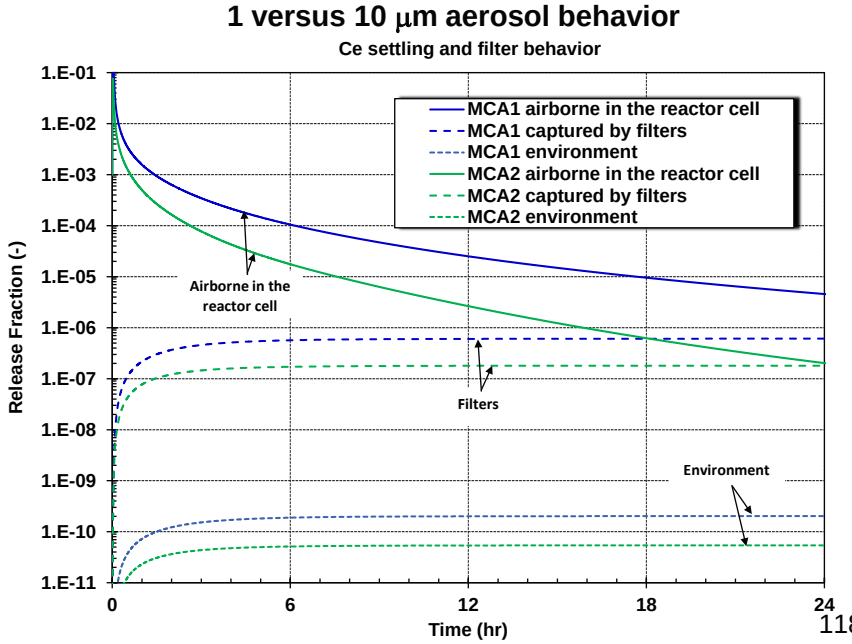
The cerium aerosol release to the environment without a water spill were very low

- MCA3, MCA4, and MCA5 releases to the environment were approximately the same and larger than MCA1
  - MCA4 and MCA5 included continuous venting of very small aerosols from the reactor cell through the auxiliary filter
  - MCA3 results show impact of nominal leakage from the reactor building (i.e., no filtration)
  - MCA1 included filtration of the reactor building but no auxiliary filter flow
- MCA2 had larger aerosols, which settled faster and the smallest amount released to the environment

Cases without a water spill

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 μm	Yes	No	No
MCA2	10 μm	Yes	No	No
MCA3	1 μm	No	No	No
MCA4	1 μm	Yes	Yes	No
MCA5	1 μm	No	Yes	No





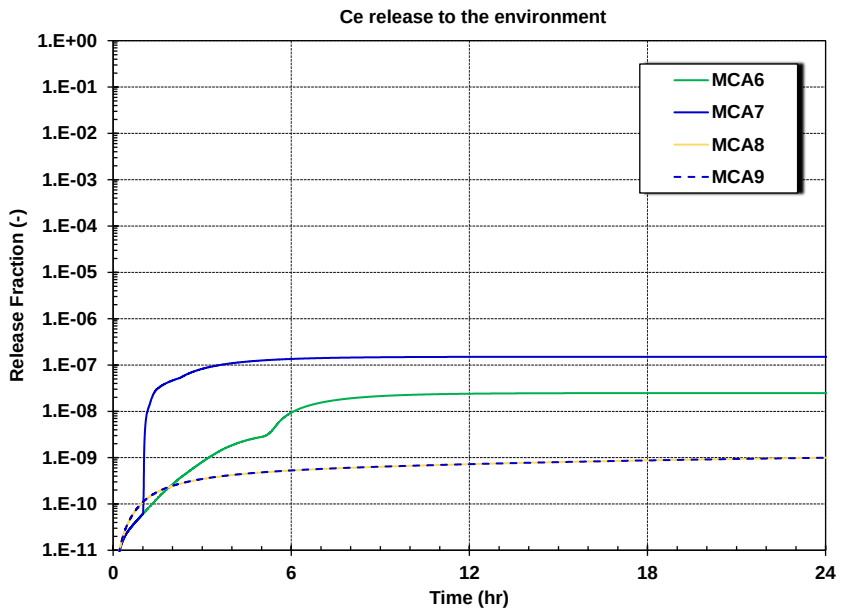
Note: The capture efficiency of the absolute filters for aerosols below <0.3 μm was assumed to be zero.

Results of the sensitivity studies

Cerium aerosol release to the environment with a water spill

- MCA6 and MCA7 had the higher releases release due the HVAC flow through the reactor building
  - The auxiliary filter flow increased releases to the environment due to non-perfect capture by the absolute filters
  - MCA6 and MCA7 were higher than the corresponding dry cases (MCA1 and MCA4) due to higher leakage from the reactor cell
- MCA8 and MCA9 are essentially identical releases to the environment (explained on next slide)
  - MCA8 and MCA9 did not have the building HVAC flow

Cases with a water Spill



Cases with a water spill

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA6	1 μm	Yes	No	Yes
MCA7	1 μm	Yes	Yes	Yes
MCA8	1 μm	No	Yes	Yes
MCA9	1 μm	No	No	Yes

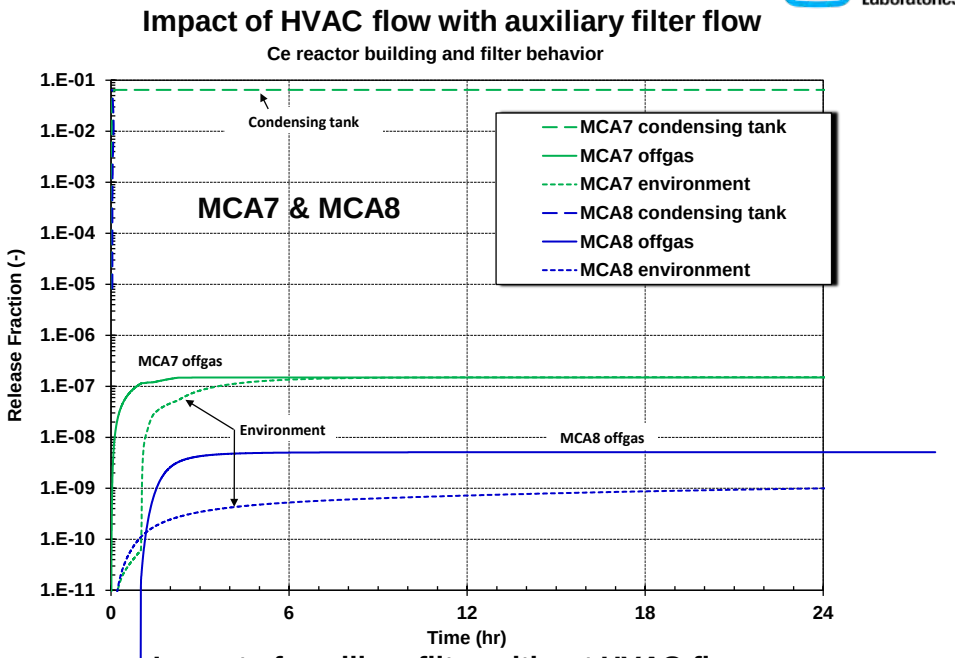
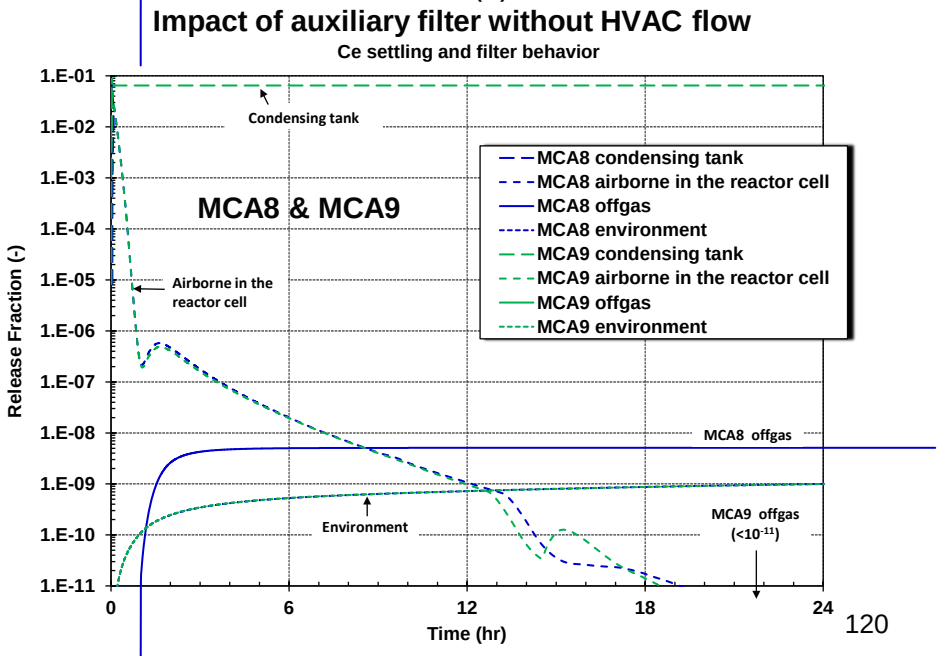
Results of the sensitivity studies

Comparison of MCA7 and MCA8 shows the HVAC flow sweeps a portion of the small aerosols through the filters and out the stack

- Most aerosols in the condensing tank
- Stack flow capture and aerosol pass-through is more important than only the auxiliary filter flow

Comparison of MCA8 and MCA9 shows the auxiliary filter has a negligible impact on the environmental release

- Capture in the condensing tank, rapid settling in the reactor cell, and retention in the offgas system (filter pit and stack) overwhelms the importance of the auxiliary flow when the HVAC is not operating

Cases with a water spill

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA6	1 μm	Yes	No	Yes
MCA7	1 μm	Yes	Yes	Yes
MCA8	1 μm	No	Yes	Yes
MCA9	1 μm	No	No	Yes