

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

September 13, 2022



# U.S. NRC



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# Outline

NRC strategy for non-LWR source term analysis

Project scope

Overview of Molten Salt Reactor (MSR)

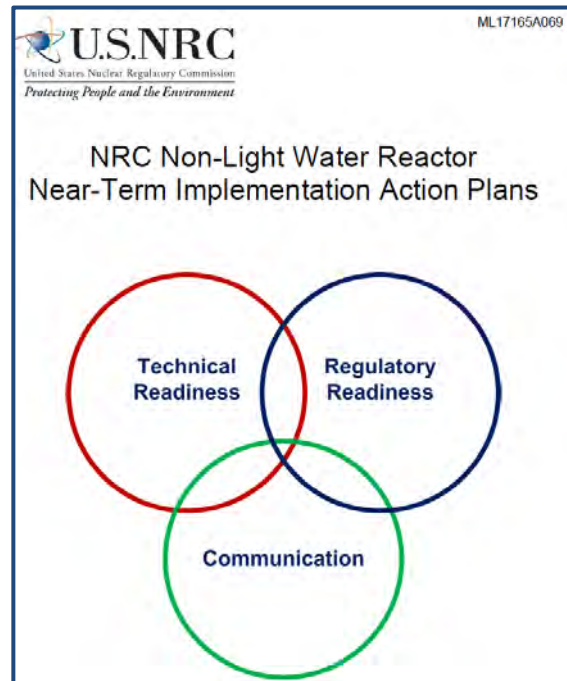
MSR reactor fission product inventory/decay heat methods & results

MELCOR molten salt models

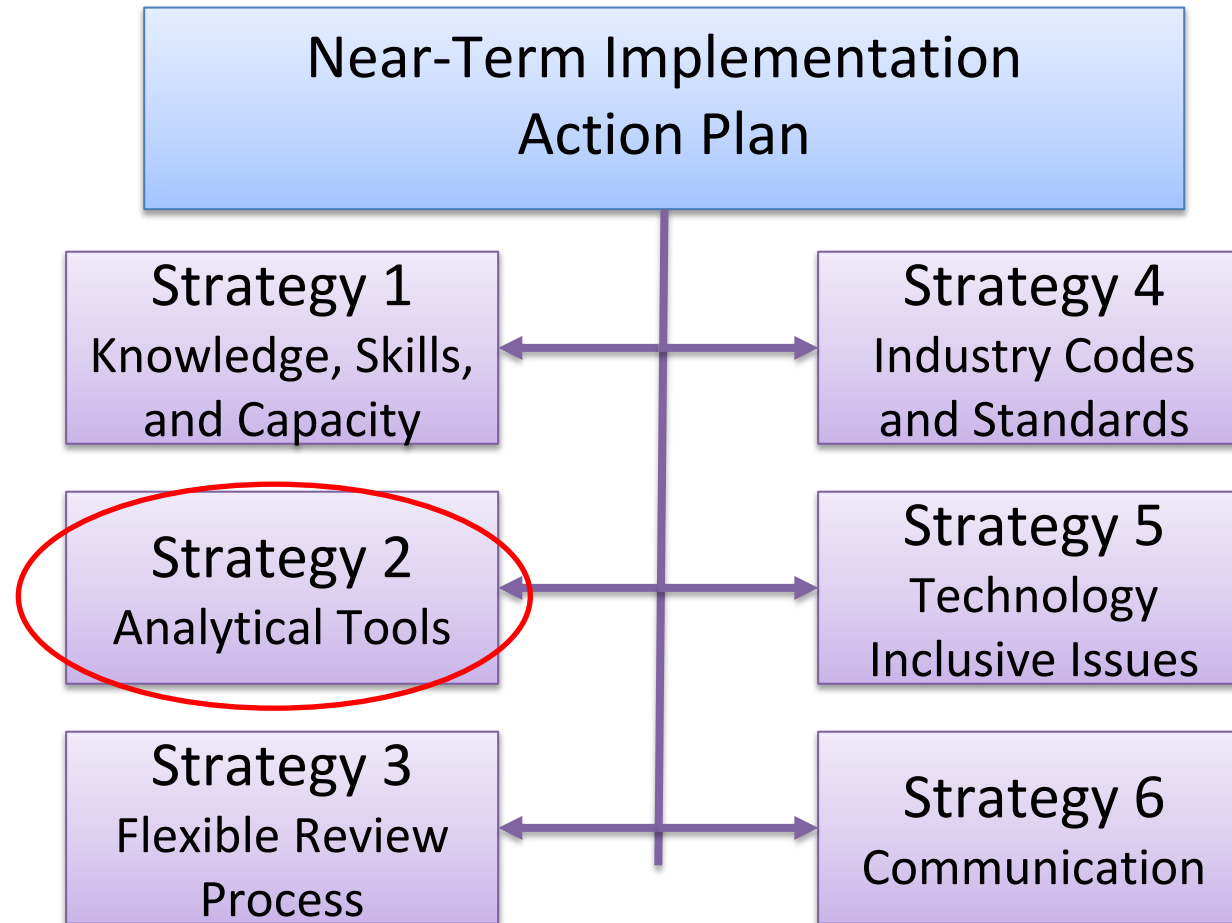
MSR plant model and source term analysis

Summary

# Integrated Action Plan (IAP) for Advanced Reactors

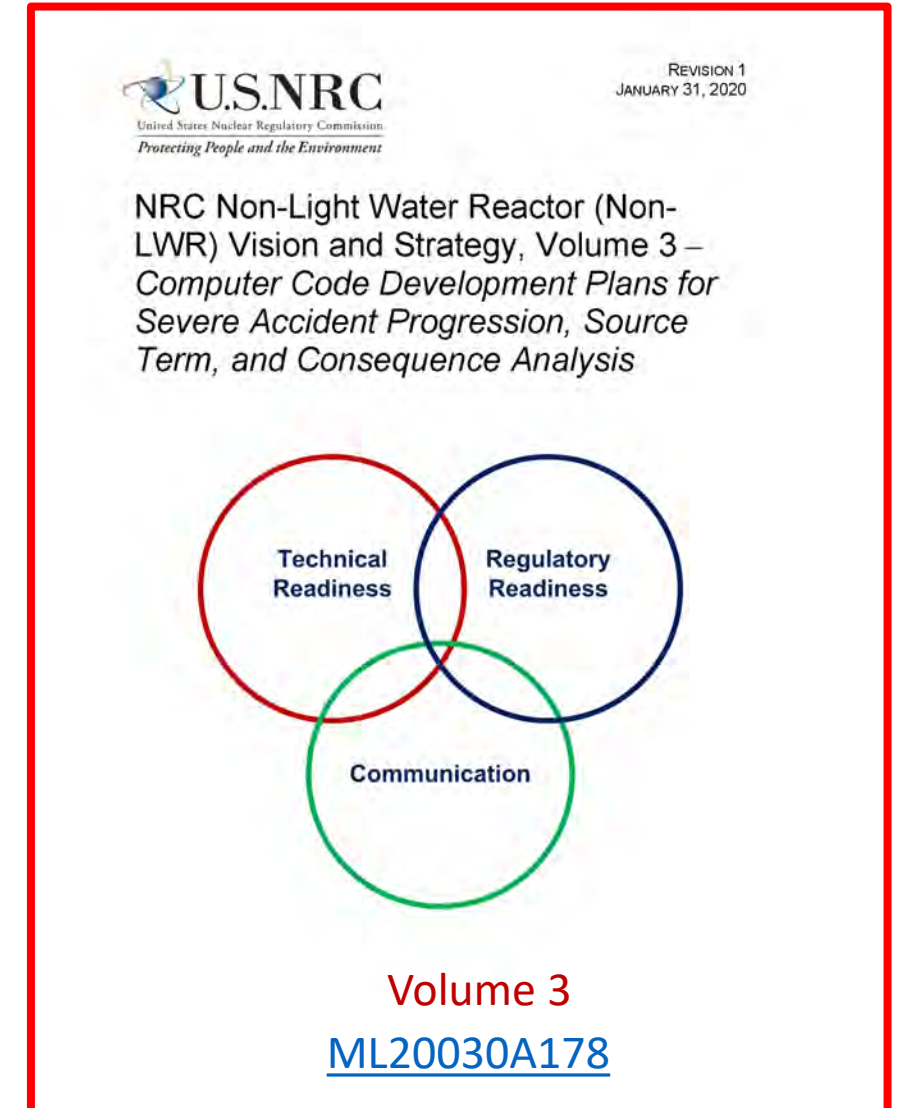
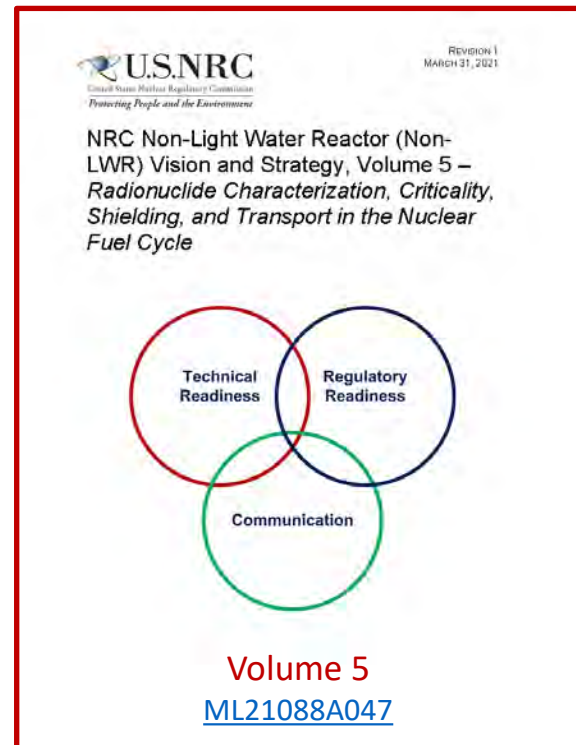
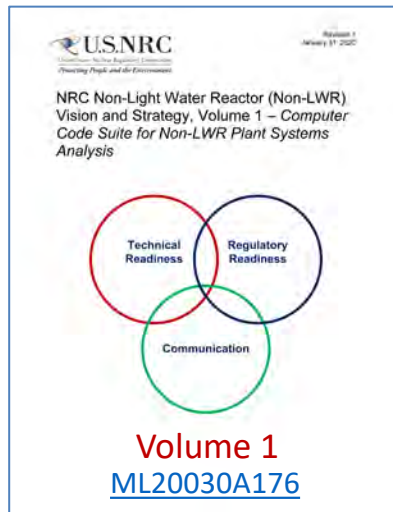
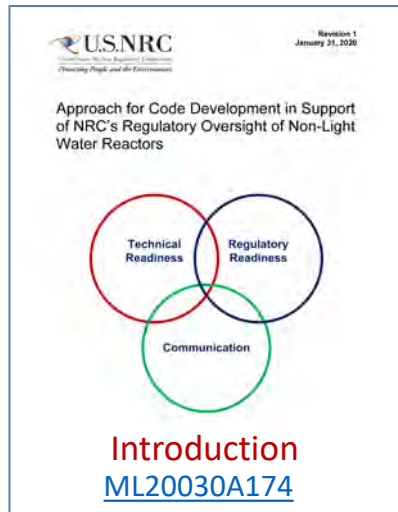


[ML17165A069](#)



# IAP Strategy 2 Volumes

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.



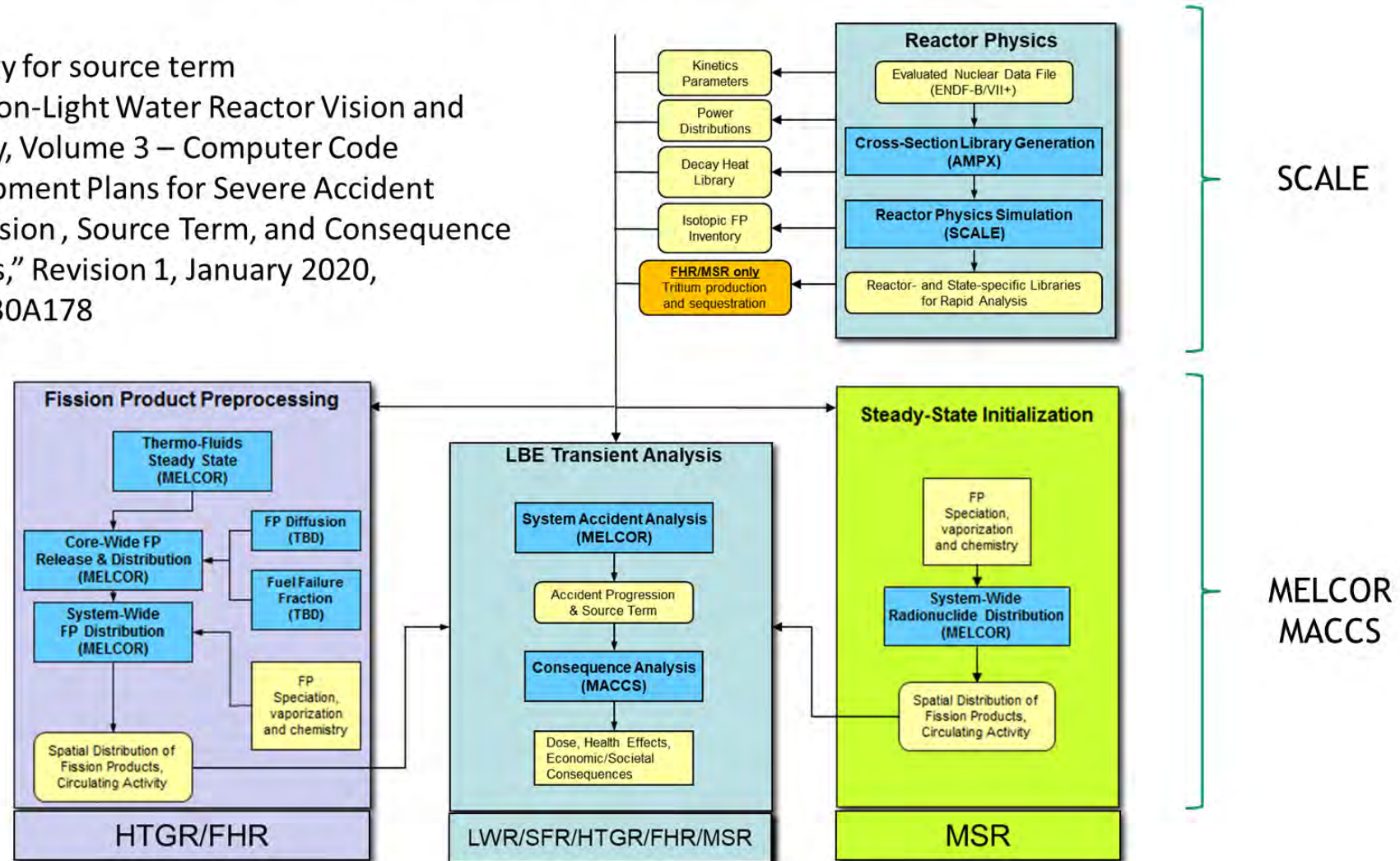


# NRC strategy for non-LWR analysis (Volume 3)

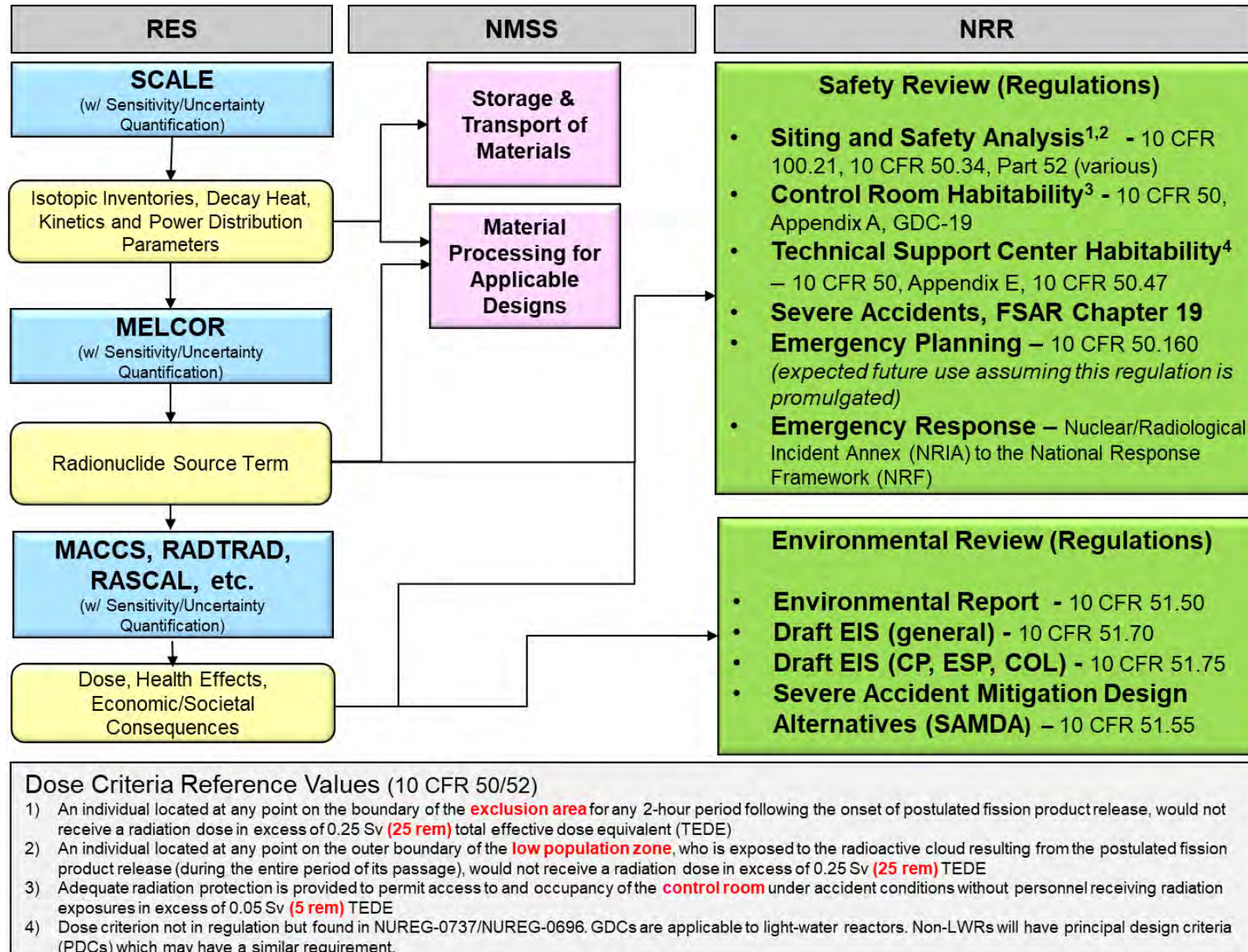
## Evaluation Model and Suite of Codes

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

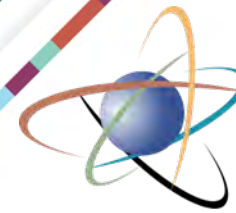


# Role of NRC severe accident codes





# Project Scope



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# 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)



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# 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](https://en.wikipedia.org/wiki/Convair_NB-36H#/media/File:NB36H-1.jpg)]



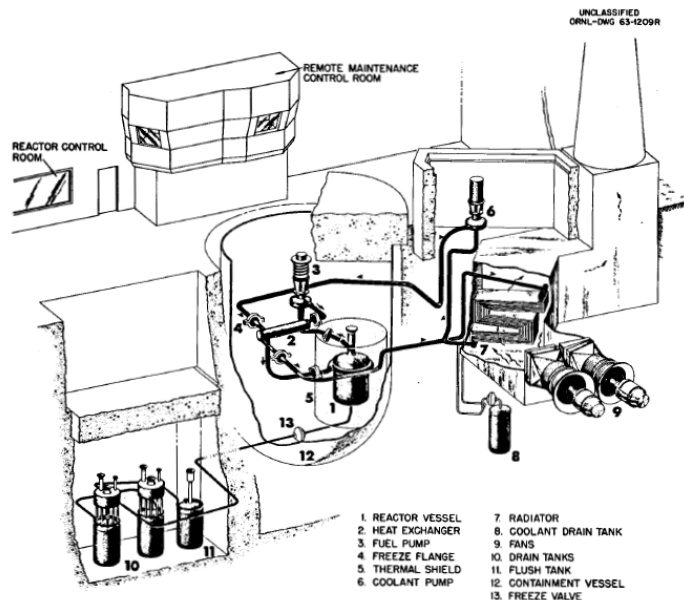
**Heat Transfer Reactor Experiment #3**

[[https://en.wikipedia.org/wiki/Aircraft\\_Nuclear\\_Propulsion#/media/File:HTRE-3.jpg](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<sub>th</sub>
- Used for SCALE MELCOR source term demonstration calculations



**MSRE**  
[ORNL-TM-0728]

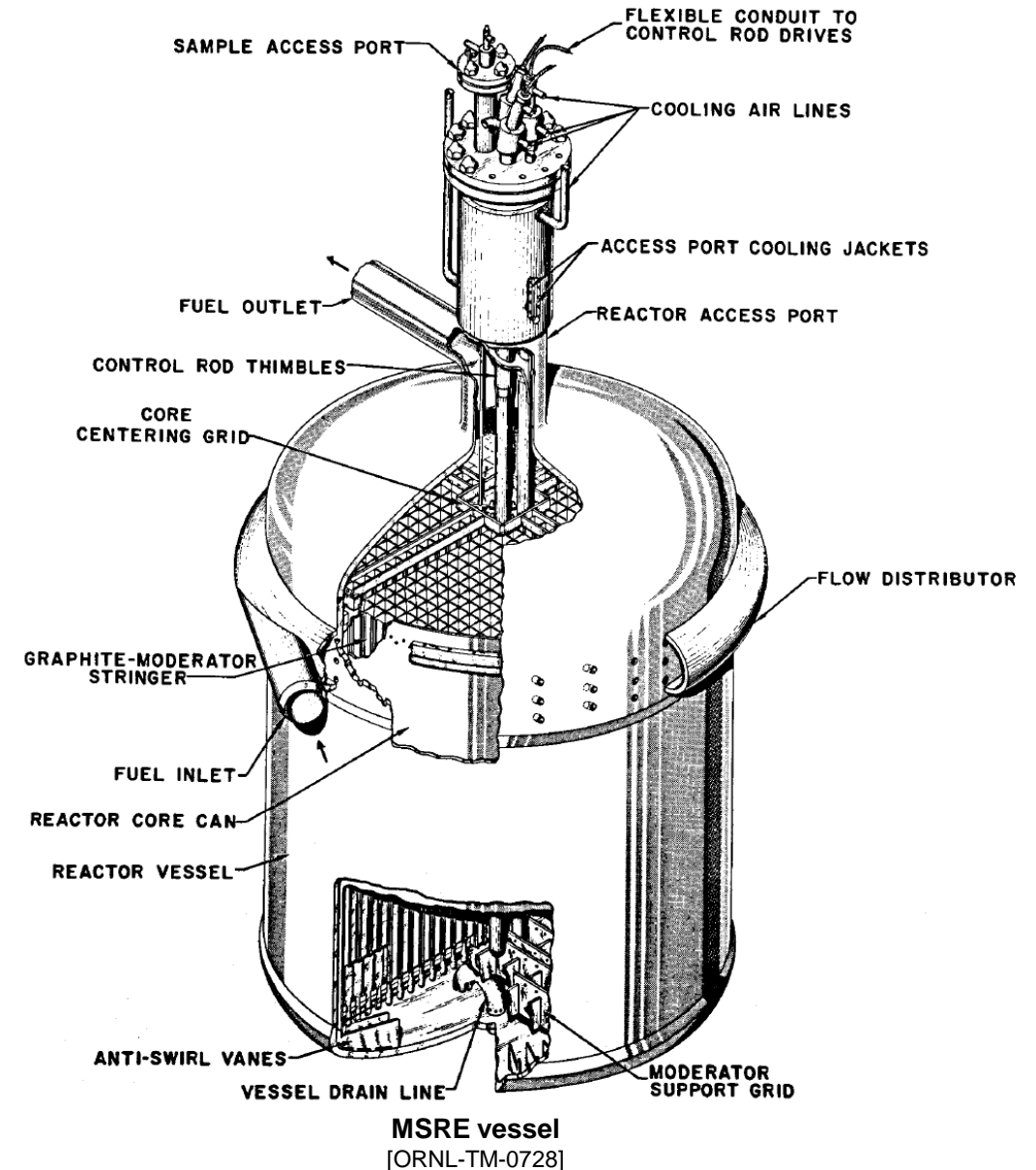


**MSRE Graphite Core Structure**  
[[https://en.wikipedia.org/wiki/Molten-Salt\\_Reactor\\_Experiment](https://en.wikipedia.org/wiki/Molten-Salt_Reactor_Experiment)]

# MSRE (1/5)

## Reactor

- 10 MW<sub>th</sub>
- 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<sup>3</sup>/s (1200 gpm) core flowrate
- 635°C core inlet
- 668°C 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



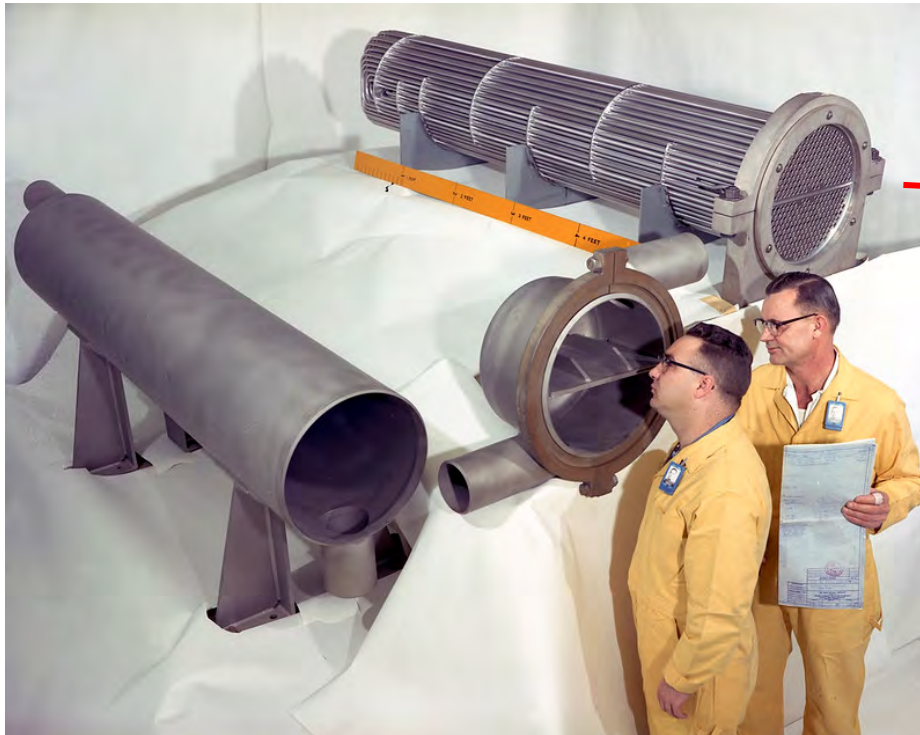


# MSRE (2/5)

## Coolant salt circulation

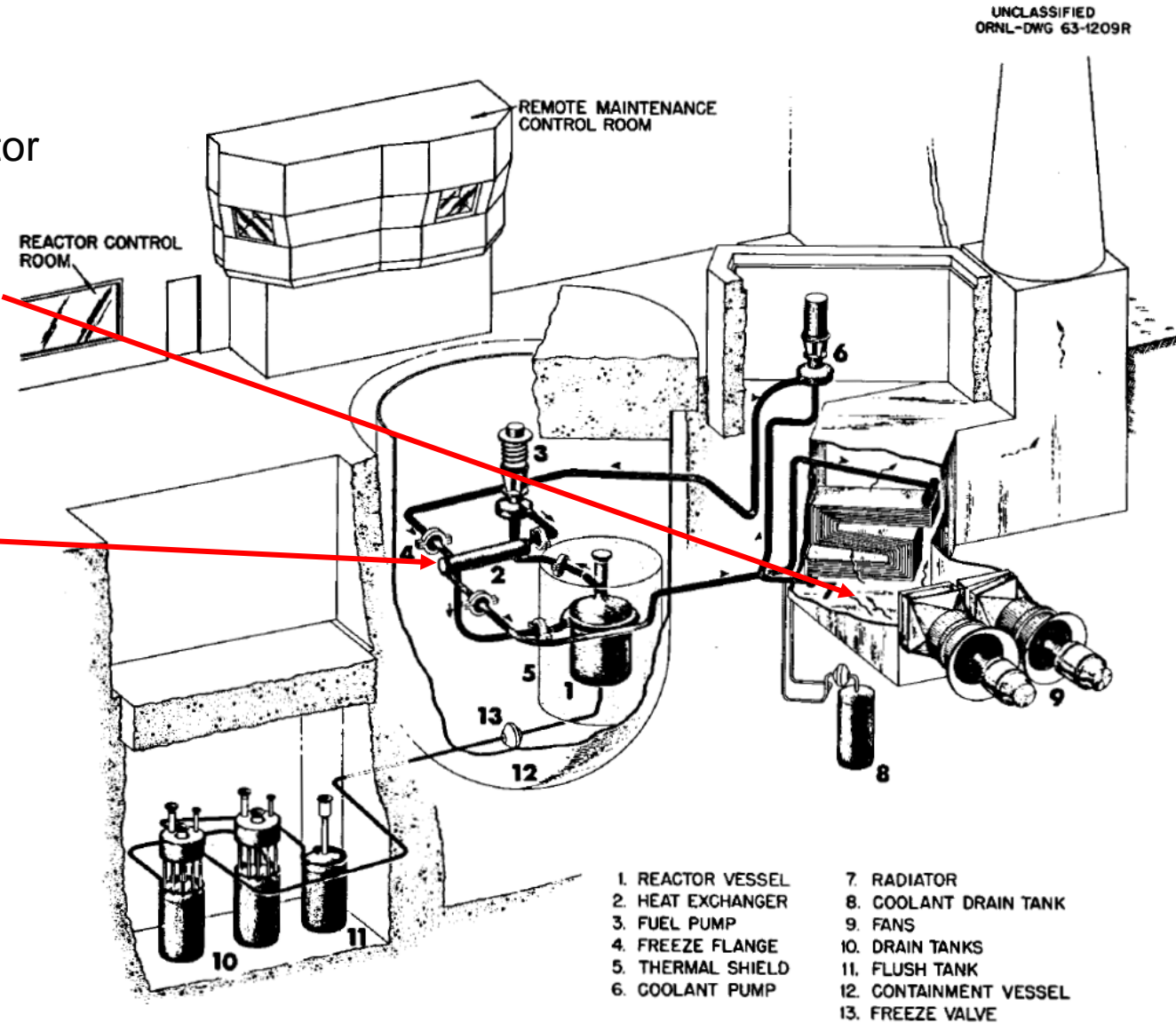
- Primary loop with pump and heat exchanger
- Intermediate loop with pump and air-cooled radiator
- No fuel in intermediate loop

Air-cooled radiator rejects heat to the plant stack



MSRE primary heat exchanger

[<https://www.flickr.com/photos/oakridgelab/albums/72157659472696880/with/21573745744/>]

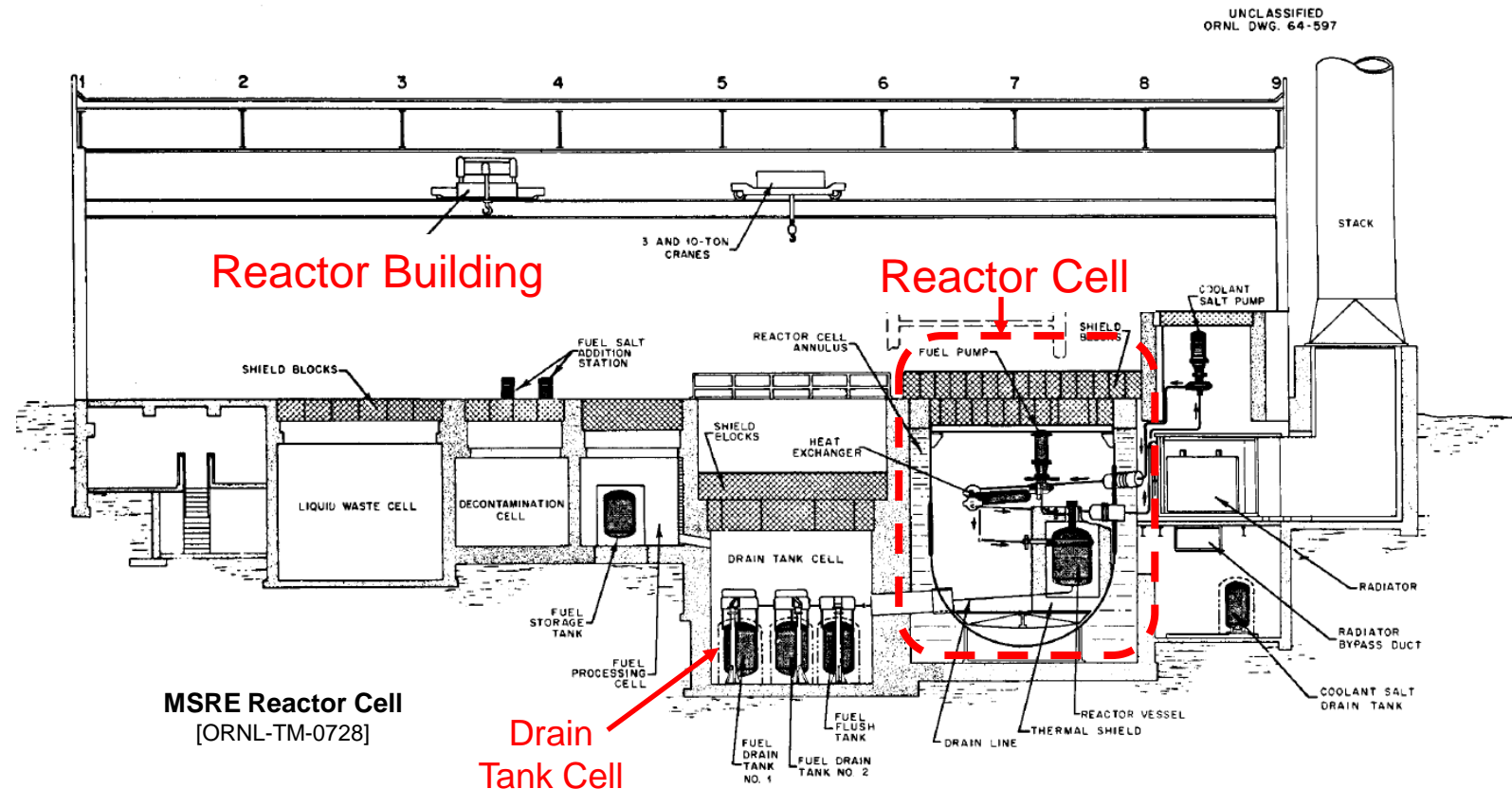


MSRE schematic  
[ORNL-TM-0728]

# MSRE (3/5)

## Reactor Cell acts as containment

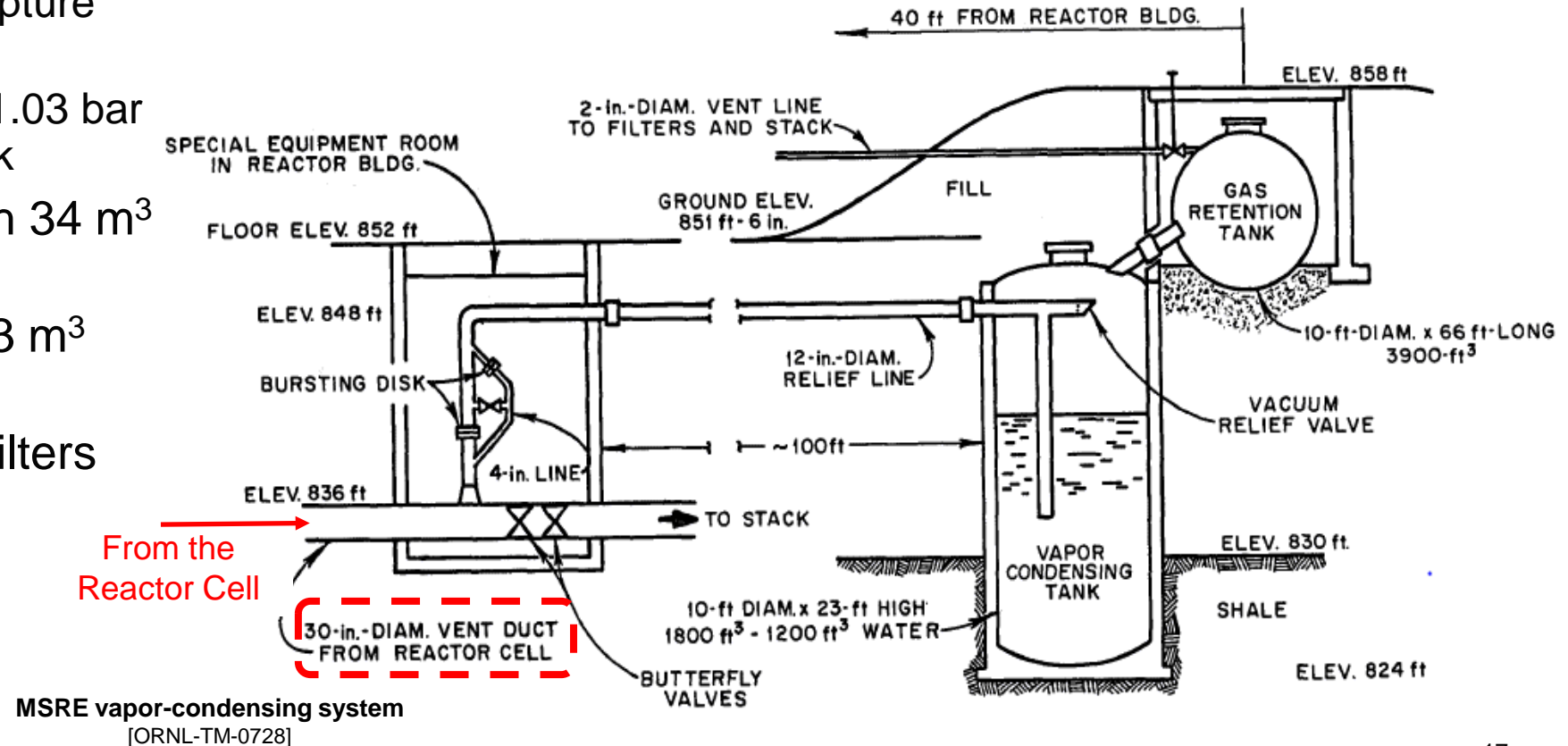
- Contains the reactor vessel, the primary circulating fuel loop, and most of the coolant salt loop
- Circulating salt to air-cooled radiators located outside of the reactor cell
- 95% N<sub>2</sub>
- 0.875 bar absolute
- 320 m<sup>3</sup>
- Leak rate = 0.42 standard liters per hour at 0.875 bar (12.7 psia) (0.23 mm dia.)
- Attached by a tunnel to the drain tank cell



# MSRE (4/5)

## Vapor-condensing system

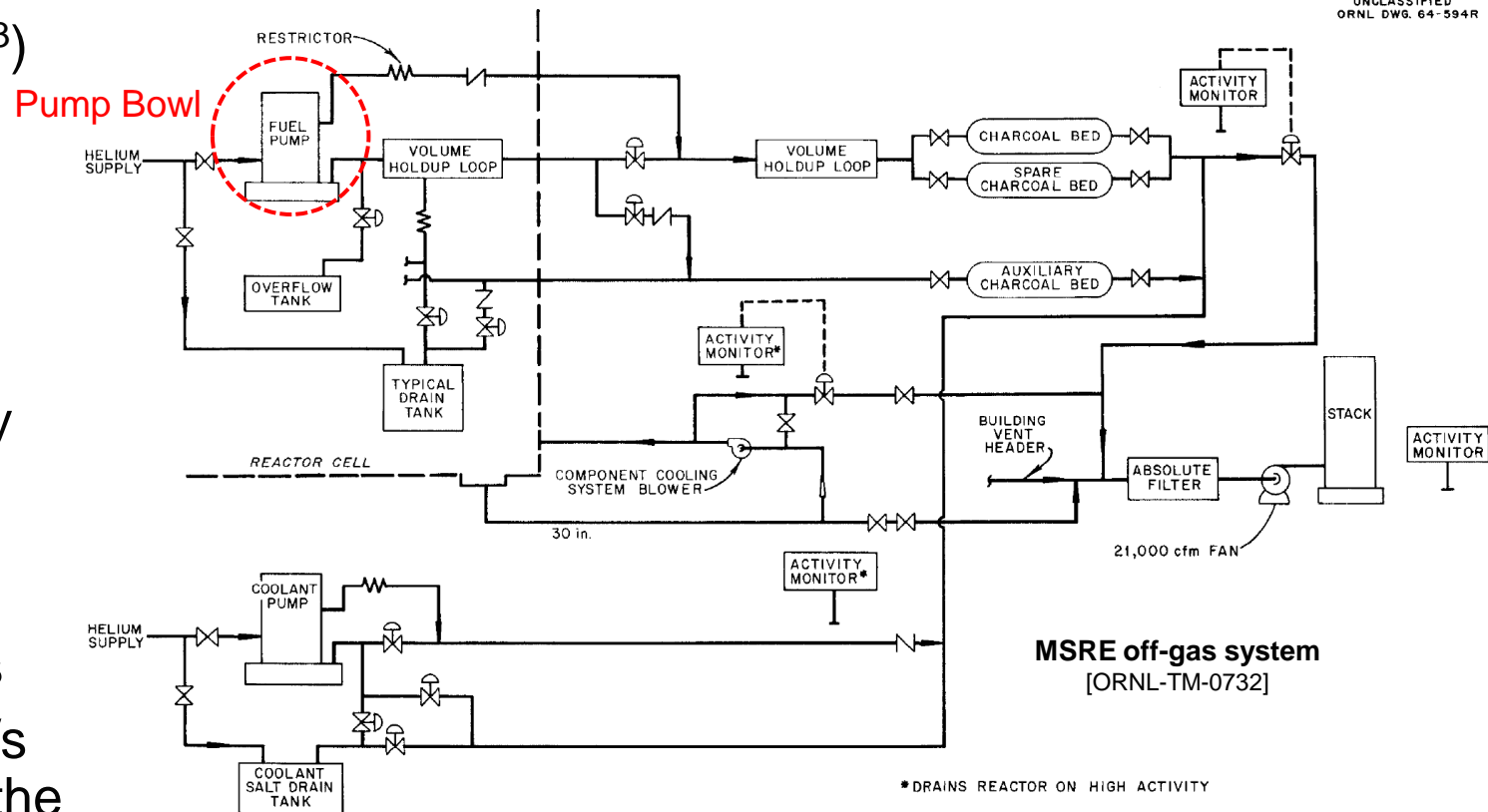
- Connects to the reactor cell via a 30" pipe
- Normally isolated from the stack with 2 rupture disks
  - 30.5 cm (12") line with 1.38 bar (20 psig) rupture disk
  - 10 cm (4") line with 1.03 bar (15 psig) rupture disk
- Condensing tank with 34 m<sup>3</sup> (1200 ft<sup>3</sup>) of water
- Gas retention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



# 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<sup>3</sup> (22 ft<sup>3</sup>) of charcoal
  - One train typically isolated
  - Auxiliary charcoal filter for reactor cell venting
- 3x32 m<sup>2</sup> (3x350 ft<sup>2</sup>) fiberglass roughing filters 90-95% efficiency for dust
- 3x2.23 m<sup>2</sup> (3x24 ft<sup>2</sup>) HEPA “absolute” filters with 99.7% efficiency for 0.3 micron particles
- Filtered flow merges with 9.9 m<sup>3</sup>/s (21,000 cfm) building HVAC out the plant stack for dilution





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



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# NRC SCALE/MELCOR Non-LWR Demonstration Project

## Objectives:

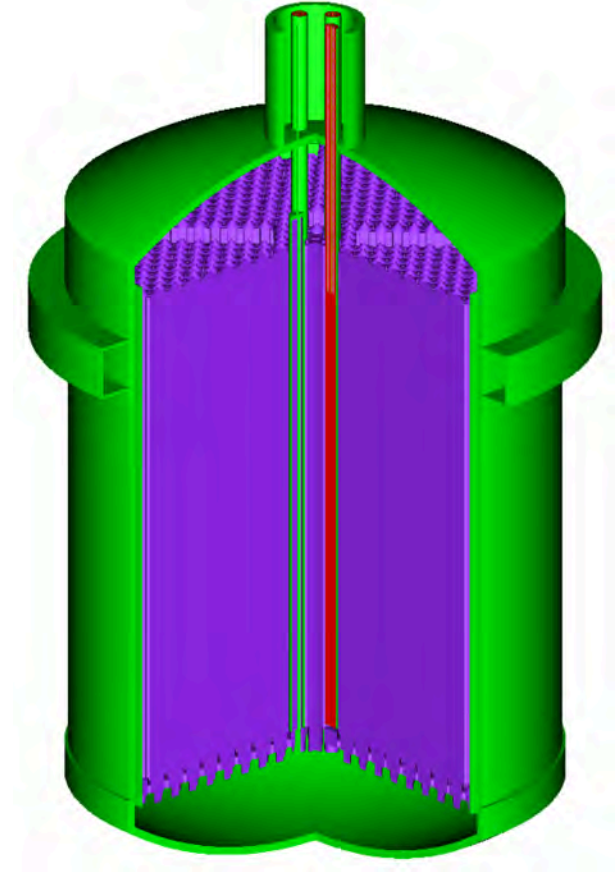
- Develop approach and models for SCALE analysis to obtain:
  - Radionuclide inventory
  - System decay heat
  - Power profiles
  - Reactivity coefficients

## Key differences to LWR analysis:

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

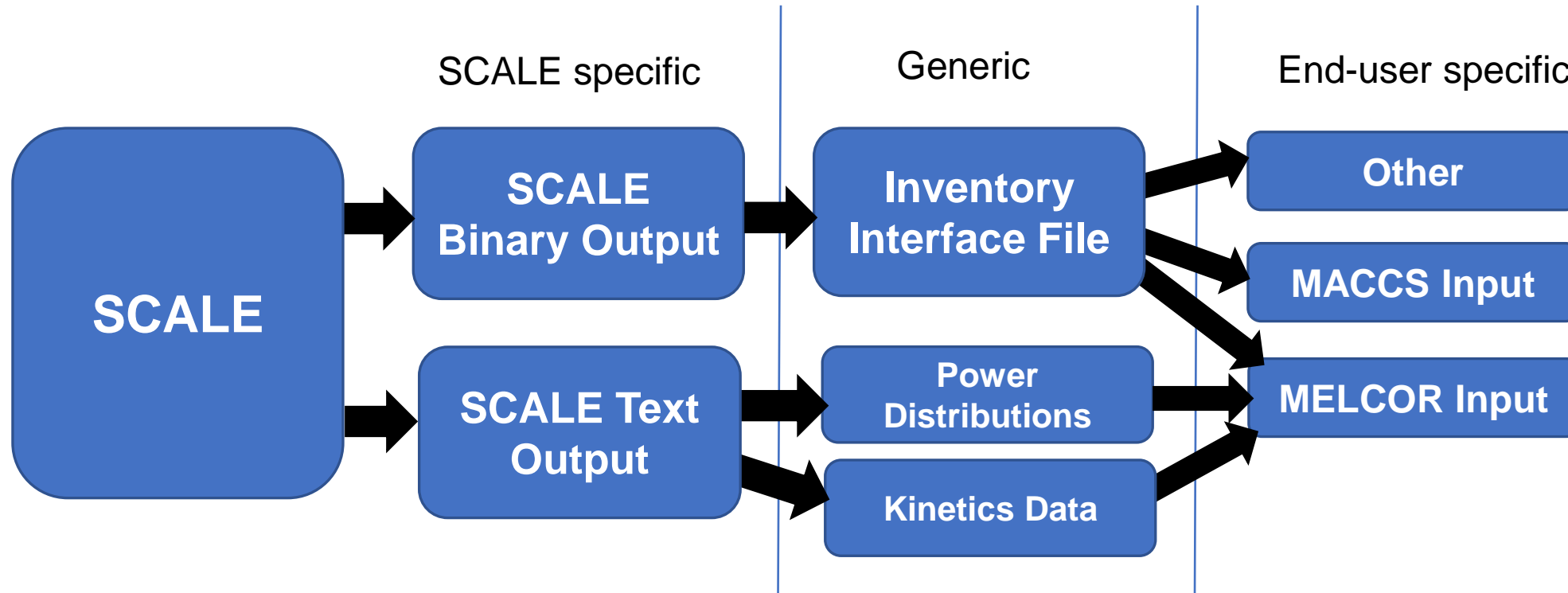
## Approach:

- 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:

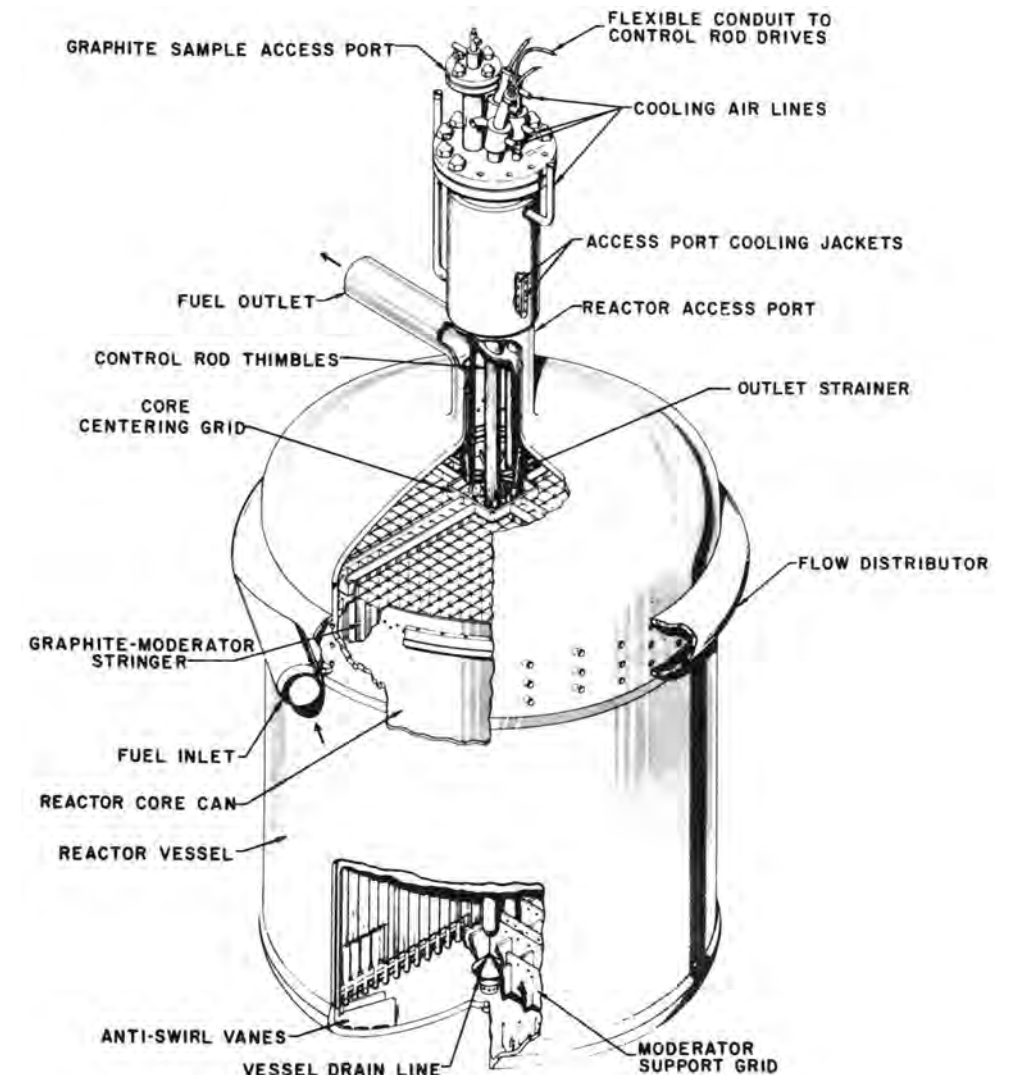
- CSAS for criticality/reactivity
- TRITON for reactor physics & depletion

\* 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 <sub>2</sub> -ZrF <sub>2</sub> -UF <sub>2</sub>
Enrichment	34.5 wt.% <sup>235</sup> U
Moderator	Graphite
Structure	Nickel-based alloys
Core volume	0.7 m <sup>3</sup>
System volume	2 m <sup>3</sup>
Heavy metal loading	0.233 tHM
Loop transit time	25.2 seconds
Nuclide removal	<ul style="list-style-type: none"> <li>Noble gases via Off-Gas System (OGS)</li> <li>Noble metal plate-out at heat exchanger (HX)</li> </ul>
Re-fueling	Irregular re-fueling by capsules with HEU fuel salt
Operating time	~375 equivalent full-power days with <sup>235</sup> U fuel

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



MSRE reactor vessel [1]

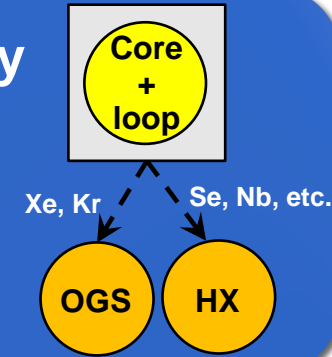
[1] R. C. Robertson (1965), "MSRE Design and Operations Report Part I: Description of Reactor Design," ORNL-TM-0728, ORNL.

[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

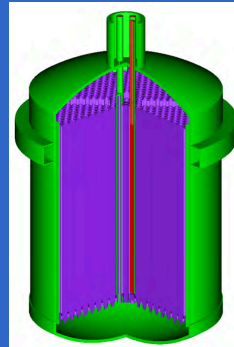


*System-average inventory at point in time*



## Core power/flux distribution

- Predicts neutron flux and power profiles at point in time

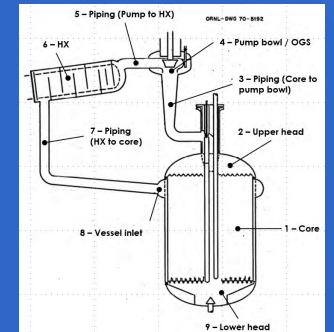


*Power/flux profile*



## Location-dependent inventory in loop

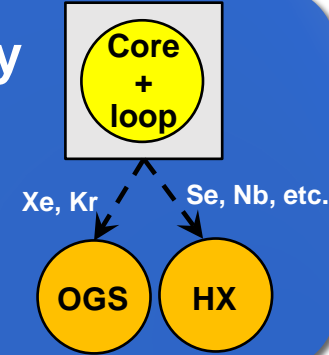
- Considers power profile and off-gas
- Predicts inventory in each region of the loop



# SCALE analysis approach

## Time-dependent inventory

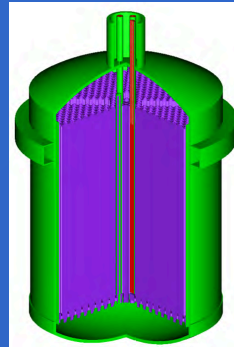
- Considers core + loop + off-gas + plating-out
- Predicts system-average inventory over time



*System-average inventory at point in time*

## Core power/flux distribution

- Predicts neutron flux and power profiles at point in time



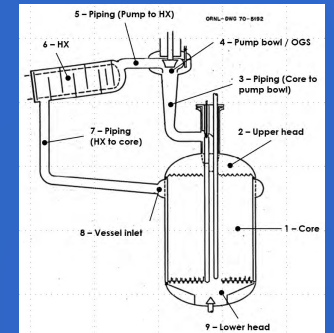
*Sensitivity study:  
Region-dependent  
nuclide inventory*

*Power/flux  
profile*

*System-average inventory at point in time*

## Location-dependent inventory in loop

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

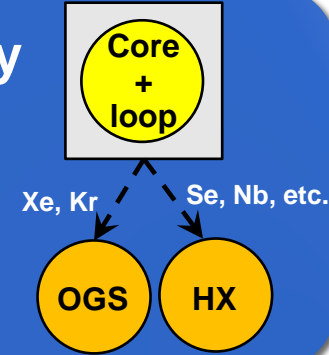




# SCALE analysis approach

## Time-dependent inventory

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

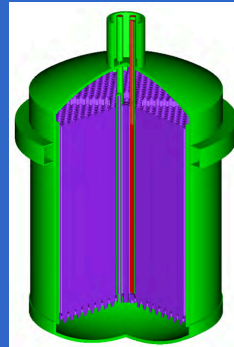


*System-average inventory at point in time*



## Core power/flux distribution

- Predicts neutron flux and power profiles at point in time



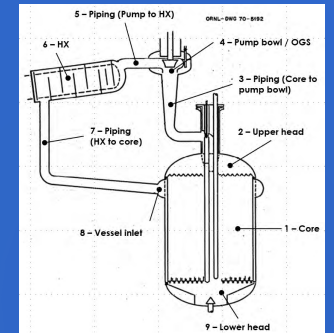
*Consistency assessment on removal rates*



*System-average inventory at point in time*

## Location-dependent inventory in loop

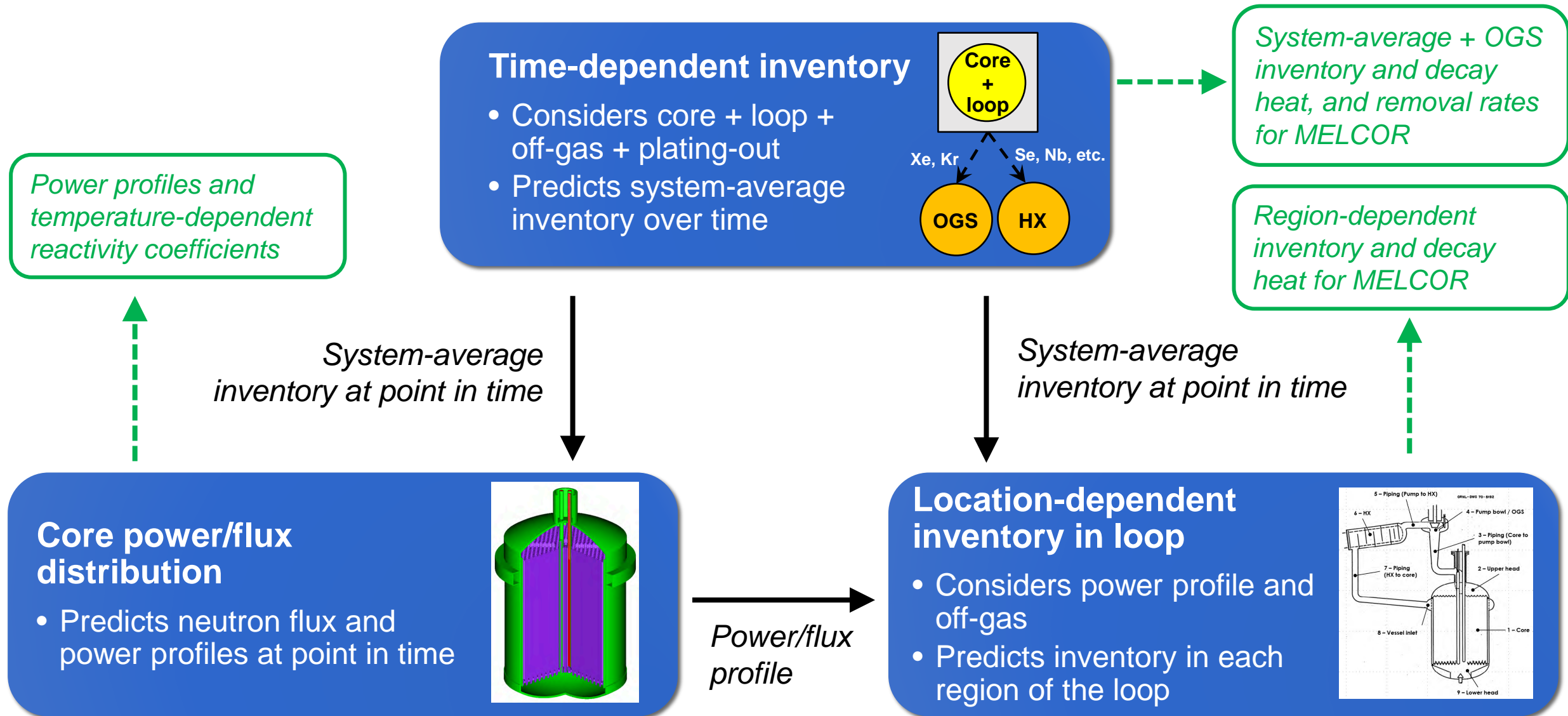
- Considers power profile and off-gas
- Predicts inventory in each region of the loop



*Power/flux profile*



# SCALE analysis approach



# SCALE MSRE full core model



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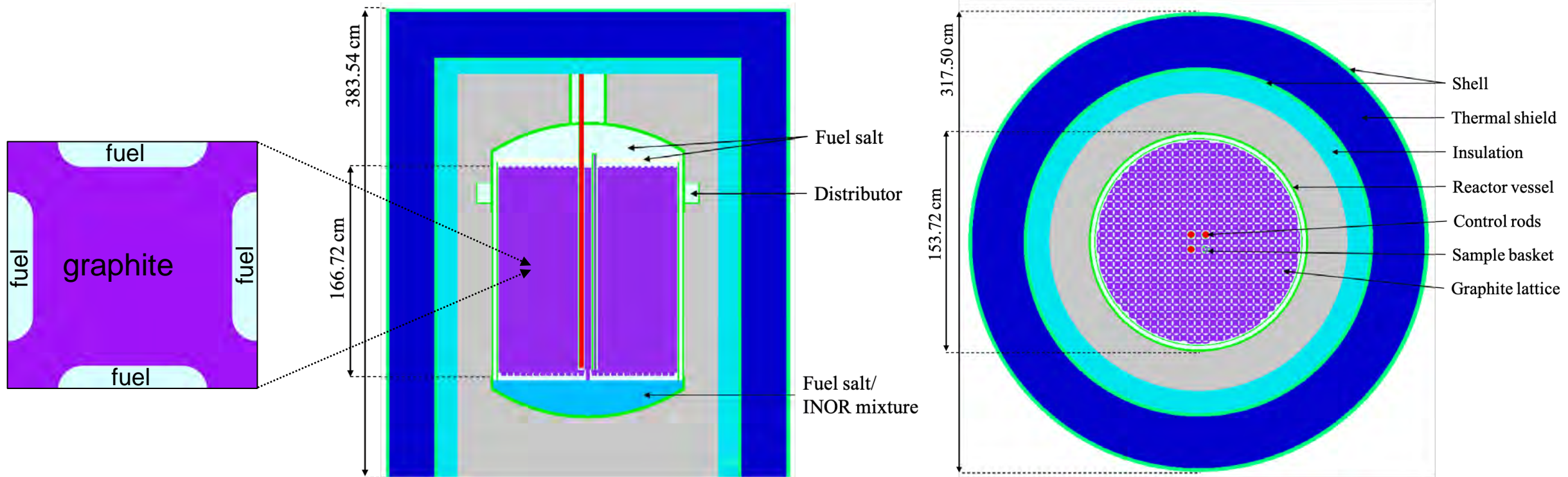
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# MSRE full core model

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



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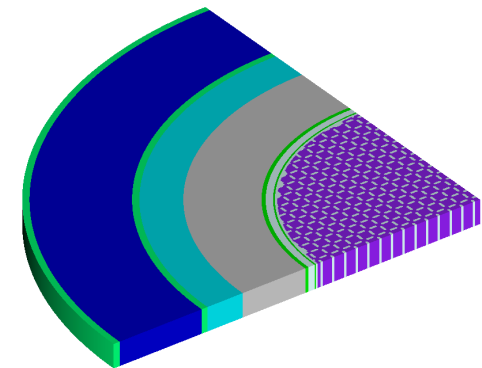
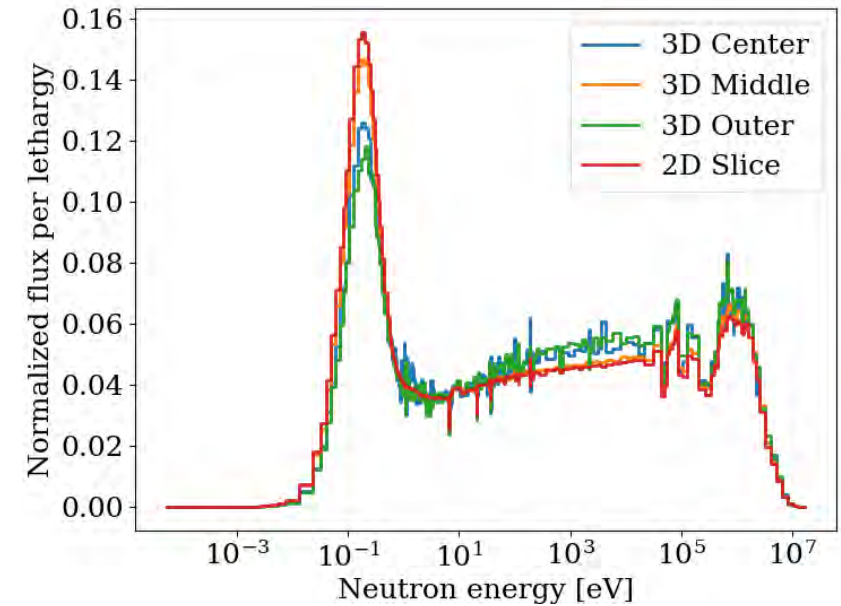


# Time-dependent inventory – model development

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  $^{235}\text{U}$  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”<sup>1,2</sup> (next slide)



**SCALE “2D” slice model**

[1] B. R. Betzler, et 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:

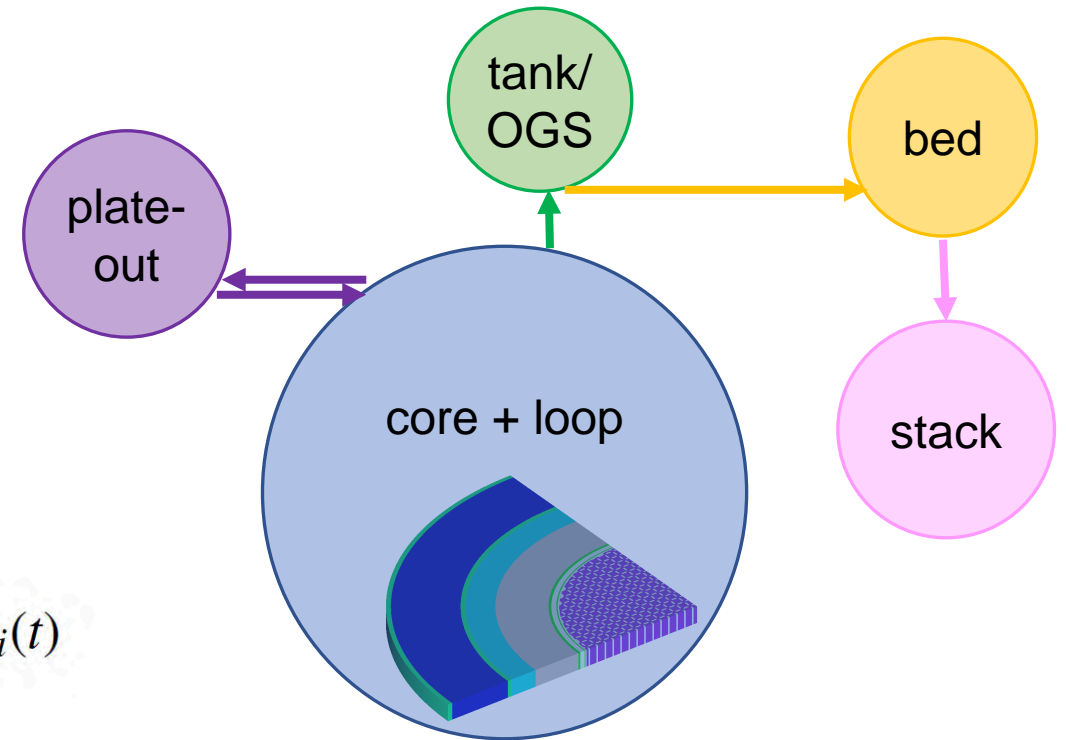
$$\frac{dN_i}{dt} = \sum_{j \neq i} (l_{ij}\lambda_j + f_{ij}\sigma_j\Phi)N_j(t) - (\lambda_i + \lambda_{i,rem} + \sigma_i\Phi)N_i(t) + S_i(t)$$

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  $i$



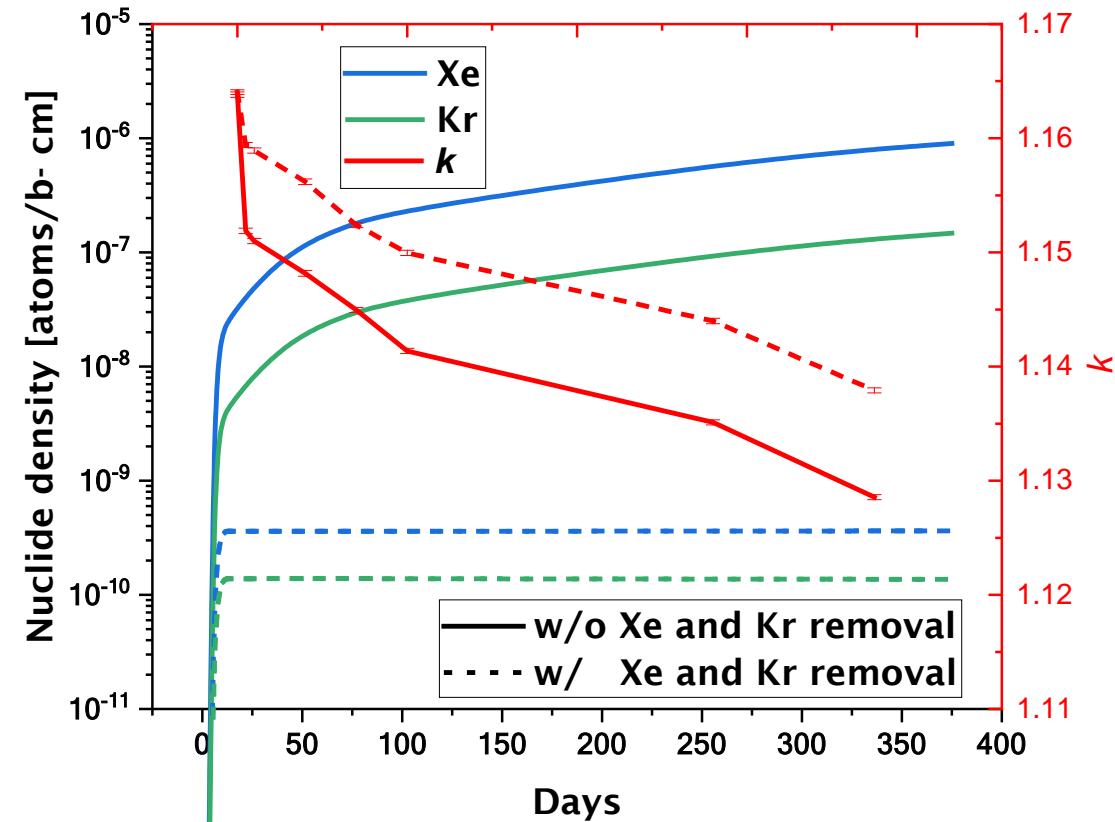
# Time-dependent inventory – nuclide removal

- Noble gas removal in the off-gas system:
  - Main experimental basis is the xenon poison fraction (ratio of absorption by  $^{135}\text{Xe}$  to absorption by  $^{235}\text{U}$ ), 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  $1.88 \cdot 10^{13}$  n/cm<sup>2</sup>-s
- No re-fueling in this depletion calculation
- At 375 days:
  - 5.627% <sup>235</sup>U consumed,
  - 0.455% <sup>238</sup>U consumed,
  - 13.76 GWd/tHM burnup achieved

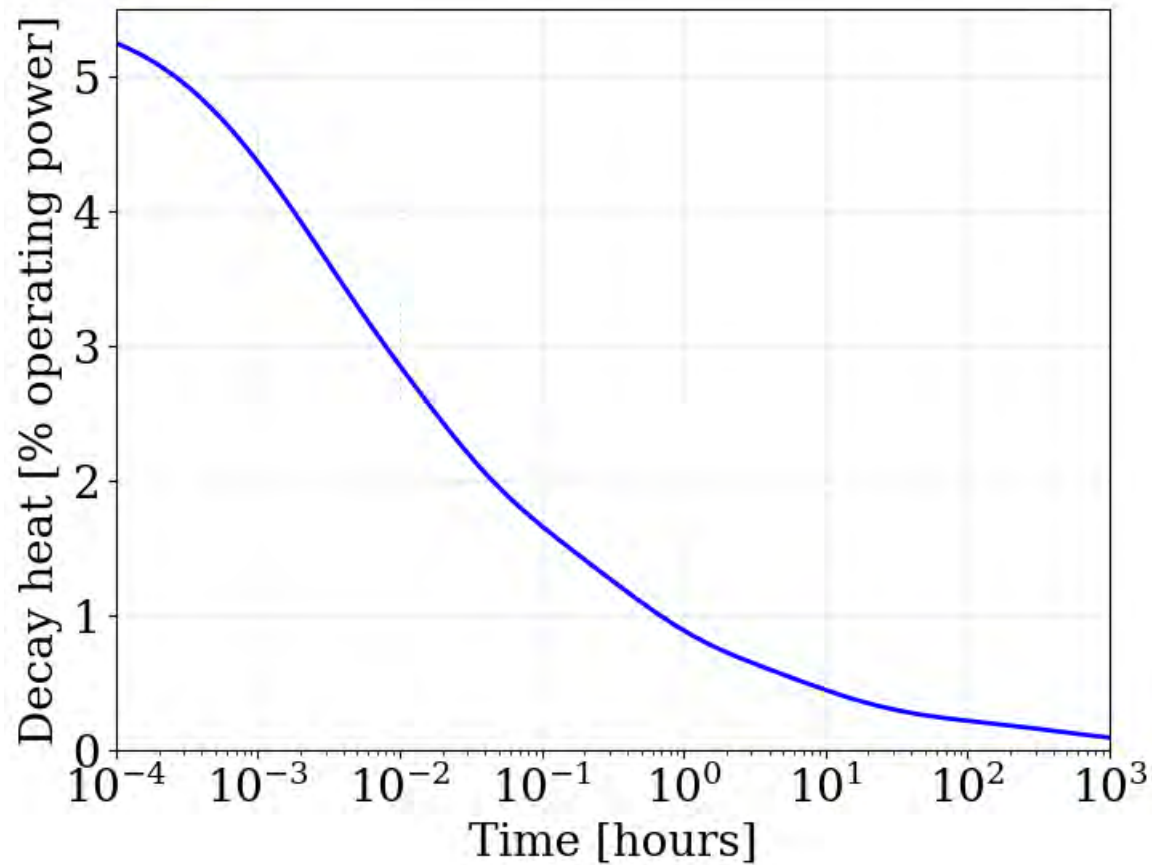
	Amount removed after 375 days
Noble gas (Xe + Kr)	0.170 kg / 30.6 L
Insoluble metals (Mo + Tc + Ru + Rh + Pd + Ag + Sb)	0.611 kg
Sometimes soluble metals (Se + Nb + Te)	0.057 kg



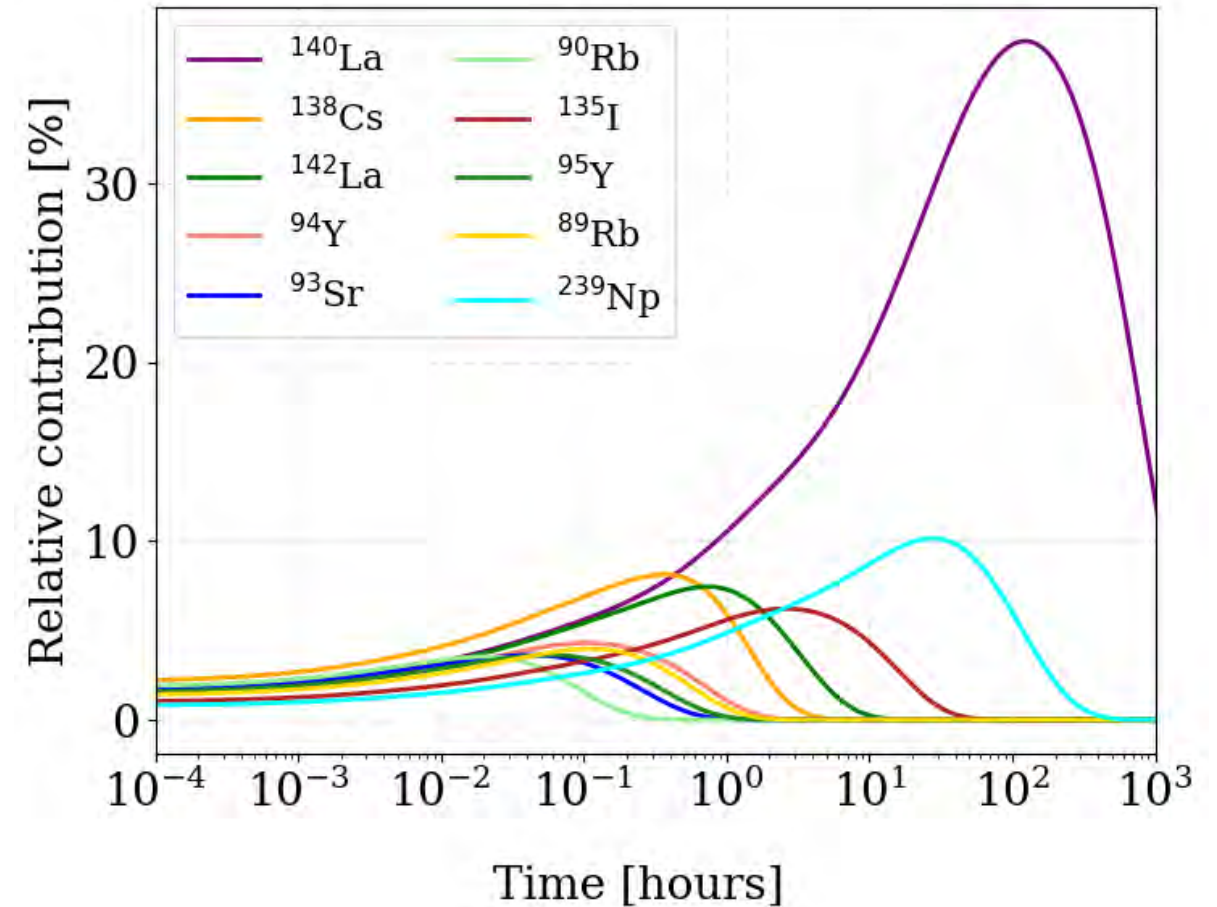
**Comparison of Xe and Kr nuclide densities with and without Xe/Kr removal**

# Decay heat after shutdown at 375 days

System decay heat [% operating power]

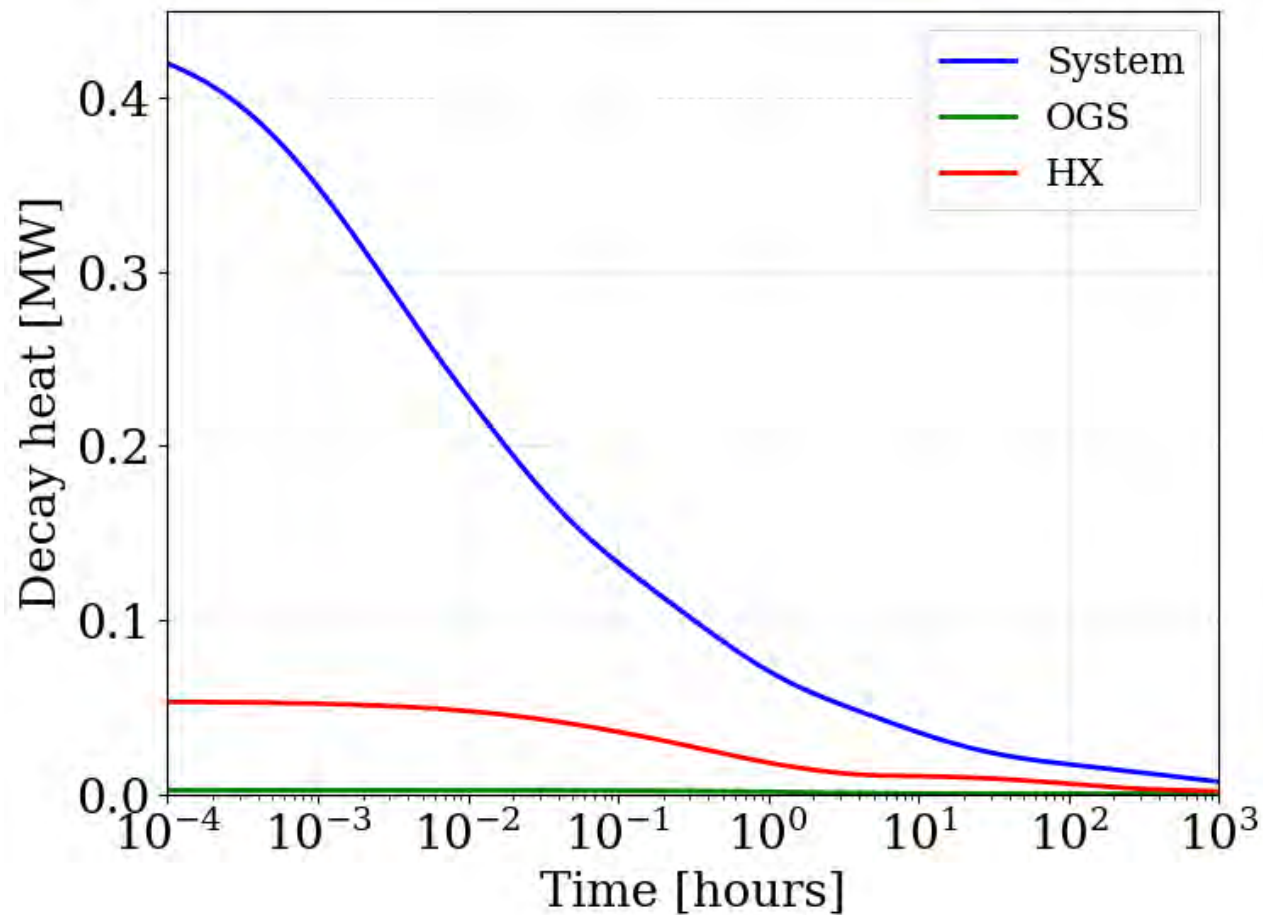


Top contributors

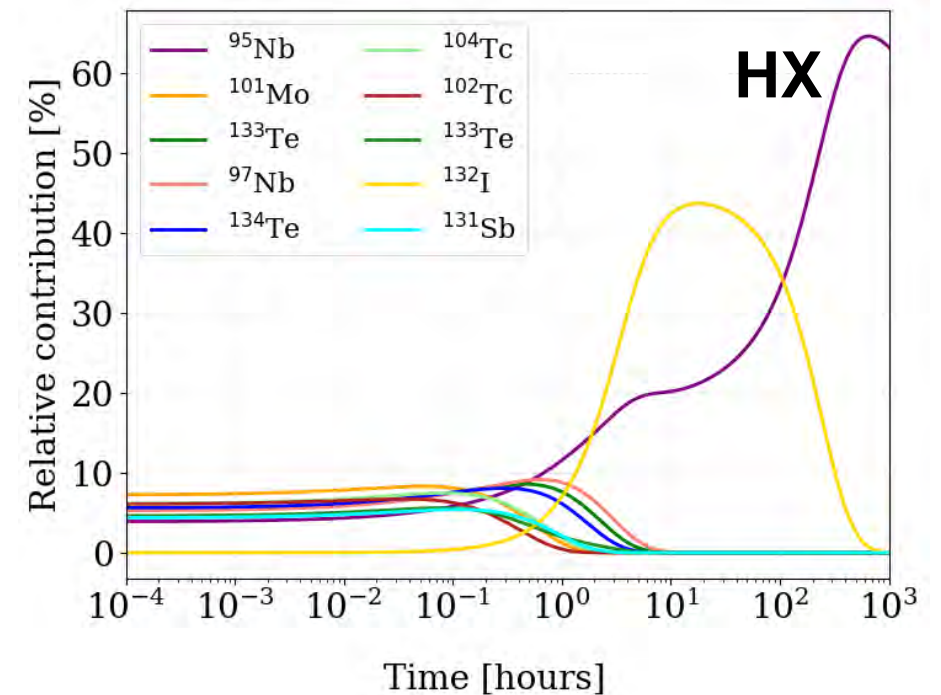
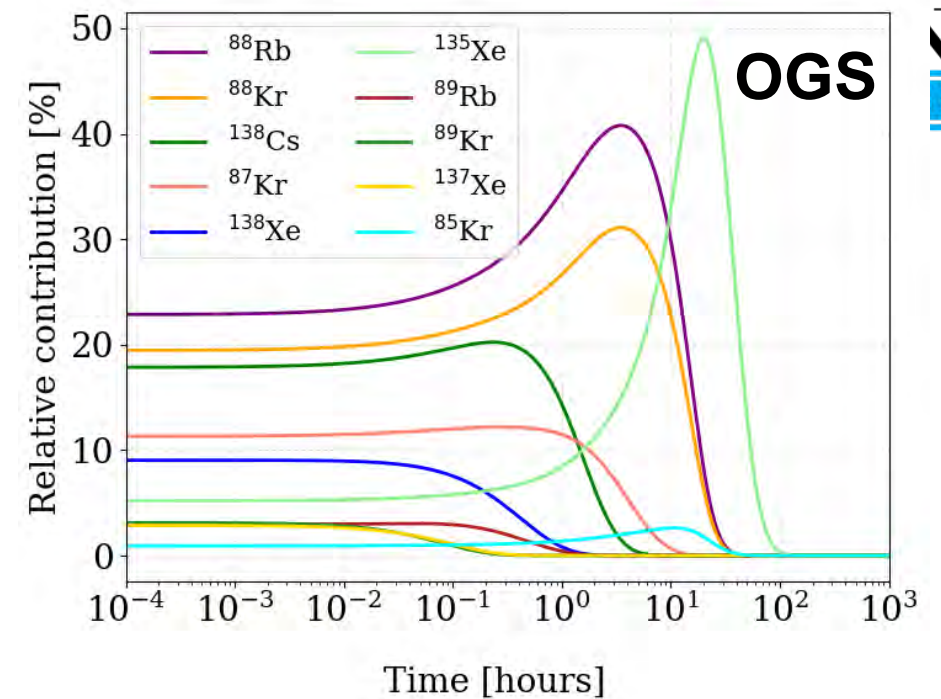




# Decay heat after shutdown at 375 days

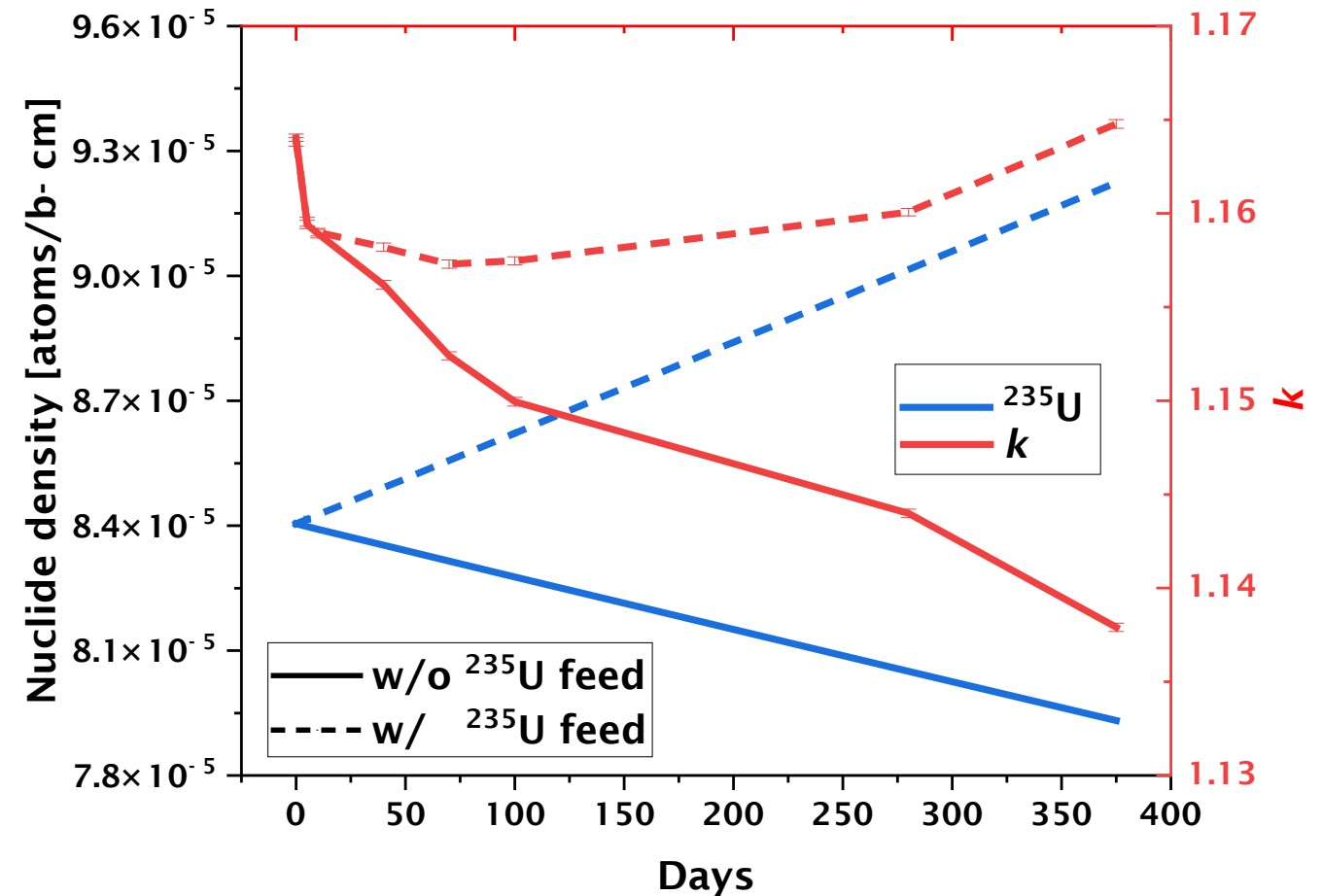


MSRE operating power: 8 MWth



# Demonstration of continuous feed / refueling

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



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

# Core power/flux distribution



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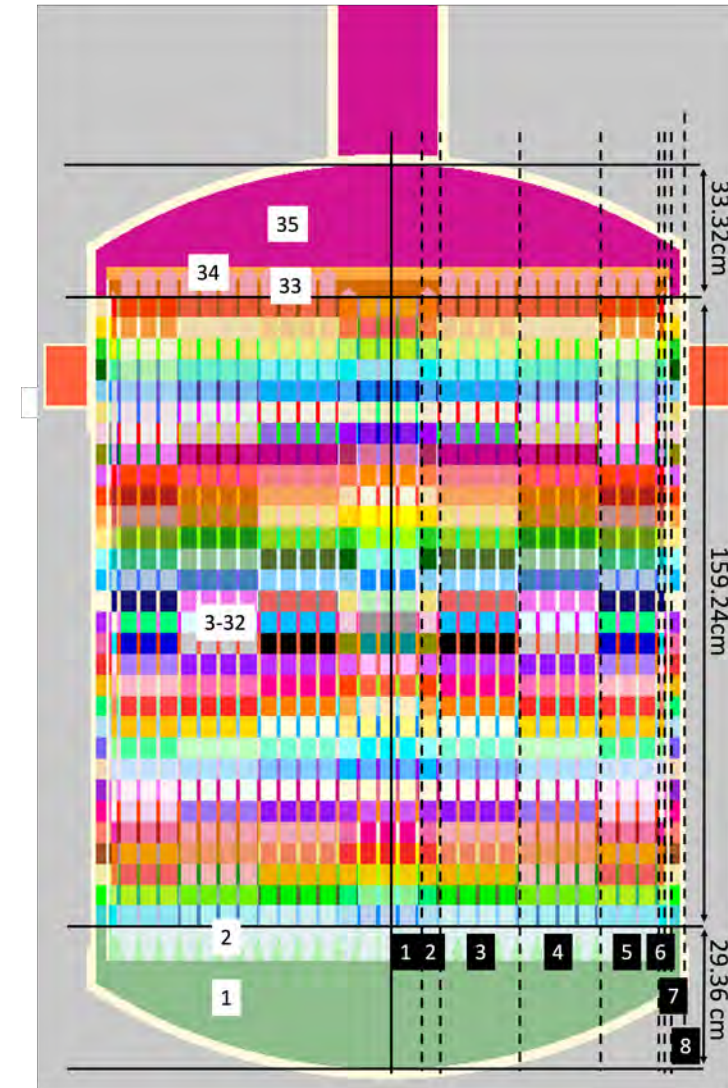
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# Core power/flux distribution – model development

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

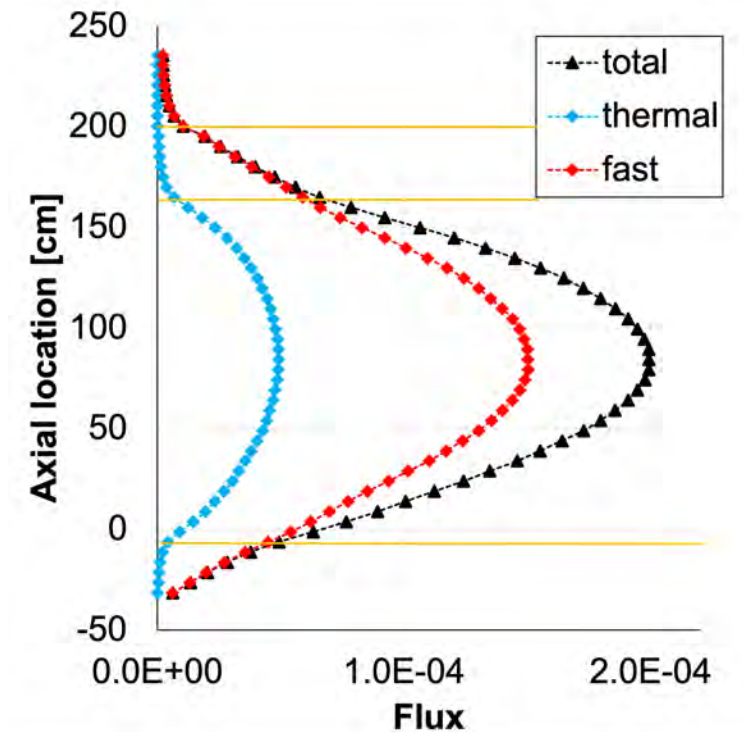
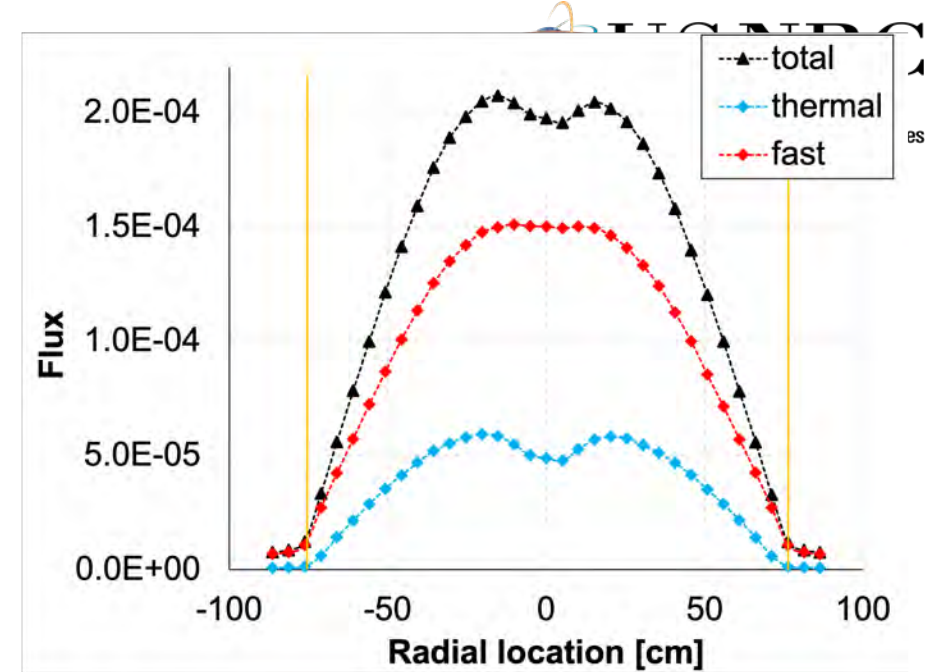
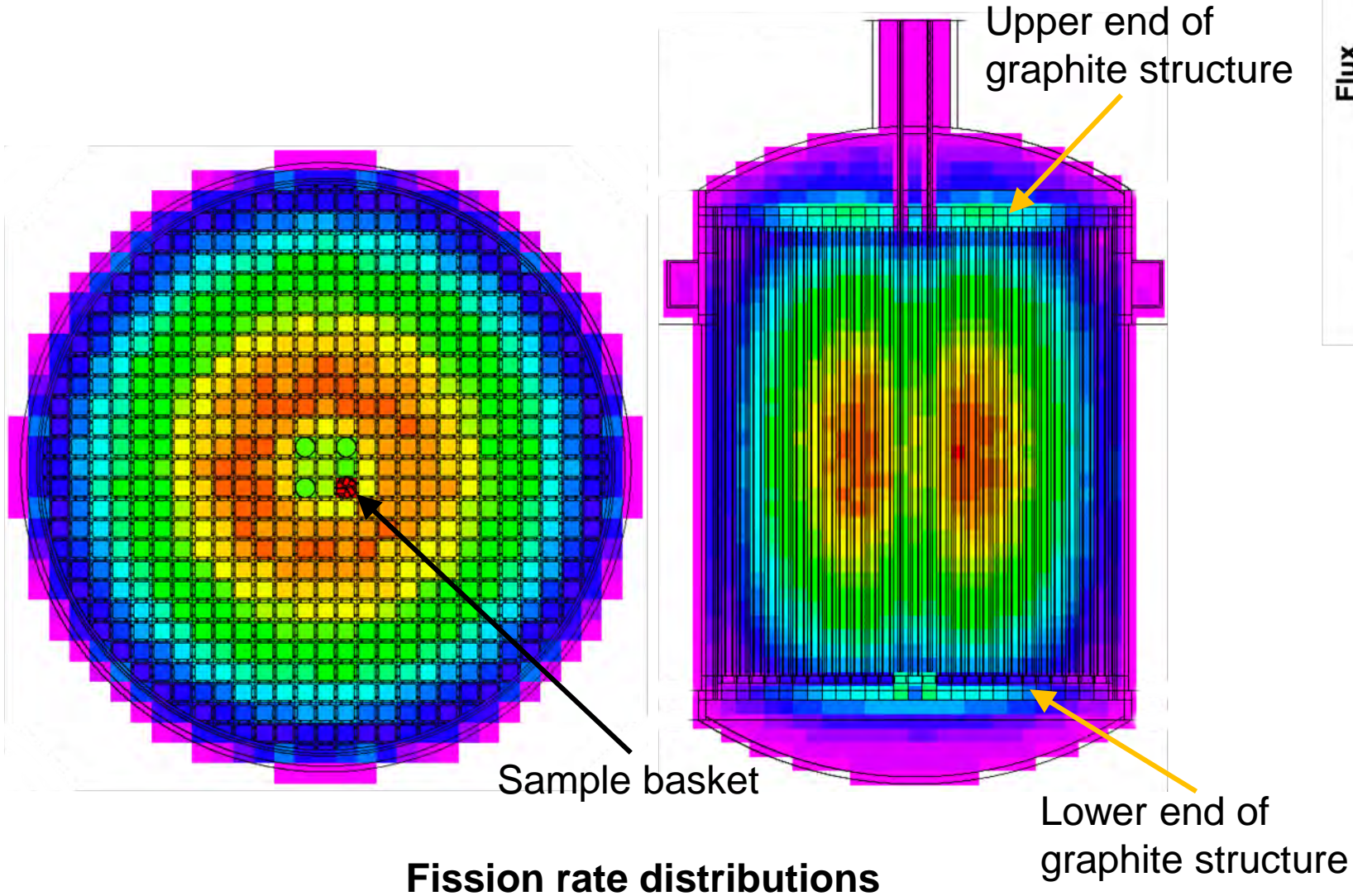
Discretized model uses 34 axial and 8 radial zones



Discretized model

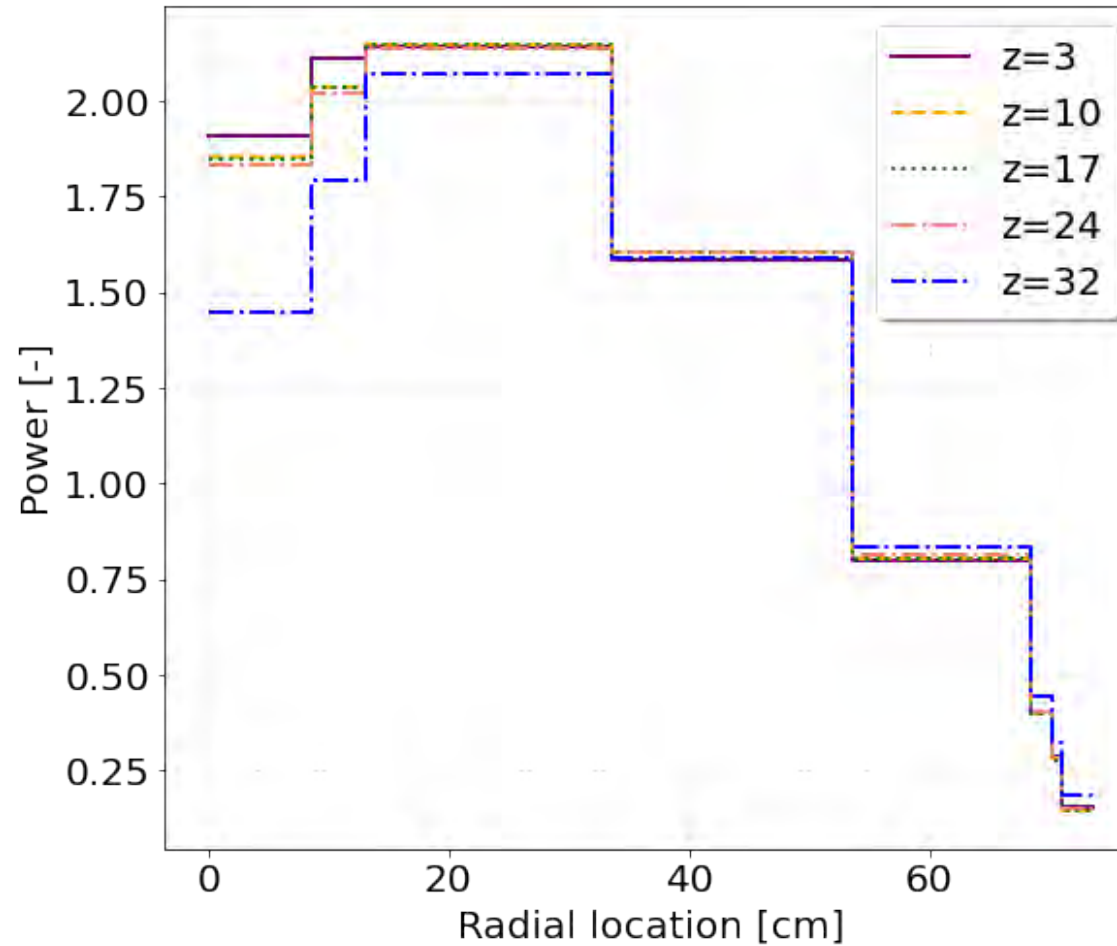


# Core power/flux distribution – fission rate and flux



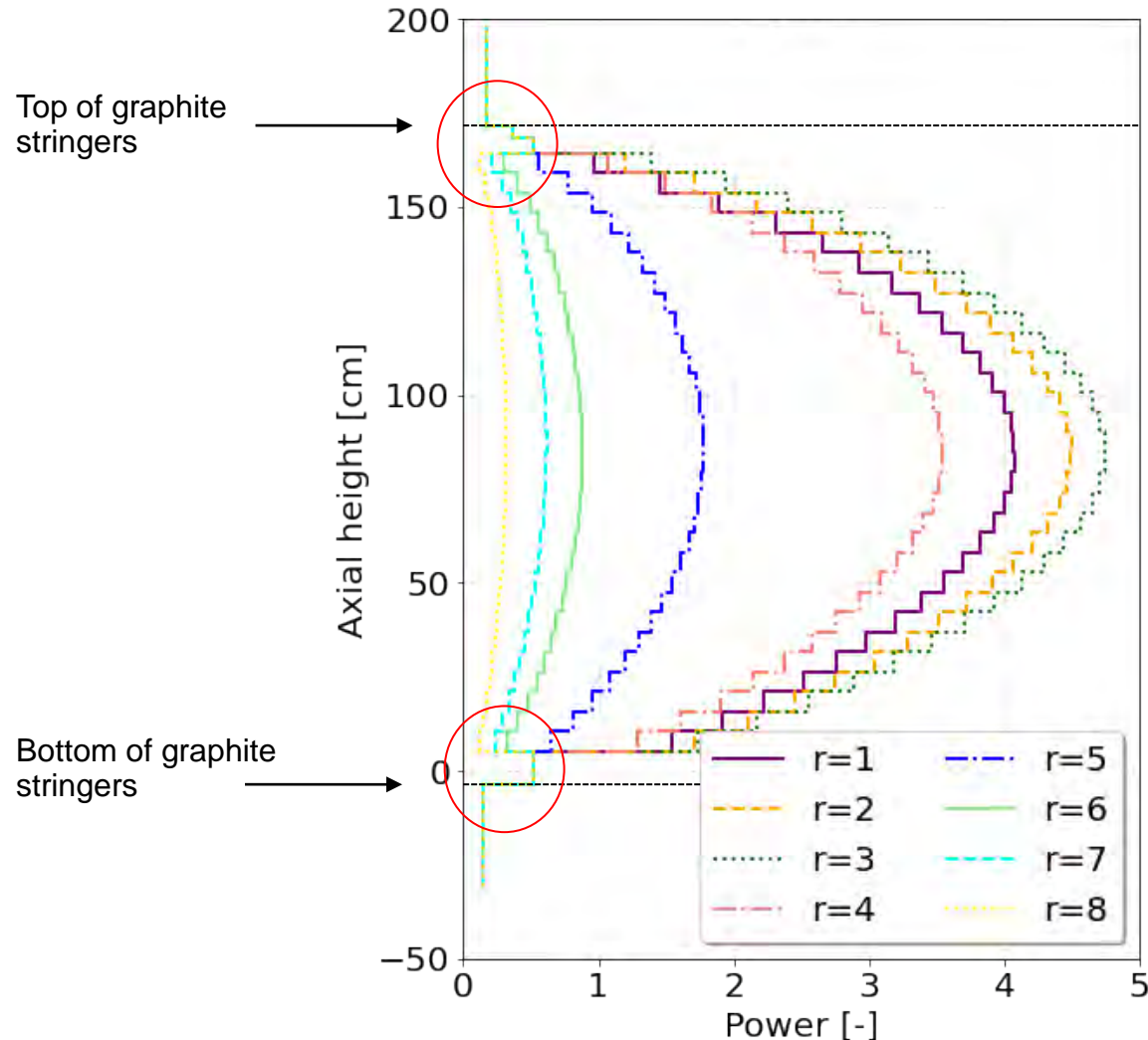


# Core power/flux distribution – power

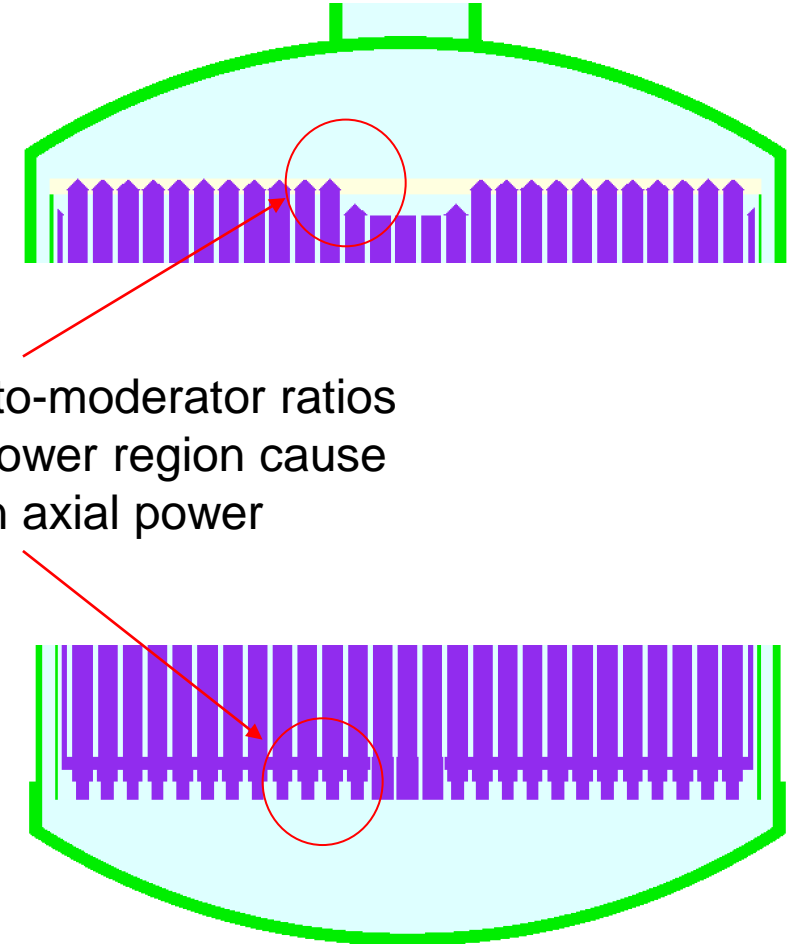


Normalized radial power

# Core power/flux distribution – power



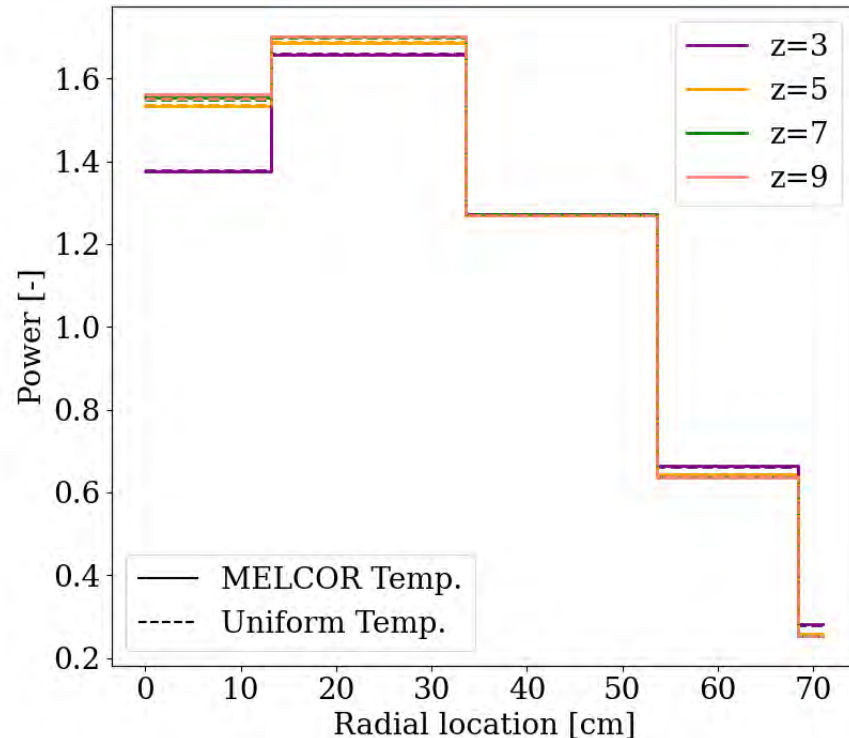
Different fuel-to-moderator ratios in upper and lower region cause small peaks in axial power



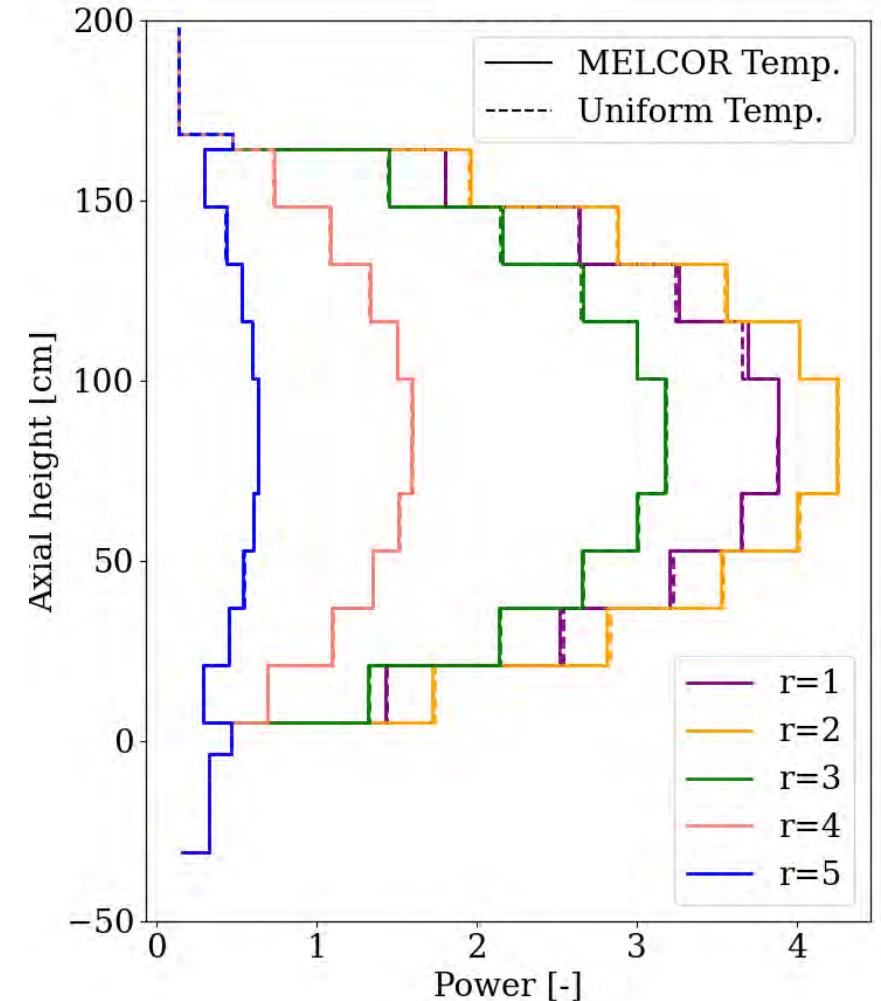
# Core power/flux distribution – power

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**



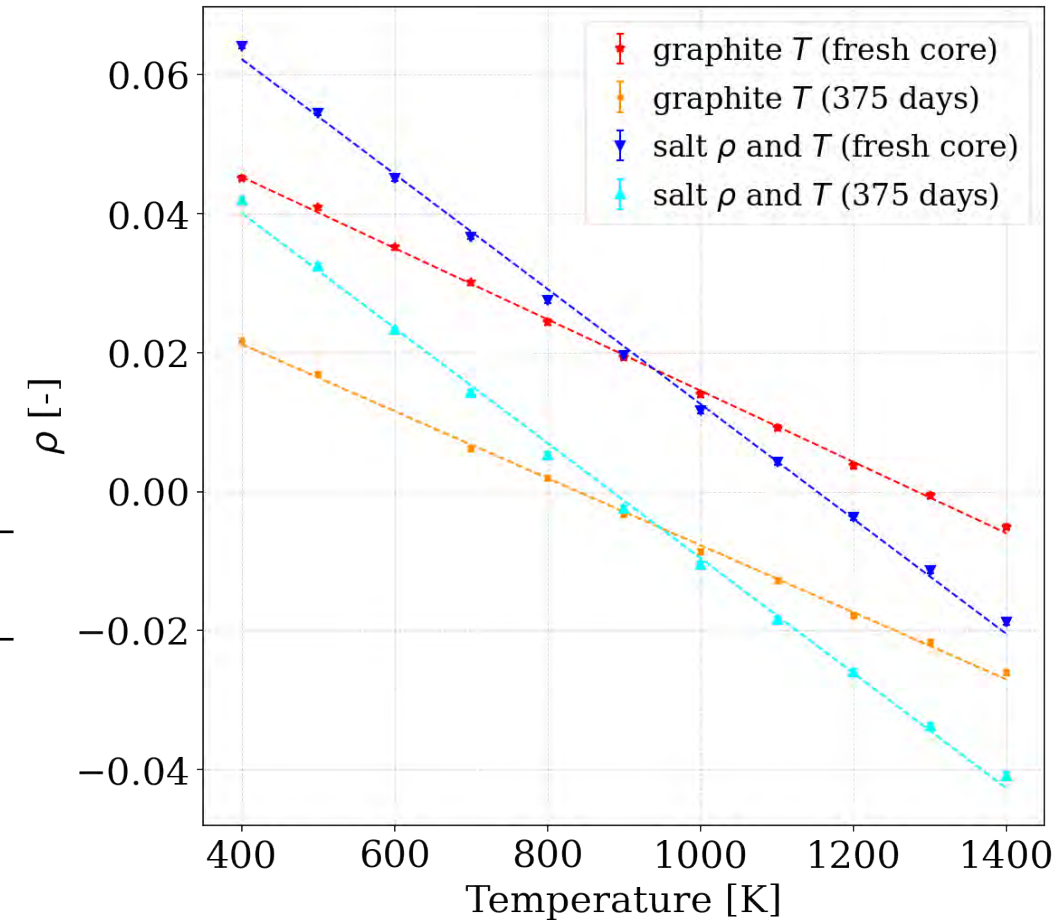
**Normalized axial power profile**

# 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
$\beta_{eff}$ [pcm]	$704 \pm 14$	$697 \pm 22$
Graphite temperature reactivity coefficient [pcm/K]	$-5.13 \pm 0.05$	$-4.83 \pm 0.07$
Fuel salt temperature <i>and density</i> reactivity coefficient [pcm/K]	$-8.27 \pm 0.12$	$-8.28 \pm 0.12$



# Location-dependent inventory in loop



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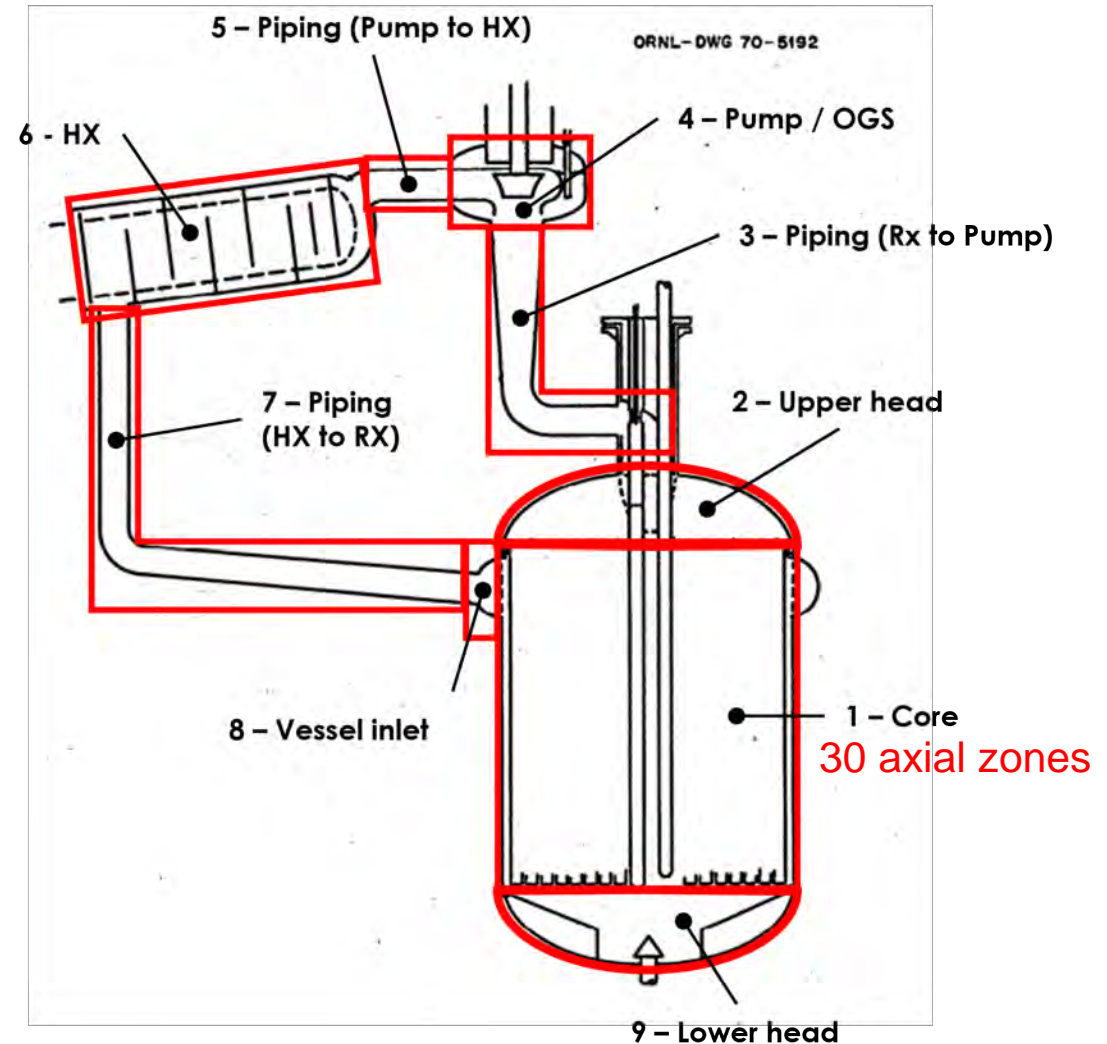
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# Location dependent inventory – model development

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



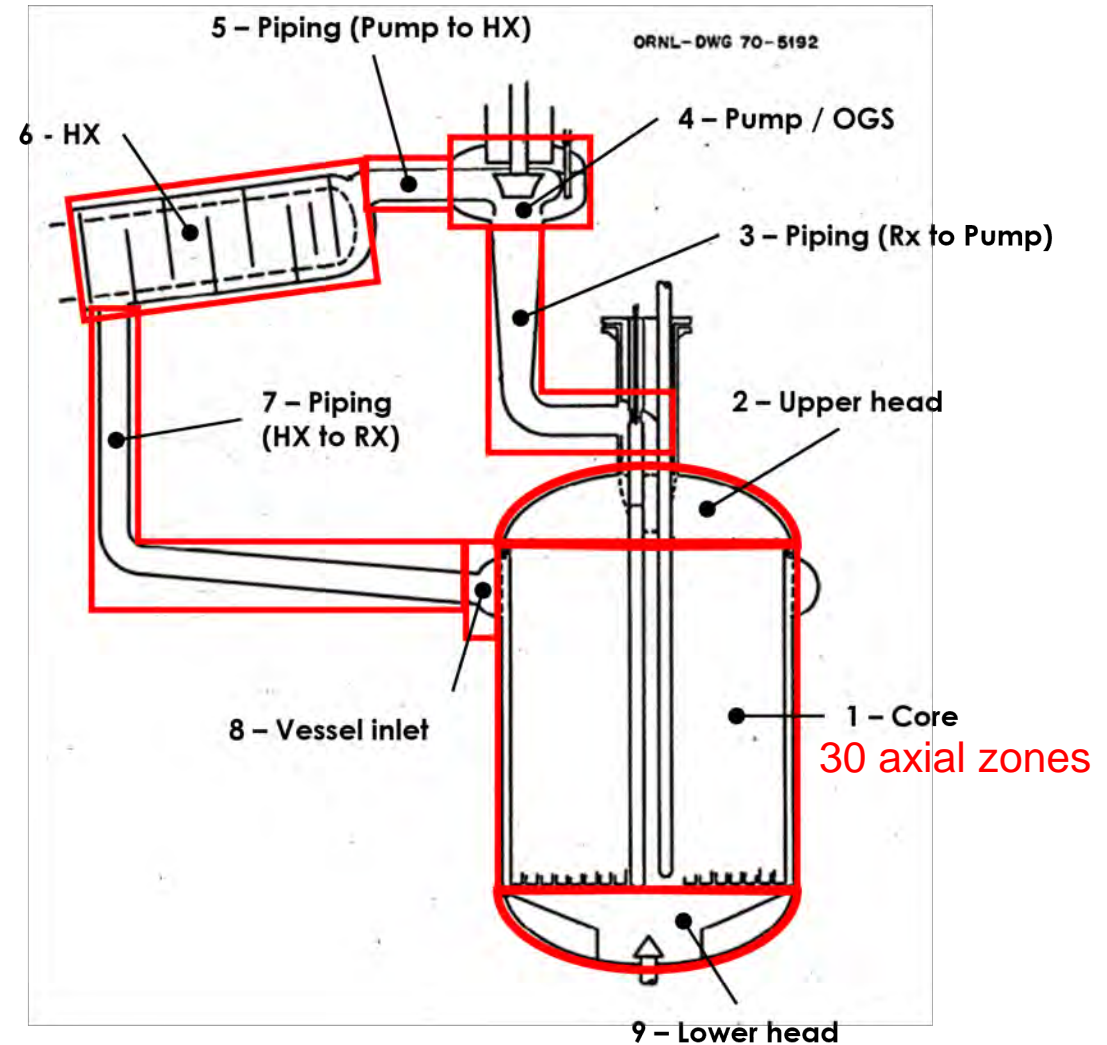
Regions in MSRE system for  
ORIGEN model

# 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)

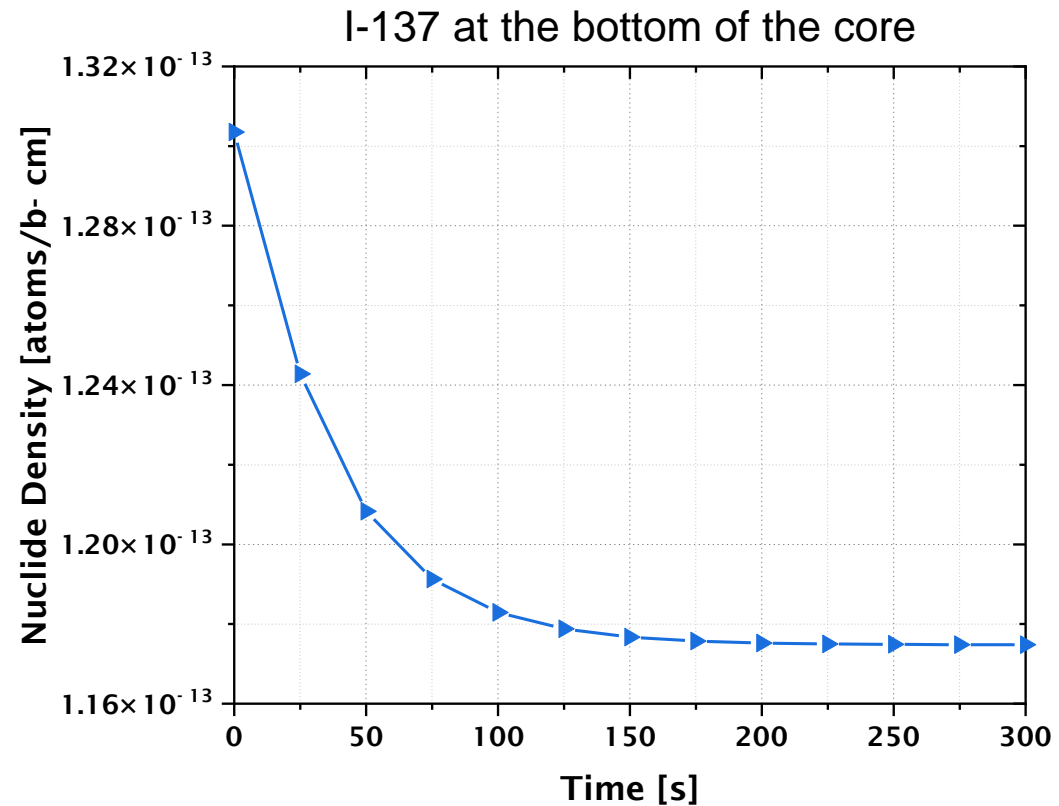
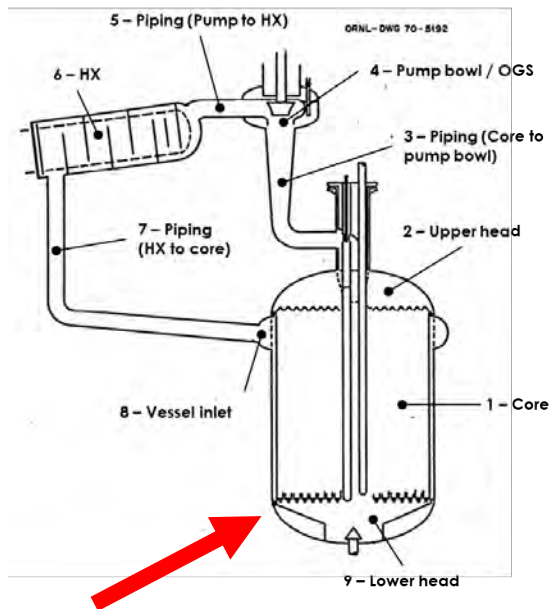


Regions in MSRE system for  
ORIGIN model

# Location dependent inventory analysis example

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

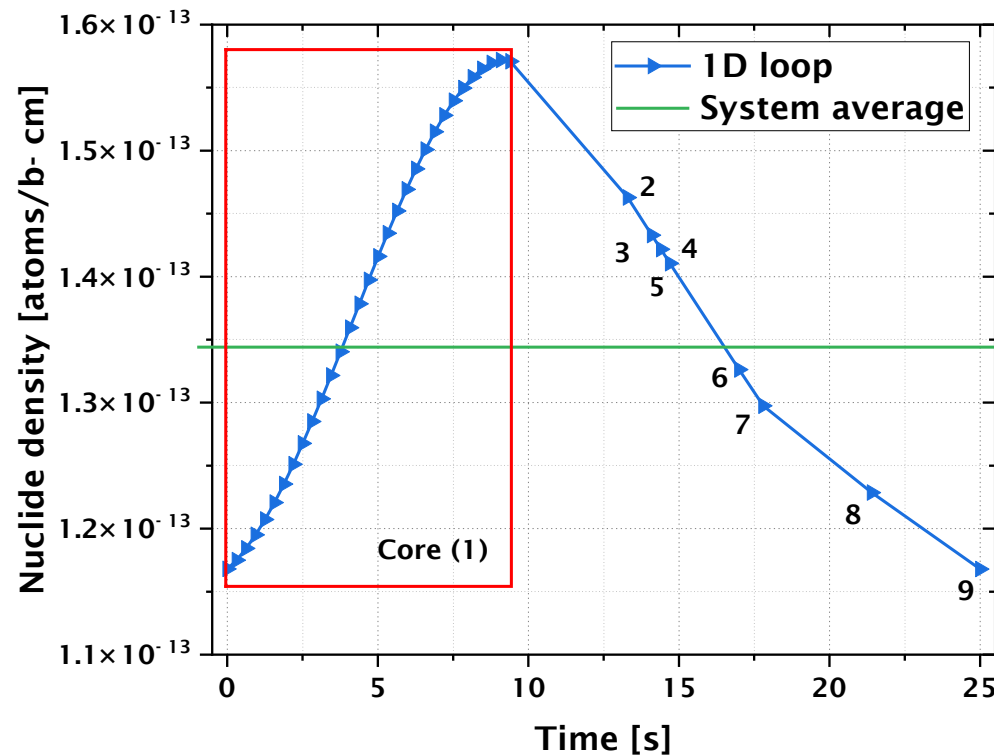
Example: Short-lived nuclide (I-137,  $t_{1/2}=24.5\text{s}$ ) as a function of time at the bottom of the core



# 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

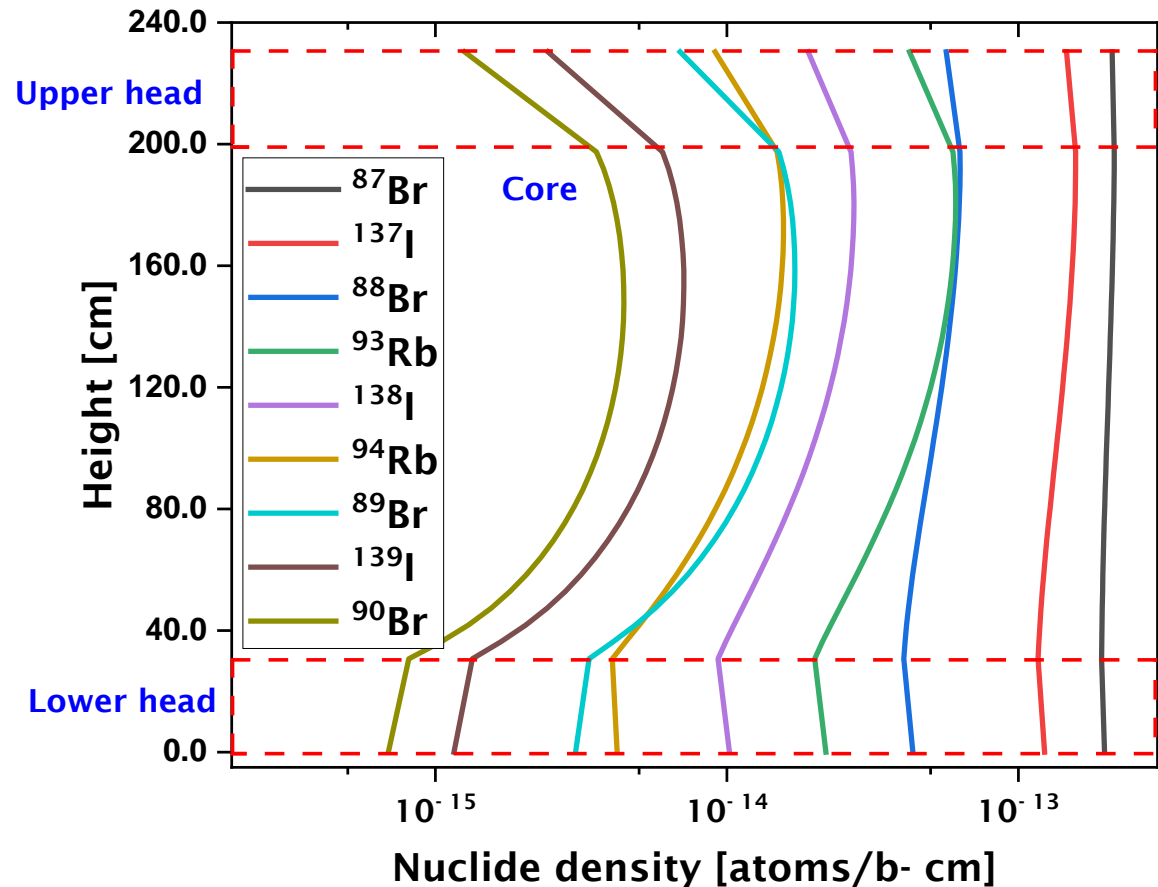
Example: Short-lived nuclide (I-137,  $t_{1/2}=24.5\text{s}$ )  
as a function of location  
in the loop



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  $\beta_{eff} \sim 700$  pcm without drift
  - $\beta_{eff}$  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

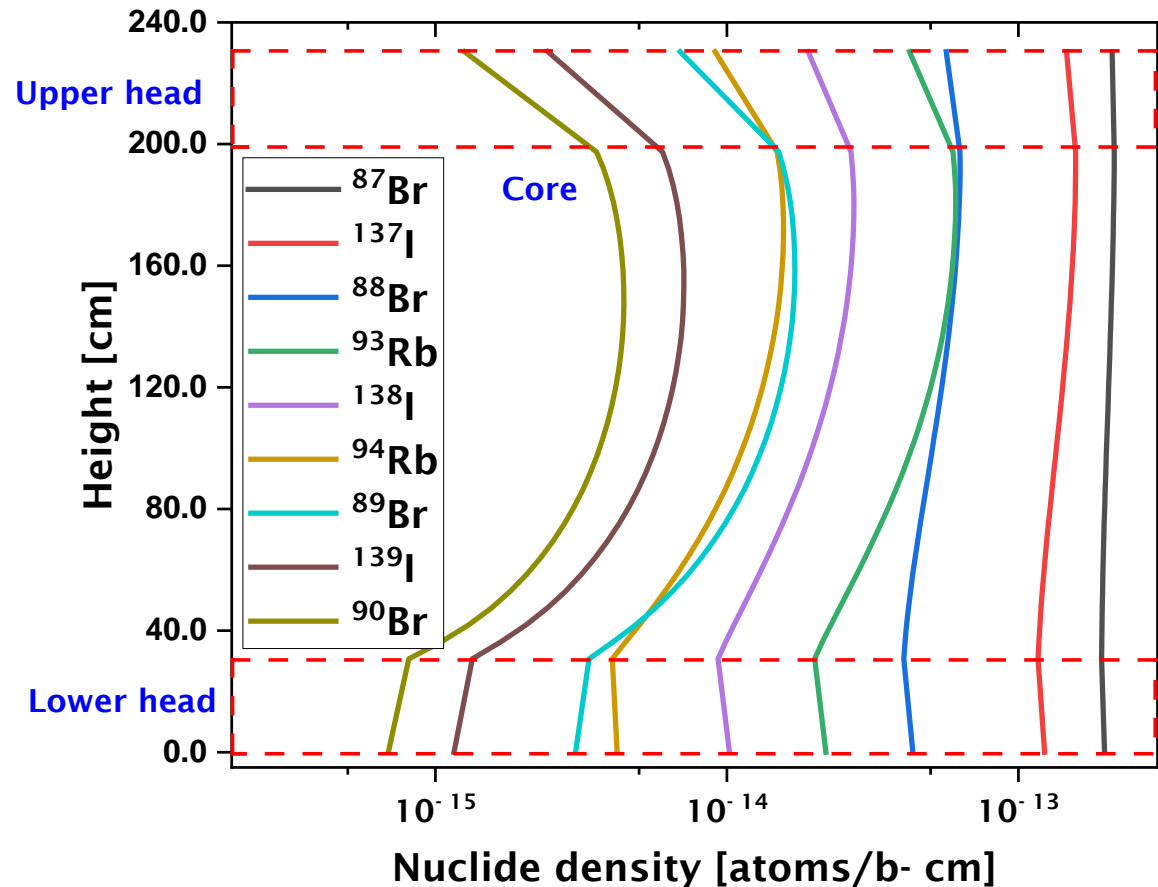


Selected delayed neutron precursors  
calculated by ORIGEN



# 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



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# 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



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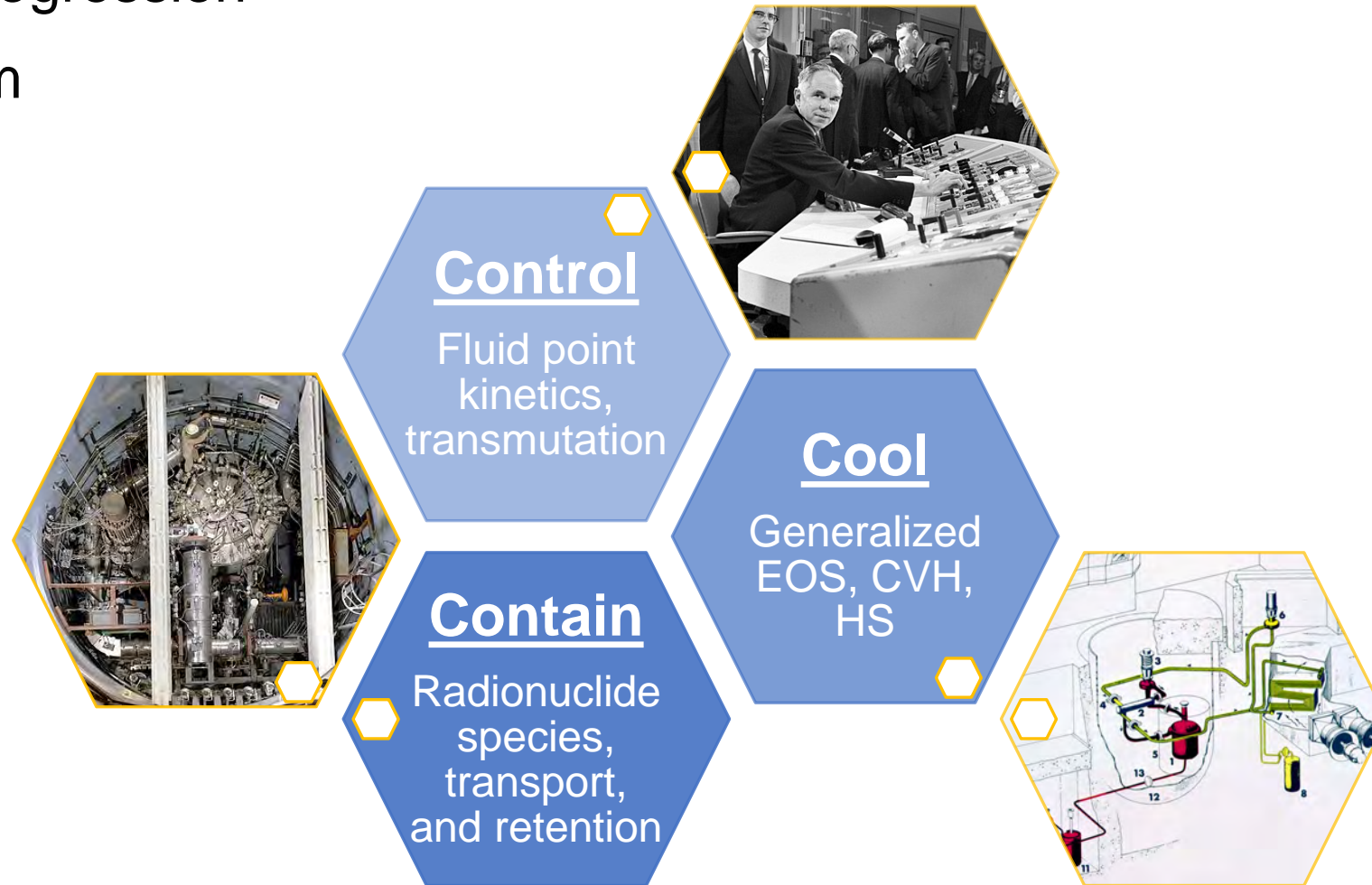


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# Molten Salt Reactor Modeling

## 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

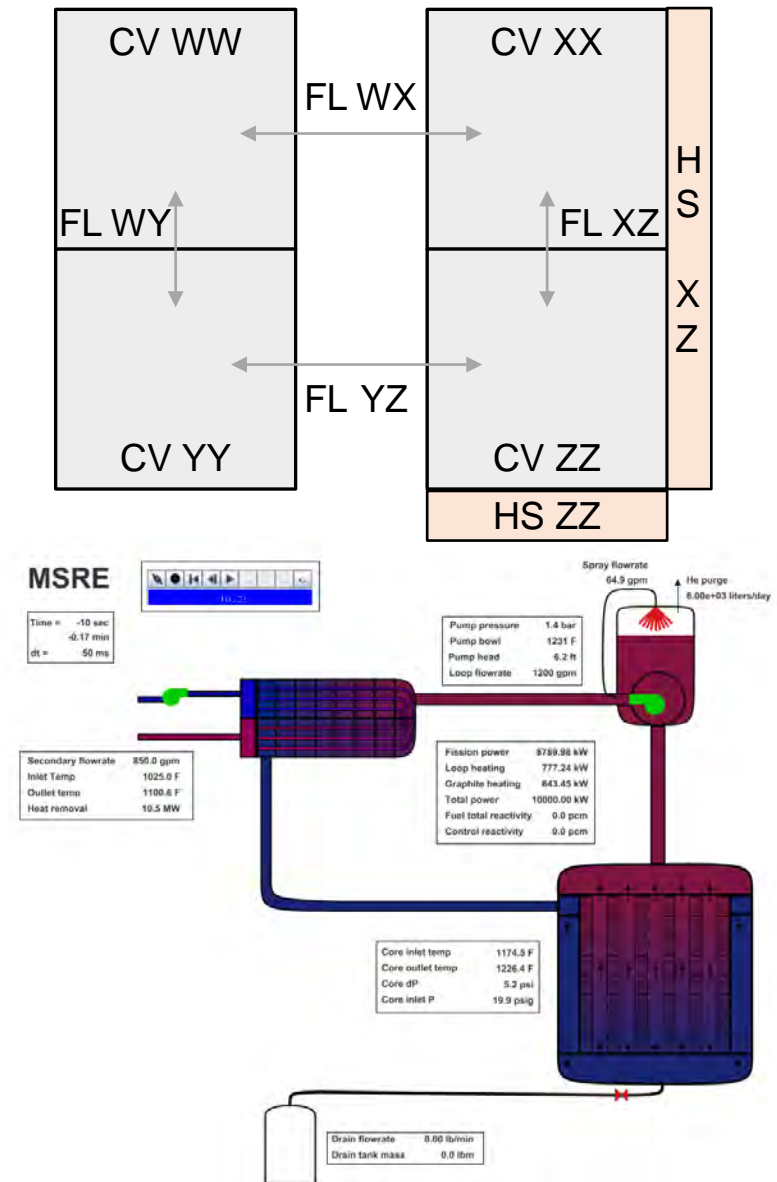
- Leverage existing thermal hydraulics modeling in MELCOR
- Utilize fundamental *two-phase* thermal hydraulic equations
- Introduce new thermo-physical properties and phase diagram of fluid specific to FLiBe
  - Generalized EOS – Equations of state for multiple working fluids are presently available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

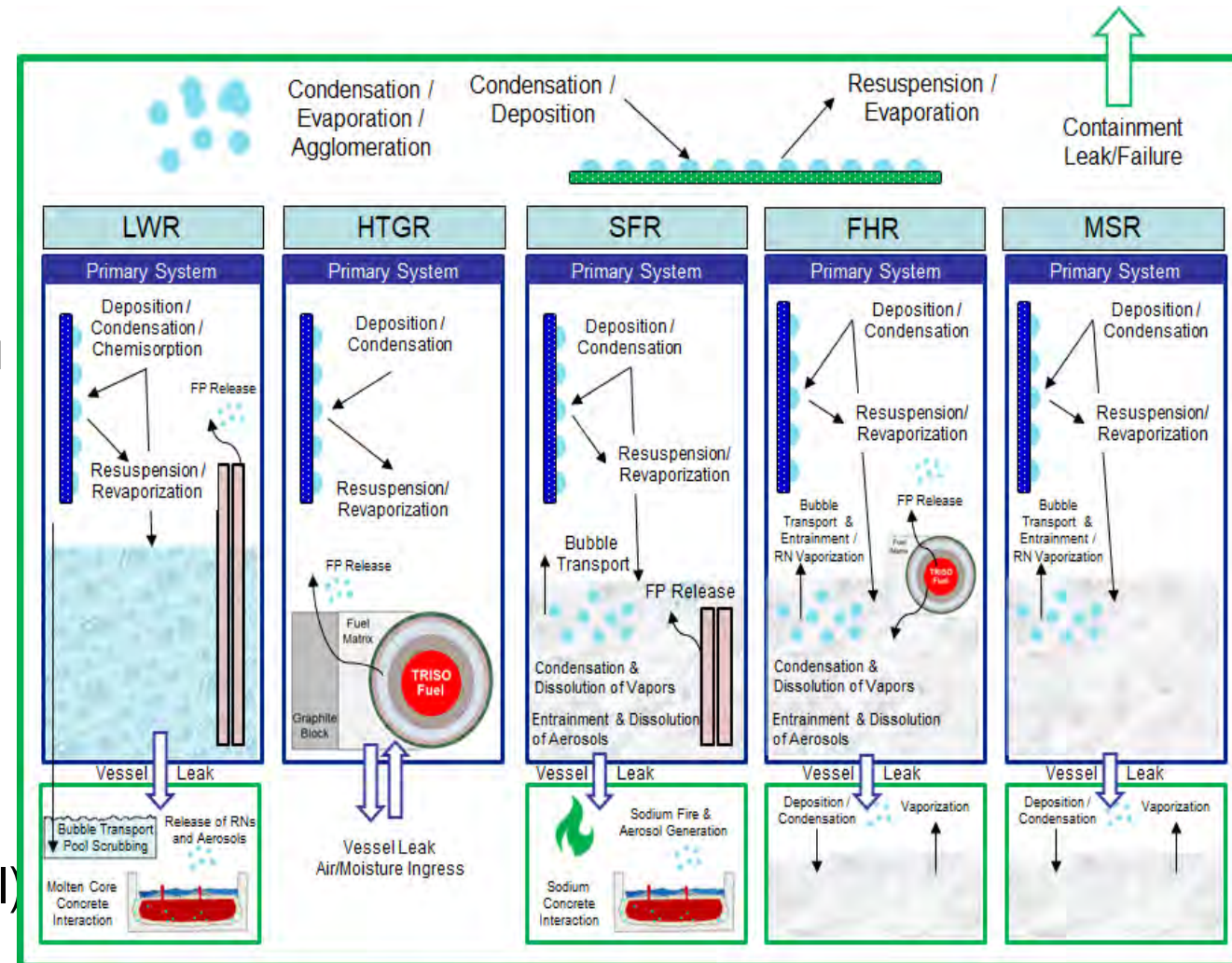
Molten salt serves as a potential means of fission product retention

## 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

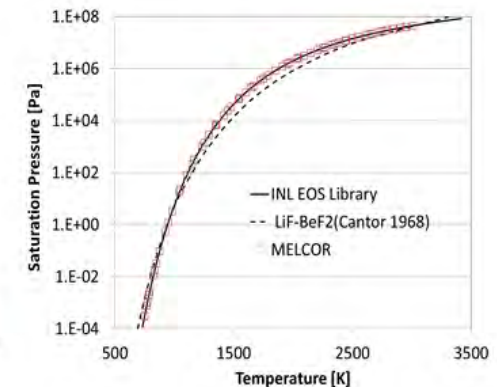
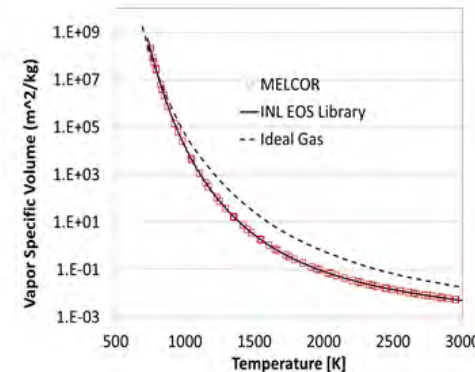
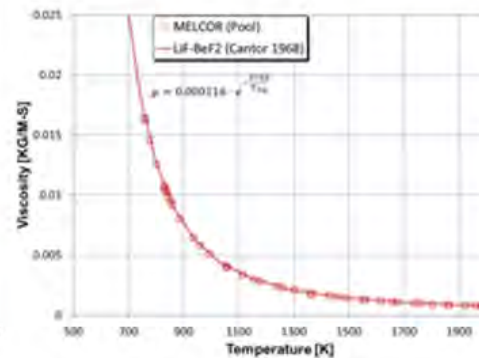
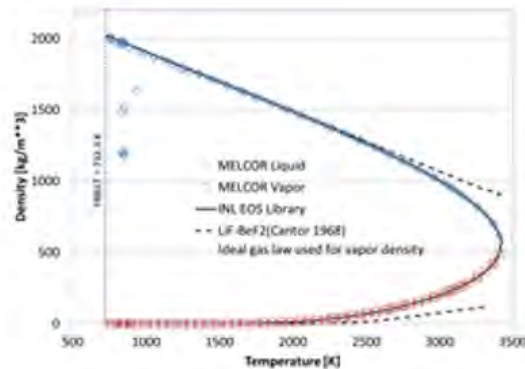
- Generalized Radionuclide Transport and Retention (GRTR) modeling framework
- Molten salt chemistry and physics pertaining to radionuclide transport
- GRTR for MSRs but generalized and applicable to other systems (e.g., liquid metal)



# 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)



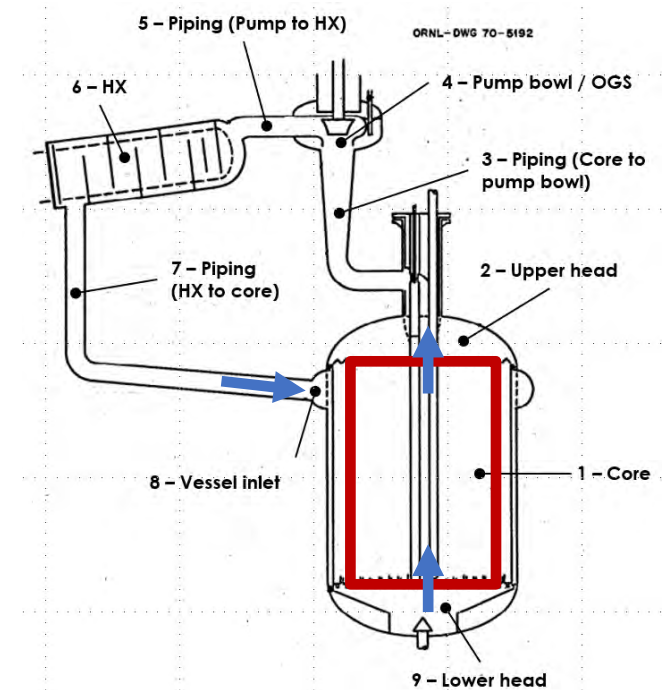
# Fluid Core and Power Distribution

Fluid fuel core defined within the graphite stringers

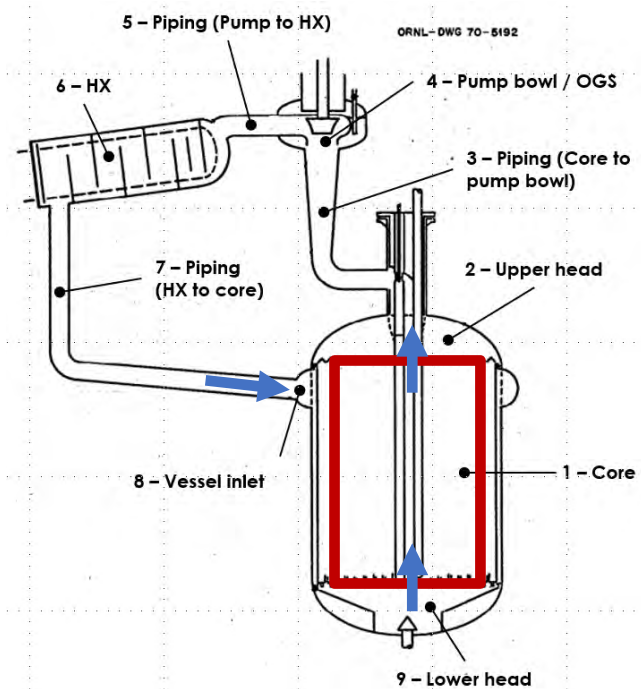
- The fluid volume within the graphite stringers comprise the active “Core”
- “Loop” volumes comprise a portion of the primary fuel flow loop OUTSIDE the active core
- Allows specification of the axial and radial power distribution from SCALE
  - Feedbacks and power governed by flowing fluid fuel point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

- 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

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

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

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

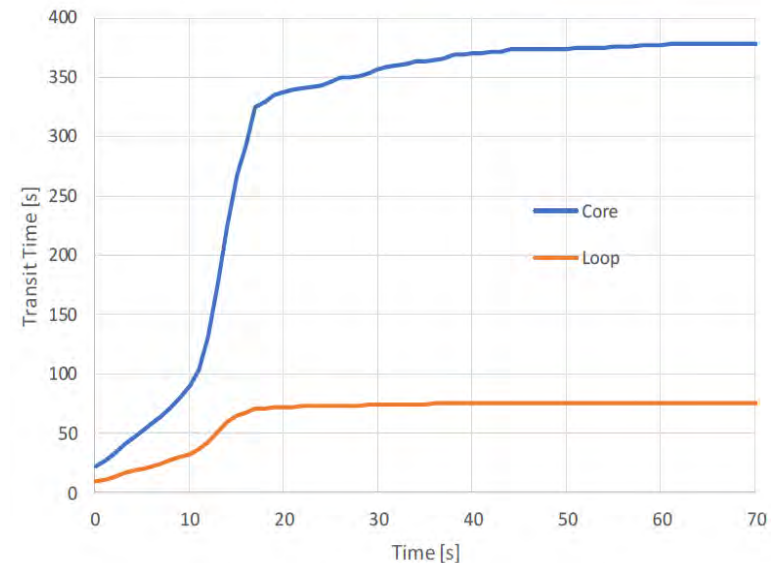
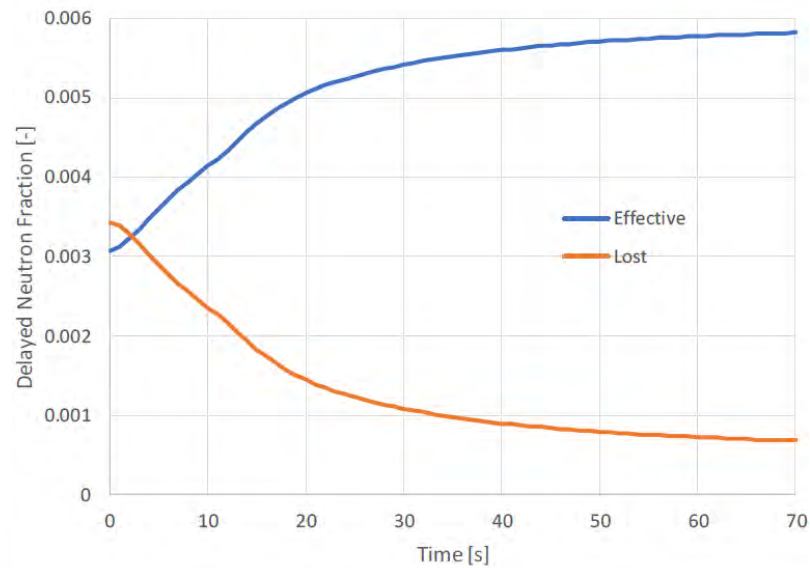
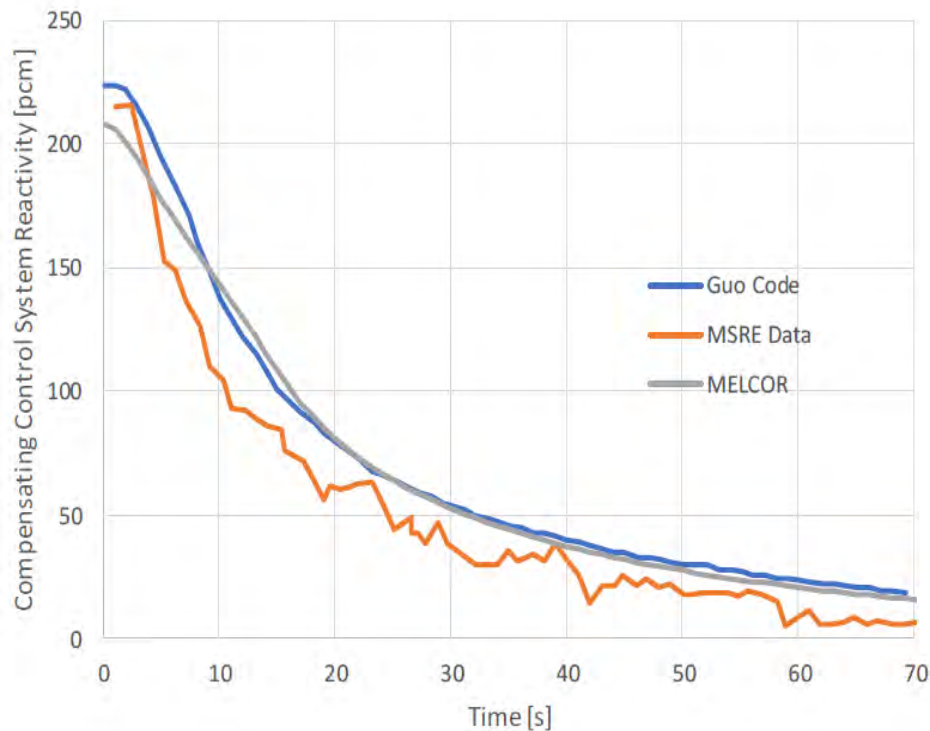
$$\bar{\beta} = \beta - \left( \frac{\Lambda}{P(t)} \right) \sum_{i=1}^6 \lambda_i C_i^L(t)$$

# 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

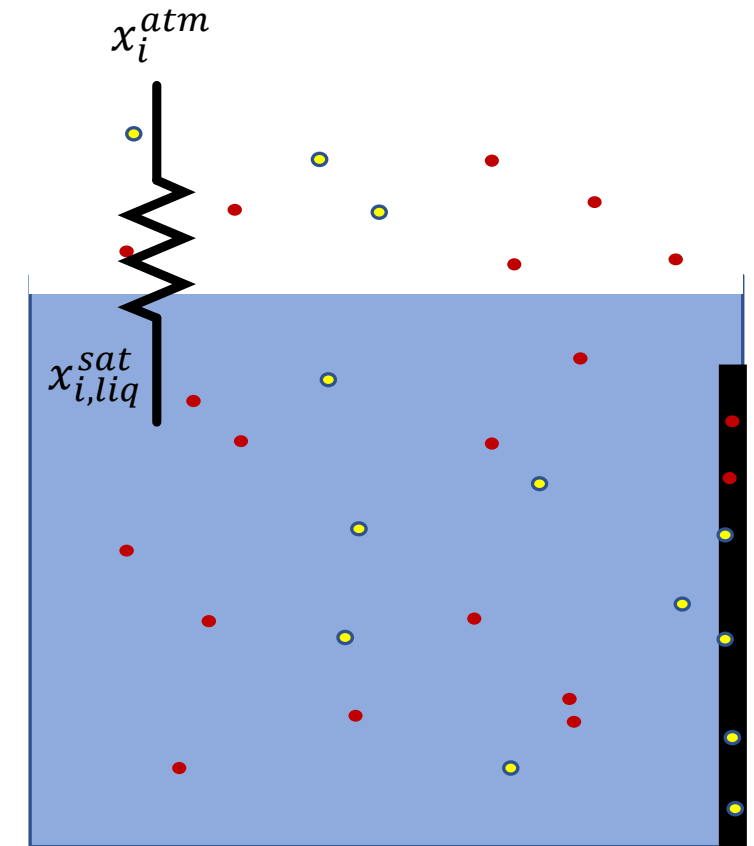
Track where fission products are and how much is released from liquid to atmosphere

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

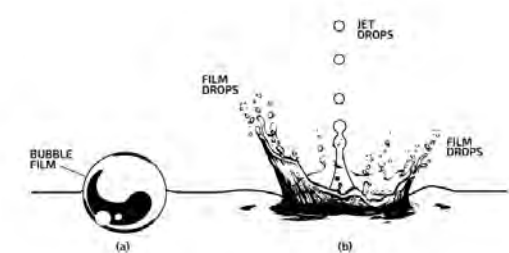
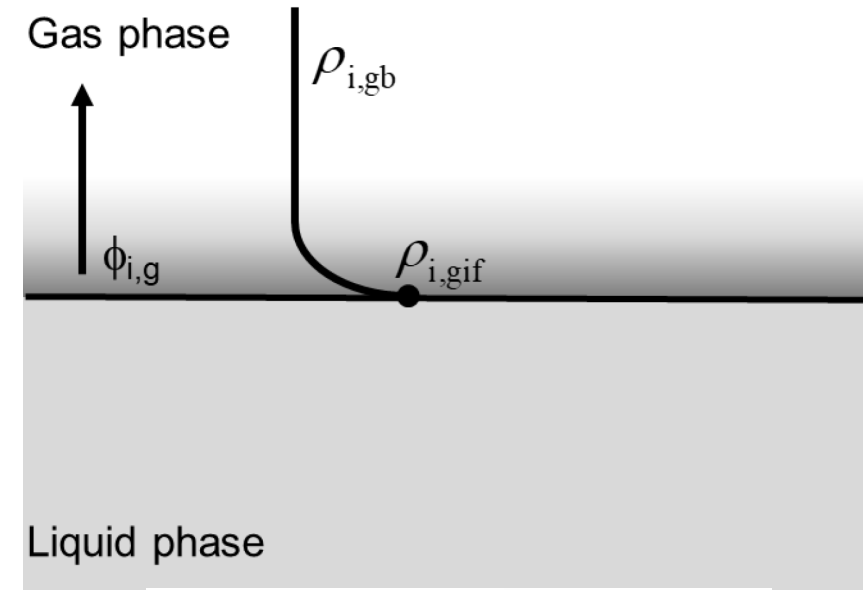
- Provides ability to perform best estimate evaluations of release from molten salts
- Demonstration calculations have focused on direct comparison to MSRE for the maximum hypothetical accident
- Exercise of model will be performed next year

Mass transfer interfaces

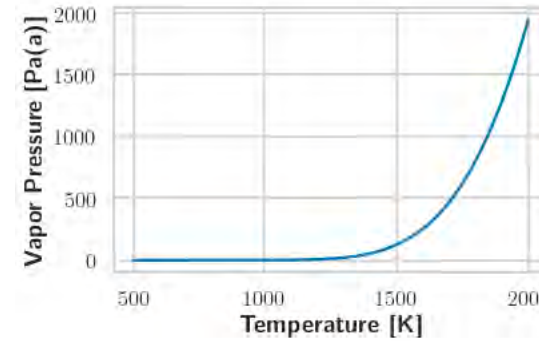
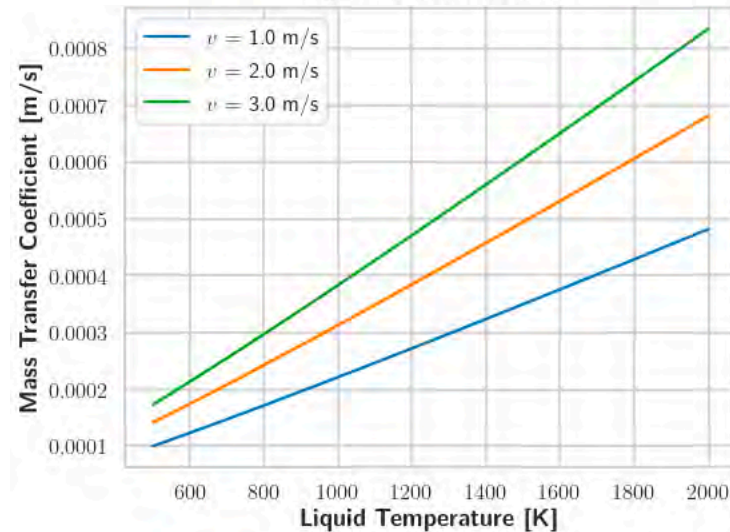
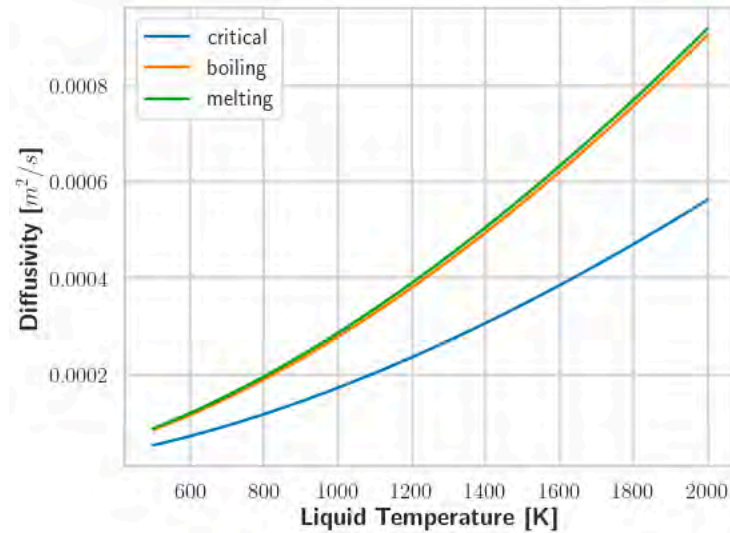
- Liquid-gas atmosphere interfaces
- Liquid-solid structure interfaces
- Gas atmosphere-solid structure interfaces
- Model allows new interfaces to be defined

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

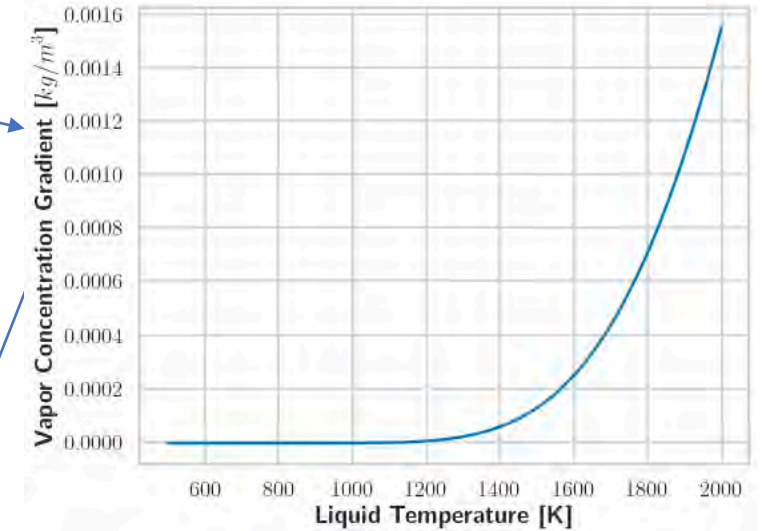
Jet breakup when contaminated fluids are released into a gas atmosphere (e.g., due to a pipe break)



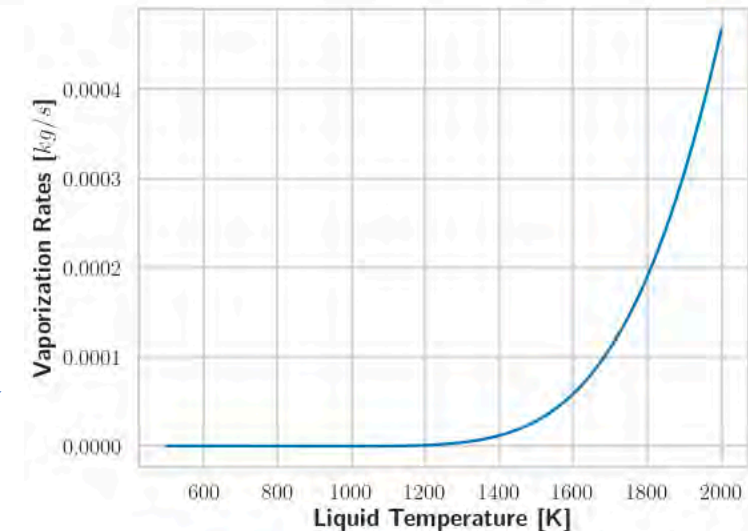
# Illustrating Components of Vaporization Mass Transfer



Example CsF vapor pressure – subject to change as thermochemistry evolves



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



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

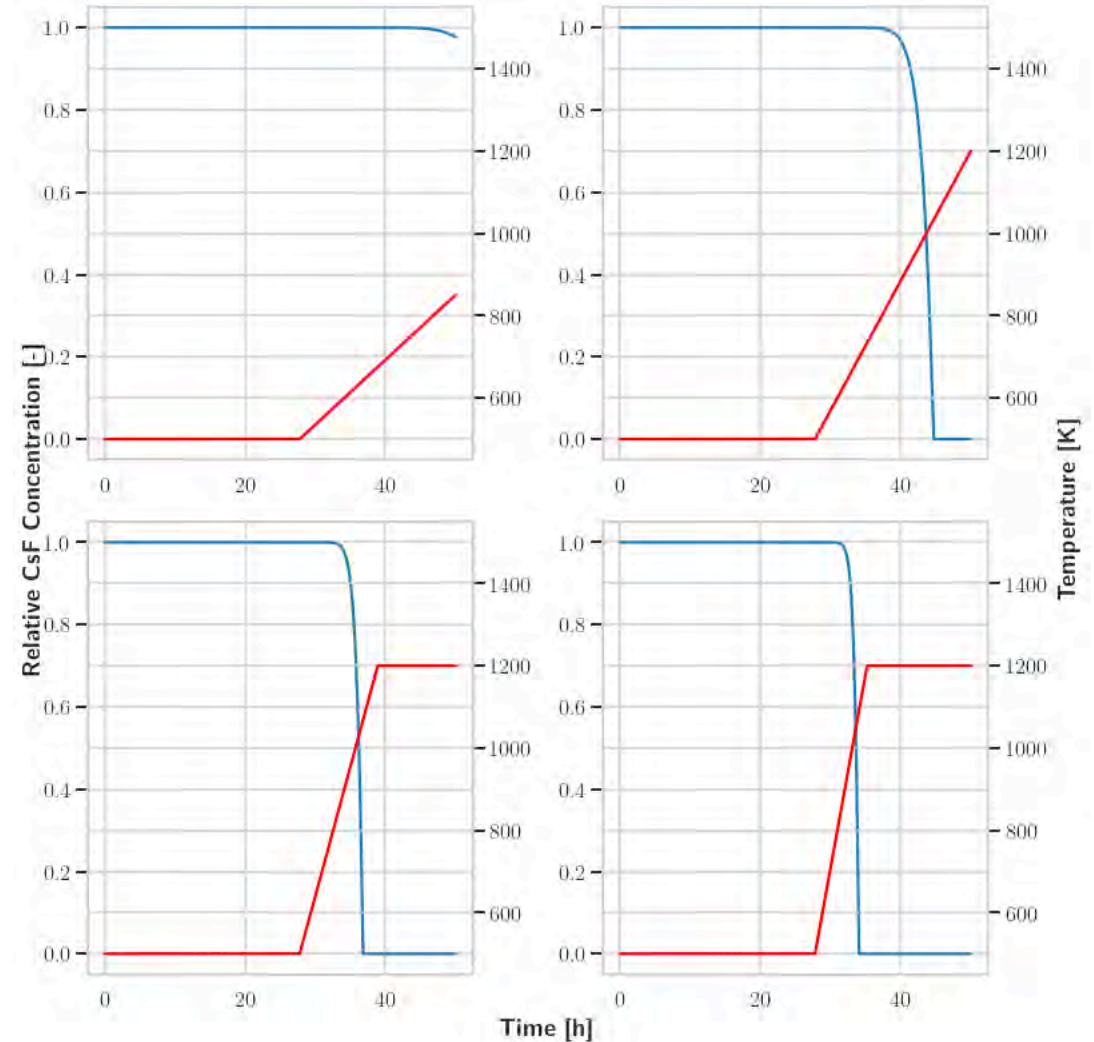
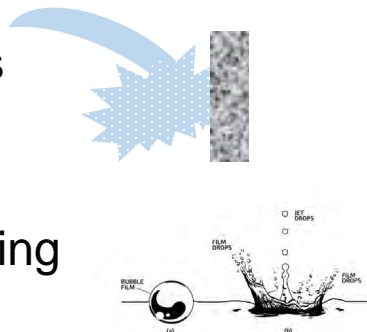
Focus of modeling efforts evolving based on insights from current demonstration calculations

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

- Relatively low temperature molten salt temperature leads to a very low vaporization ( $\ll 10^{-6}$ )
- 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



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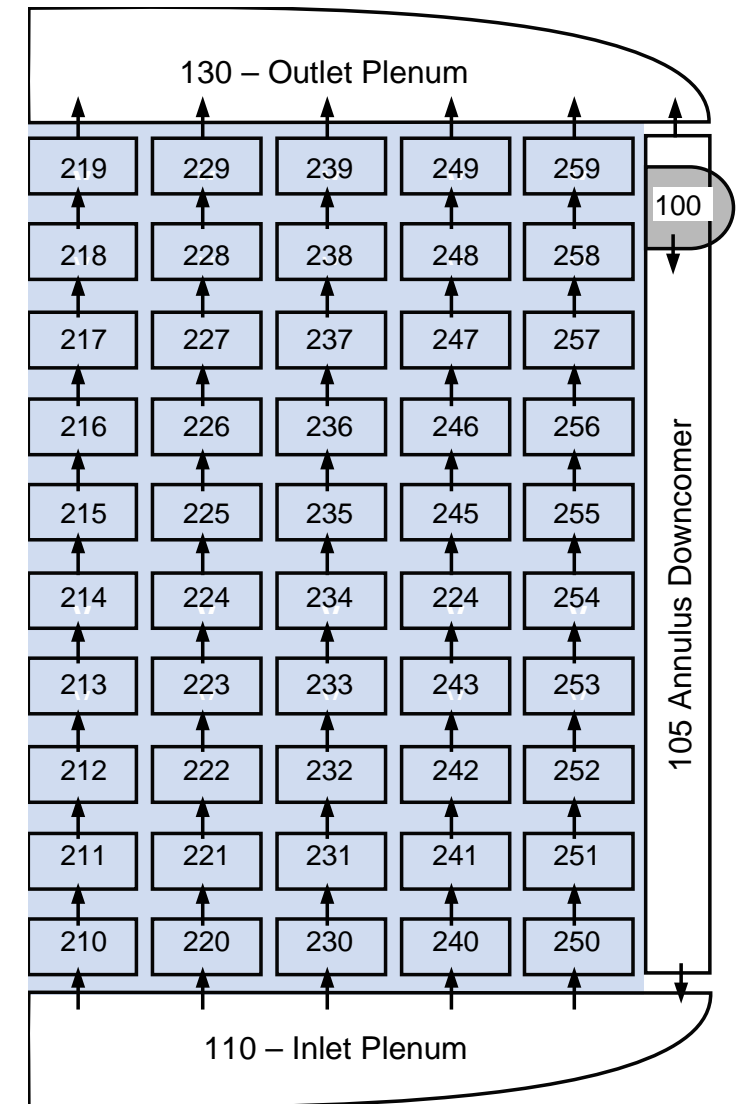
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# MELCOR nodalization - core and reactor vessel

## 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

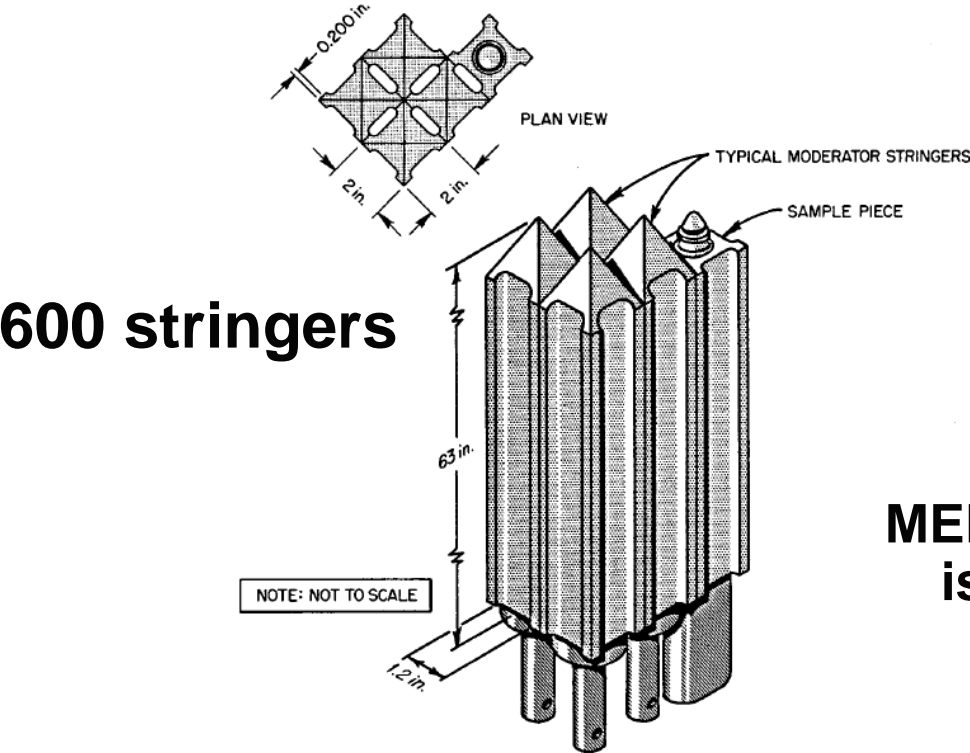
Core region





# MELCOR core region mapping to SCALE

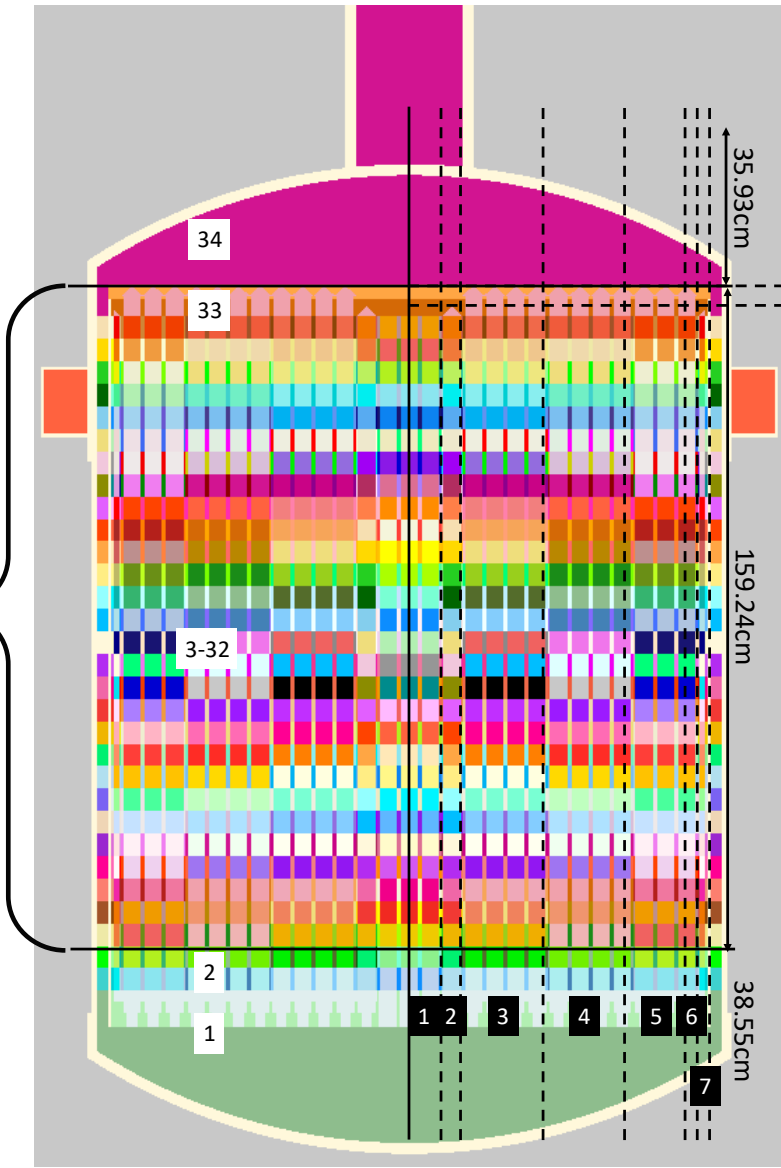
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ORNL-LR-DWG 56874 R



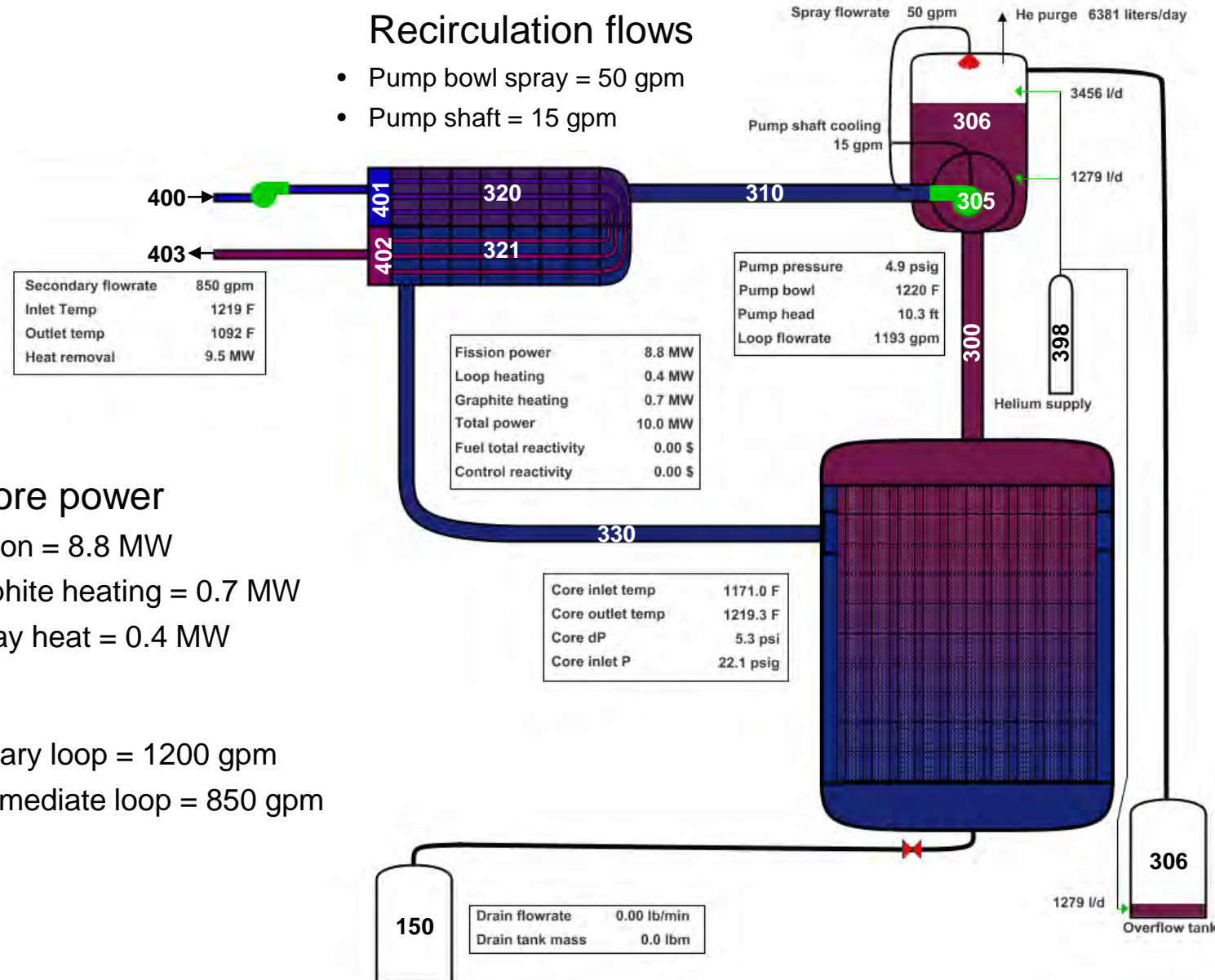
MELCOR axial mapping  
is 3 SCALE levels per  
1 MELCOR level

## 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



## Helium off-gas flows

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

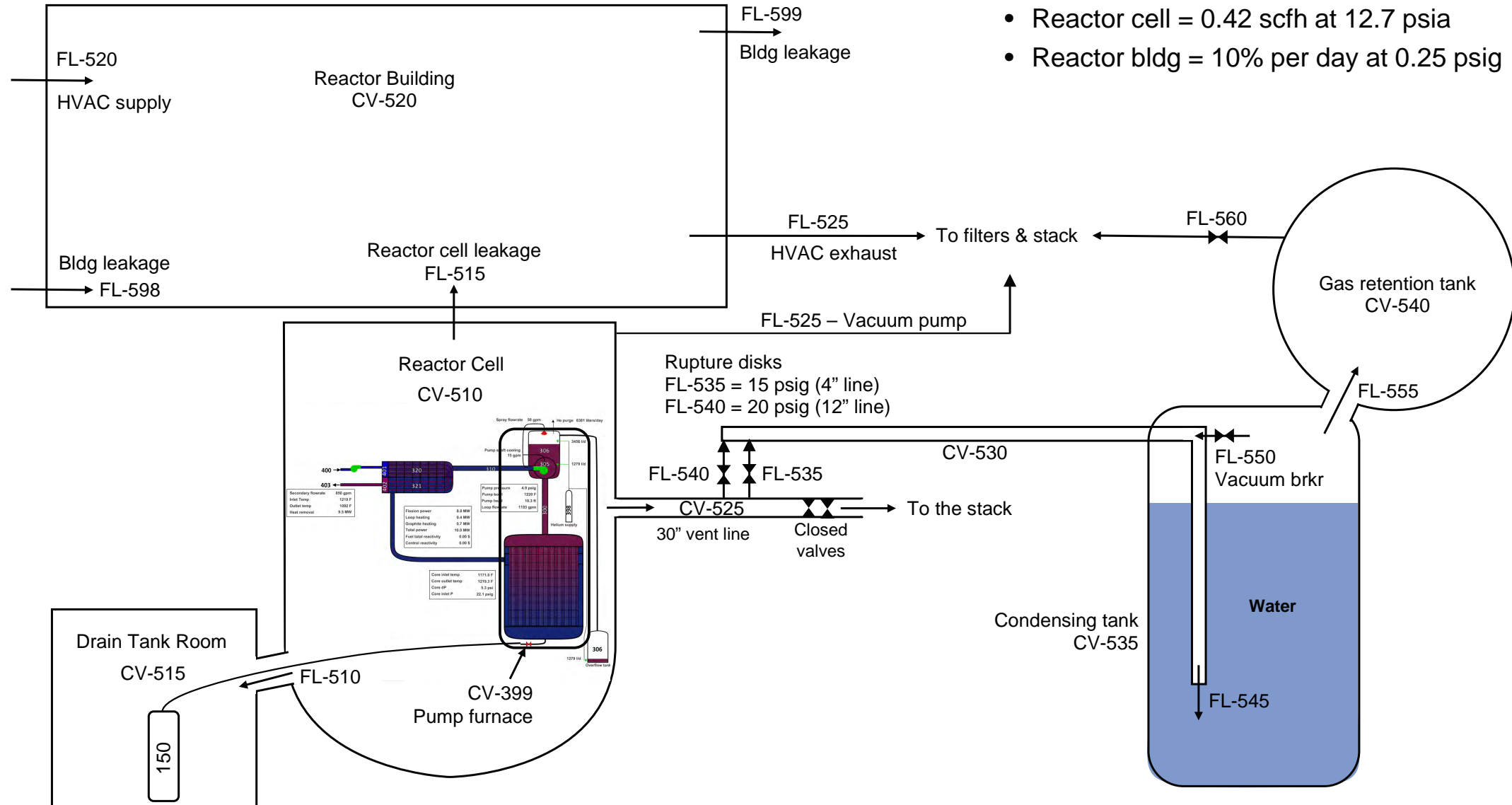
## Total core power

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

## Flows

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

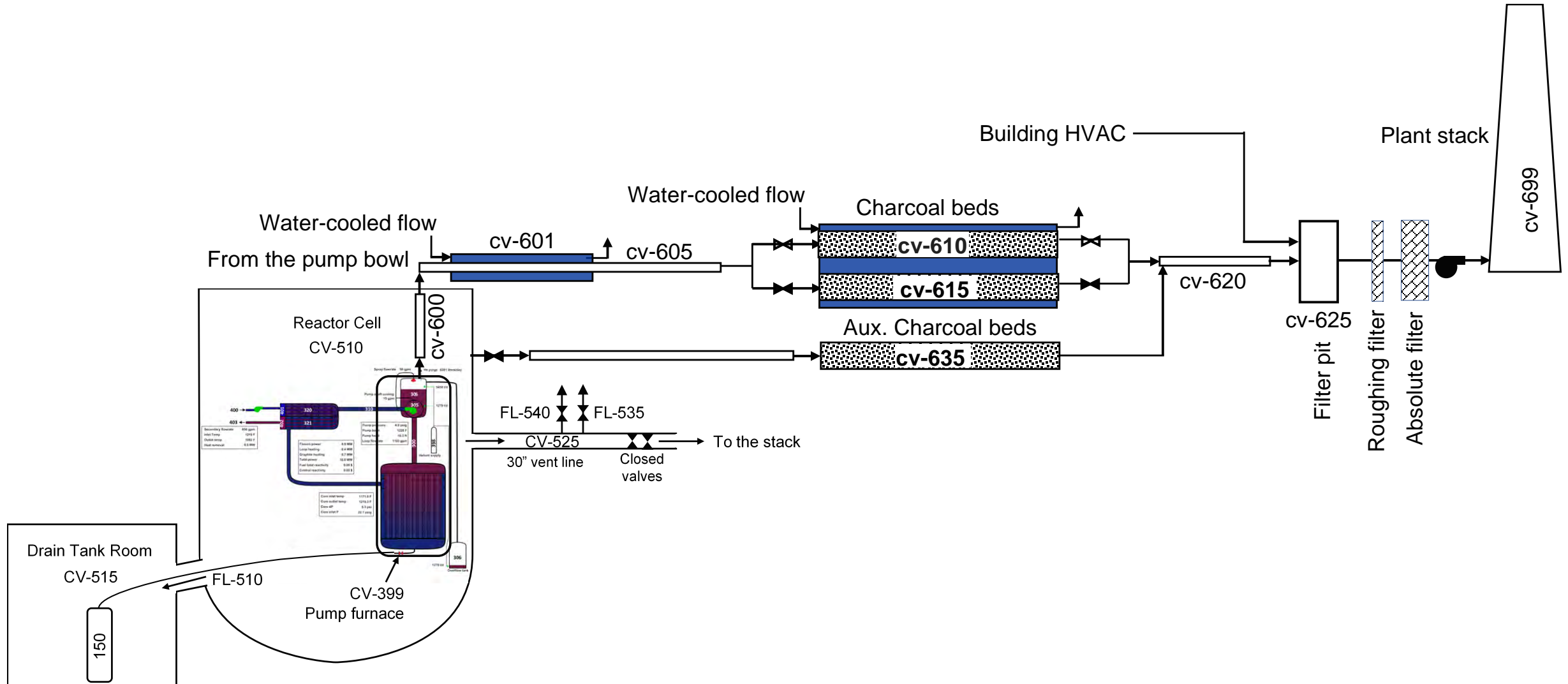
# MELCOR nodalization – reactor cell, condensing tank, and reactor building



## 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 and suggestions by Britt (ORNL)
- Insoluble elements isolated into two groups (next slide)

Antoine coefficient estimates for few species (Cs, CsF)

- Cesium and cesium fluoride estimated using MSTDB-TC



## 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

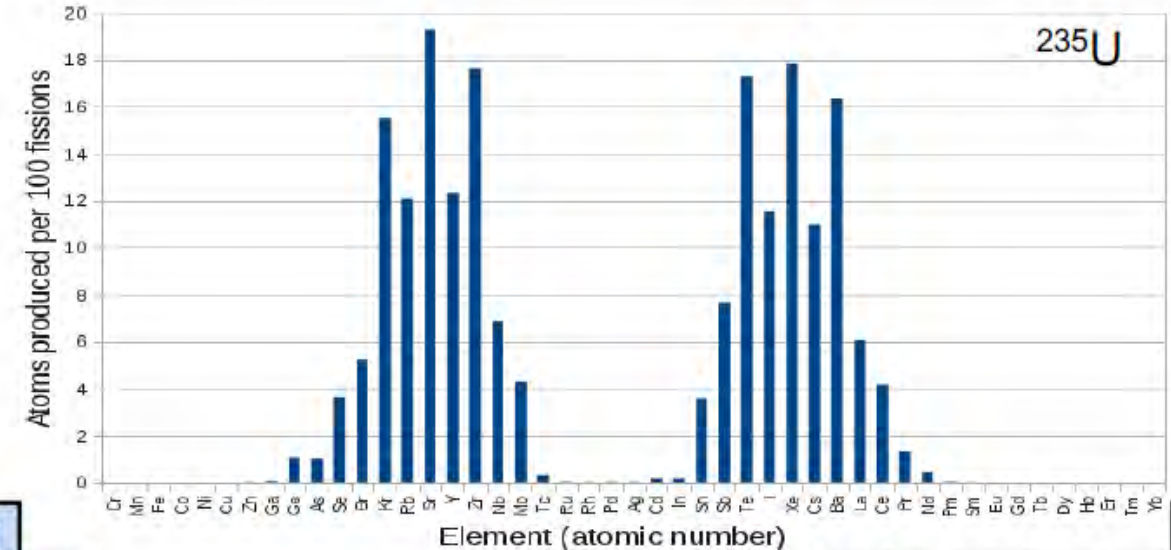
La : Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy,  
Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf

$$U : U$$

Cd : Hg, Ga, In

Ag : Pb, Tl, Bi

B : B, Si, P



Element (atomic number)																		He			
H																	He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
Fr	Ra	Ac-Lr																			
always soluble			sometimes soluble					insoluble					gaseous								

Mo class assumed to be insoluble

# 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

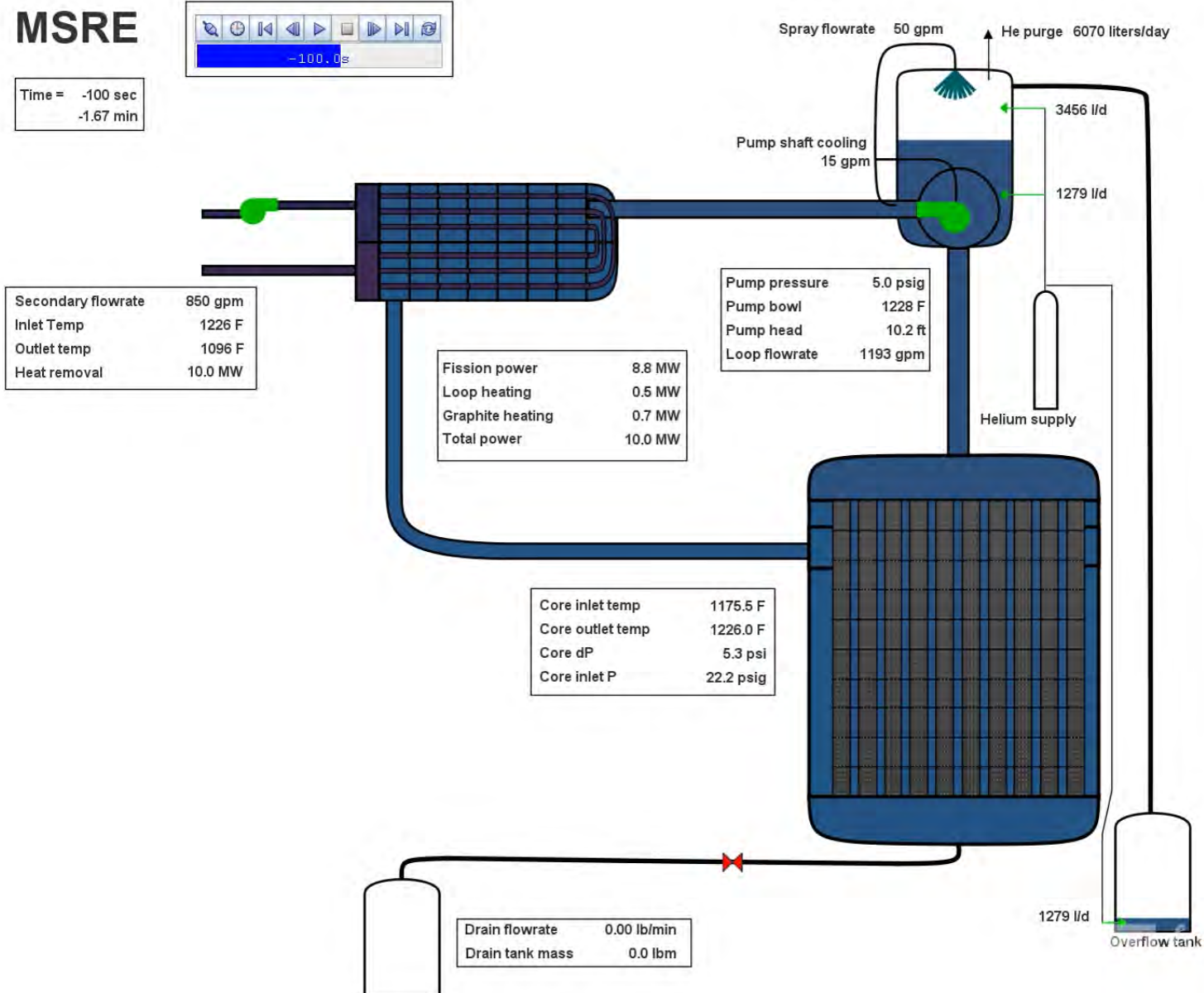
# Salt spill cases

## Walk-through MCA1 (base case)

- Spill creates aerosols with 1  $\mu\text{m}$  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 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No
MCA6	1 $\mu\text{m}$	Yes	No	Yes
MCA7	1 $\mu\text{m}$	Yes	Yes	Yes
MCA8	1 $\mu\text{m}$	No	Yes	Yes
MCA9	1 $\mu\text{m}$	No	No	Yes

# MCA1 salt spill base case – Primary System Response



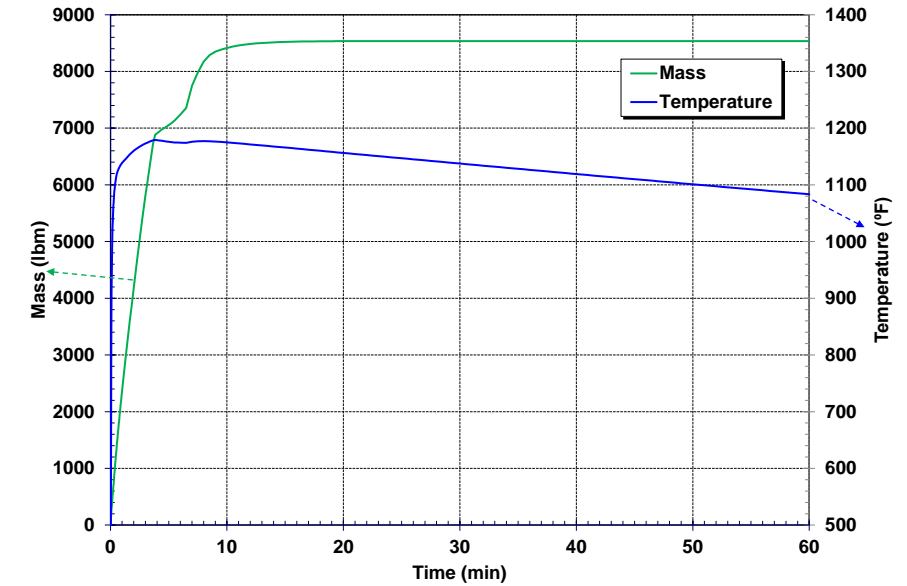




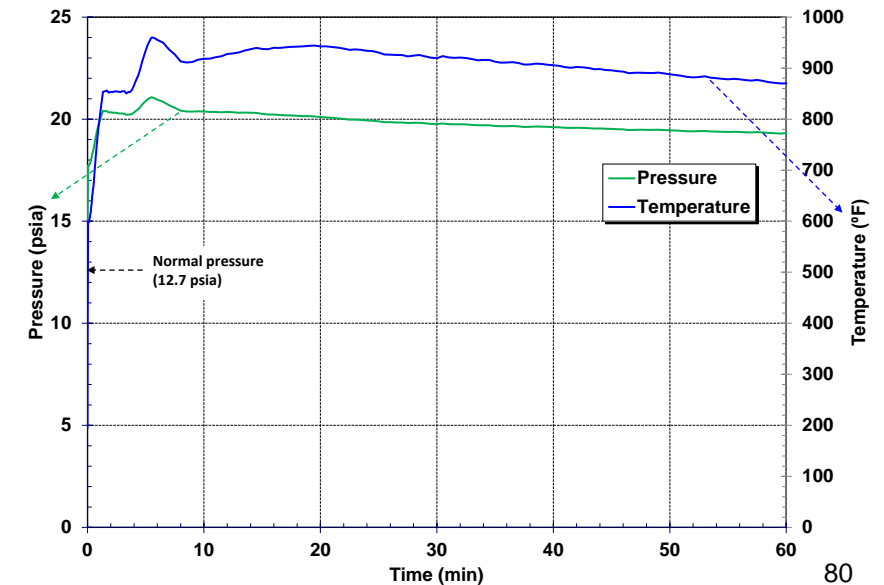
# MCA1 reactor cell thermal-hydraulic response

- 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 (~1100°F)
  - Heating due to the released radionuclides
- Reactor cell gas temperature initially rises to over 900°F and then slowly cools

Mass of molten salt spilled and its temperature



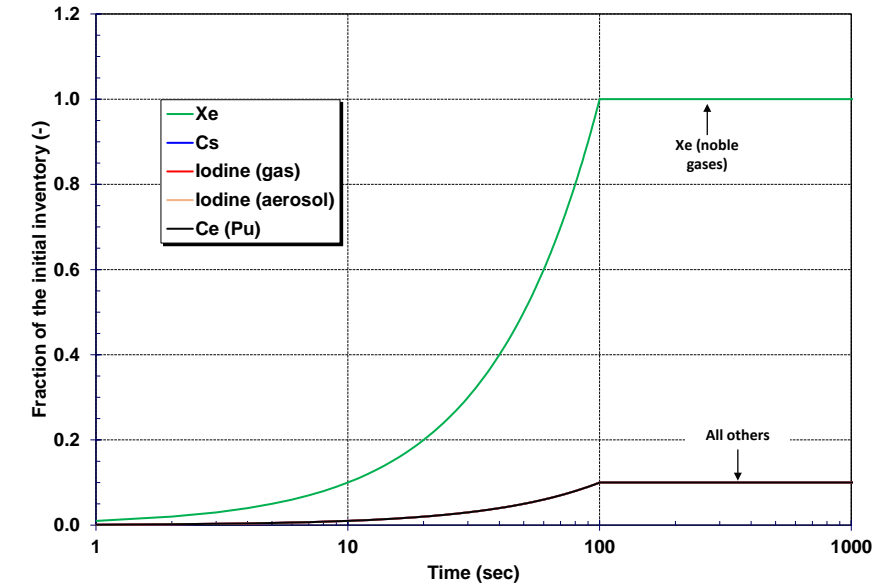
Reactor cell pressure and temperature



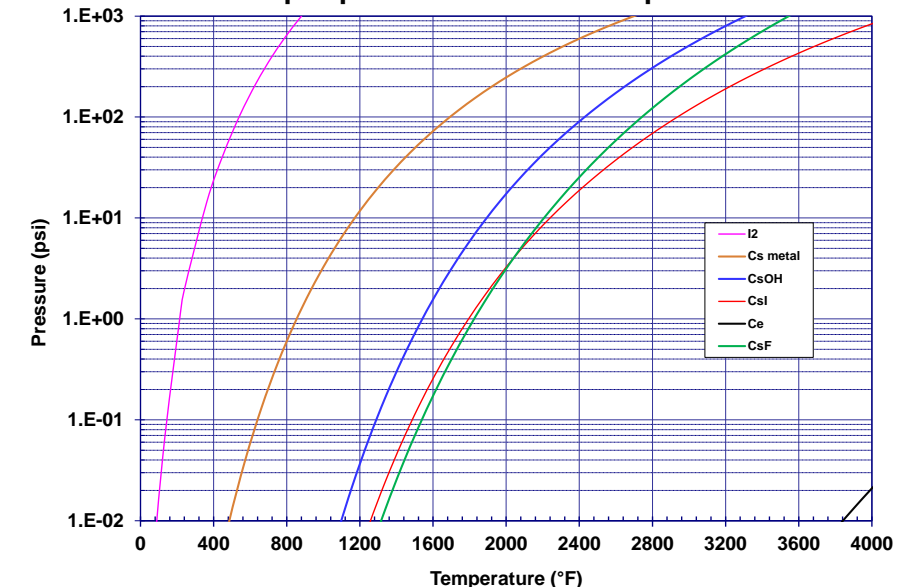
# MCA1 reactor cell radionuclide releases

- 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
  - Analysis used some modification for likely MSR chemical forms
    - Some gaseous iodine (5%)
    - Cesium and iodine combine (CsI)
    - Remaining cesium as CsF
  - MELCOR allows exploration of alternate chemical forms for the MSR

Radionuclide airborne release



Vapor pressure in the atmosphere



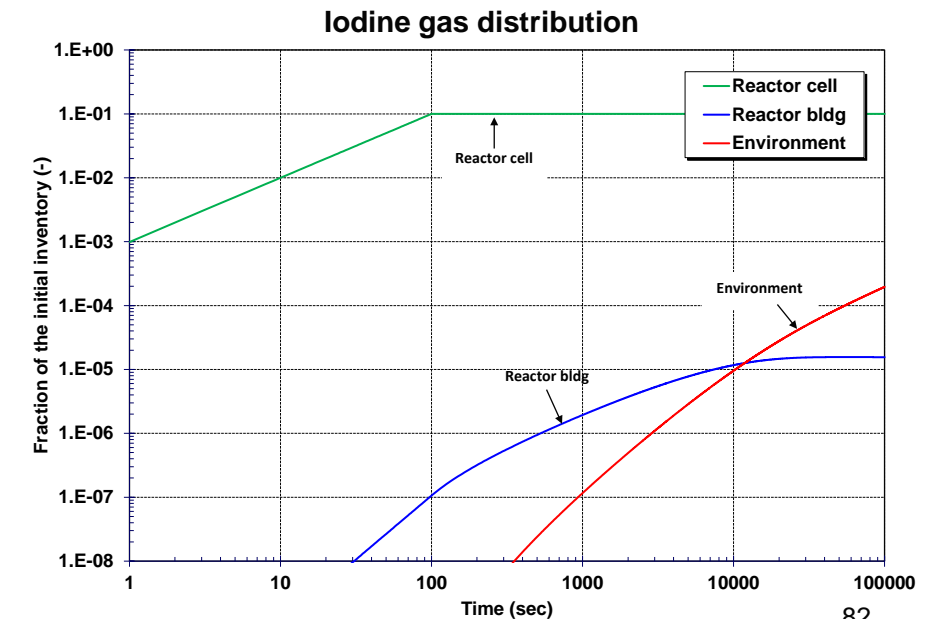
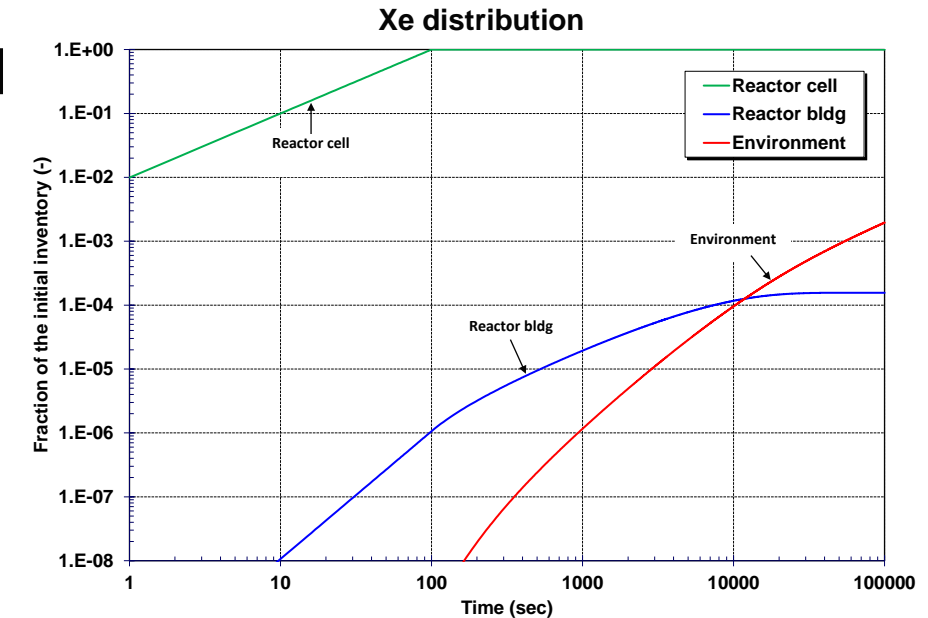
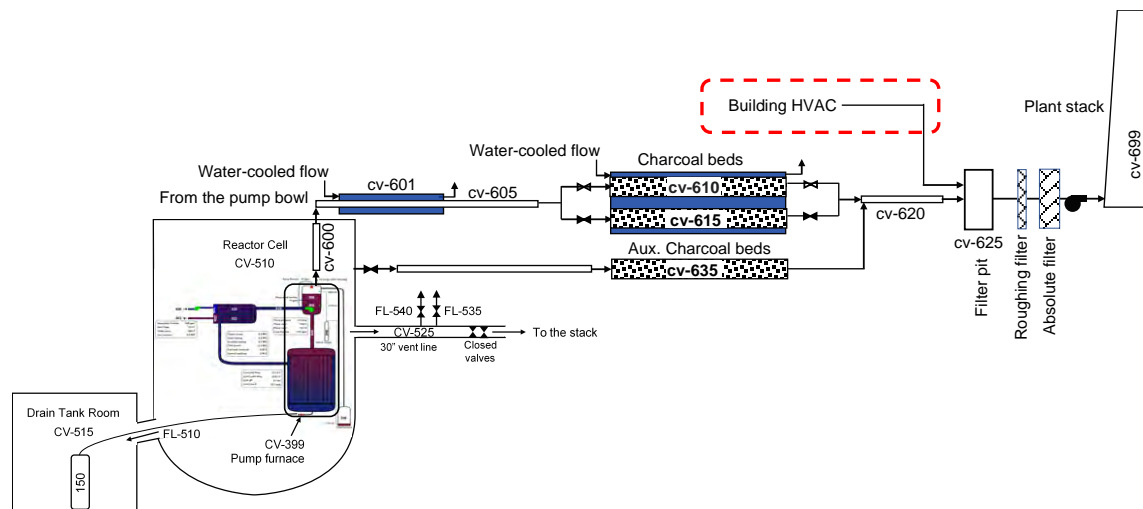
# MCA1 gaseous radionuclide distributions

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

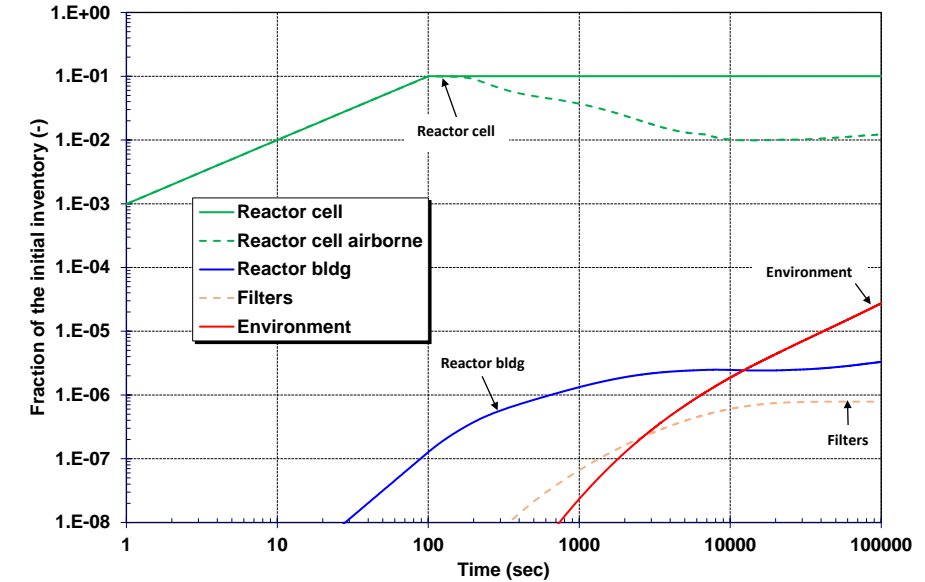


# MCA1 aerosol radionuclide distributions

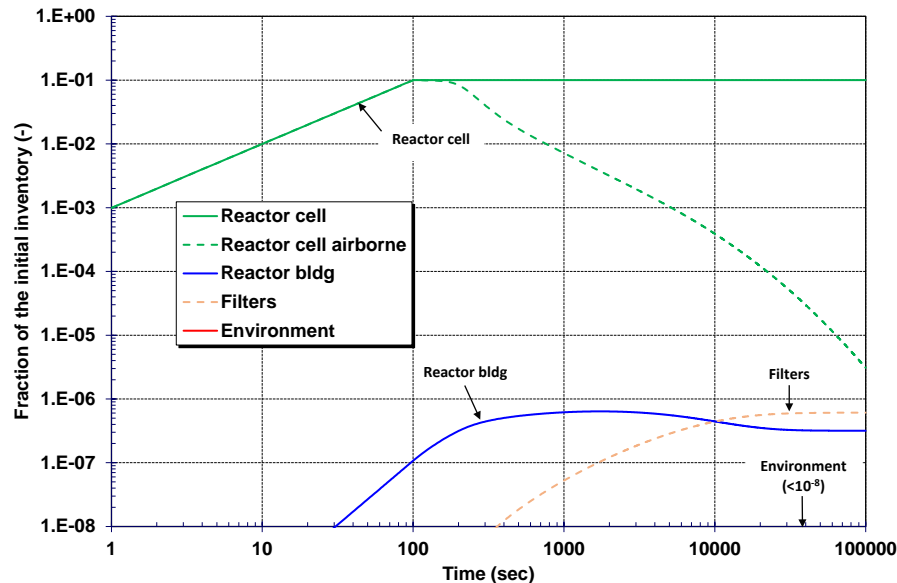
Release fractions of radionuclides that form aerosols in the reactor building

- CsF and CsI illustrate radionuclide chemical forms that include both vapor and aerosol forms in the reactor cell
  - Higher leakage of vapors → formation of small aerosols in the reactor building → more to environment & the filters
- Ce is an aerosol that primarily settles in the reactor cell and captured by the absolute filters

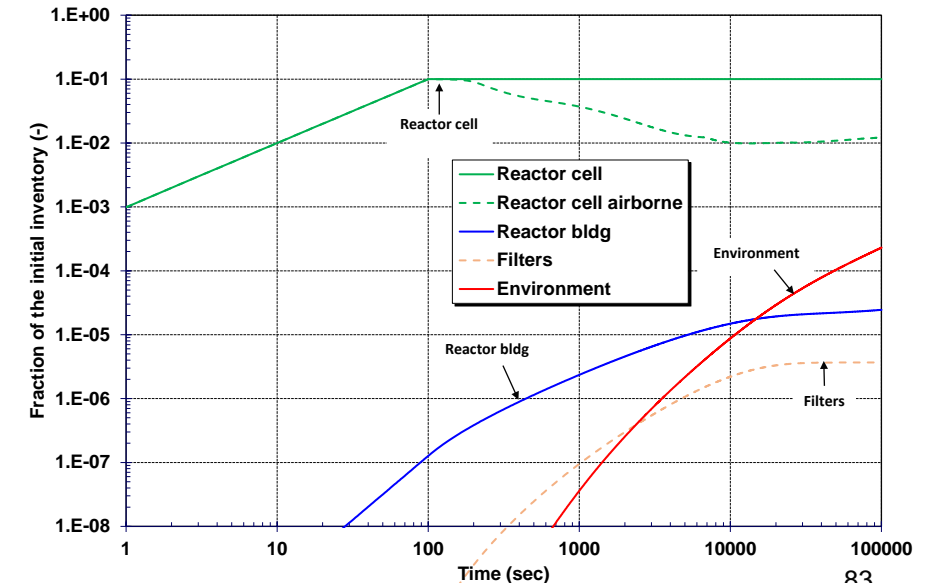
CsF distribution



Ce distribution



CsI distribution



# Salt spill with water base case

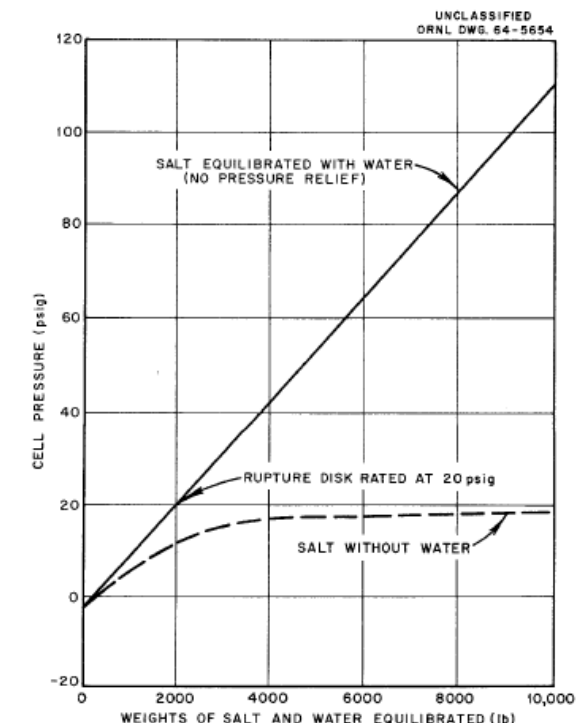
## Walk-through MCA6

- Spill creates aerosols with 1  $\mu\text{m}$  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

*“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]

Case	Aerosol size	Stack Fans	Aux. Filters	Water Spill
MCA1	1 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No
MCA6	1 $\mu\text{m}$	Yes	No	Yes
MCA7	1 $\mu\text{m}$	Yes	Yes	Yes
MCA8	1 $\mu\text{m}$	No	Yes	Yes
MCA9	1 $\mu\text{m}$	No	No	Yes

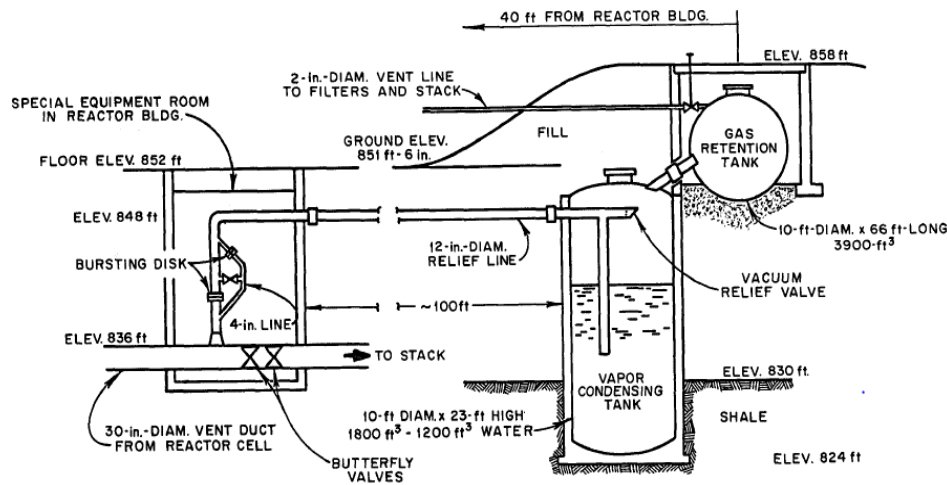


[ORNL-TM-0732]

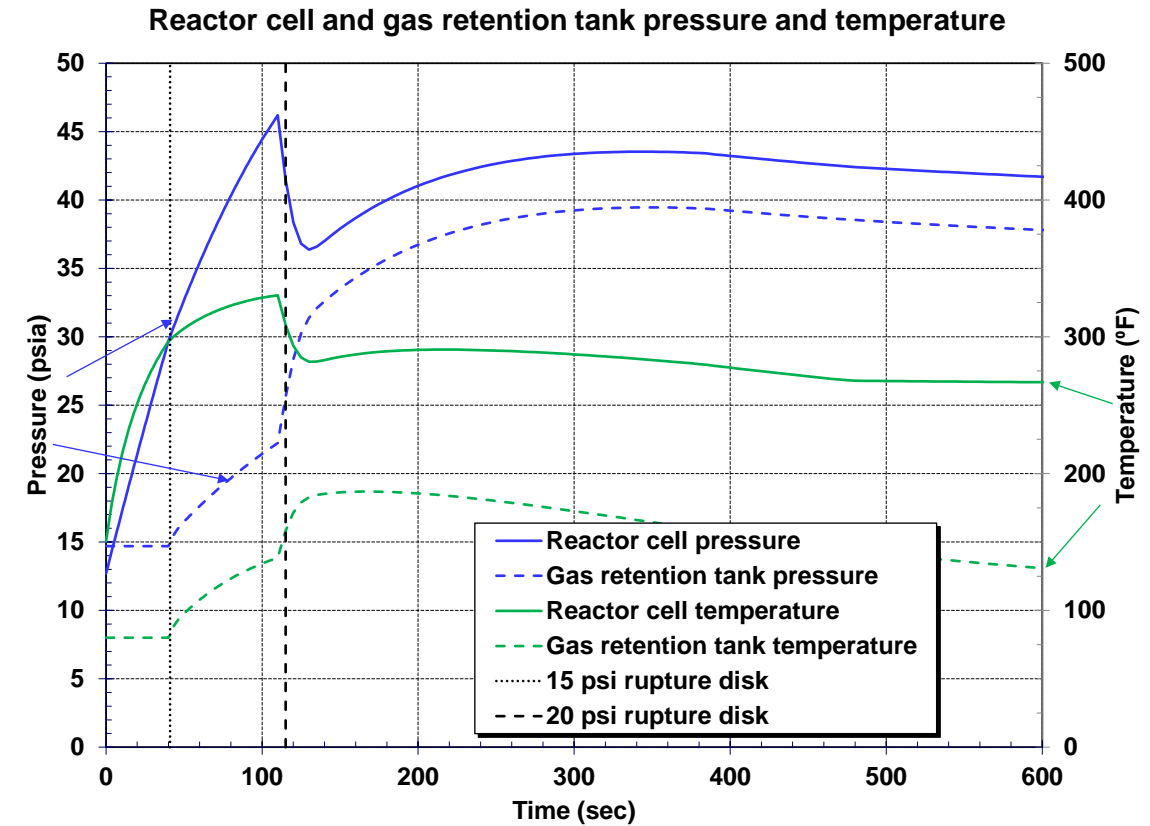


# MCA6 reactor cell thermal-hydraulic response

- 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 330°F but falls after the 20 psi rupture disk opens



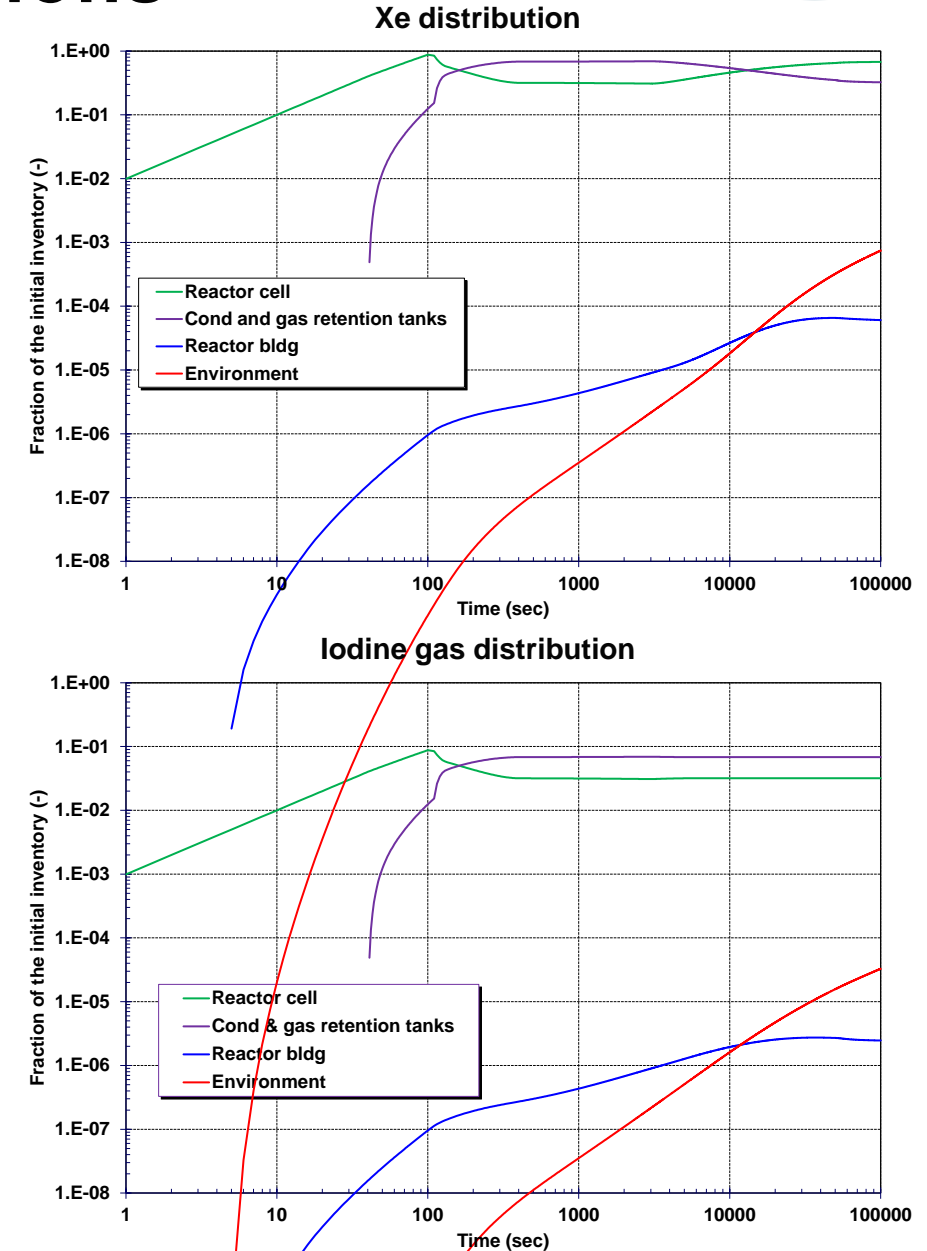
MSRE vapor-condensing system  
[ORNL-TM-0728]



# 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

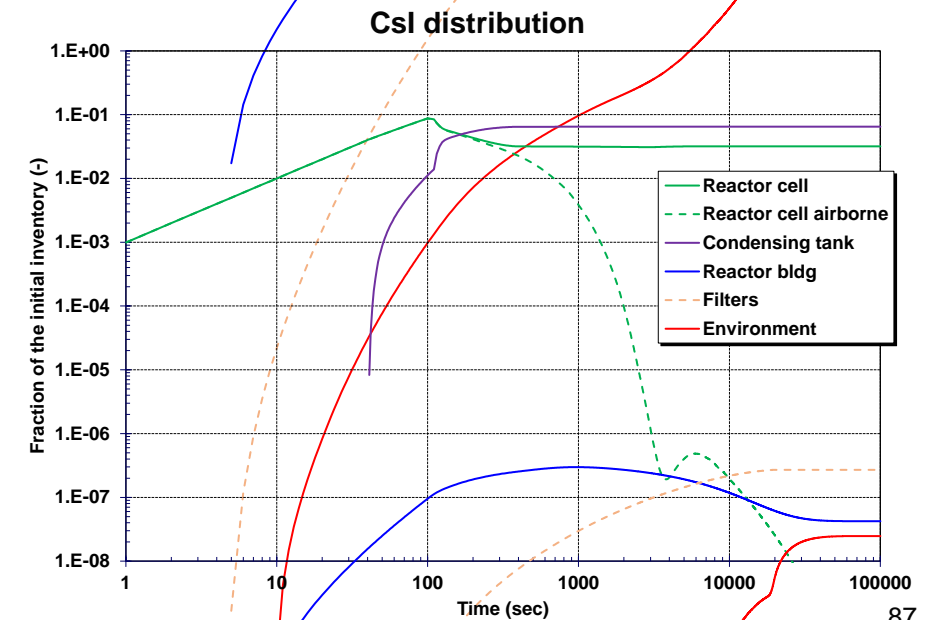
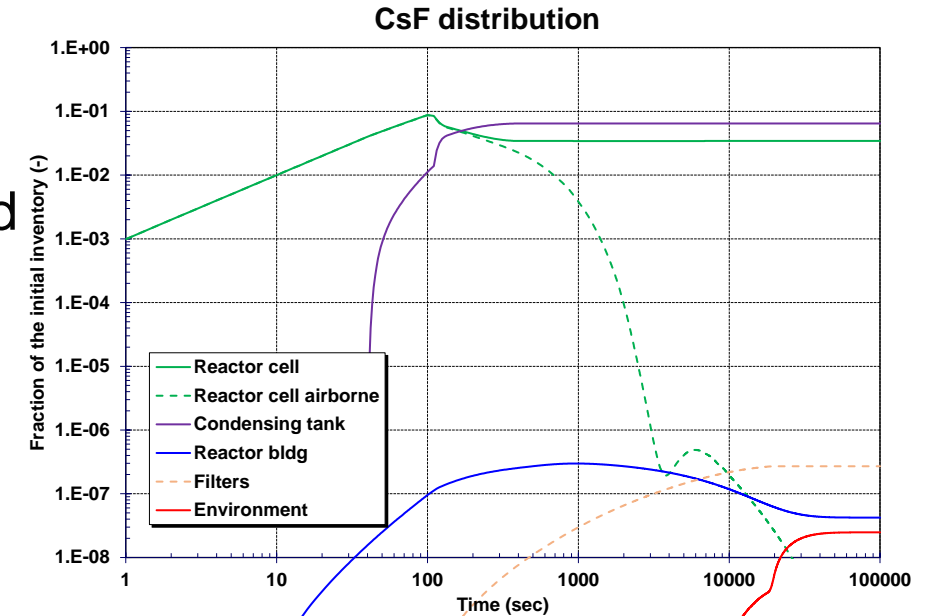
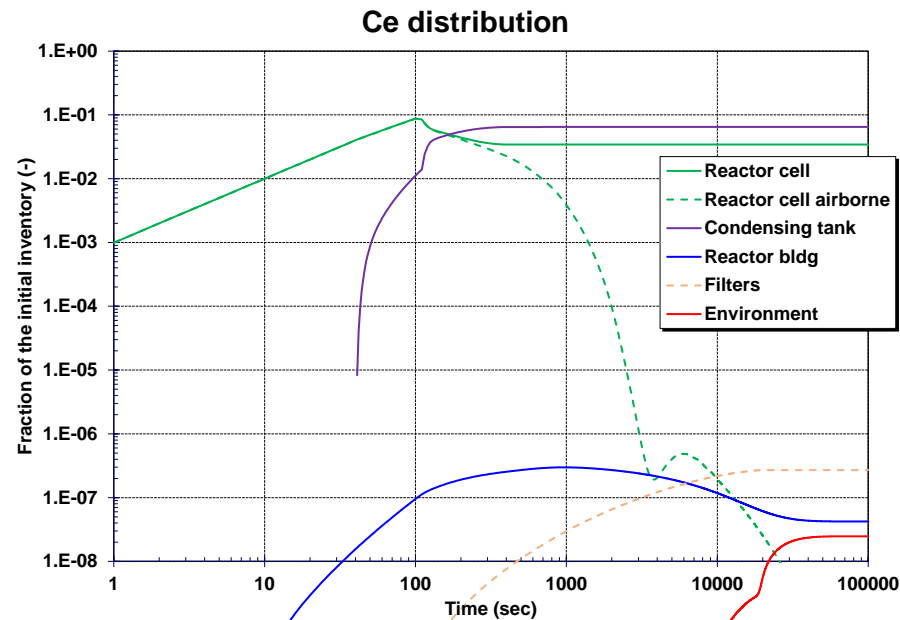


# MCA6 aerosol radionuclide distributions

Most of the aerosol releases are retained in the condensing tank

- CsF 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

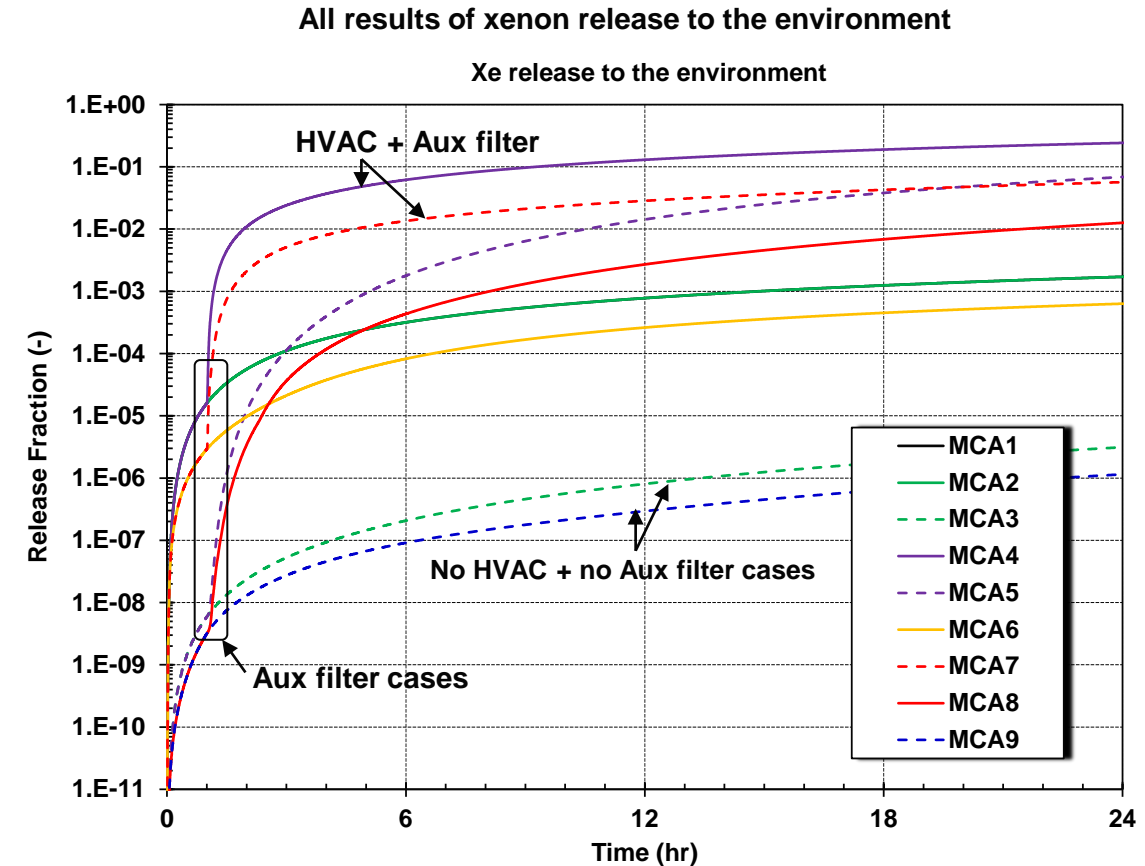


# Overall insights (1/4)

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 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No
MCA6	1 $\mu\text{m}$	Yes	No	Yes
MCA7	1 $\mu\text{m}$	Yes	Yes	Yes
MCA8	1 $\mu\text{m}$	No	Yes	Yes
MCA9	1 $\mu\text{m}$	No	No	Yes

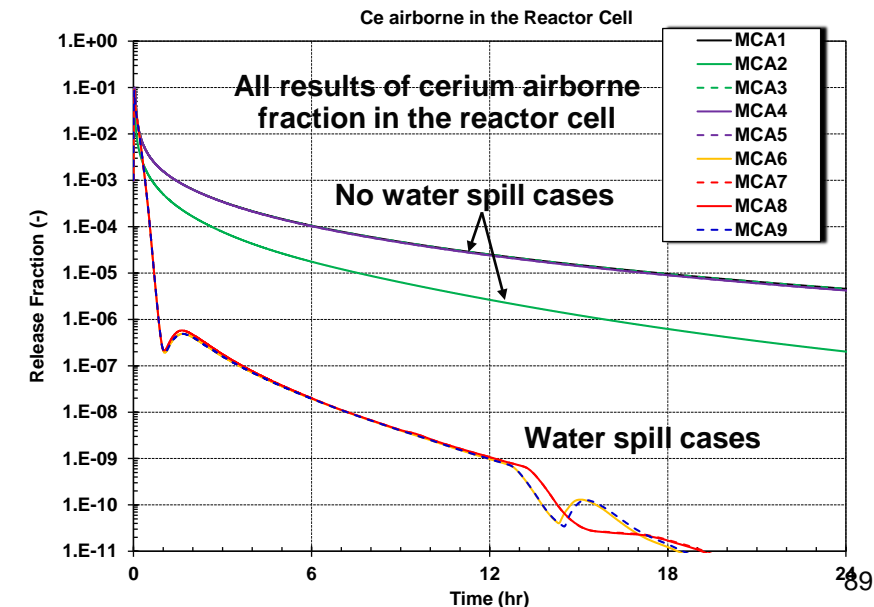
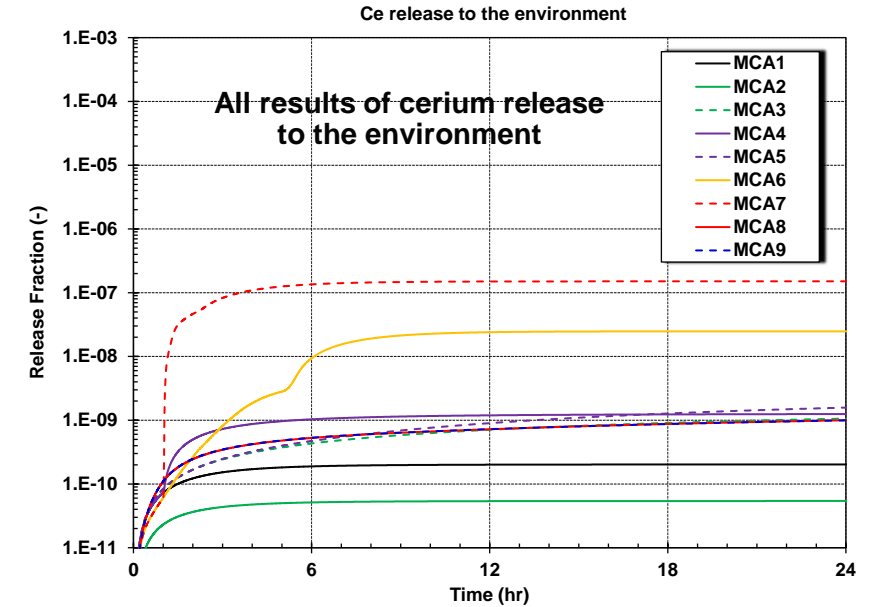
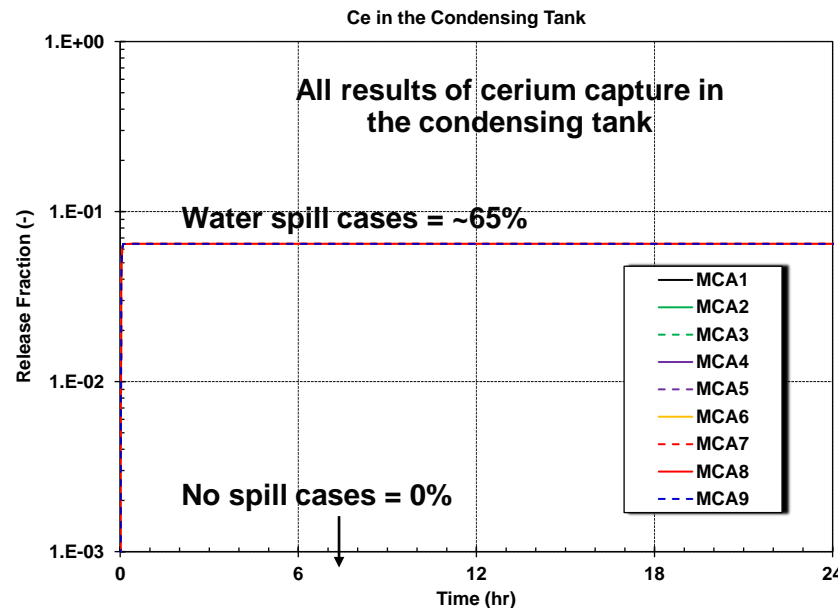


Note: Results assume no xenon retention in the charcoal filters.

# 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



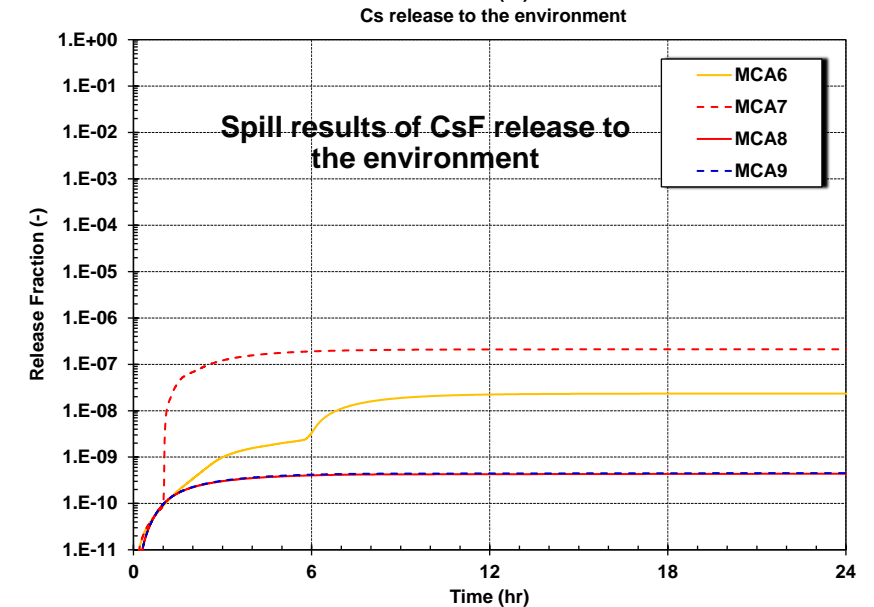
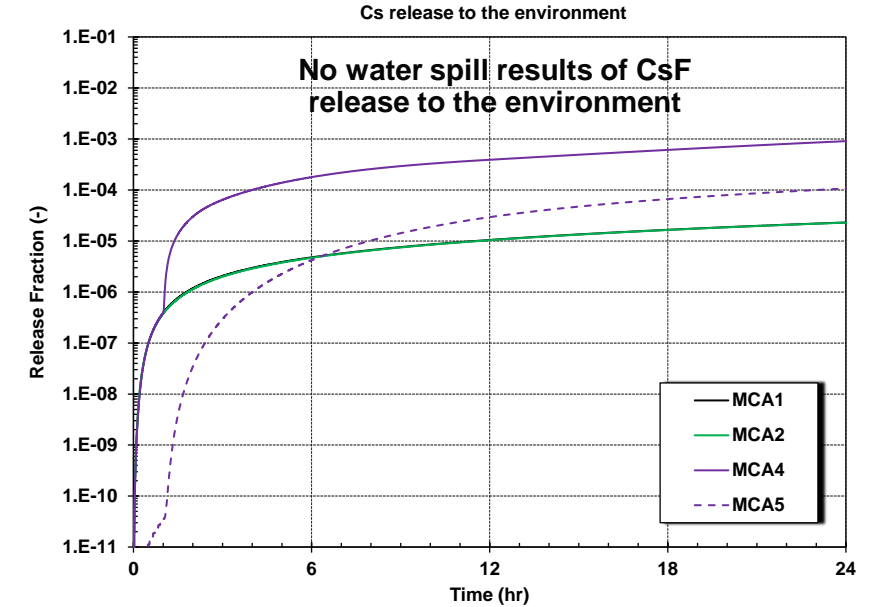
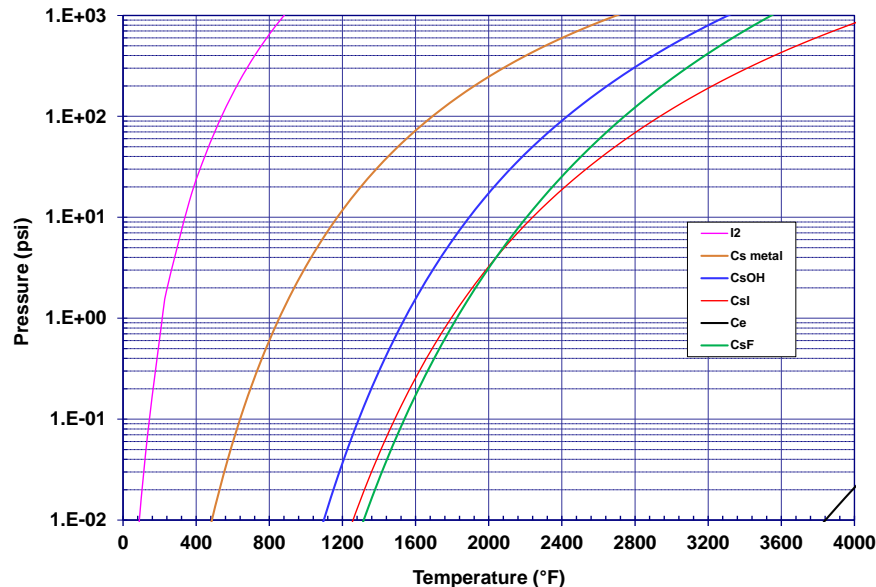


## Overall insights (3/4)

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

- Released CsI and CsF vapors subsequently condensed in the reactor building and the offgas system to form very small aerosols
- CsF and CsI vapors remained airborne in the reactor cell

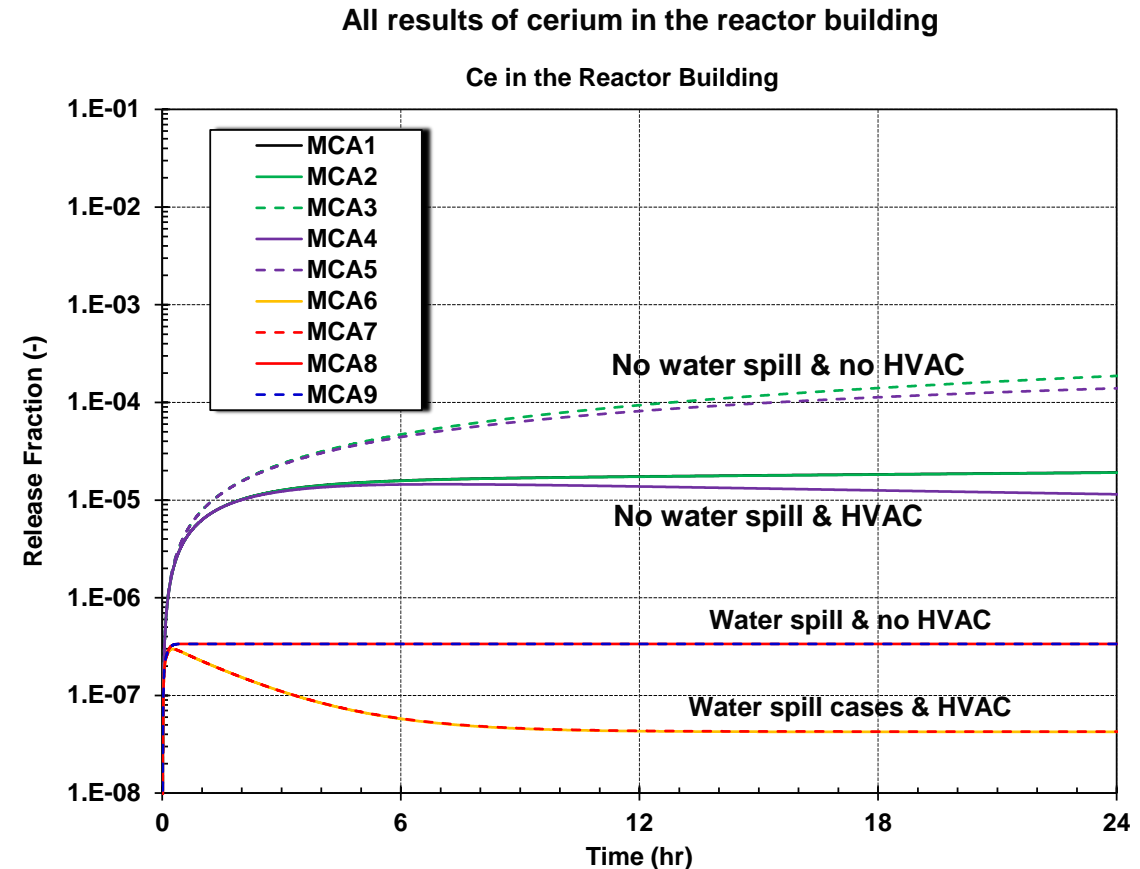
This contributed to higher cesium environmental releases than the lower temperature cases with a water spill



## Overall insights (4/4)

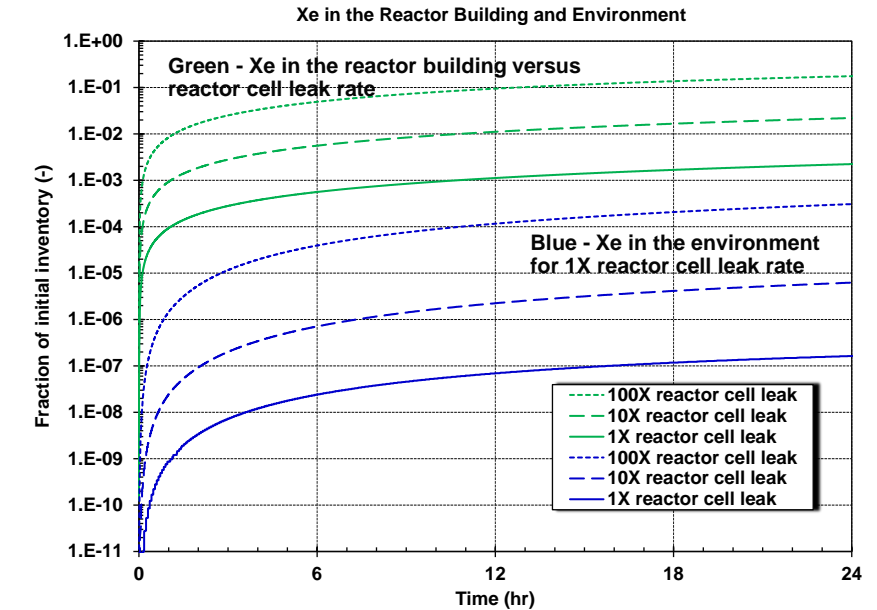
The aerosol mass in the reactor building also spanned many orders of magnitude depending on scenario assumptions

- 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 and a water spill 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



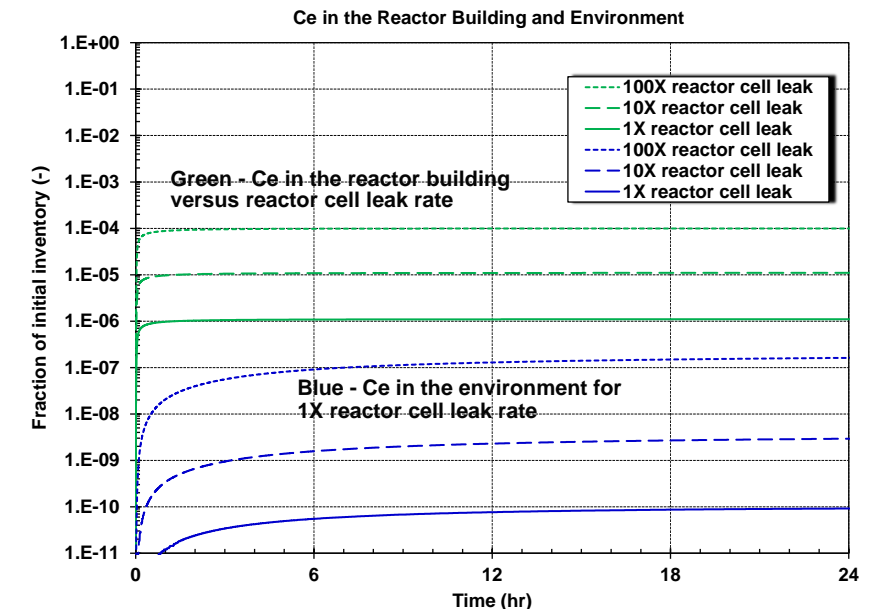
# Sensitivity to increased reactor cell leakage

- 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 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No

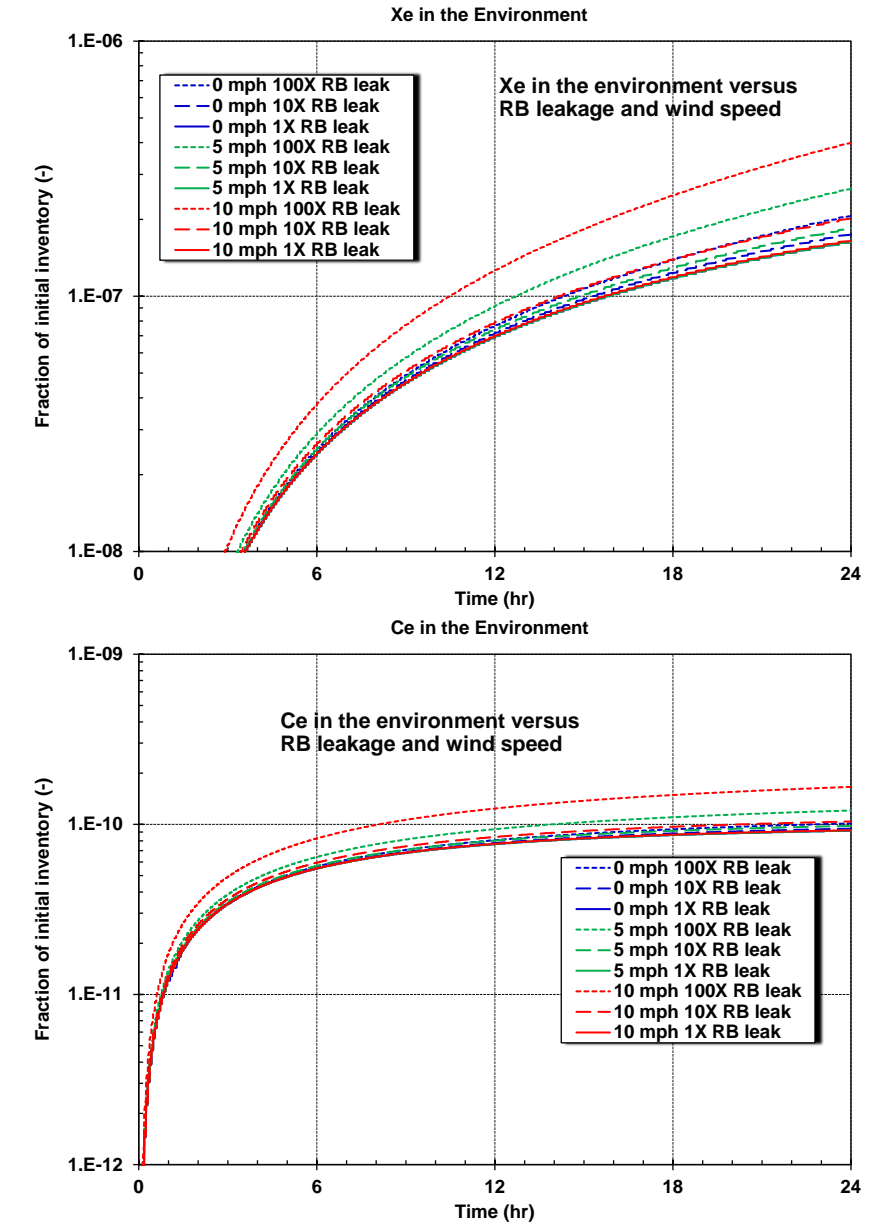


# Sensitivity to increased reactor building leakage

- 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) reactor building leakage is very low
  - Only 10% per day at 0.25 psig, 0.002 in<sup>2</sup>
  - The very large building (480,000 ft<sup>3</sup>) 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 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No



# Summary



U.S. NRC



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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



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# Further SCALE analysis details



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# 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

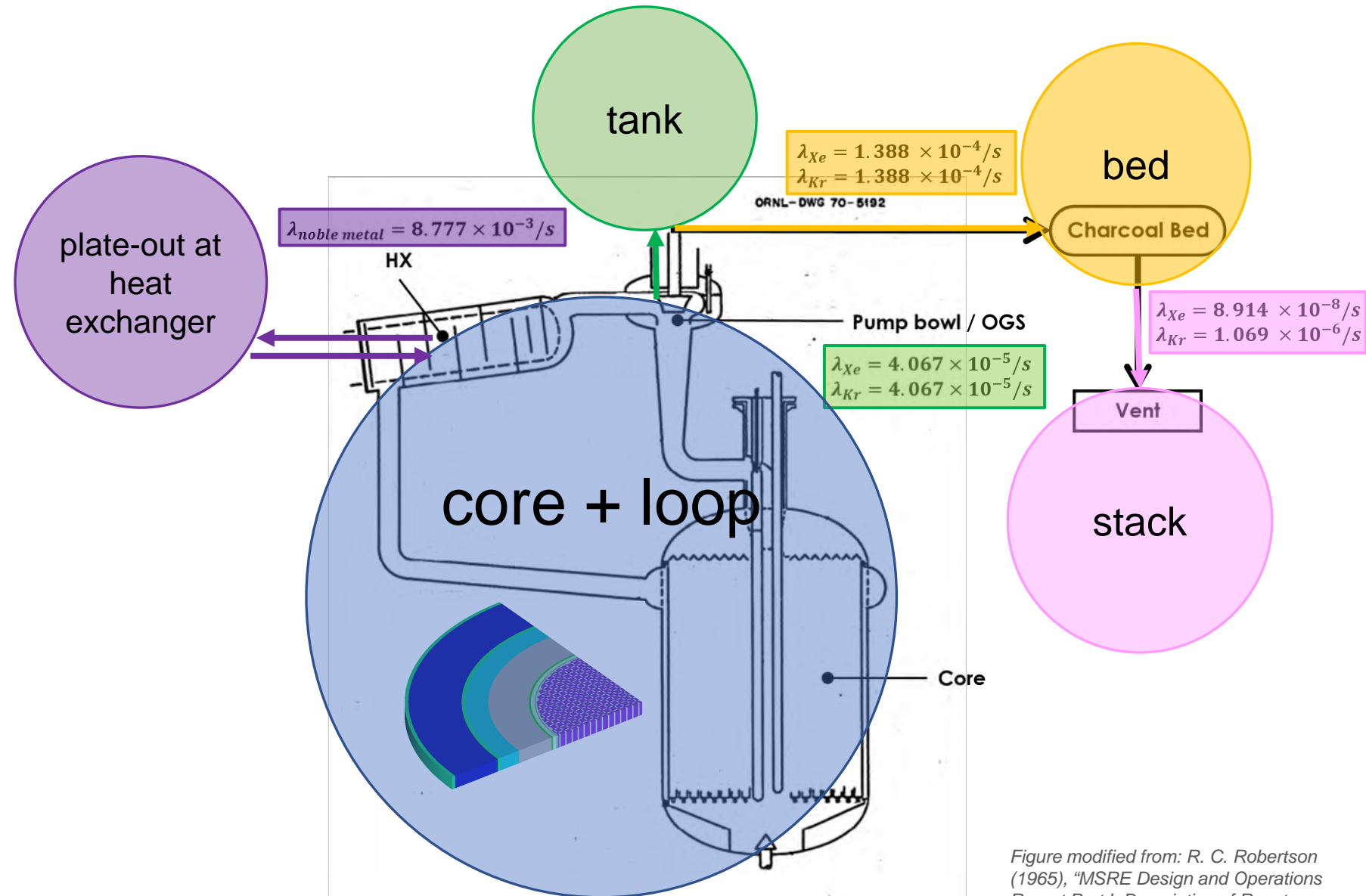
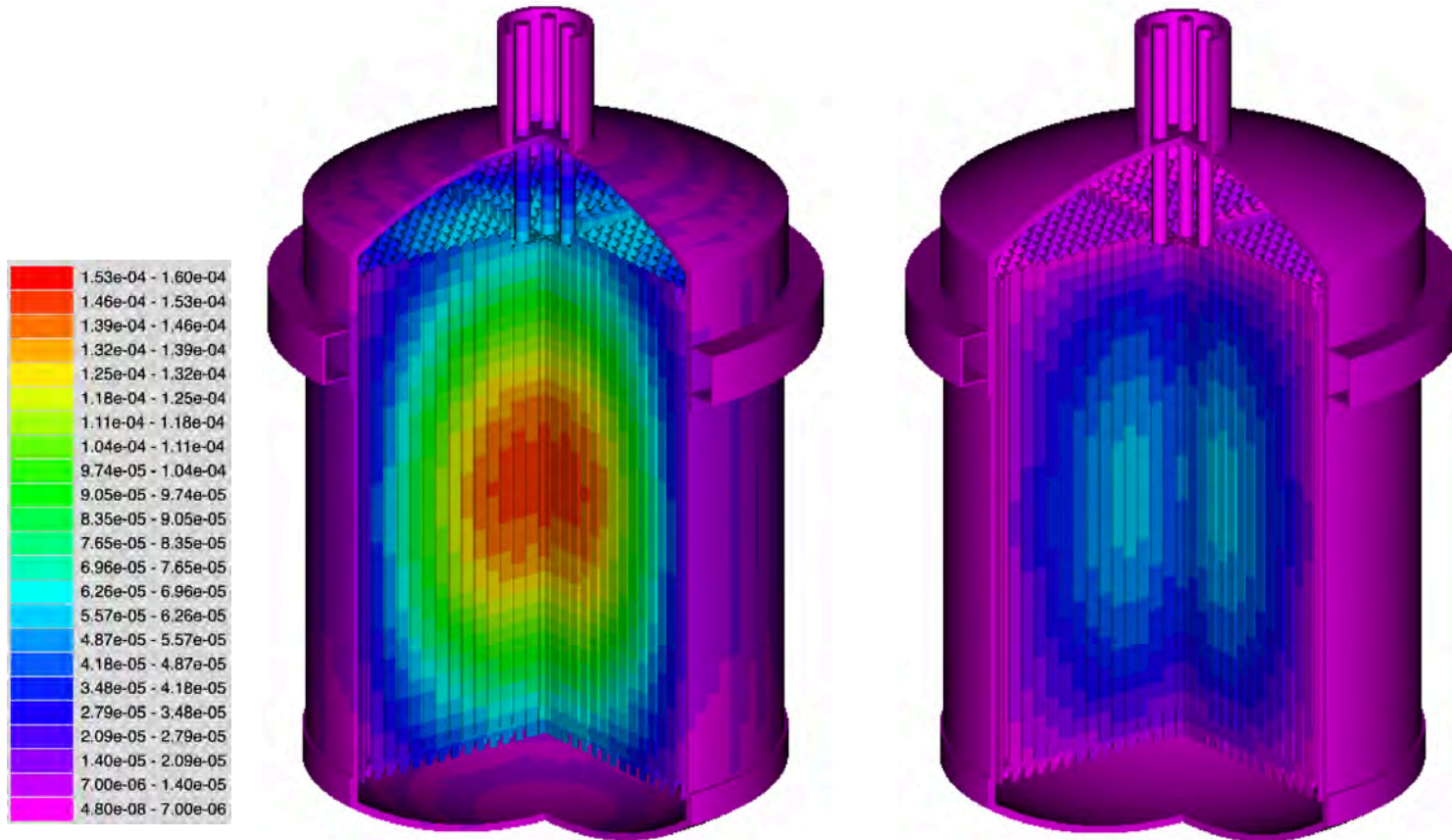


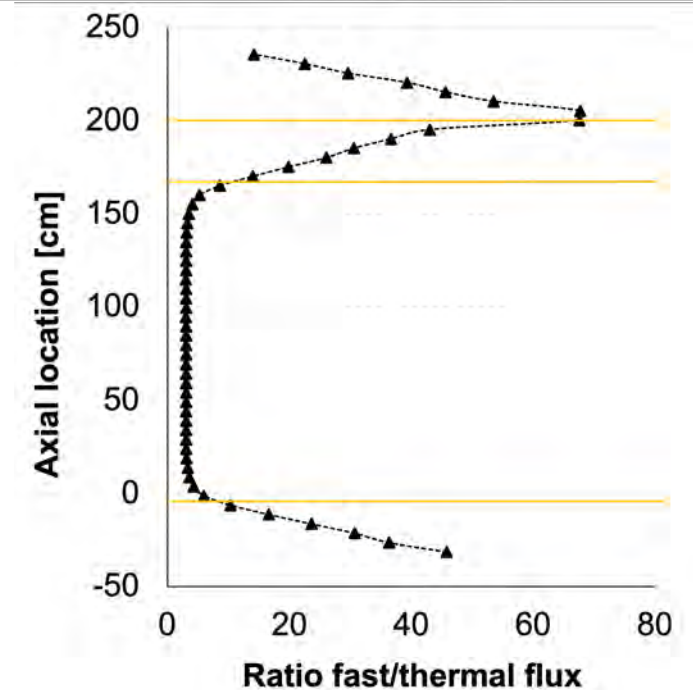
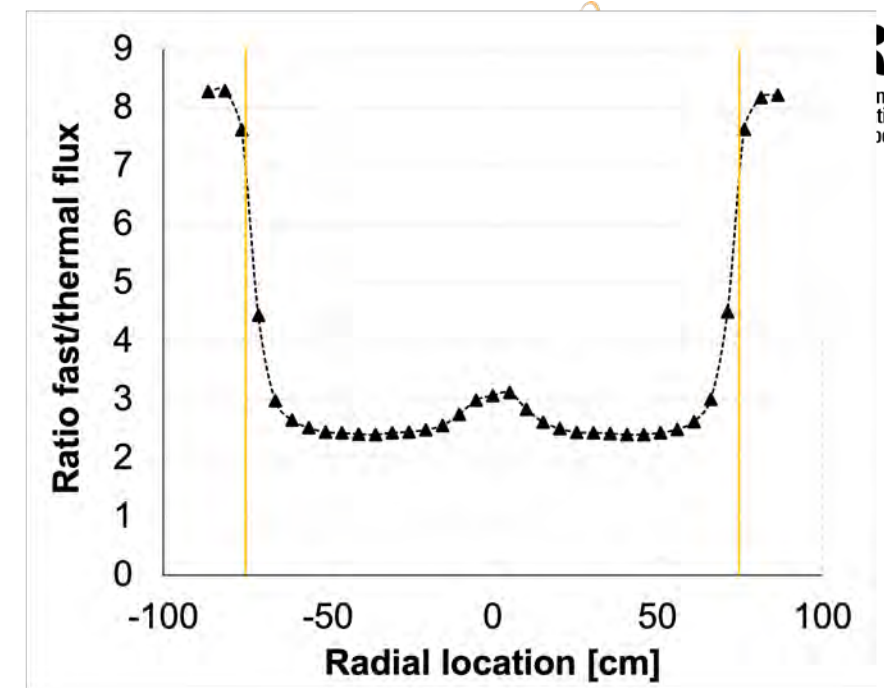
Figure modified from: R. C. Robertson (1965), "MSRE Design and Operations Report Part I: Description of Reactor Design," ORNL-TM-0728, ORNL. 98

# Core power/flux distribution – flux



**Thermal flux**  
( $< 0.625$  eV)

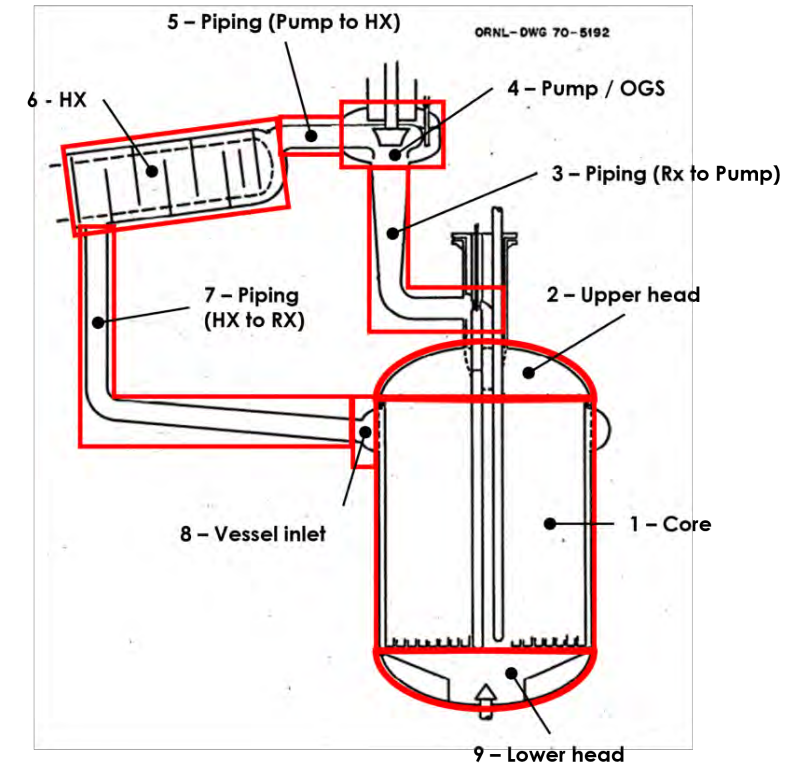
**Fast flux**  
( $> 0.625$  eV)





# Region-wise data

Region	Description	Volume (m <sup>3</sup> )	Residence Time (s)	<sup>235</sup> 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
<b>System Total</b>		<b>1.996</b>	<b>25.2</b>	<b>218</b>



# MELCOR for Accident Progression and Source Term Analysis



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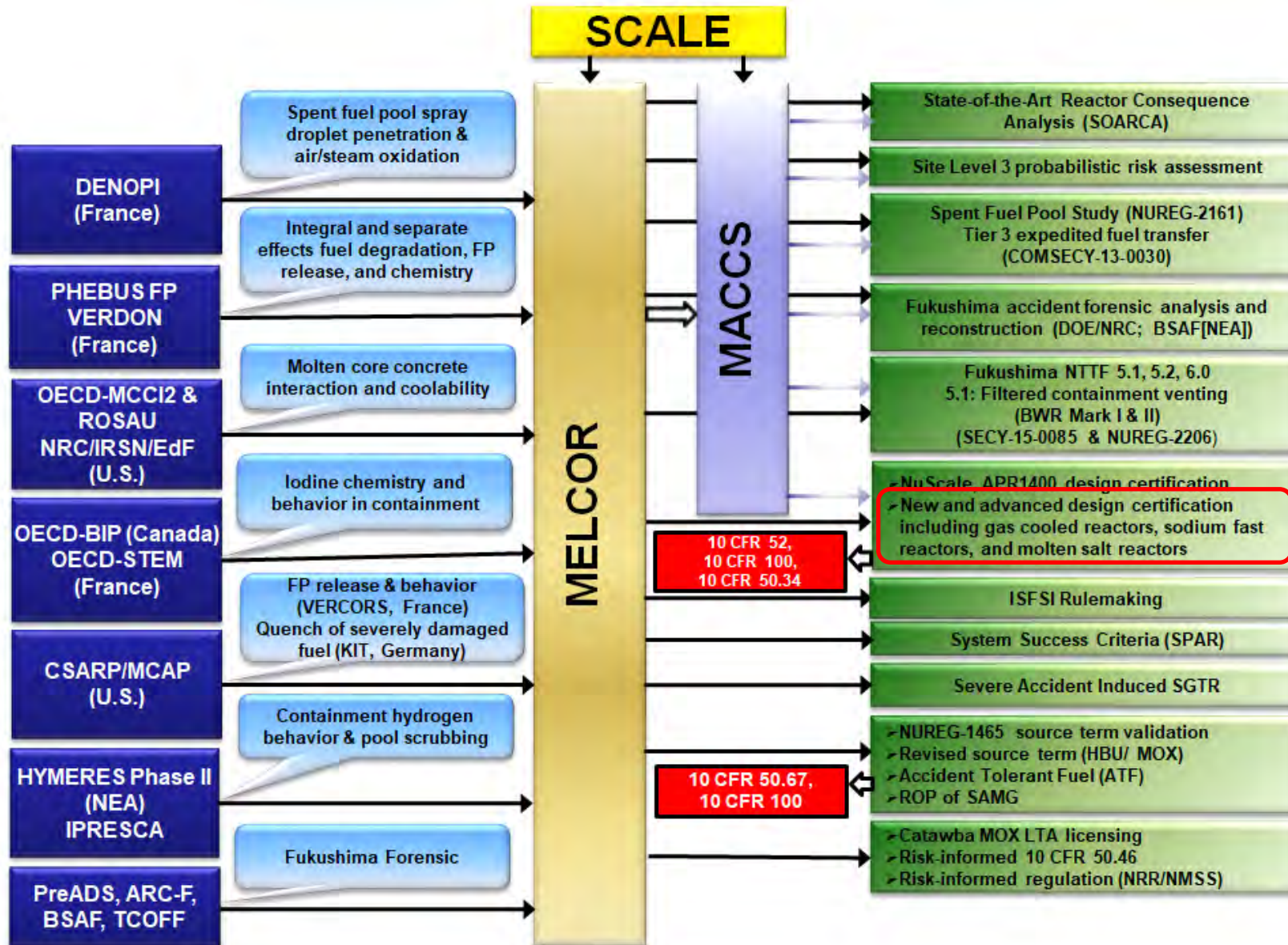


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# MELCOR Development for Regulatory Applications



## 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?

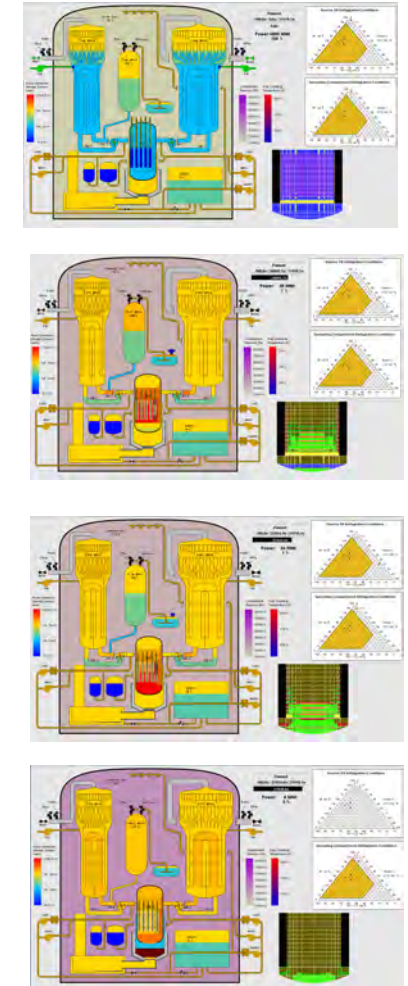
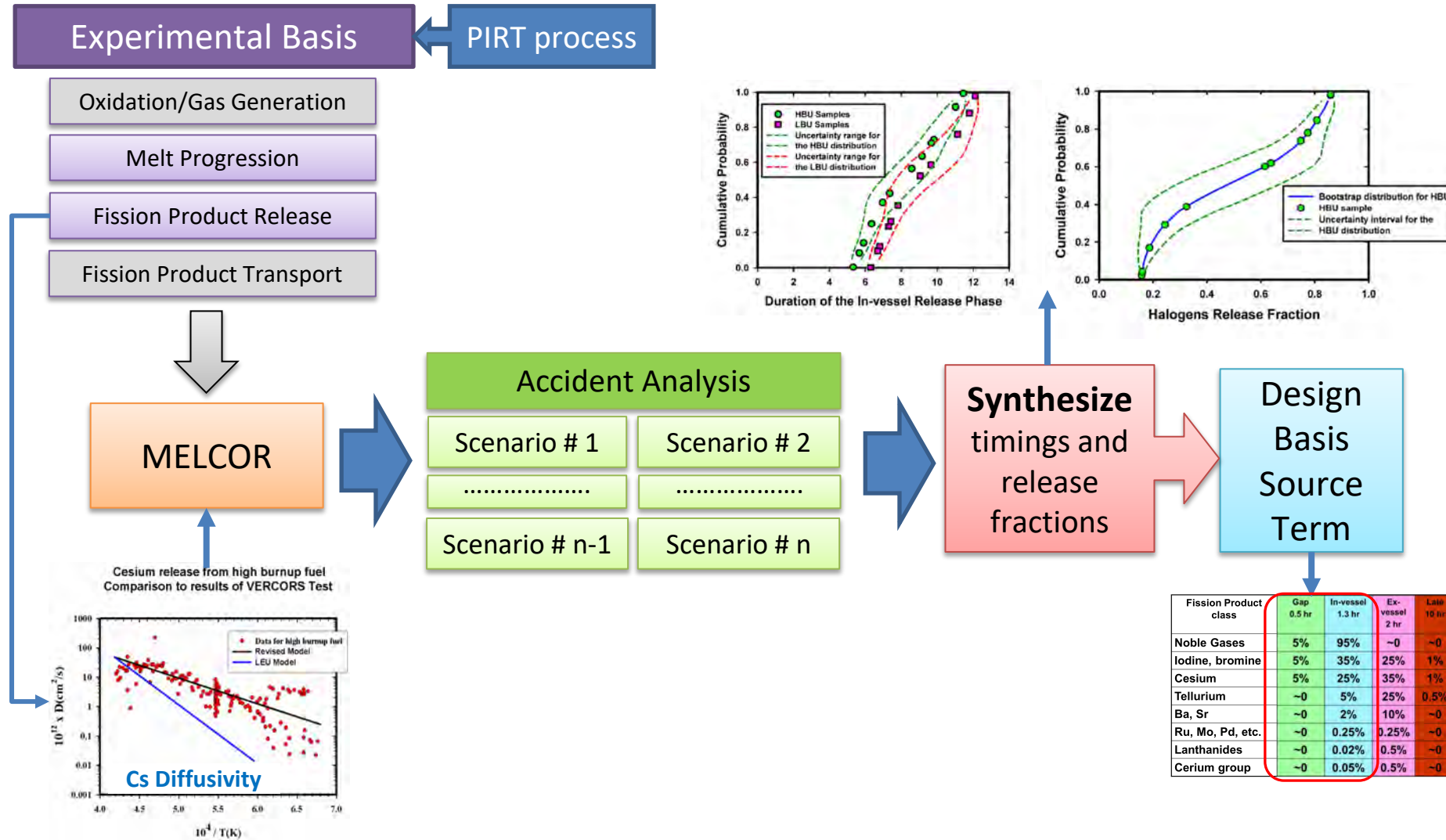
MELCOR is used to support severe accident and source term activities at NRC, including the development of regulatory source terms for LWRs, analysis of success criteria for probabilistic risk assessment models, site risk studies, and forensic analysis of the Fukushima accident.

## 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



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

## 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<sup>3</sup>)

#### 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

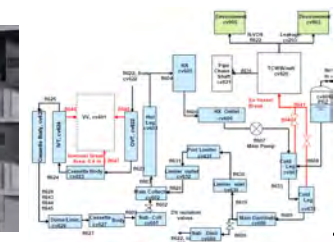
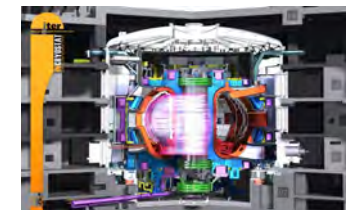
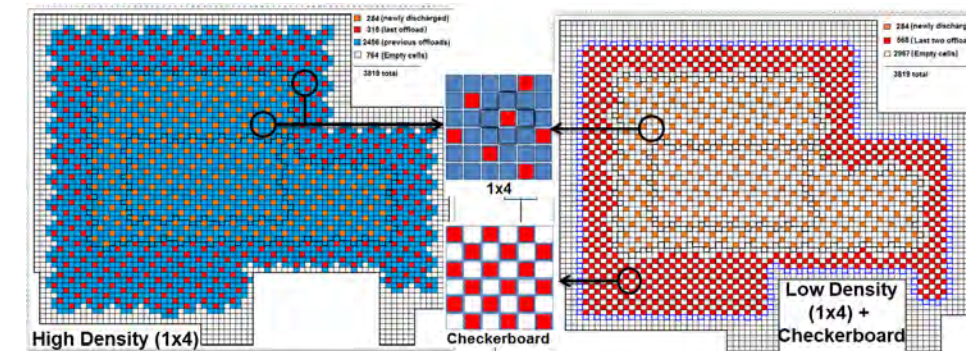
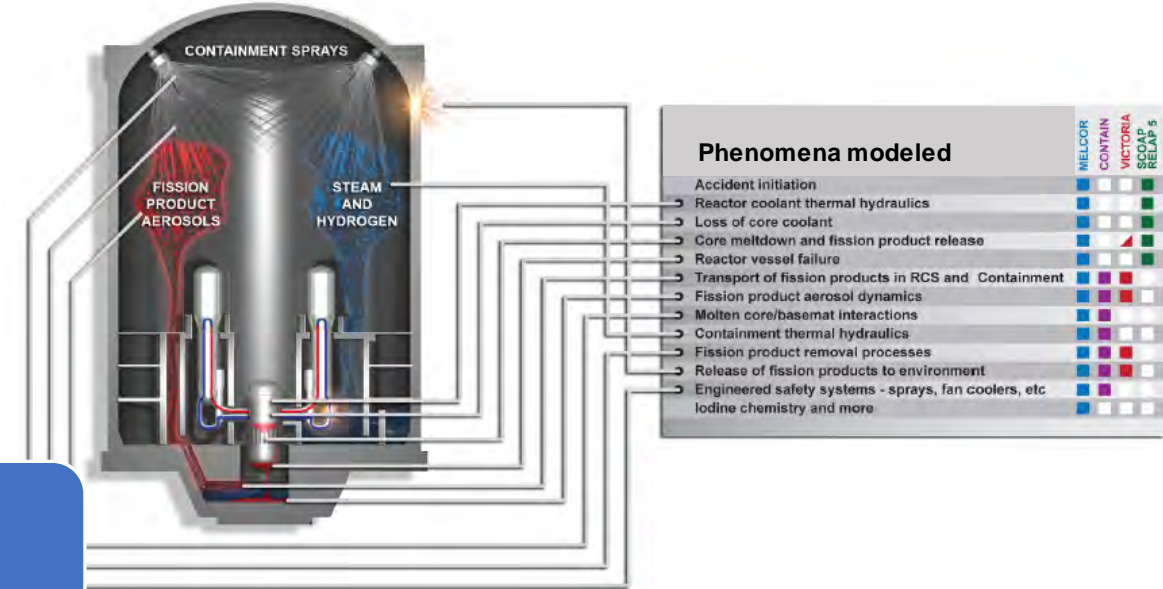
- Thermal-hydraulic response of reactor coolant system, reactor cavity, reactor enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

### 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

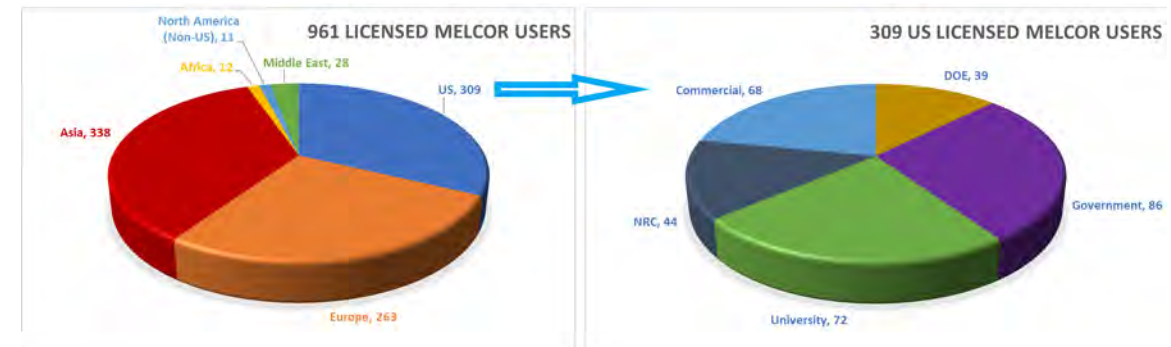
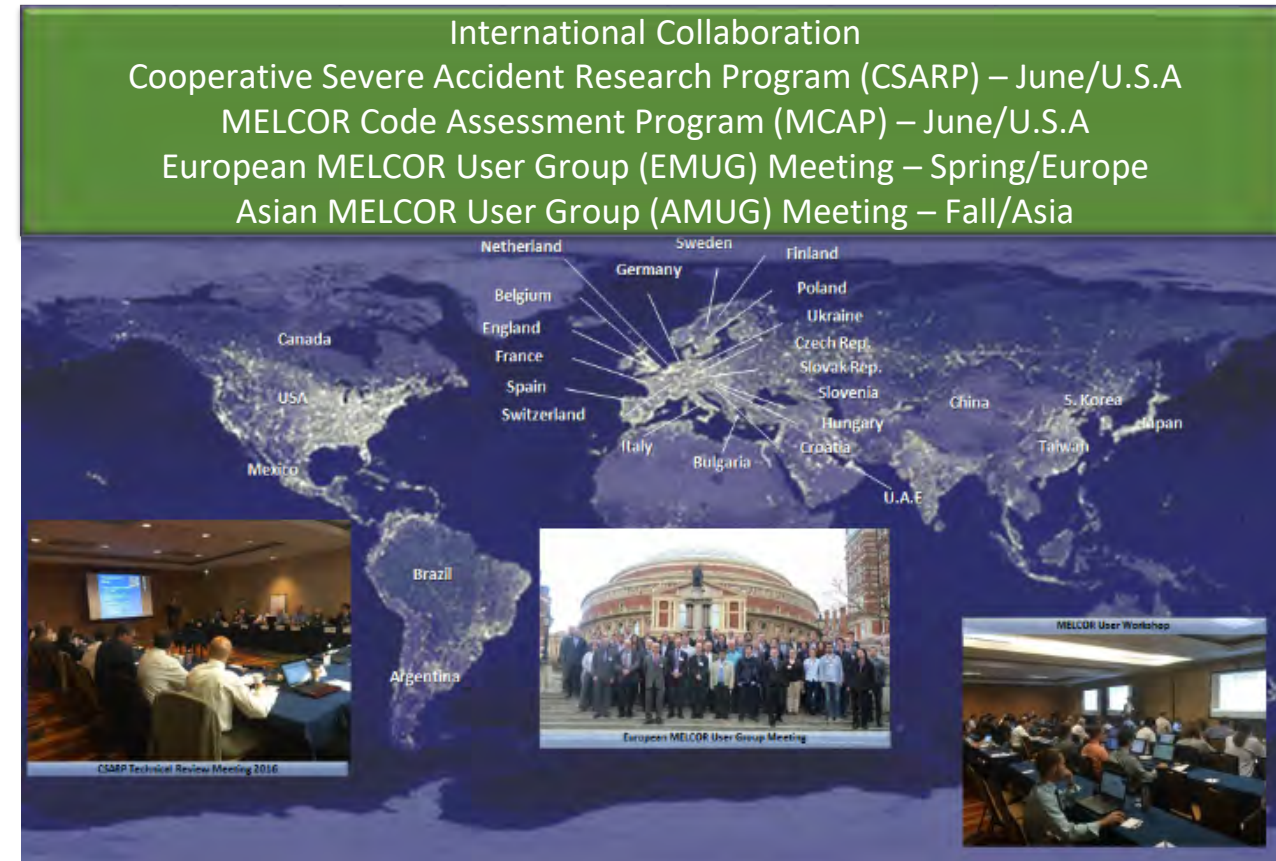
## MELCOR Pedigree

### 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

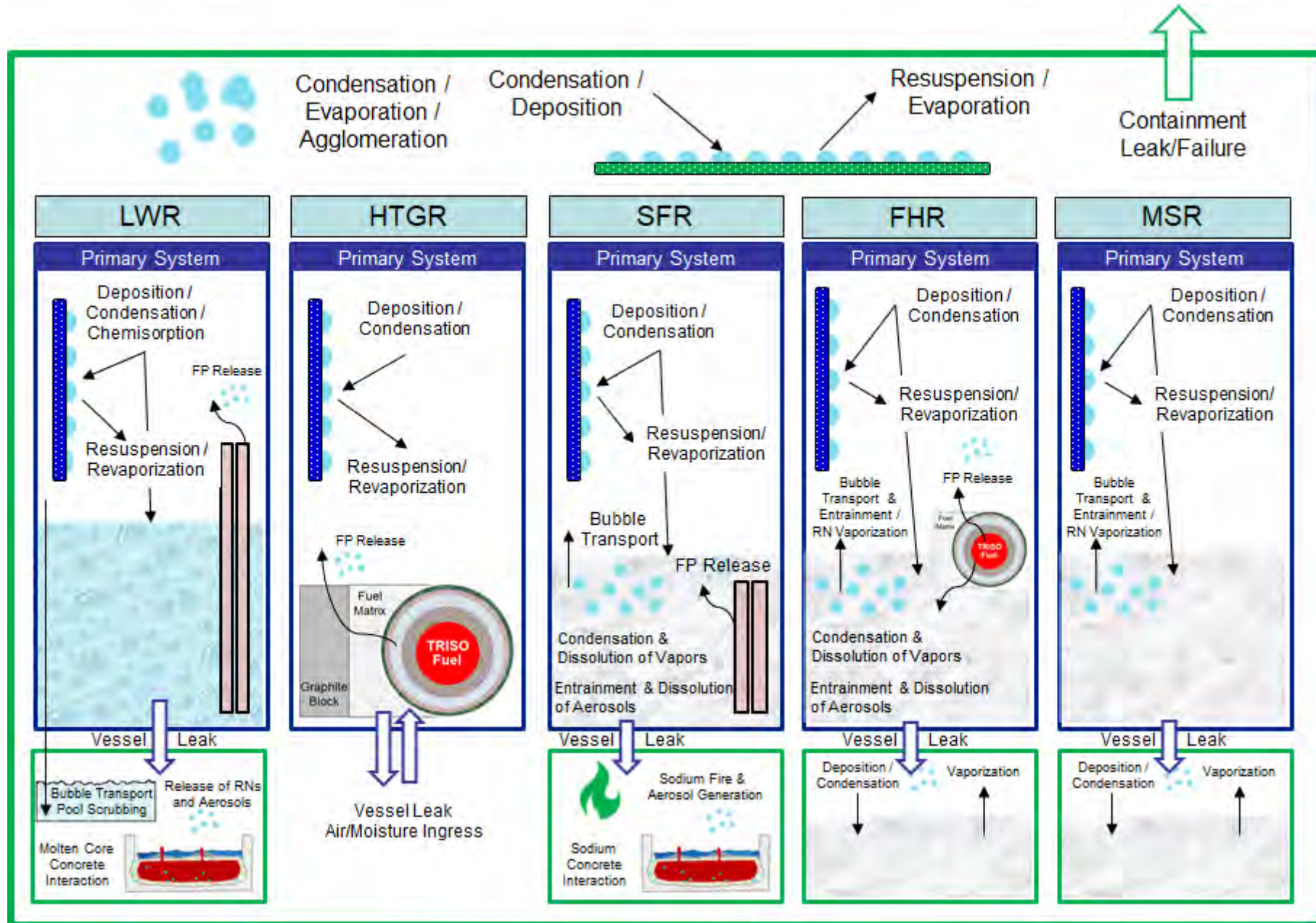
Cooperative Severe Accident Research Program (CSARP) is an NRC-sponsored international, collaborative community supporting the validation of MELCOR

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





# Common Phenomenology



# MELCOR Modeling Approach

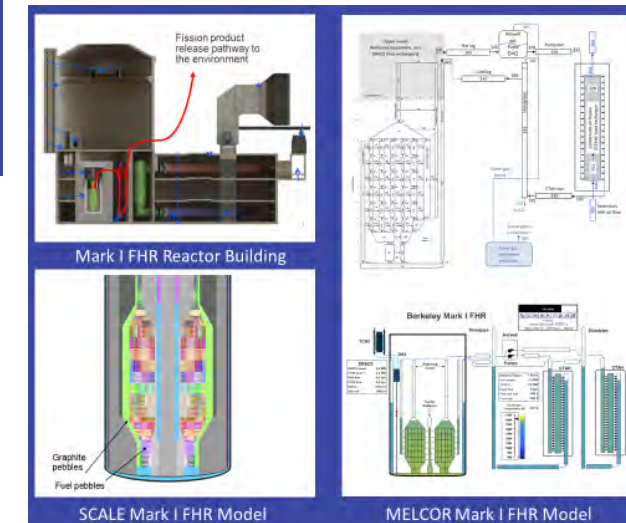
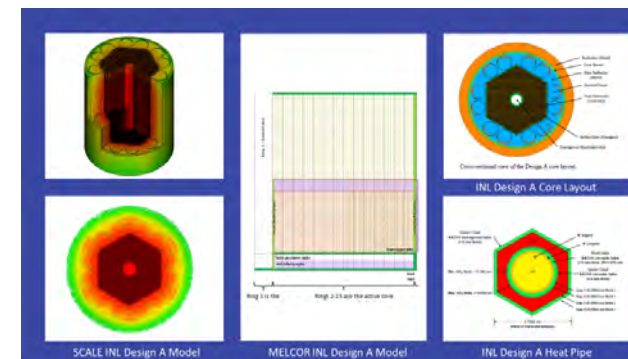
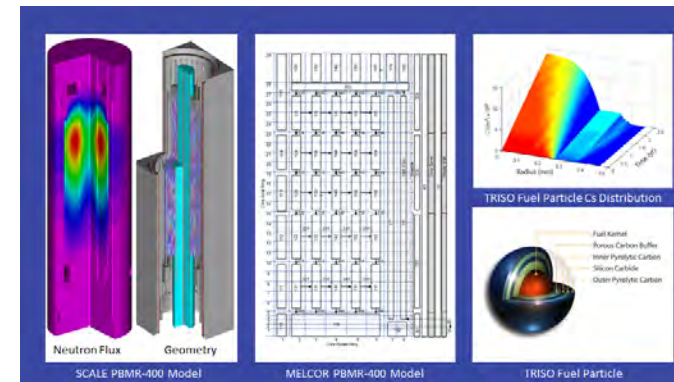
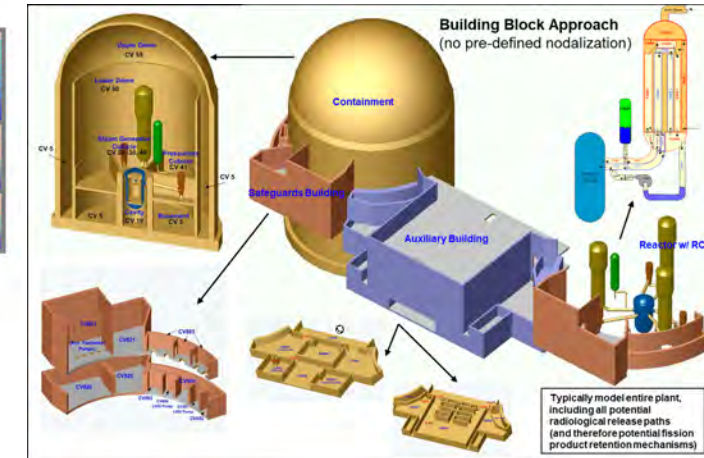
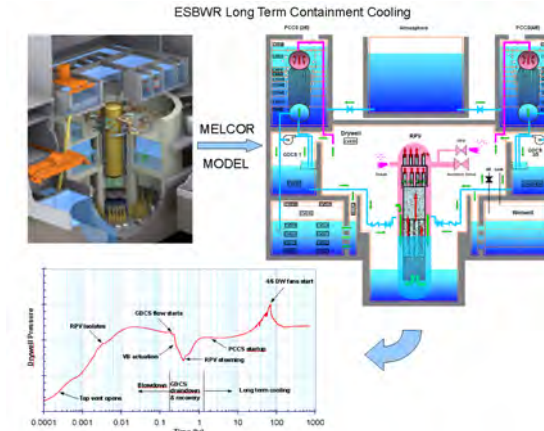
Modeling is mechanistic consistent with level of knowledge of phenomena supported by experiments

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

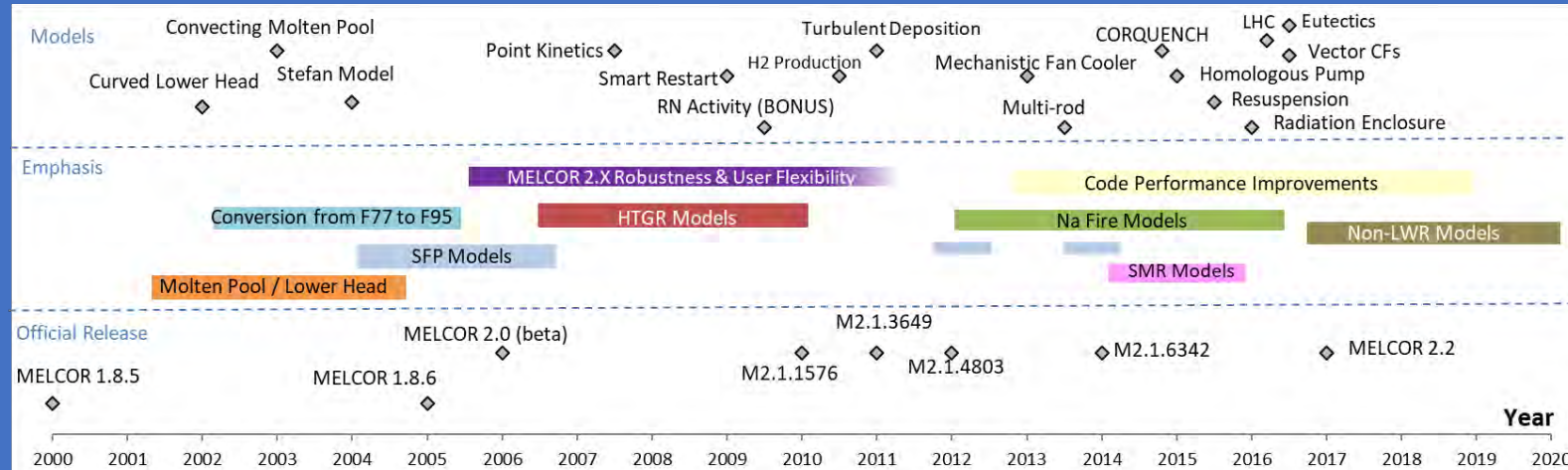
- Relatively easy to model novel designs
- All-purpose thermal hydraulic and aerosol transport code





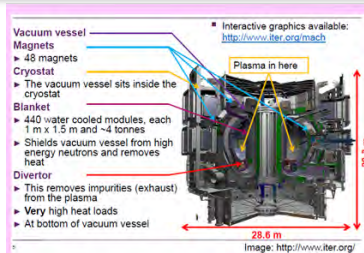
# MELCOR State-of-the-Art

## 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

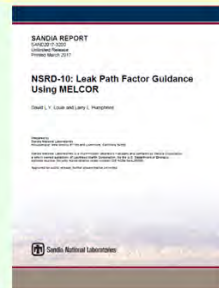
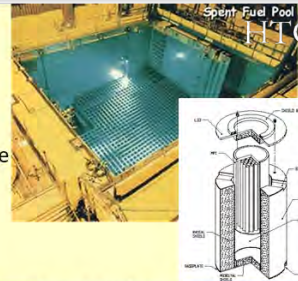


### Fusion

- 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

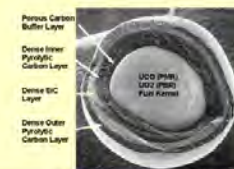


### Non-Nuclear Facilities

- 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



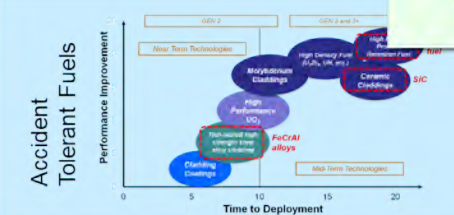
### Sodium Reactors

- 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
  - Thermo-mechanical properties





# MELCOR Software Quality Assurance – Best Practices

## 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

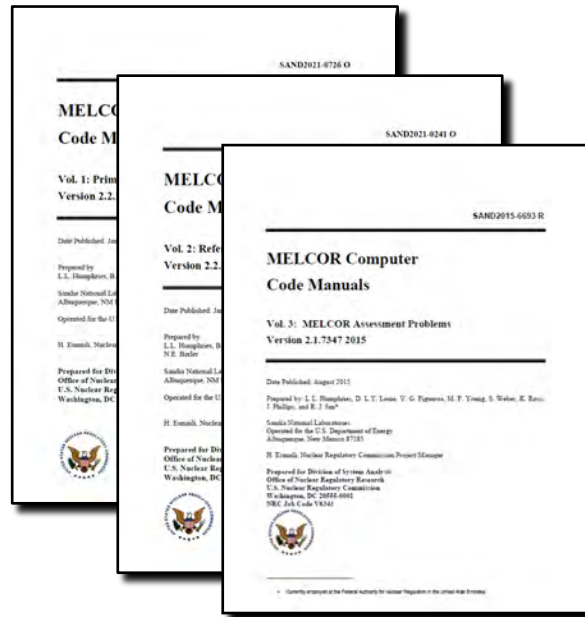
- External web page
- MELCOR workshops
- MELCOR User Groups (EMUG & AMUG)



	BUR	CAV	CF	COR	CVH	DCH	FCL	FDI	FL	HS	NCG	PAR	RN	SPR
Case														
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	

Table 1-1: Physics Package Coverage

# MELCOR Verification & Validation Basis



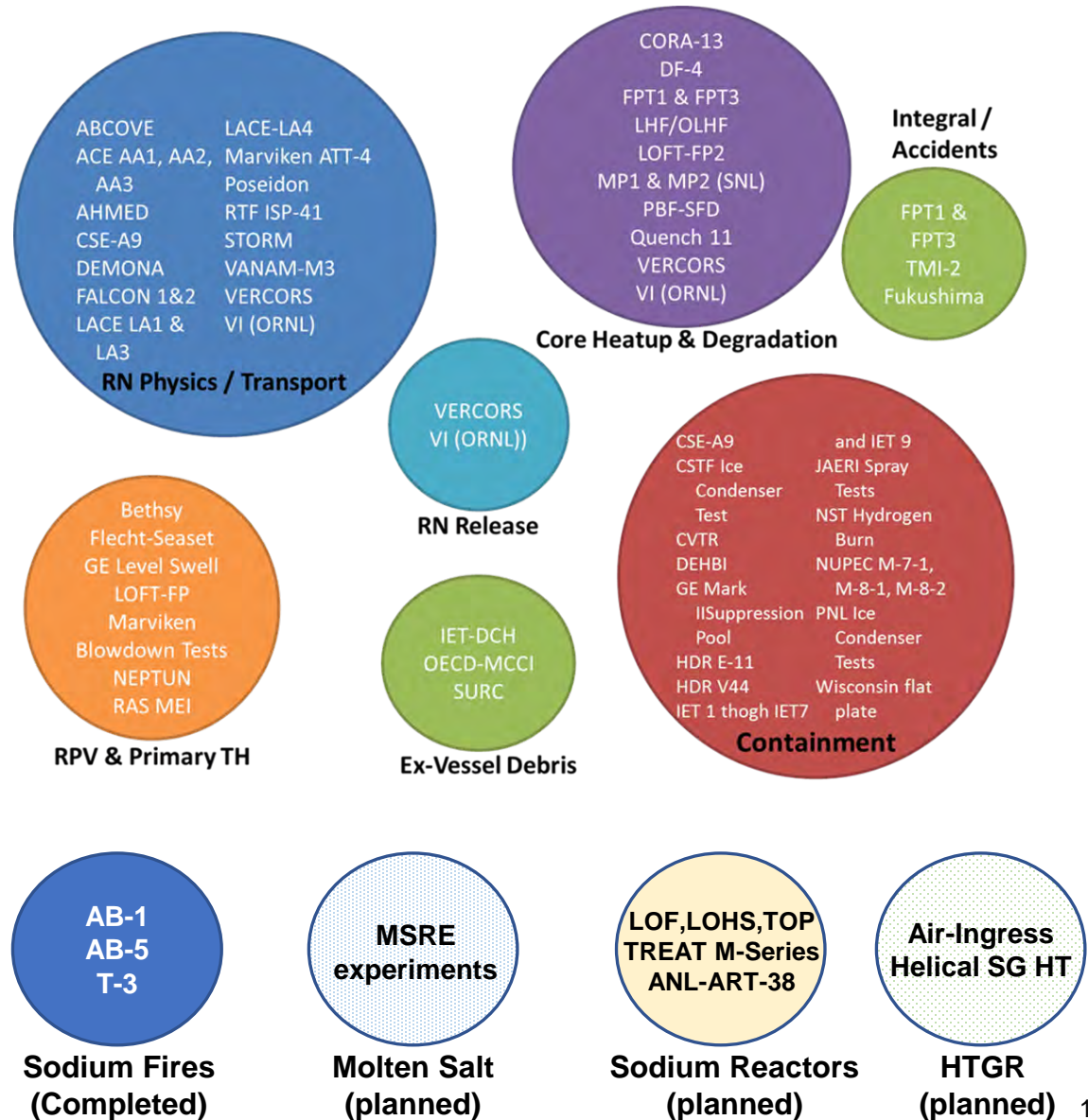
**Volume 1: Primer & User Guide**  
**Volume 2: Reference Manual**  
**Volume 3: MELCOR Assessment Problems**  
 [SAND2015-6693 R]

## 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

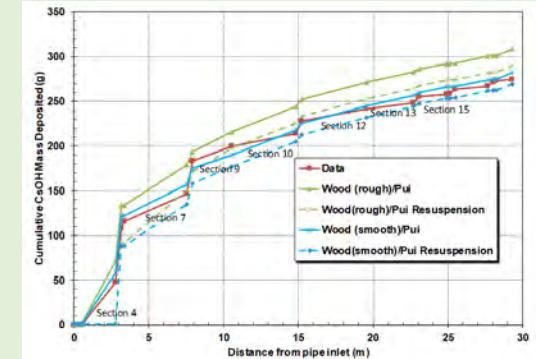
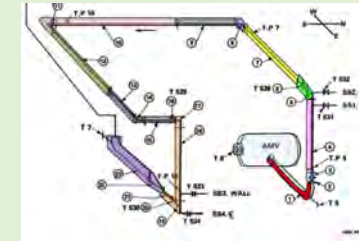
Case	1a	1b	2a	2b	3a	3b
US/INL	0.467	1.0	0.026	0.996	1.32E-4	0.208
US/GA	0.453	0.97	0.006	0.968	7.33E-3	1.00
US/SNL	0.465	1.0	0.026	0.995	1.00E-4	0.208
US/NRC	0.463	1.0	0.026	0.989	1.25E-4	0.207
France	0.472	1.0	0.028	0.995	6.59E-5	0.207
Korea	0.473	1.0	0.029	0.995	4.72E-4	0.210
Germany	0.456	1.0	0.026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

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

## Turbulent Deposition

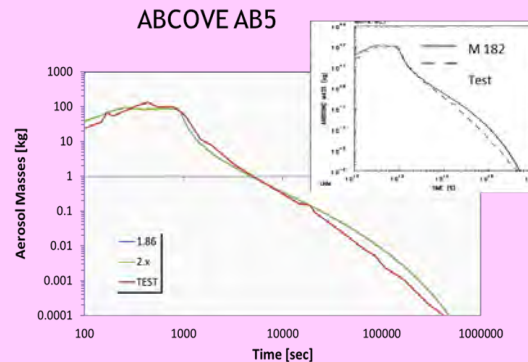


## Aerosol Physics

- Agglomeration
- Deposition
- Condensation and Evaporation at surfaces

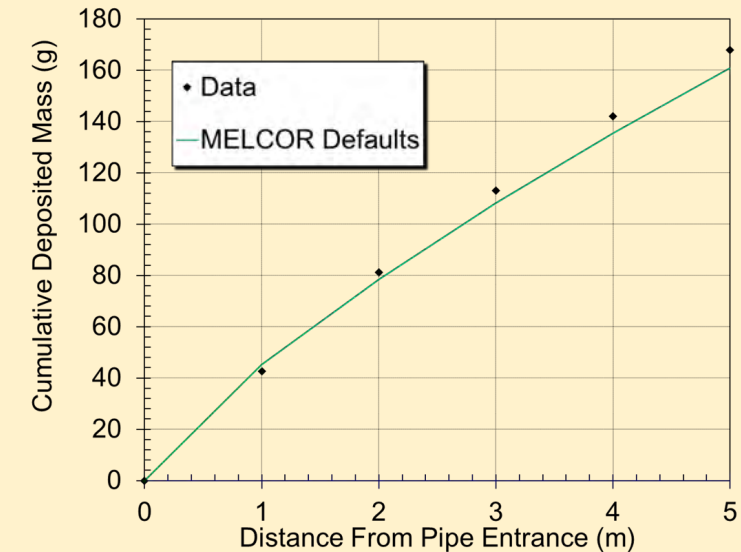
### Validation Cases

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



## Resuspension

STORM (Simplified Test of Resuspension Mechanism) test facility



# MELCOR Modernization

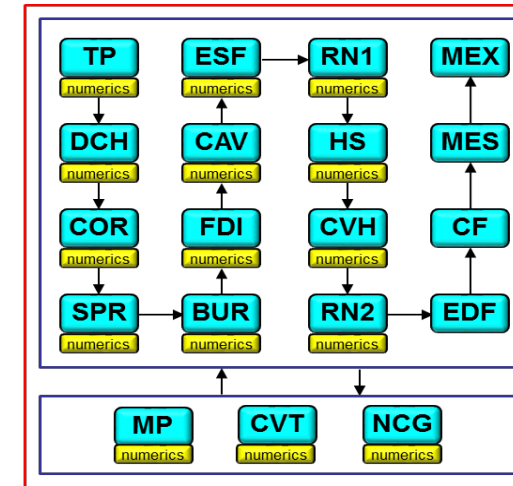
Generalized numerical solution engine

Hydrodynamics

In-vessel damage progression

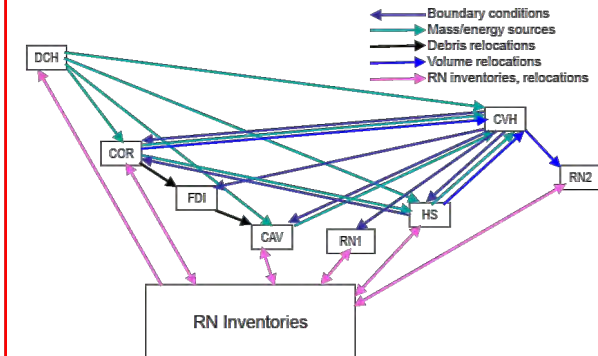
Ex-vessel damage progression

Fission product release and transport

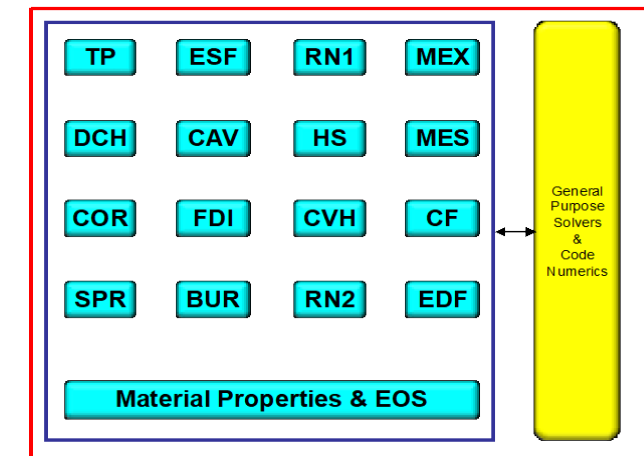


TP = Transfer Process  
DCH = Decay Heat  
COR = Core  
SPR = Containment Spray  
BUR = Gas Combustion  
FDI = Fuel Dispersion Interaction  
CAV = Cavity (MCCI)  
ESF = Engineered Safety Features  
MP = Material Properties

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 Condensable Gas

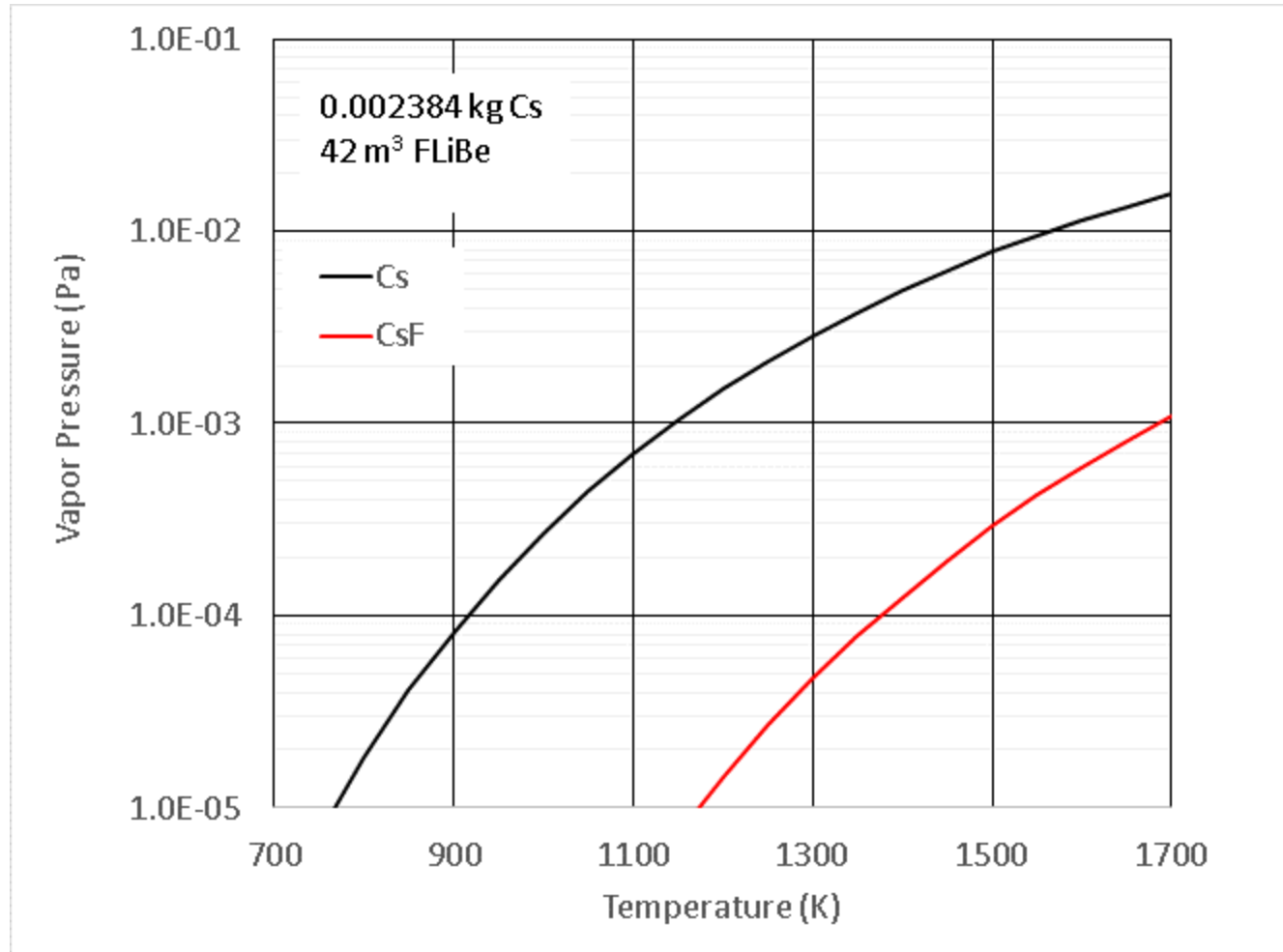


Separate **Physics** & **Numerics**





# 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

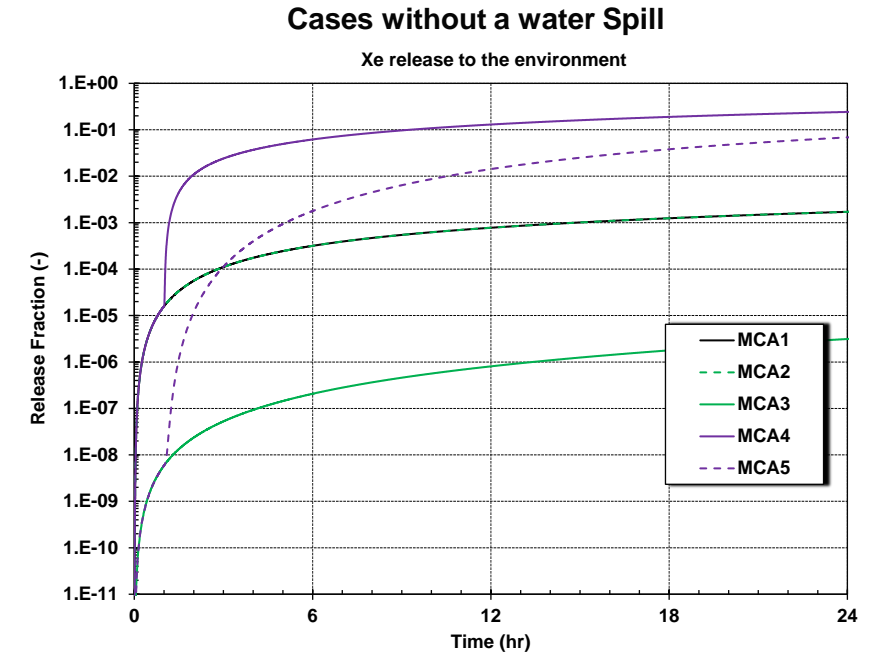
- Soluble fission products
- Insoluble/colloidal fission products
- Deposited fission products
- Gaseous fission products

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 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No

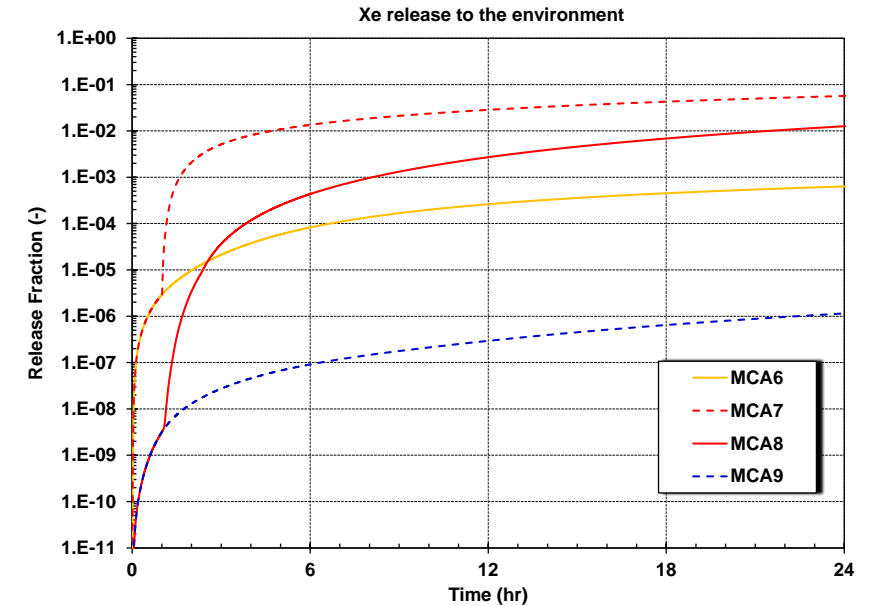
Note: Results assume no xenon retention in the charcoal filters.

# 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



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

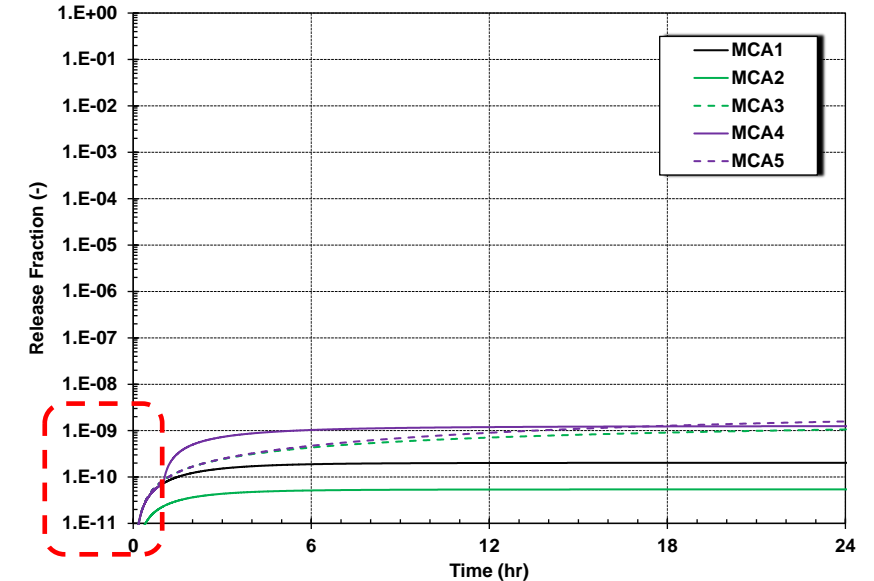
- MCA3, MCA4, and MCA5 releases to the environment were approximately the same and larger than MCA1
  - MCA4 and MCA5 included continuous venting of very small aerosols from the reactor cell through the auxiliary filter
  - MCA3 results show impact of nominal leakage from the reactor building (i.e., 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 $\mu\text{m}$	Yes	No	No
MCA2	10 $\mu\text{m}$	Yes	No	No
MCA3	1 $\mu\text{m}$	No	No	No
MCA4	1 $\mu\text{m}$	Yes	Yes	No
MCA5	1 $\mu\text{m}$	No	Yes	No

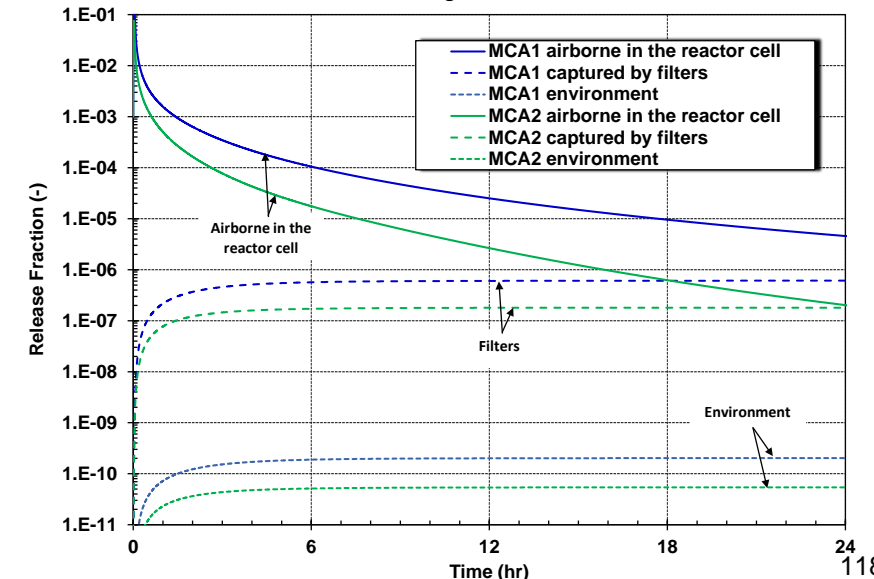
Note: The capture efficiency of the absolute filters for aerosols below  $<0.3 \mu\text{m}$  was assumed to be zero.

Cases without a water Spill  
Ce release to the environment



1 versus 10  $\mu\text{m}$  aerosol behavior

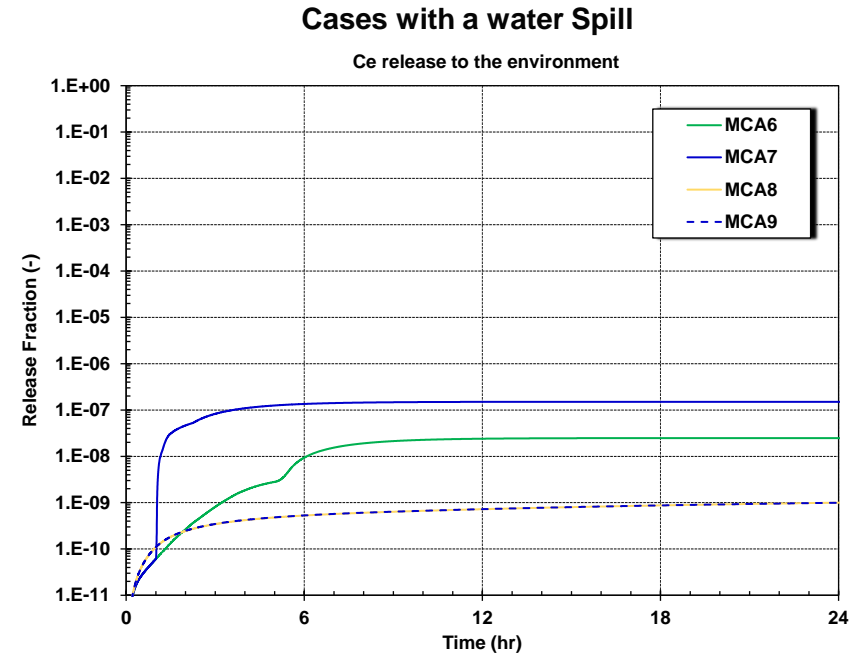
Ce settling and filter behavior



# 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**

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 $\mu\text{m}$	Yes	No	Yes
MCA7	1 $\mu\text{m}$	Yes	Yes	Yes
MCA8	1 $\mu\text{m}$	No	Yes	Yes
MCA9	1 $\mu\text{m}$	No	No	Yes

