

# SCALE/MELCOR Non-LWR Source Term Demonstration Project – Fluoride-Salt-Cooled High-Temperature Reactor (FHR)

September 14, 2021



# U.S. NRC



**Sandia  
National  
Laboratories**

# Outline

NRC strategy for non-LWR source term analysis

Project scope

Overview of Fluoride-salt-cooled High-temperature Reactor (FHR)

FHR reactor fission product inventory/decay heat methods & results

MELCOR molten salt models

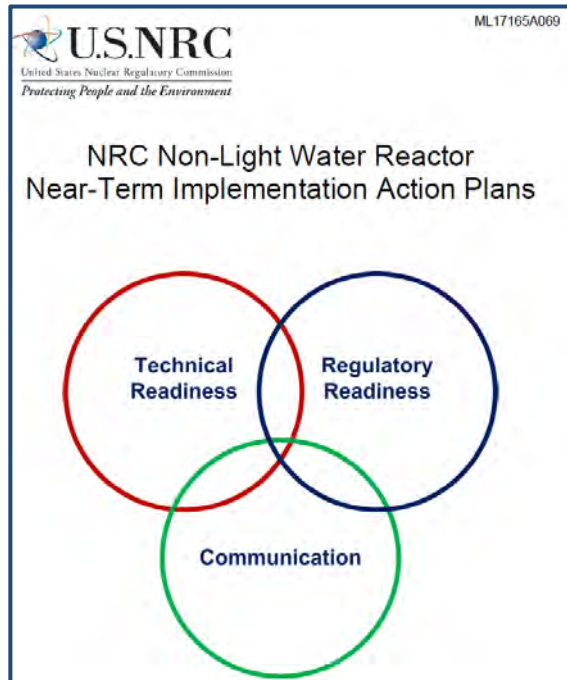
FHR plant model and source term analysis

Summary

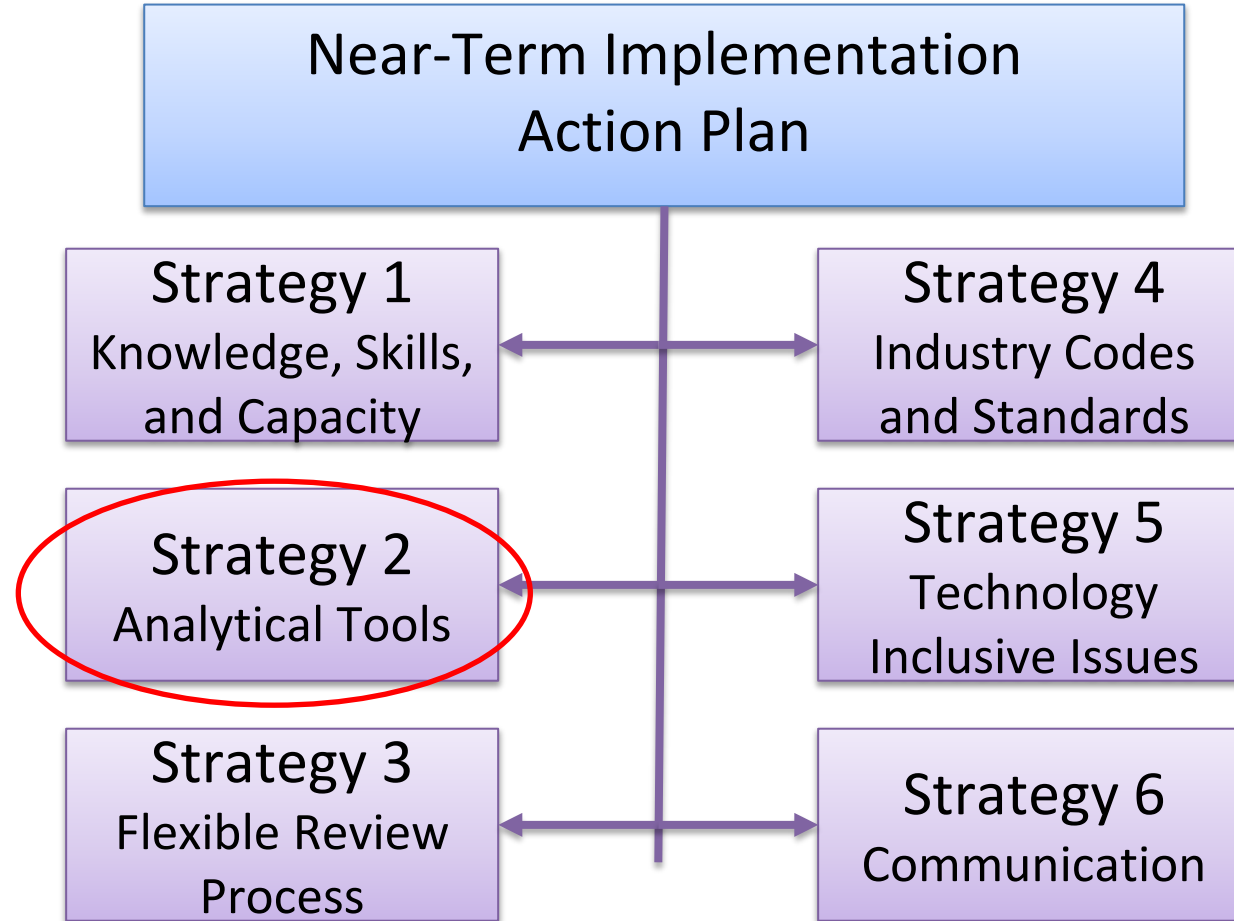
Background slides

- SCALE
- MELCOR

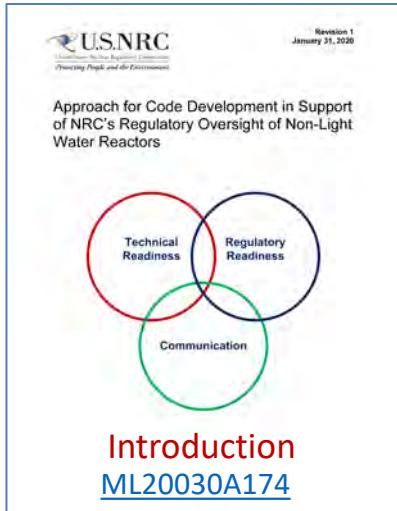
# Integrated Action Plan (IAP) for Advanced Reactors



[ML17165A069](#)

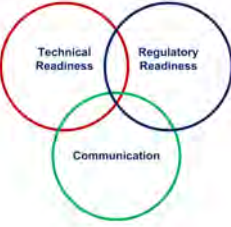


# IAP Strategy 2 Volumes



U.S. NRC  
Revision 1  
January 31, 2020

Approach for Code Development in Support of NRC's Regulatory Oversight of Non-Light Water Reactors



**Introduction**  
[ML20030A174](#)



U.S. NRC  
Revision 1  
January 31, 2020

NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 1 – Computer Code Suite for Non-LWR Plant Systems Analysis



**Volume 1**  
[ML20030A176](#)



U.S. NRC  
Revision 1  
January 31, 2020

NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 2 – Fuel Performance Analysis for Non-LWRs



**Volume 2**  
[ML20030A177](#)



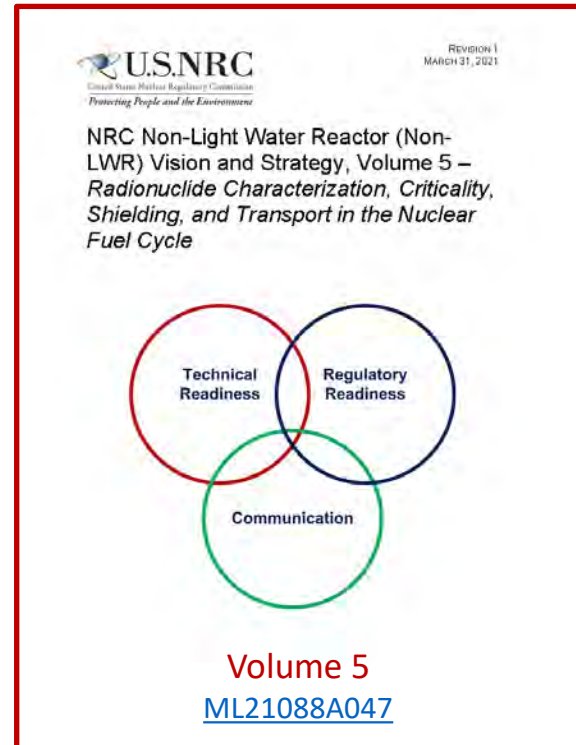
U.S. NRC  
Revision 1  
March 31, 2021

NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 4 – Licensing and Siting Dose Assessment Codes



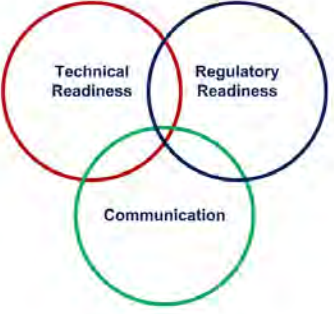
**Volume 4**  
[ML21085A484](#)

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

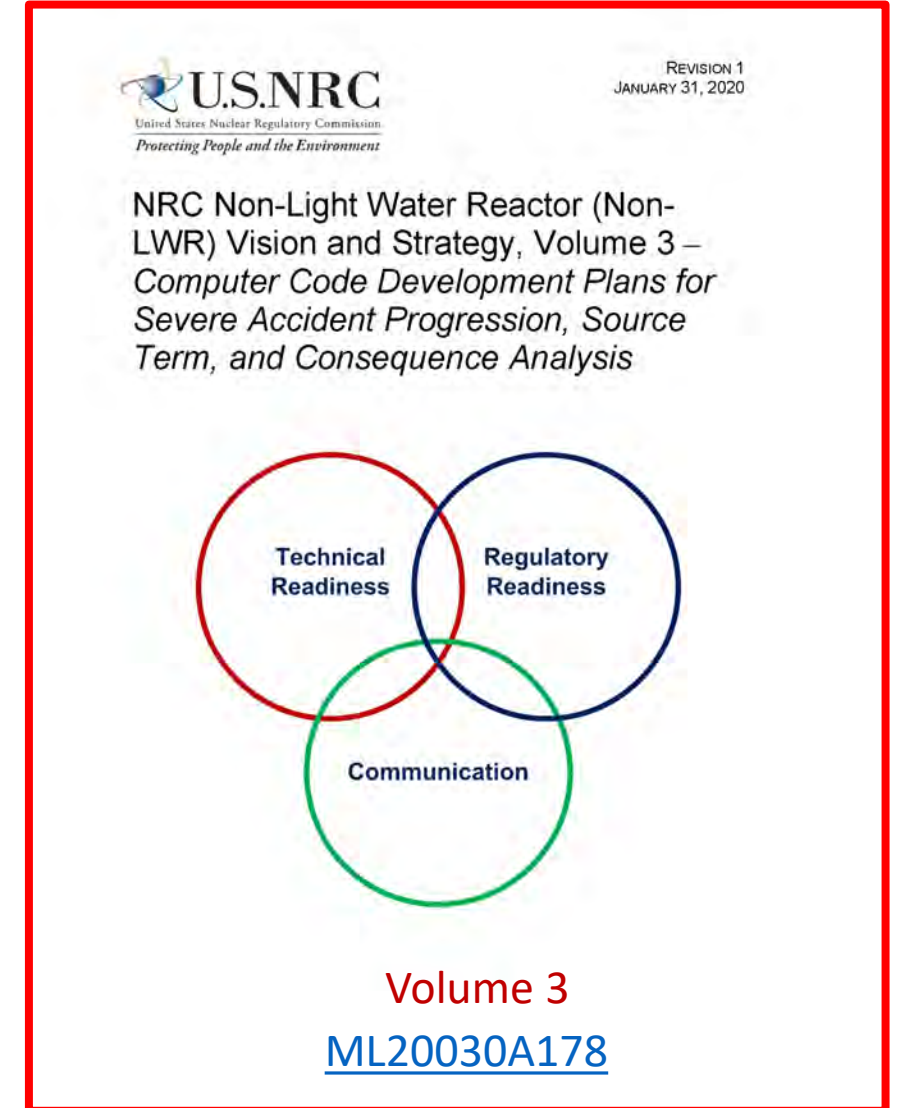


U.S. NRC  
Revision 1  
MARCH 31, 2021

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



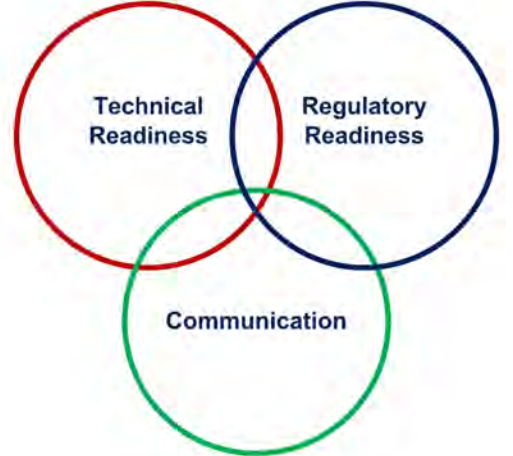
**Volume 5**  
[ML21088A047](#)



U.S. NRC  
United States Nuclear Regulatory Commission  
Protecting People and the Environment

REVISION 1  
JANUARY 31, 2020

NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 3 – Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis



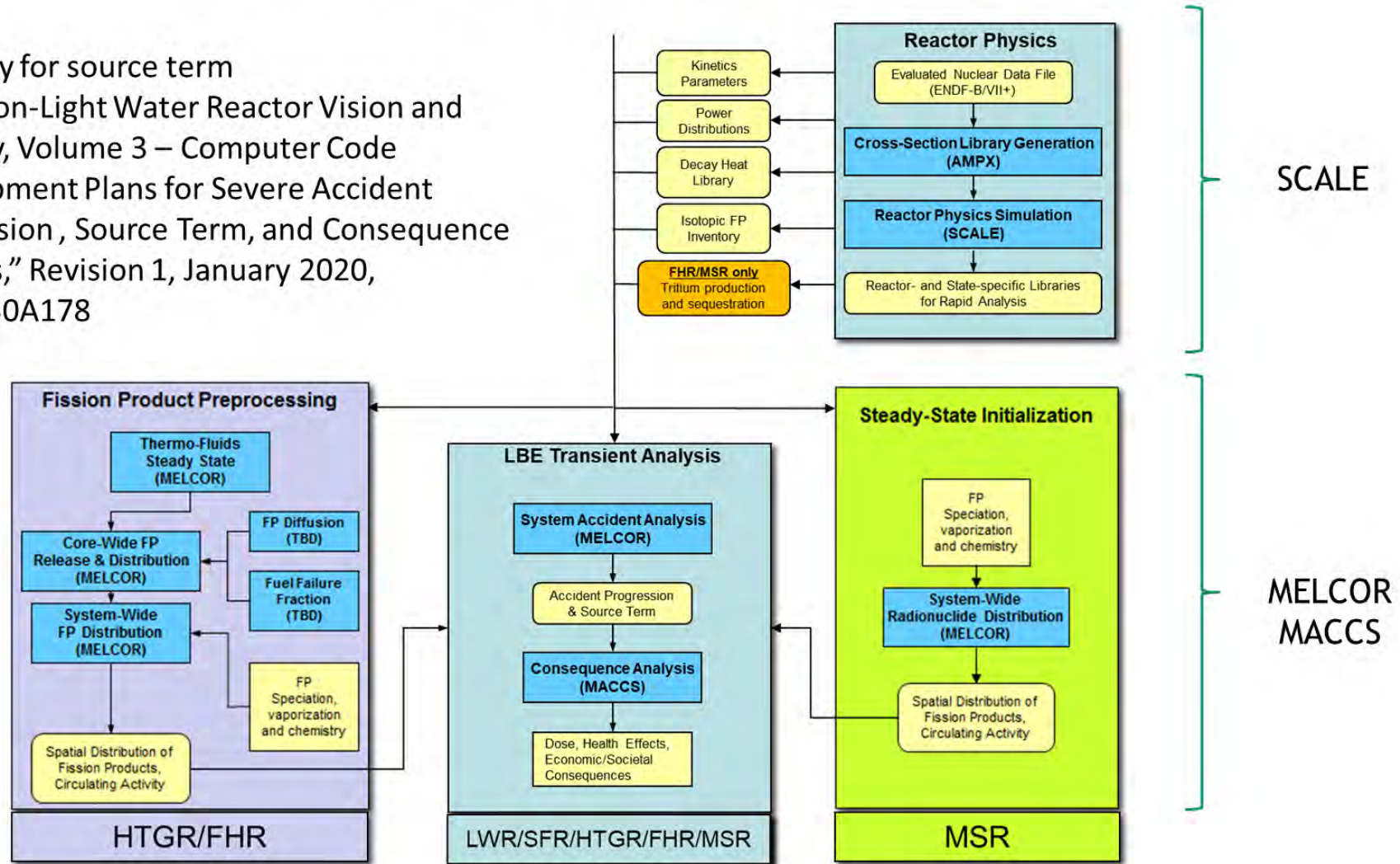
**Volume 3**  
[ML20030A178](#)



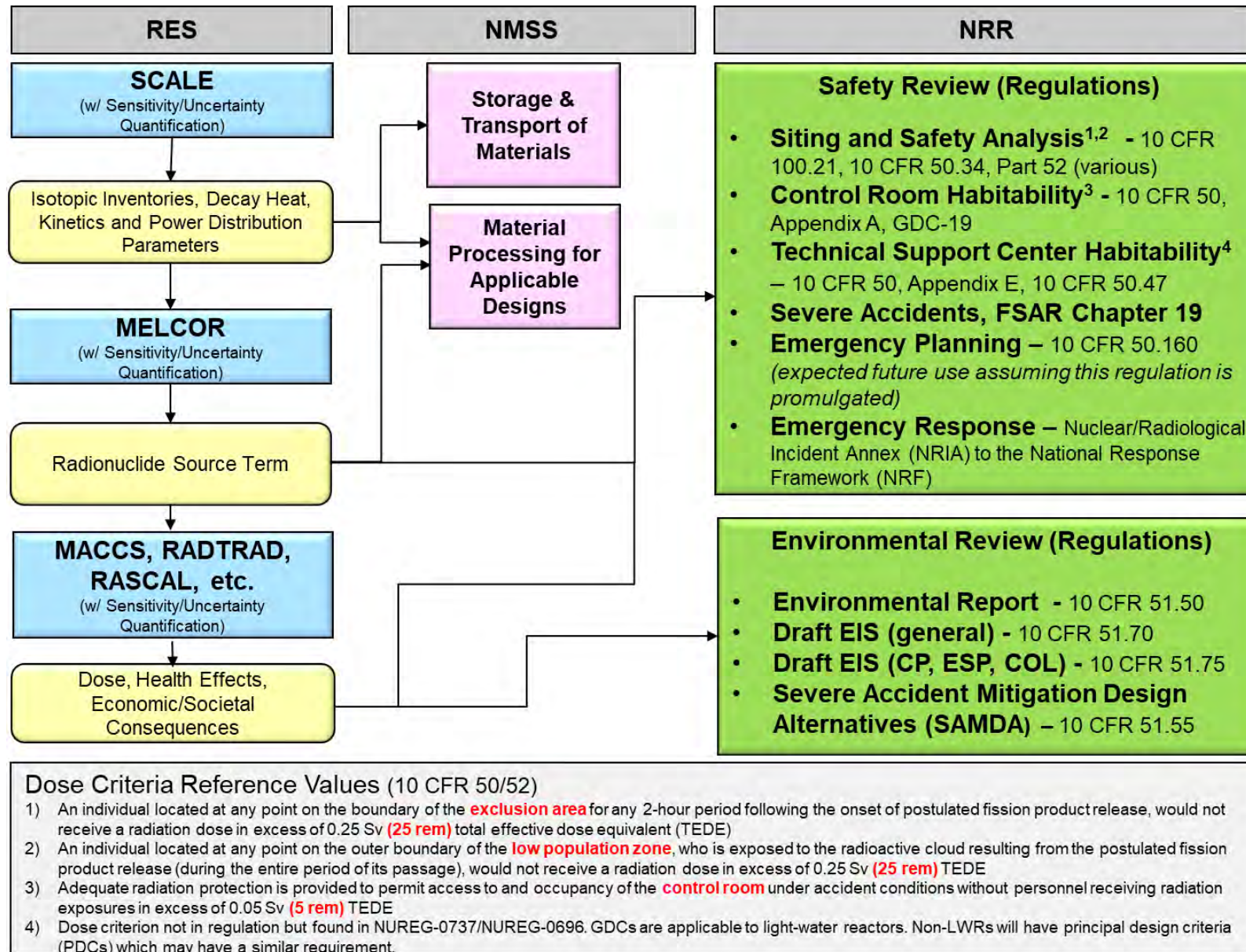
# NRC strategy for non-LWR analysis (Volume 3)

## Evaluation Model and Suite of Codes

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



# Role of NRC severe accident codes





# 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 for three representative non-LWRs (FY21)

- Heat pipe reactor – INL Design A
- Pebble-bed gas-cooled reactor – PBMR-400
- Pebble-bed molten-salt-cooled – UCB Mark 1

FY22

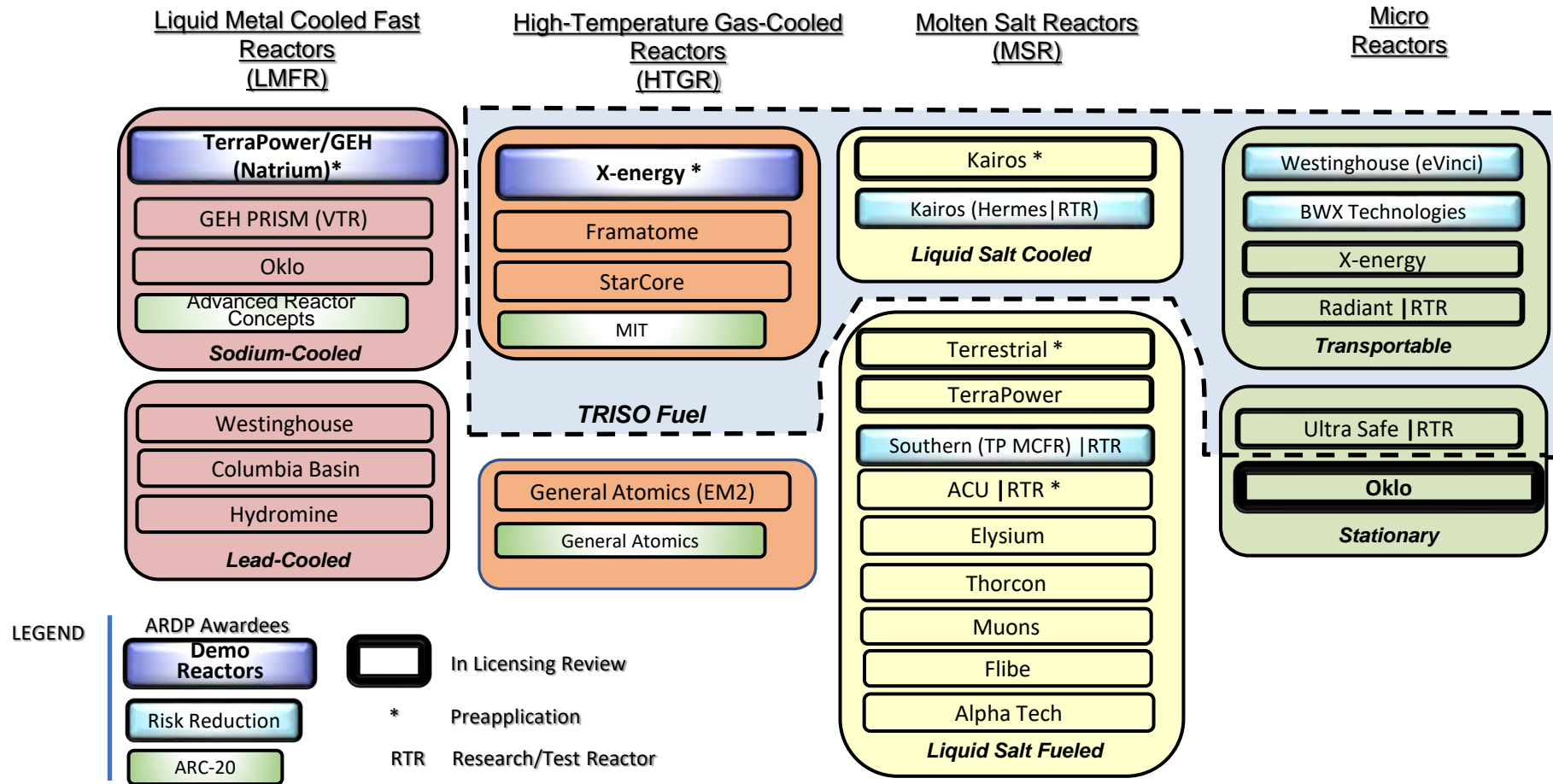
- Molten-salt-fueled reactor – MSRE
- Sodium-cooled fast reactor – To be determined



# Project approach

1. Build MELCOR full-plant input model
  - Use SCALE to provide decay heat and core radionuclide inventory
2. Scenario selection
3. Perform simulations for the selected scenario and debug
  - Base case
  - Sensitivity cases

# Advanced Reactor Designs



# Fluoride-Salt-Cooled High-Temperature Reactor (FHR)



**U.S. NRC**



# Molten-salt reactors (1/3)

## 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)]



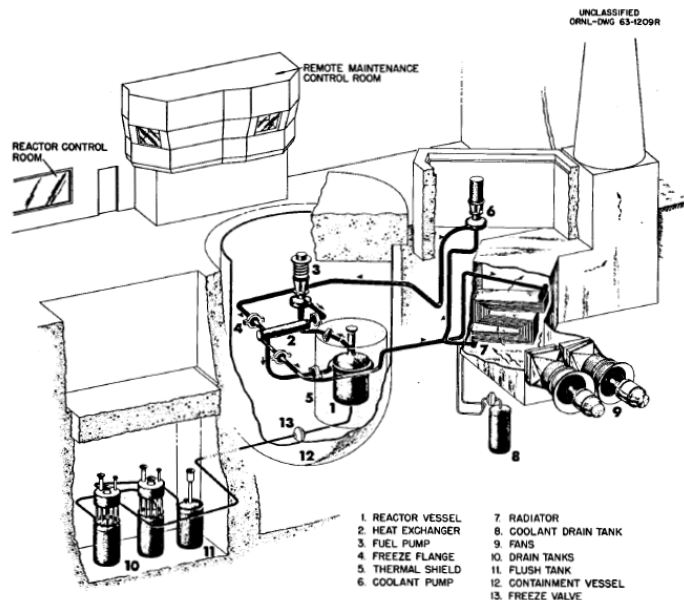
**Heat Transfer Reactor Experiment #3**

[[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 (2/3)

## ORNL Molten Salt Reactor (MSR)

- AEC funded the Molten Salt Reactor Experiment (MSRE)
- Operated from 1965 to 1969
- 30 MWt
- Coolant was FLiBe molten salt
- Fuel was dissolved in coolant (molten fuel)



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



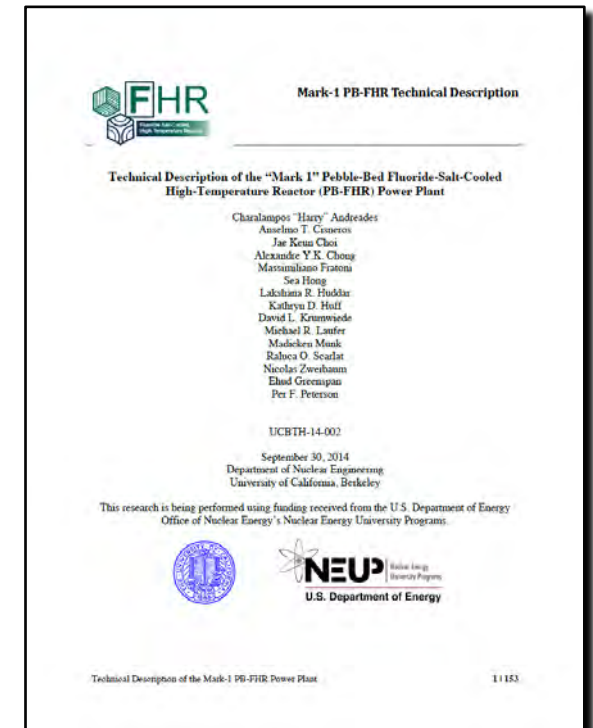
**MSRE Graphite Core Structure**  
[[https://en.wikipedia.org/wiki/Molten-Salt\\_Reactor\\_Experiment](https://en.wikipedia.org/wiki/Molten-Salt_Reactor_Experiment)]



# Molten-salt reactors (3/3)

## UCB Mark 1 – circa 2013

- Coolant is FLiBe molten salt
- Core is TRISO fuel in a pebble-bed geometry
- Design description
  - “Technical Description of the “Mark 1” Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant,” [UCBTH-14-002]
  - “Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR),” University of California, Berkeley, 2013.
- **Used for the SCALE/MELCOR demonstration project**



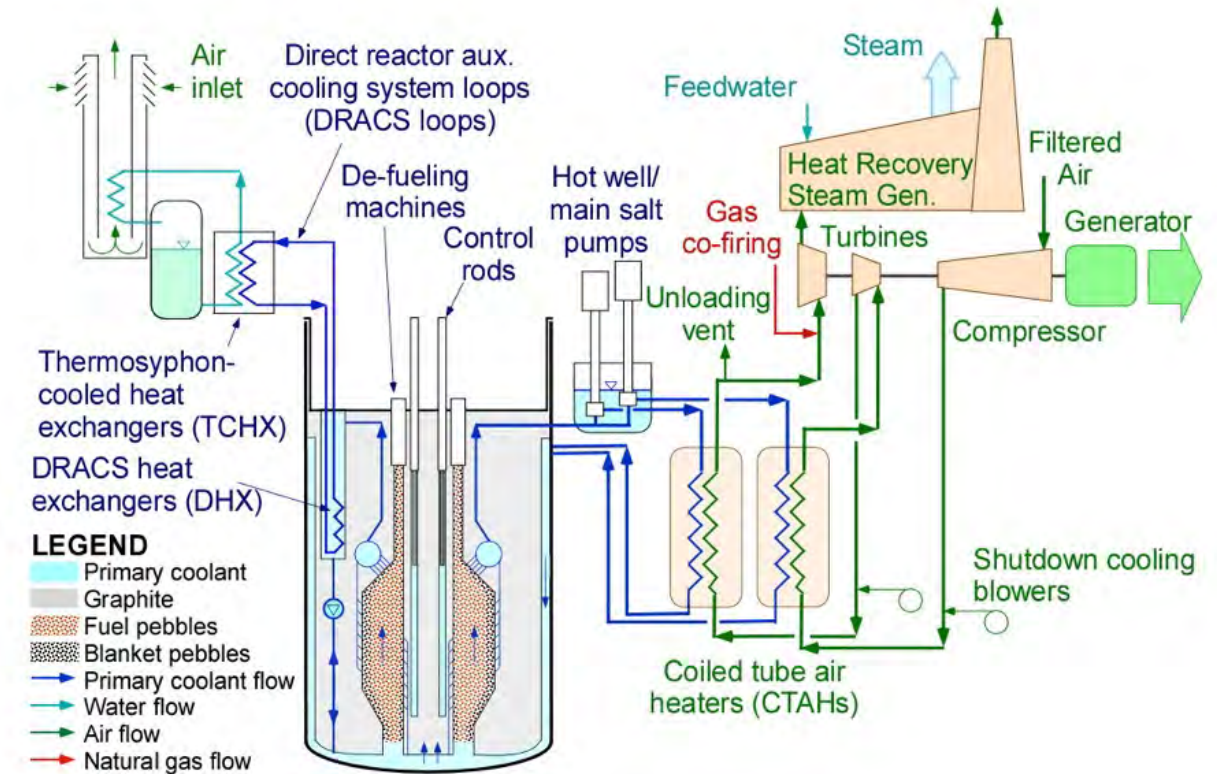
# UCB Mark 1 (1/4)

## Reactor

- 236 MW<sub>th</sub> / 100 MW<sub>e</sub>
- Atmospheric pressure
- 600°C core inlet
- 700°C core outlet
- 976 kg/s core flowrate
- FLiBe molten salt coolant

## Core

- 470,000 fueled pebbles + 218,000 unfueled pebbles in core and defueling chute
- 180 MWd/kgHM discharge burnup
- 19.9% enrichment
- Online refueling



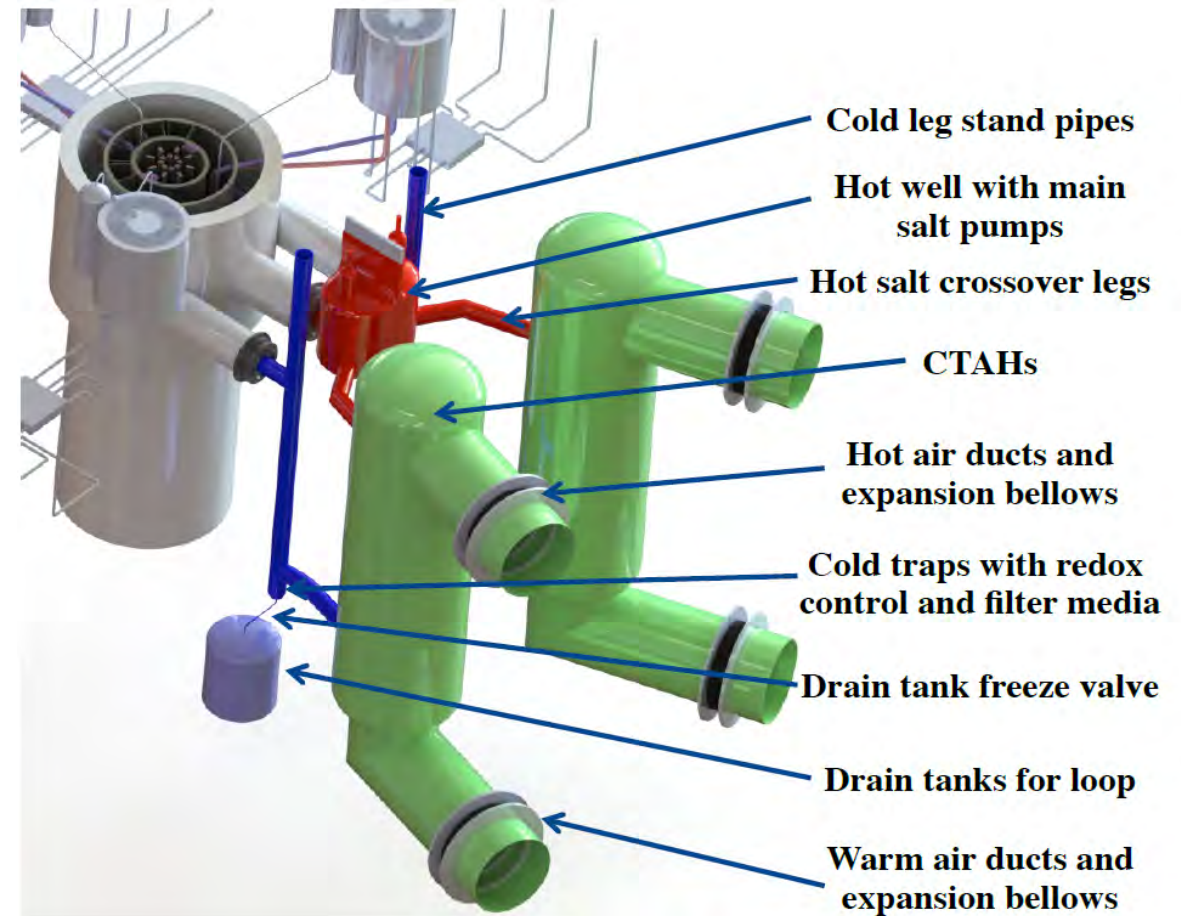
UCB Mark 1 schematic  
[UCBTH-14-002]

Secondary system: gas-turbine at 18.6 bar with natural gas co-firing capability

# UCB Mark 1 (2/4)

## Recirculation loops

- Salt pumps in the hot well with FLiBe free surface
- 2X cross-over legs to coiled tube air heaters (CTAH)
- 2X cold legs with standpipes with free surface
- Drain tank with freeze valve

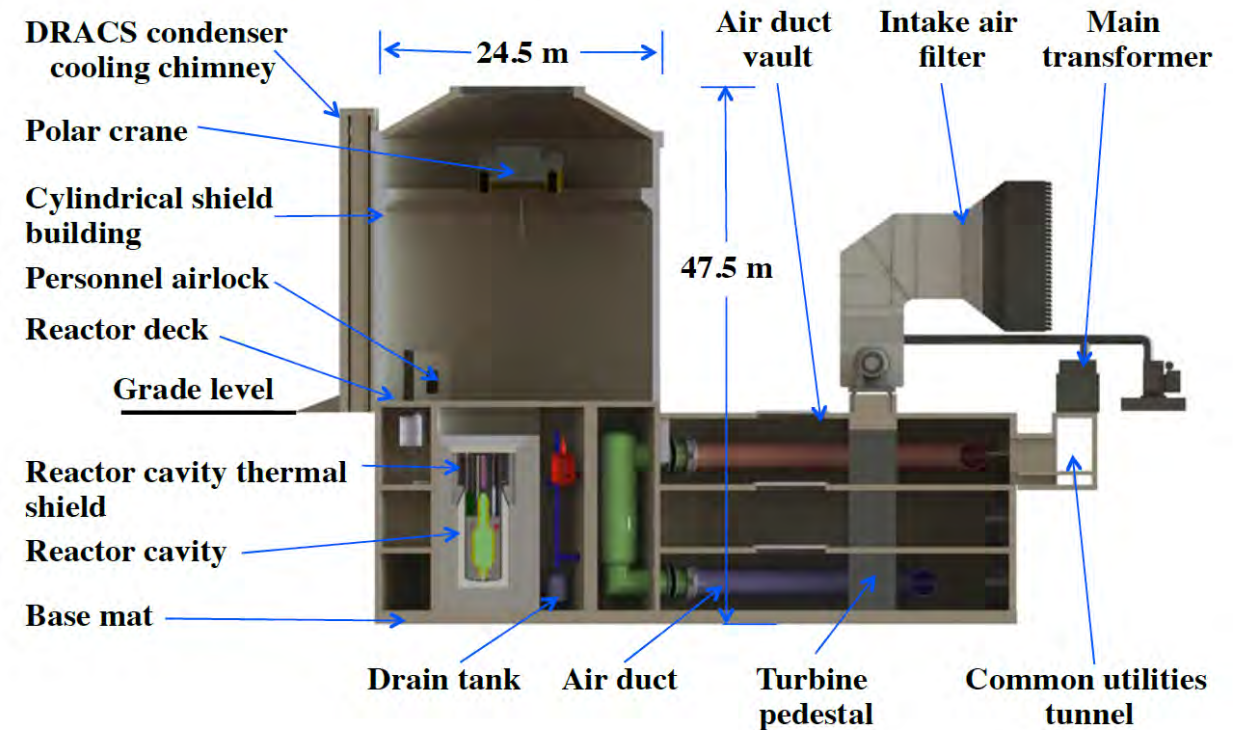


UCB Mark 1 schematic  
[UCBTH-14-002]

# UCB Mark 1 (3/4)

## Containment

- Most reactor and secondary components below-grade
- Compartmentalized building
- Low-free-volume reactor cavity with fire-brick insulation, steel liner, and concrete walls
- Shield building (above grade)



Elevation view of UCB Mark 1 containment  
[UCBTH-14-002]



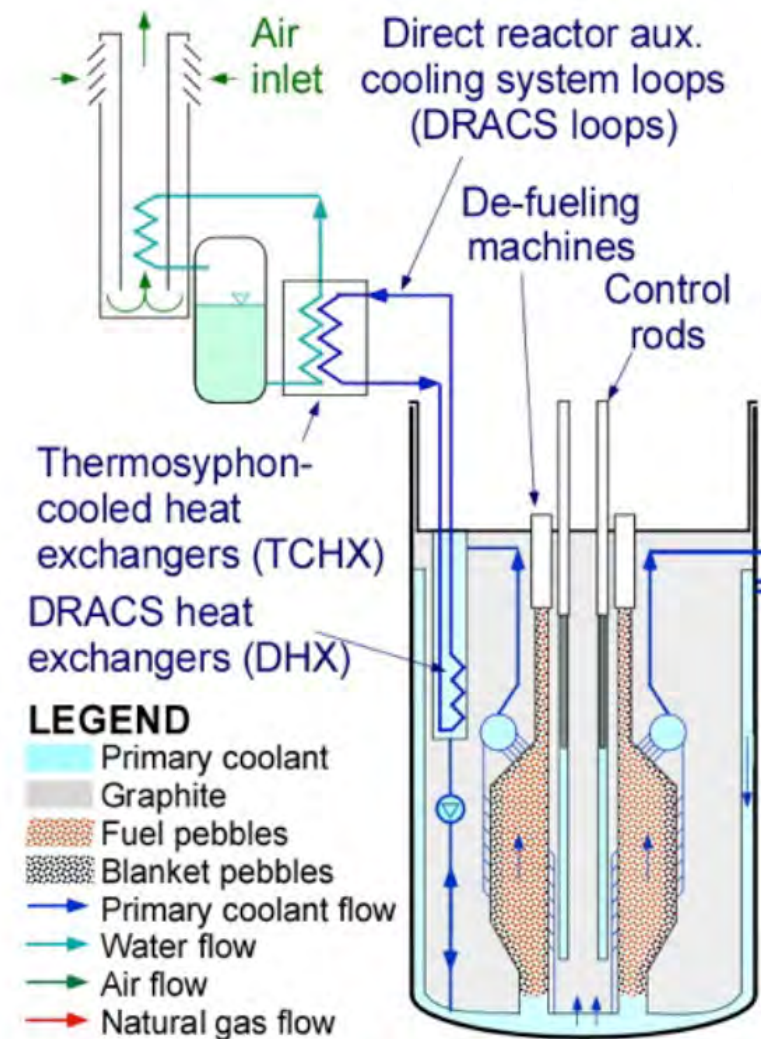
# UCB Mark 1 (4/4)

## Direct Reactor Auxiliary Cooling System (DRACS)

- 3 trains – 2.36 MW/train
  - 236 MWt reactor
- Each train has 4 loops in series
  - Primary coolant circulates to DRACS heat exchanger
  - Molten-salt loop circulates to the thermosyphon-cooled heat exchangers (TCHX)
  - Water circulates adjacent to the secondary salt tube loop in the TCHX
  - Natural circulation air circuit cools and condenses steam
- Start-up: Reactor coolant pump trip causes ball in valve to drop

## Reactor cavity cooling subsystem (RCCS) surrounds reactor cavity

- Thermal protection of the concrete



UCB Mark 1 DRACS  
[UCBTH-14-002]



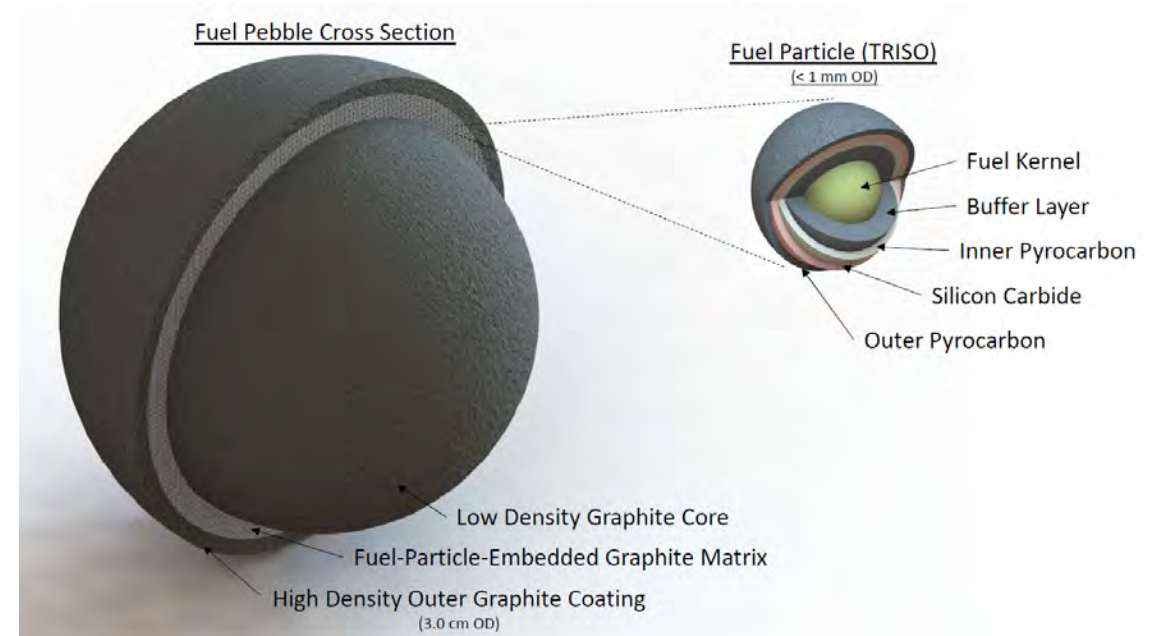
# UCB Mark 1 fuel

## TRISO particle

- TRISO is a portmanteau of **tr**istructural **i**sotropic
- Kernel – 1.5 g of UCO, 200  $\mu\text{m}$  radius
- Porous carbon buffer layer
- 3 coatings to contain fission products

## TRISO pebble

- Contains 4730 TRISO particles
- 30 mm diameter
- 1 mm graphite outer shell
- TRISO particles are distributed in the carbon matrix region between the solid core and outer shell



**TRISO in a Fuel Pebble**

[<http://fhr.nuc.berkeley.edu/wp-content/uploads/2014/10/PEBBLE-SCHEMATIC-V2.png>]

# Fluoride-salt-cooled High-Temperature Reactor Fission Product Inventory/Decay Heat Methods and Results

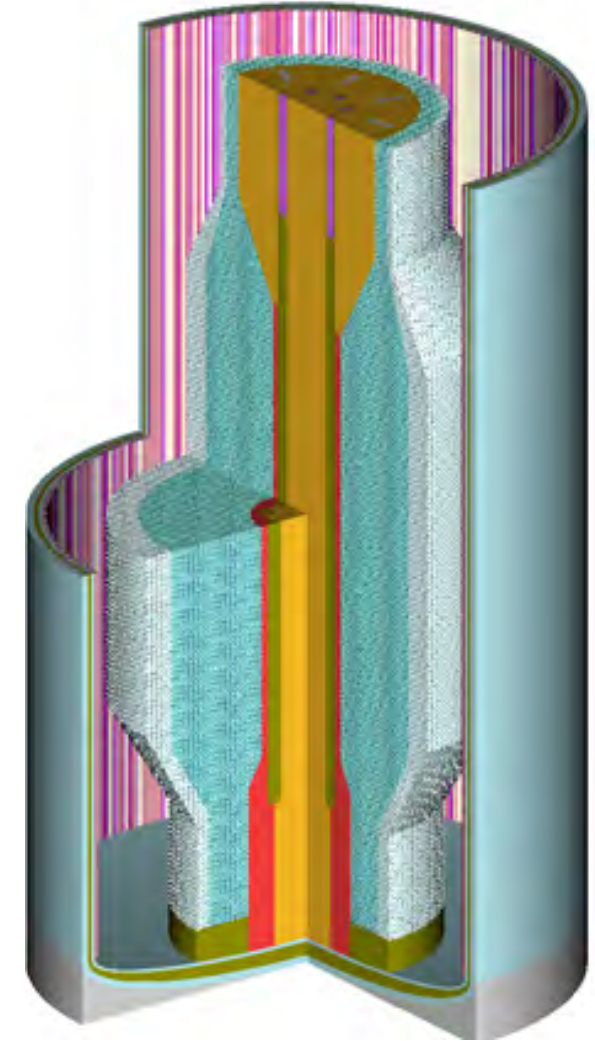


**U.S. NRC**



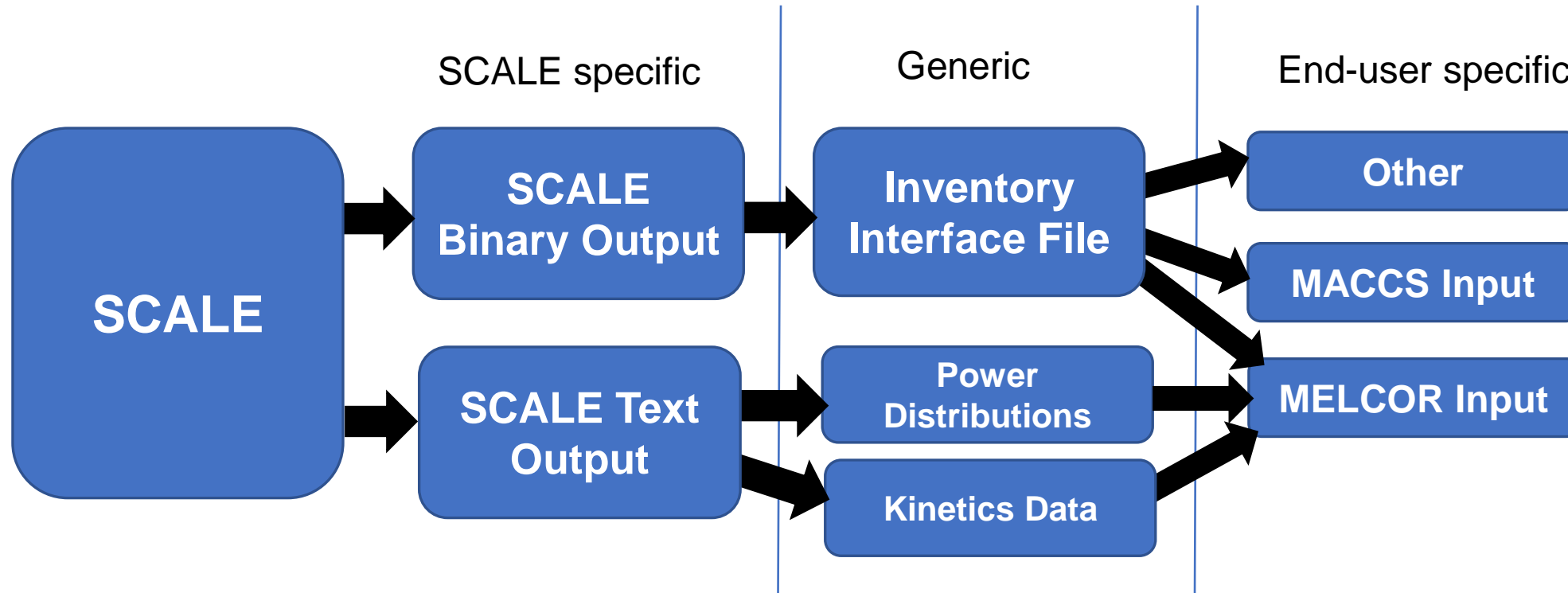
# FHR analysis with SCALE

- Objective
  - Provide input for MELCOR accident simulation
    - Radionuclide inventory
    - Decay heat profile
    - Reactivity feedback coefficients
    - Reactivity from xenon transient
- Approach
  - Apply SCALE to generate fuel composition for an equilibrium core
  - Equilibrium core – operated for several years so the average burnups are no longer changing
  - Evaluate neutronic characteristics



**SCALE model of the  
UCB Mark 1 core**

# Workflow



- **SCALE capabilities used:**

- Codes:

- ORIGEN for depletion
- KENO-VI 3D Monte Carlo neutron transport

- Data: ENDF/B-VII.1 nuclear data library\*

- Sequences:

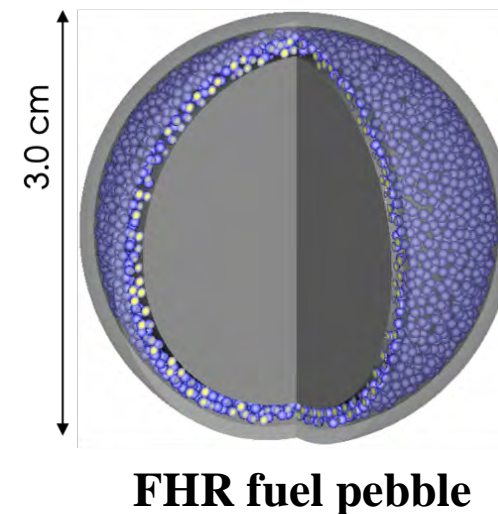
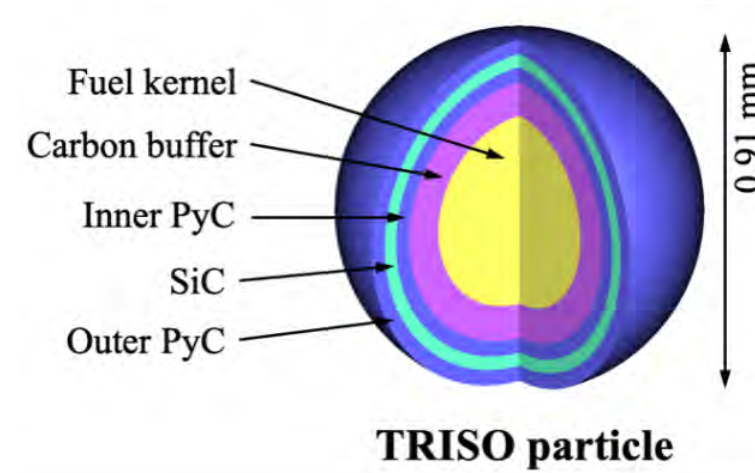
- CSAS for criticality/reactivity
- TRITON for reactor physics & depletion

\* A NUREG about *Nuclear Data Assessment for Advanced Reactors* summarizing the outcome of a recently concluded NRC-sponsored project is going to be published soon.

# Neutronics overview (1/2)

Relevant characteristics and differences to High Temperature Gas-cooled Reactors:

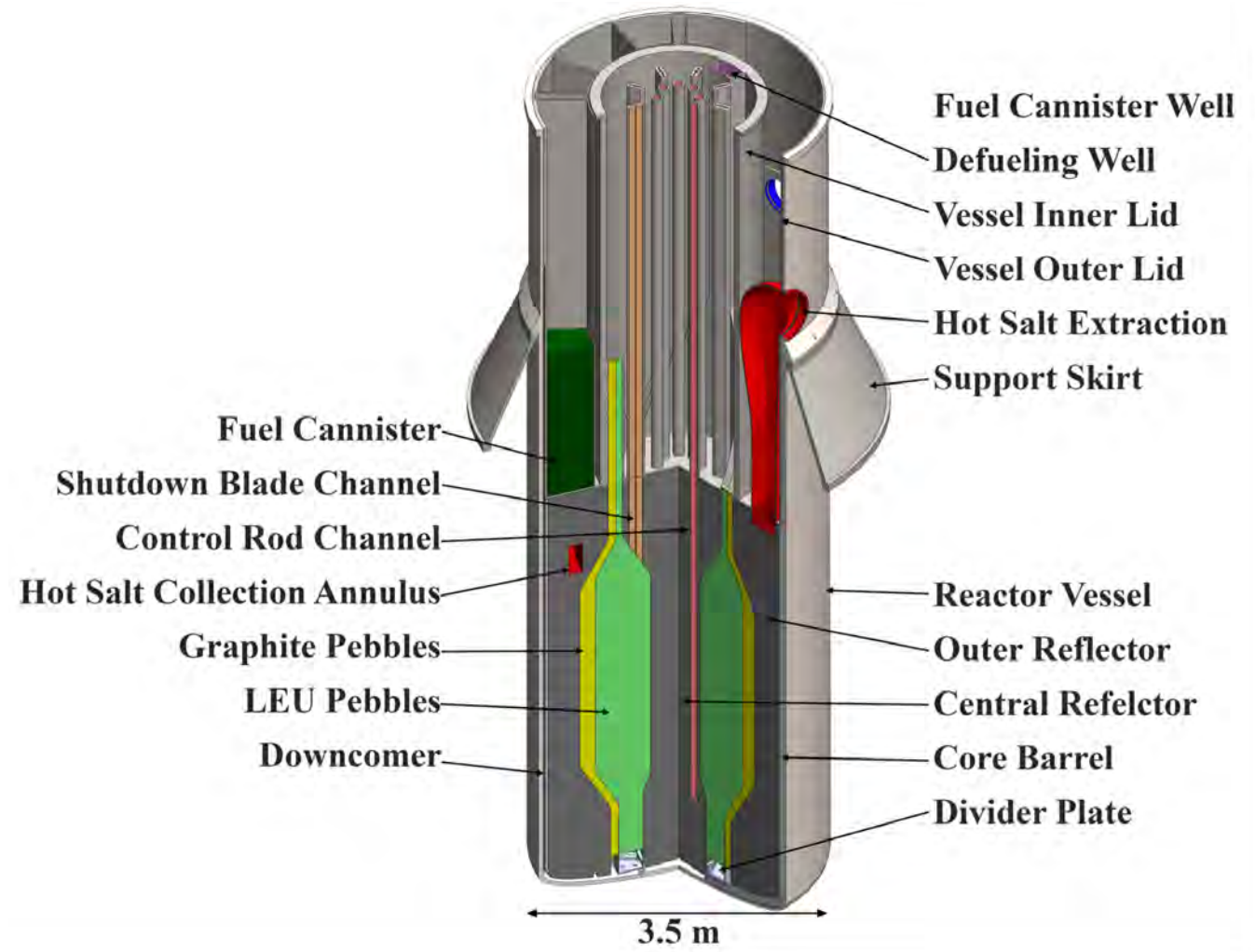
- Fuel:
  - UCO fuel in TRISO particles in fuel pebbles
  - TRISO particles located in shell instead of sphere
- Coolant: FLiBe salt instead of helium
- Moderator: graphite





# Neutronics overview (2/2)

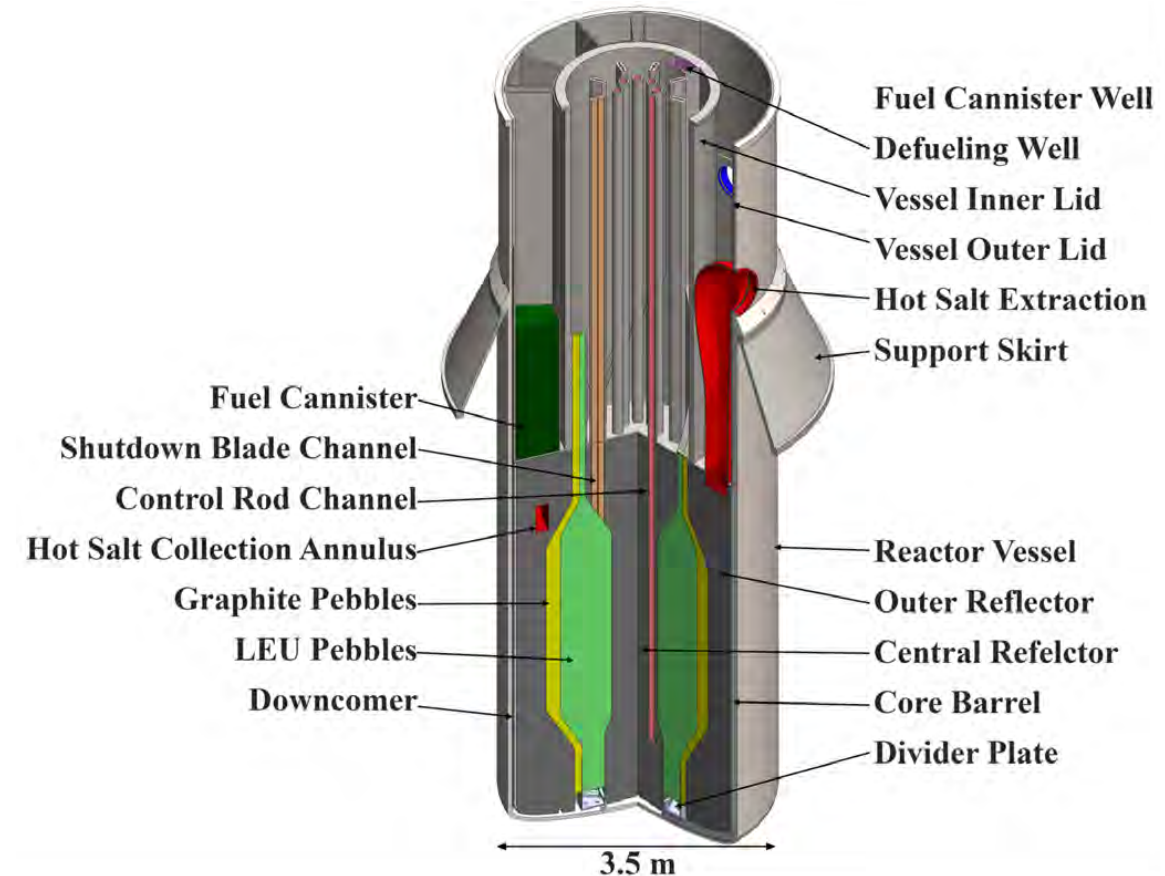
- Challenges for modeling:
  - Tritium production in FLiBe
  - TRISO particles with very high packing fraction in shell
  - Fuel pebble inlet and outlet geometry
  - Fuel and unfueled/graphite pebbles in different zones of the core
  
- Validation
  - SCALE validation with HTGR experiments partially applicable\*



\*F. Bostelmann, C. Celik, M. L. Williams, R. J. Ellis, G. Ilas, and W. A. Wieselquist, "SCALE capabilities for high temperature gas-cooled reactor analysis," *Ann. Nucl. Energy*, vol. 147, p. 107673, 2020. <https://doi.org/10.1016/j.anucene.2020.107673>

# UCB Mark 1 Model Description

Description	Value
Reactor power	236 MWth
UCO fuel density	10.5 g/cc
Uranium enrichment	<b>19.9 wt.%</b>
Fuel kernel radius	0.2 mm
Particle coating layer materials (starting from kernel)	Buffer/PyC/SiC/PyC
Fuel particle coating layer thickness	0.100/0.035/0.035/0.035 mm
Number of particles in pebble	4,730
Particle packing fraction in fuel pebble	<b>40%</b>
Radius of fuel pebble	1.5 cm
Inner/outer radius of fuel zone	1.25/1.40 cm
Number of fuel pebbles	470,000
Number of unfueled/graphite pebbles	218,000
Pebble packing fraction	<b>60%</b>
Core Inner reflector radius	35 cm
Outer fuel pebble region radius	105 cm
Outer graphite pebble region radius	125 cm
Volume of active fuel region	10.4 m <sup>3</sup>
Average pebble thermal power	500 W
Average pebble discharge burnup	<b>180 GWd/MTIHM</b>
Average pebble full-power lifetime	1.40 years

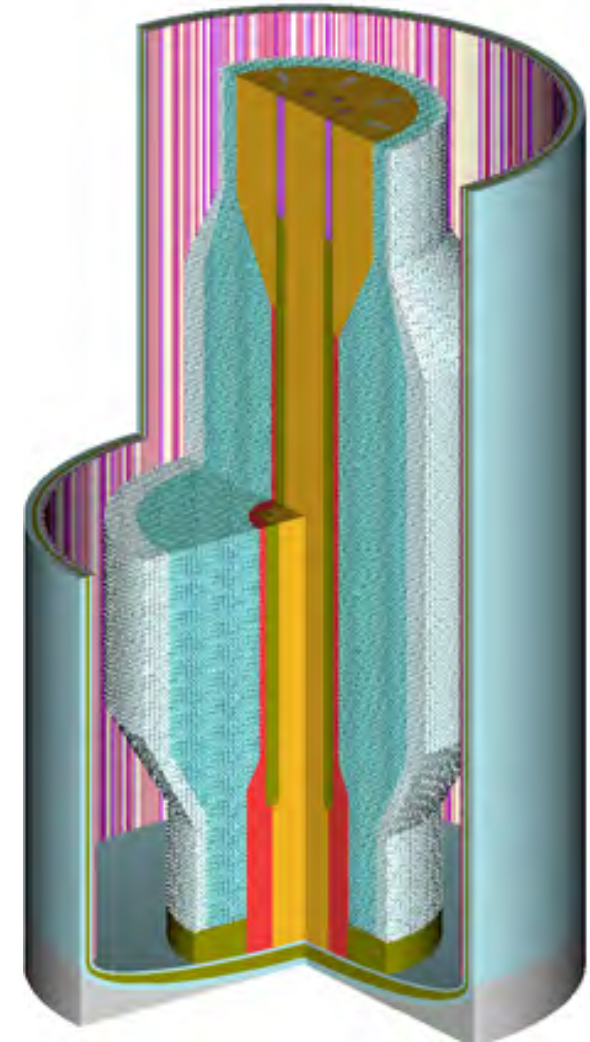


### SCALE model developed based on:

- [1] A. T. Cisneros, "Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)," University of California, Berkeley, 2013.
- [2] C. Andreades et al., "Technical Description of the "Mark 1" Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant," Berkeley, CA, UCBTH-14-002, 2014.

# Analysis areas

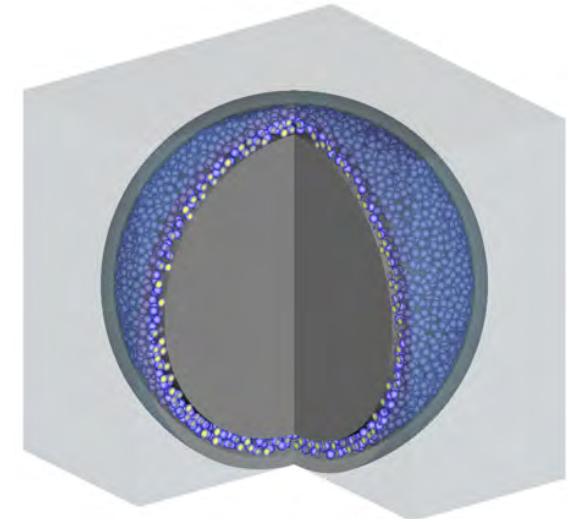
1. Verification of multigroup physics
2. Generation of equilibrium core
3. Power profile and neutron spectrum
4. Temperature feedback
5. Decay heat
6. 1-group cross sections
7. Tritium production
8. Xenon reactivity



**SCALE model of the  
UCB Mark 1 core**

# 1. Verification of multigroup physics for UCB Mark 1

- Comparison of multigroup (MG) calculation with continuous energy (CE) calculations for a pebble depletion problem
- **Why not always run CE?**
  - Significant modeling time: random distributions or particle arrays without permitting particle clipping
  - Significant computation time: many cells/surfaces (consider thousands of particles) and use of CE data
- **SCALE's MG approach for double-heterogeneous systems:**
  - Two self-shielding calculations: (1) particle in graphite matrix, (2) pebble in lattice of pebbles
  - Generation of problem-dependent cross sections for the fuel region through user-friendly input block
  - The MG calculation is 5 times faster than the CE lattice calculation, and 24 times faster than the CE calculation with a random particle distribution



**SCALE model a UCB Mark 1 pebble in a cube surrounded by FLiBe**

### Calculation:

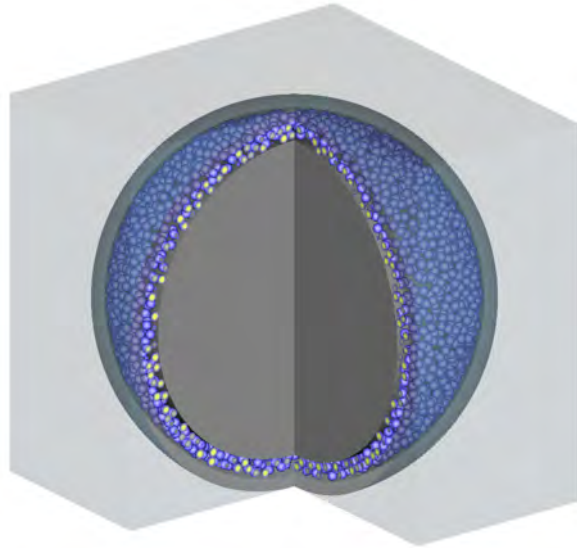
- TRITON/KENO-VI CE and MG
- Depletion calculation to reach discharge burnup of 180 GWd/tHM
- Comparison between calculations: k-eff, nuclide densities, runtime

CE, random	~79 minutes
CE, lattice	15.28 minutes
MG	3.25 minutes

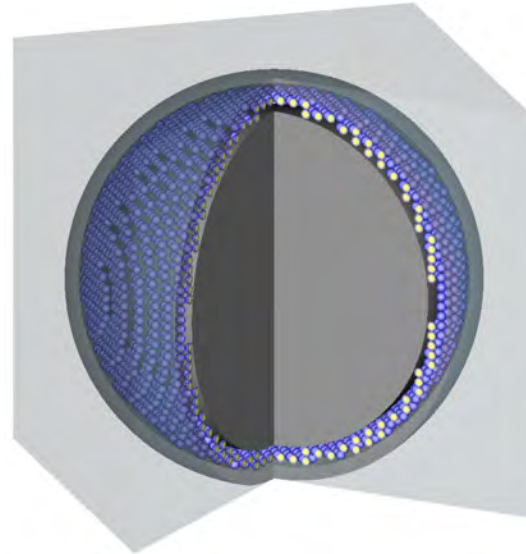




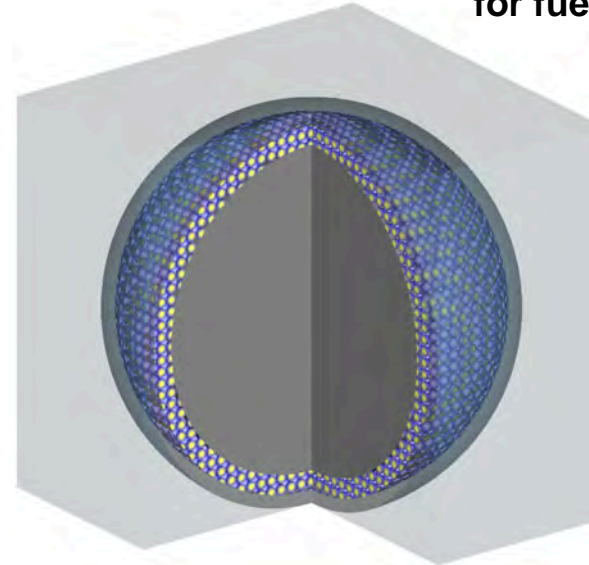
# 1. Single pebble models



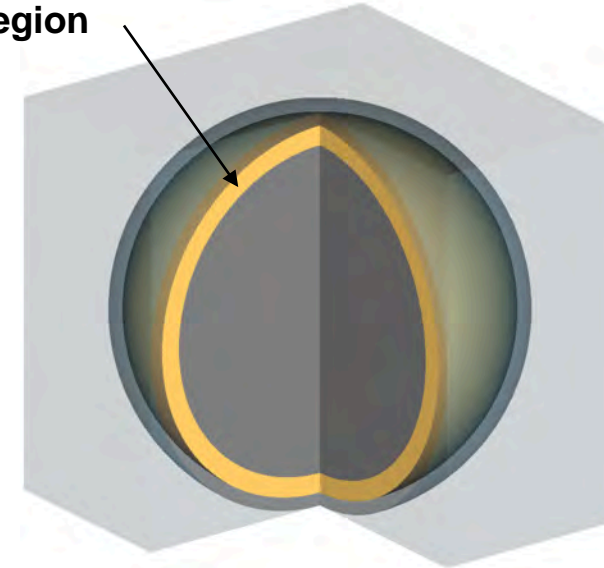
1. CE model: Random particle distribution



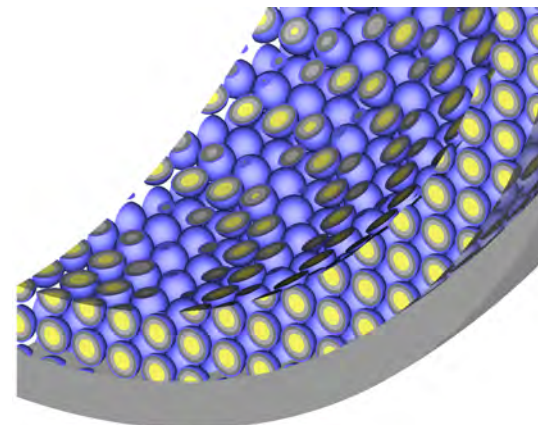
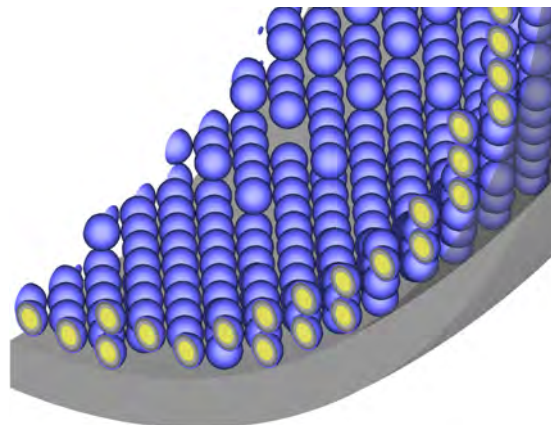
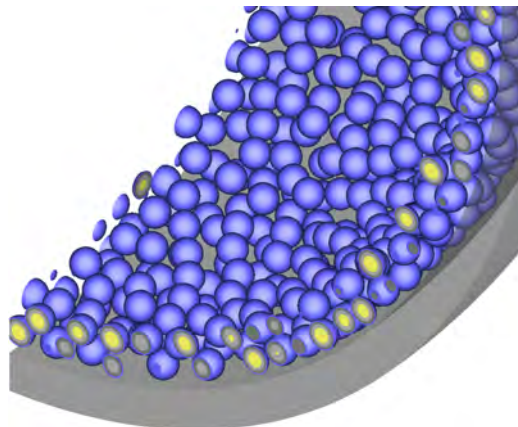
2. CE model: particle lattice (no clipping)



3. CE model: particle lattice (clipping)



4. MG model



**Note:**

- CE-random results are average of 10 realizations
- All models contain the same amount of fuel



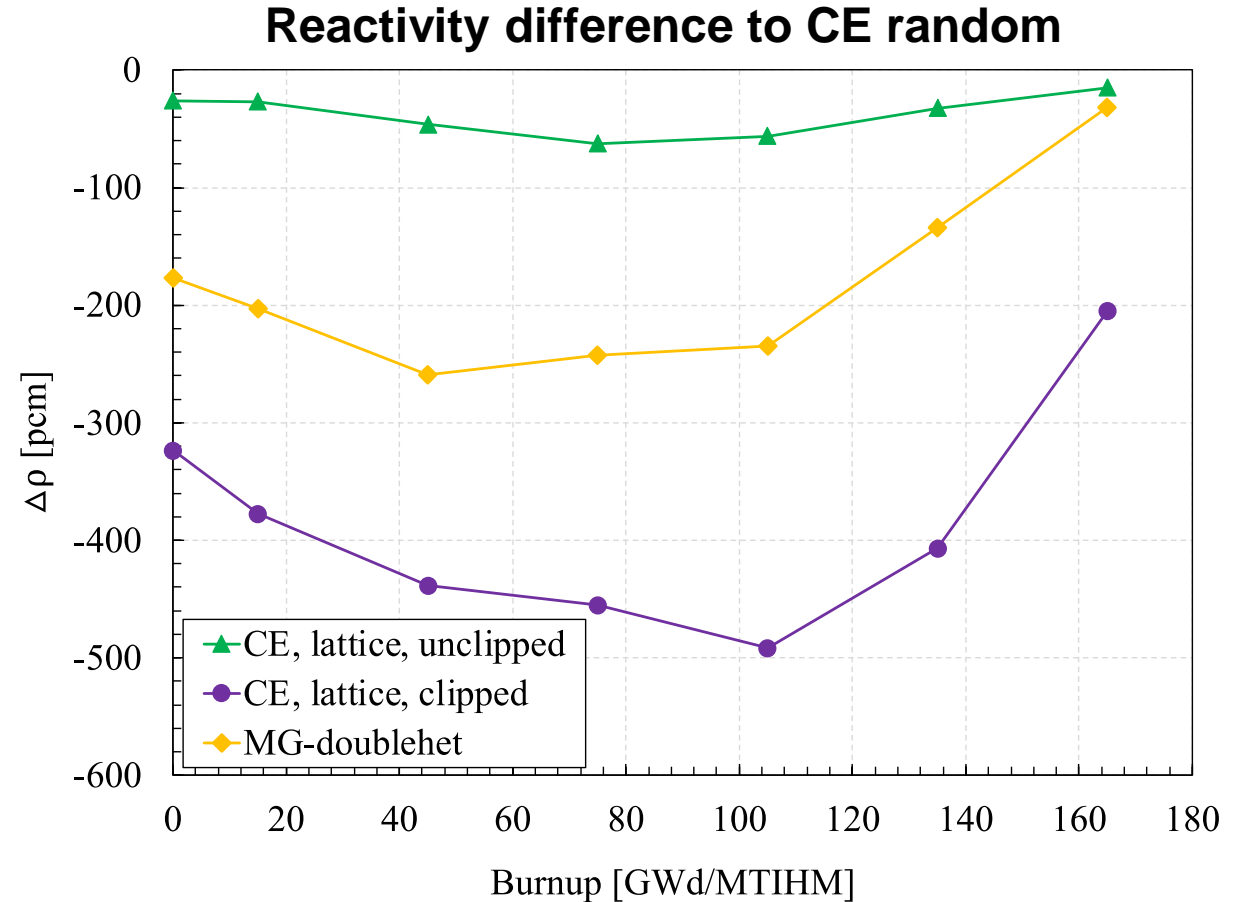
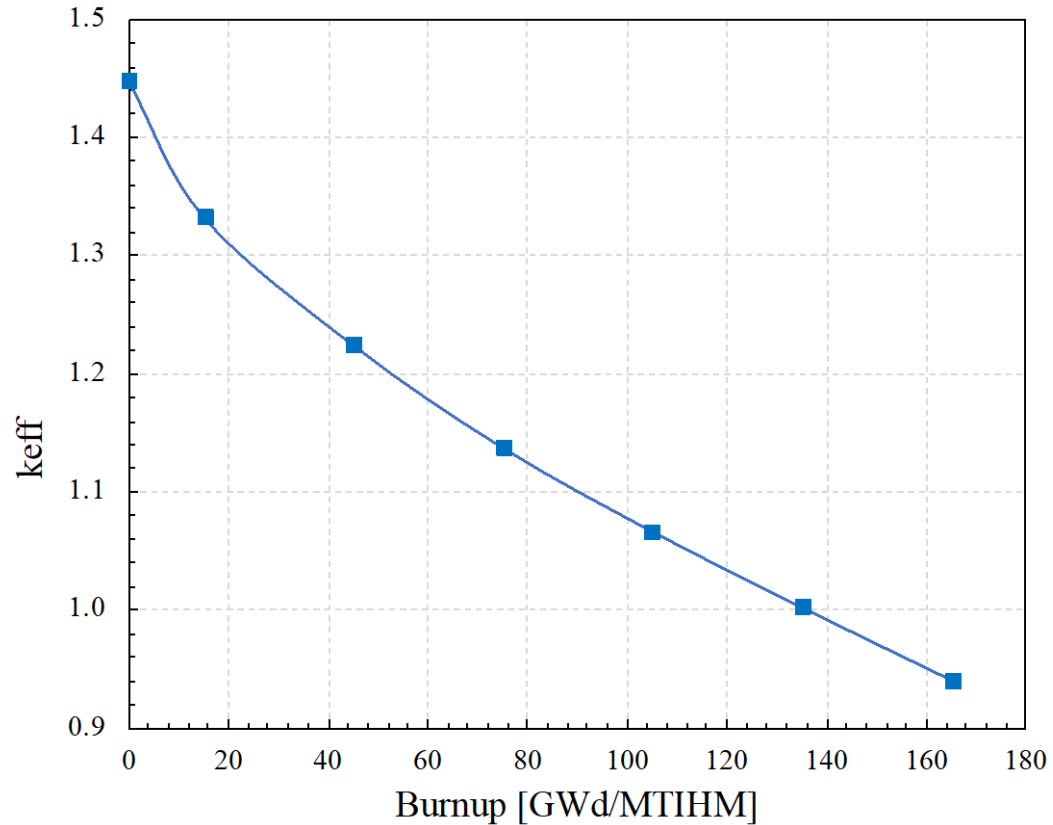
# 1. Single pebble initial criticality

Model		CZP		HFP	
		$k_{\text{eff}}$	$\Delta\rho$ [pcm]	$k_{\text{eff}}$	$\Delta\rho$ [pcm]
<b>CE, random</b>	<b>no clipping</b>	1.52539	(ref)	1.44765	(ref)
<b>CE, lattice</b>	<b>no clipping</b>	1.52449	<b>-39</b>	1.44738	<b>-13</b>
<b>CE, lattice</b>	<b>clipping</b>	1.51939	<b>-259</b>	1.44092	<b>-323</b>
<b>MG</b>		1.51986	<b>-239</b>	1.44426	<b>-162</b>

- **CZP:** all materials 300K
- **HFP:** Fuel 1003K, TRISO layers 973K, graphite center 983K, outer graphite shell 957K, coolant 923K
- All statistical errors of the Monte Carlo calculations < **20 pcm**

**Result:** MG  $k_{\text{eff}}$  calculations show good agreement with reference CE result independent of the temperature

# 1. Single pebble $k_{eff}$ over the course of depletion



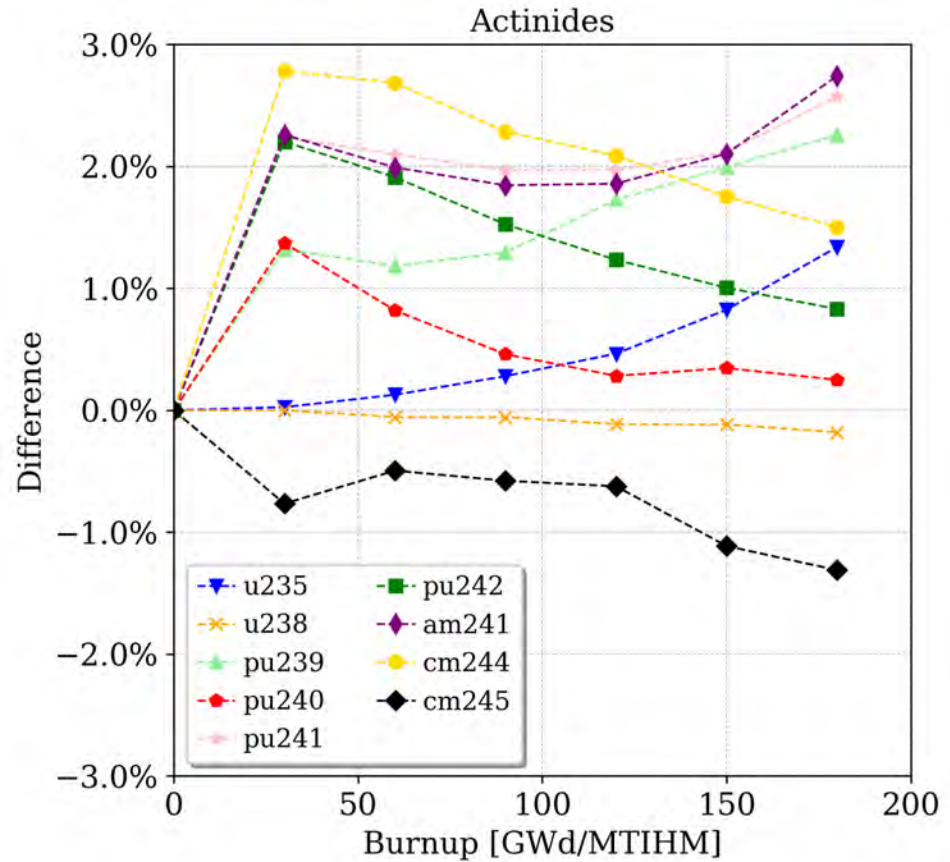
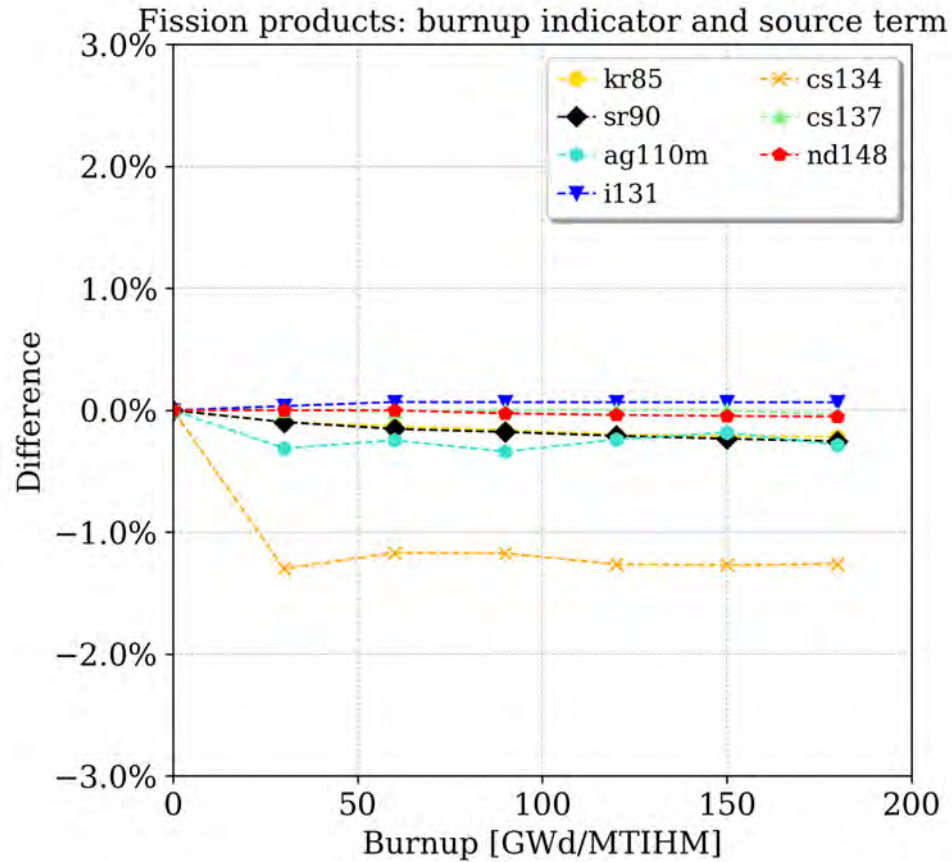
### Calculation details:

- TRITON-KENO depletion of the **HFP case**
- 540.54 days at 333 MW/MTIHM

**Result:** MG bias remains below 260 pcm over depletion

# 1. Single pebble nuclide density comparison over depletion

Comparison of MG against CE random:



**Result: MG bias remains below 3% for relevant nuclide densities over depletion**

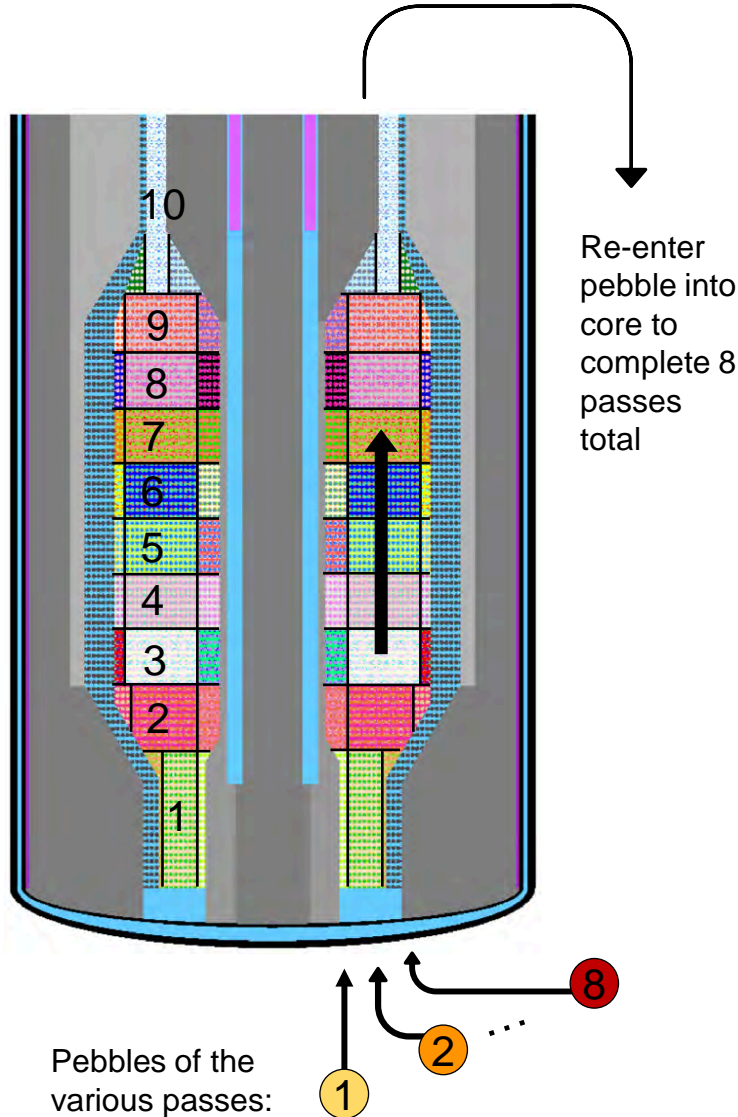
# 1. MG performance summary for UCB Mark 1

- We confirmed the performance of SCALE's MG capability for double-heterogeneous systems in terms of  $k_{\text{eff}}$  and nuclide densities in a UCB Mark 1 single pebble depletion calculation
- SCALE's MG capability permits the calculation of accurate results in a much-reduced runtime (factor of 24 when compared to reference CE calculations)





# 2. Generation of isotopics for an equilibrium state



**Fuel pebble burnup (GWd/MTIHM) in each axial zone depending on the pass through the core assuming constant axial/radial power:**

axial zone	pass through the core							
	1	2	3	4	5	6	7	8
10	21.4	43.9	66.4	88.9	111.4	133.9	156.4	178.9
9	19.1	41.6	64.1	86.6	109.1	131.6	154.1	176.6
8	16.9	39.4	61.9	84.4	106.9	129.4	151.9	174.4
7	14.6	37.1	59.6	82.1	104.6	127.1	149.6	172.1
6	12.4	34.9	57.4	79.9	102.4	124.9	147.4	169.9
5	10.1	32.6	55.1	77.6	100.1	122.6	145.1	167.6
4	7.9	30.4	52.9	75.4	97.9	120.4	142.9	165.4
3	5.6	28.1	50.6	73.1	95.6	118.1	140.6	163.1
2	3.4	25.9	48.4	70.9	93.4	115.9	138.4	160.9
1	1.1	23.6	46.1	68.6	91.1	113.6	136.1	158.6

Mix fuel compositions of these burnups to get average composition of axial zone 3

## 2. Approach to generate equilibrium inventory

1.

Depletion of surrogate pebbles in a **core slice model** to capture average spectral effects in equilibrium environment

2.

Depletion of every pebble according to its detailed **power** and spectral history (pass and zone in 3D core) based on average conditions from slice depletion

3.

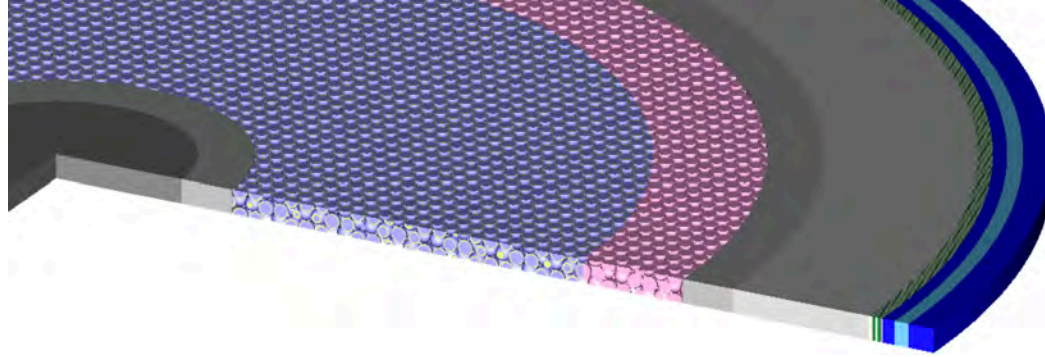
Reconstruction of 3D core equilibrium composition according to axial/radial zones

4.

Check convergence for keff and core-average fuel composition: stop or return to step 1 with new core-average fuel composition

Outer iteration:  
1. Constant power  
2. 3D power map

## 2. Slice depletion model



Pebbles containing averaged equilibrium core fuel composition  
(not changing during depletion)

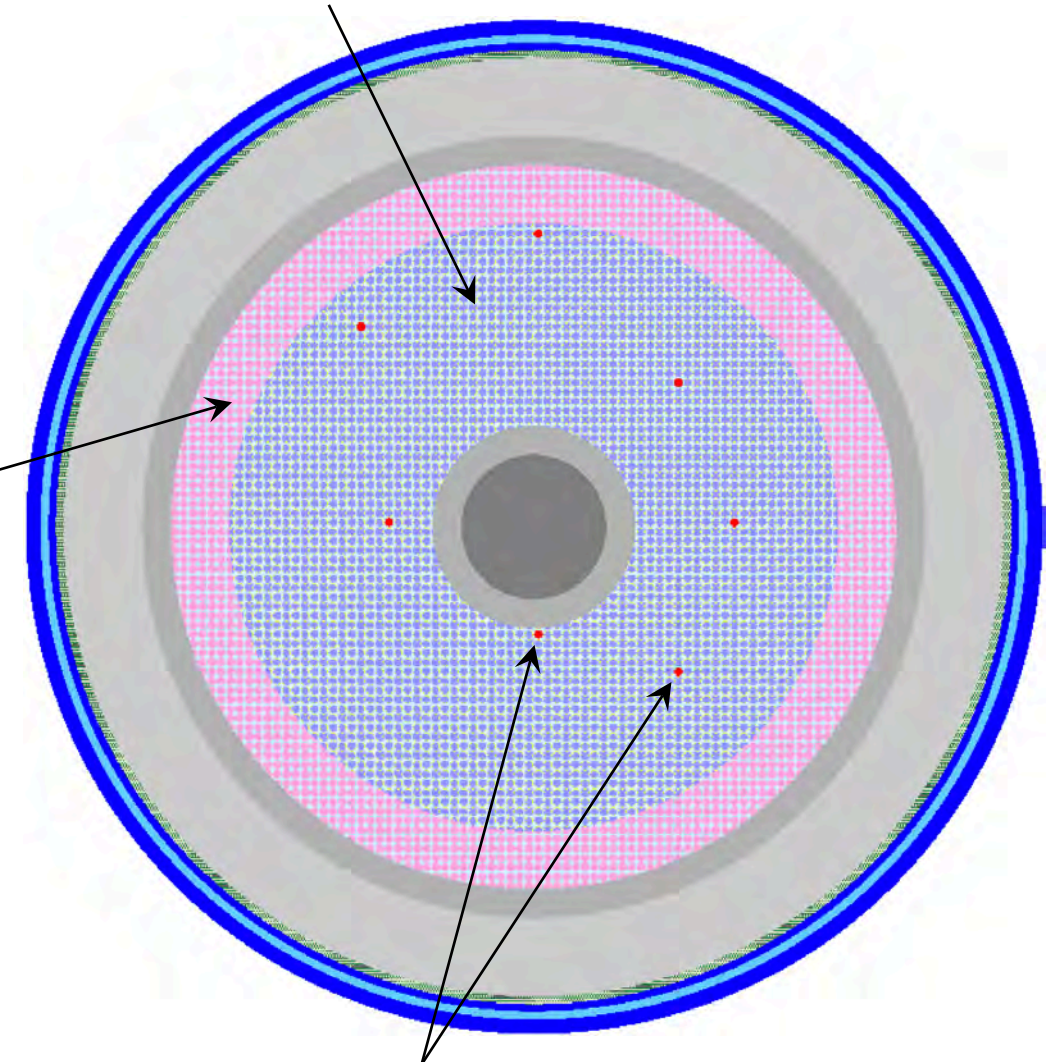
### Why a slice and not a single pebble:

- Representative moderator/fuel ratio
- Representative neighboring conditions (spectral effects)

### Depletion model:

- Slice through center of the core
- Depletion of surrogate pebbles surrounded by core-average fuel composition
- Axially reflected, radially vacuum boundary conditions

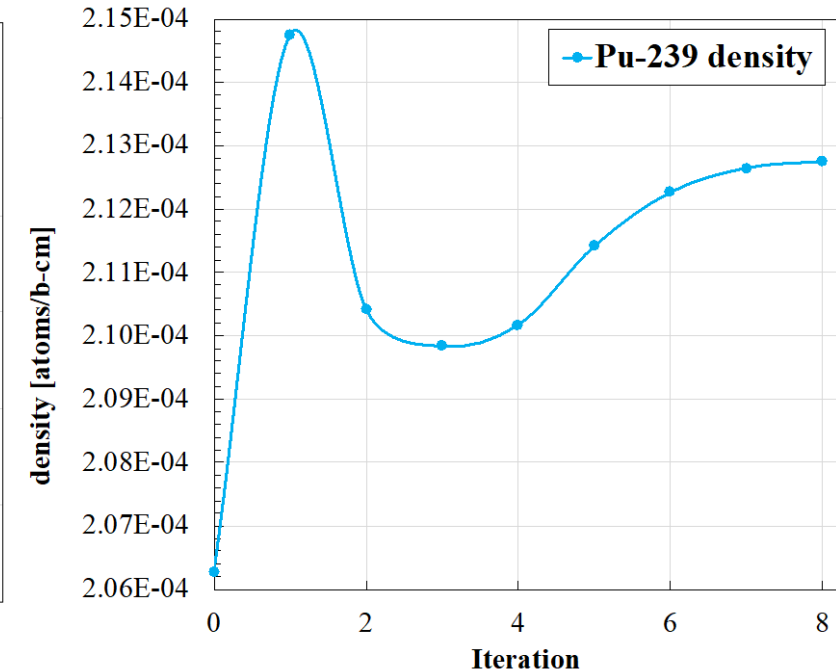
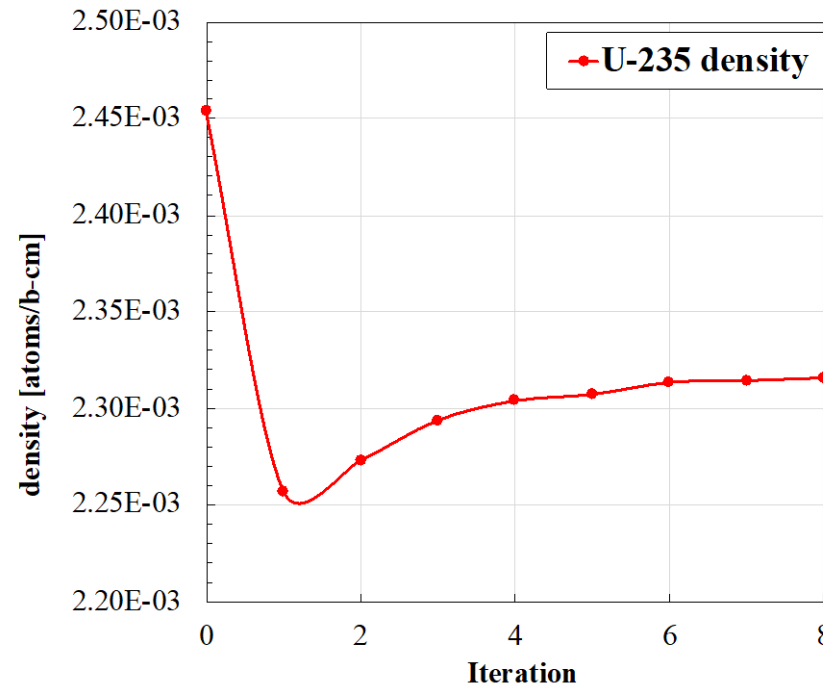
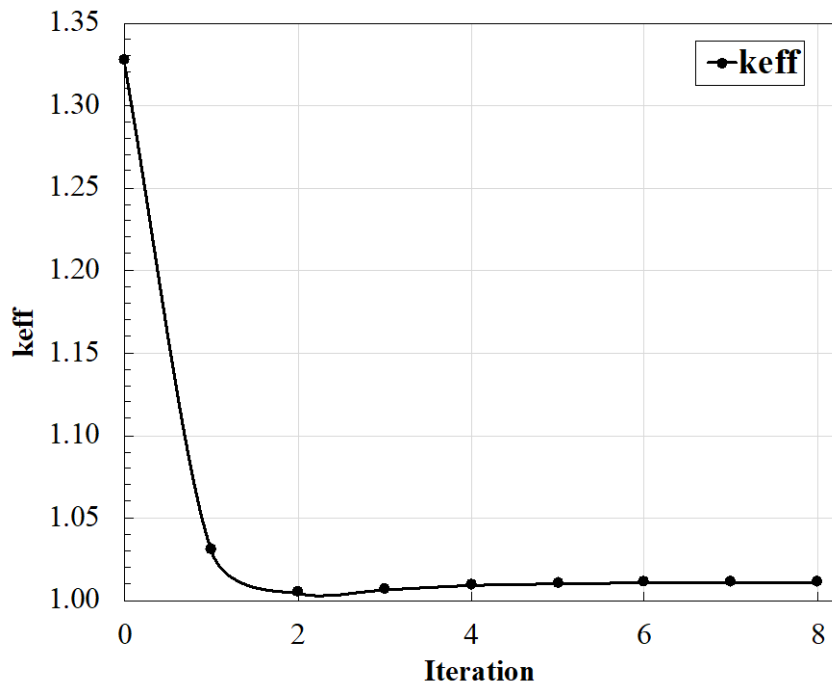
Graphite pebbles



Depletable pebbles  
(always starting with fresh fuel, depleted during depletion)

## 2. $K_{\text{eff}}$ and nuclide density convergence

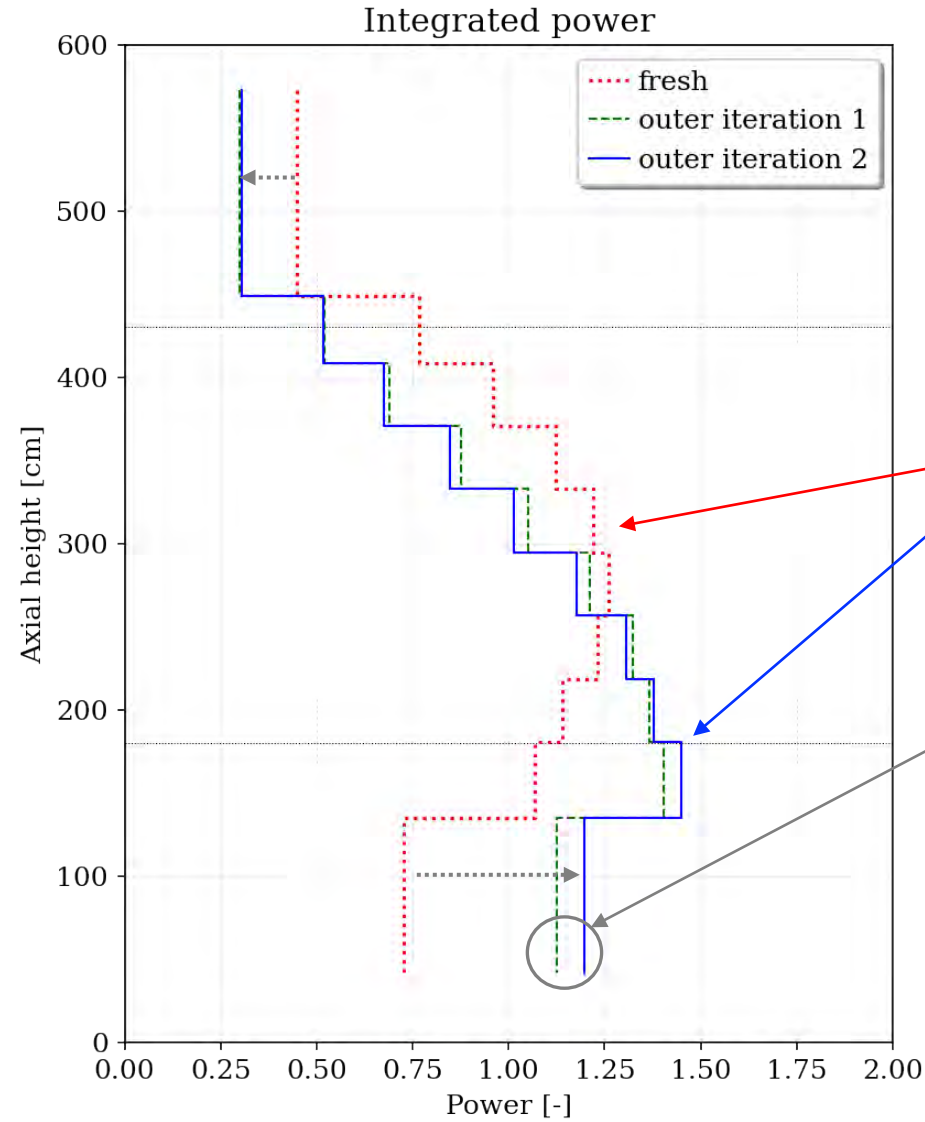
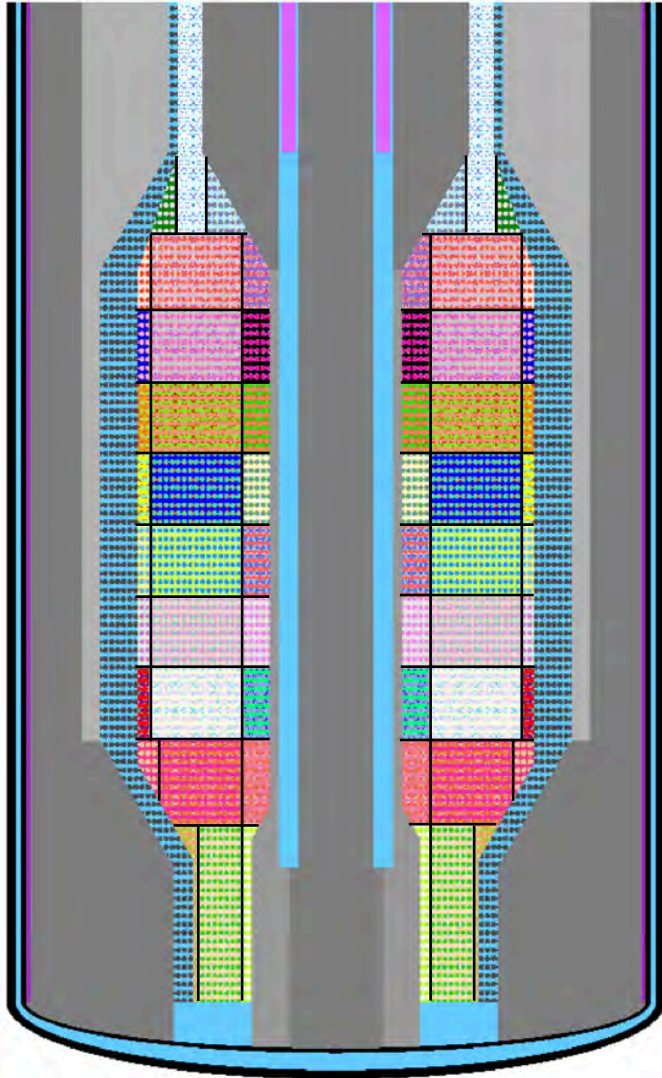
### Outer iteration 1 using constant core power



- Outer iteration 1: convergence of  $k_{\text{eff}}$  and nuclide densities achieved after 8 inner iterations
- Outer iteration 2 using 3D power map showed similar convergence behavior



# 3. Full core power profile

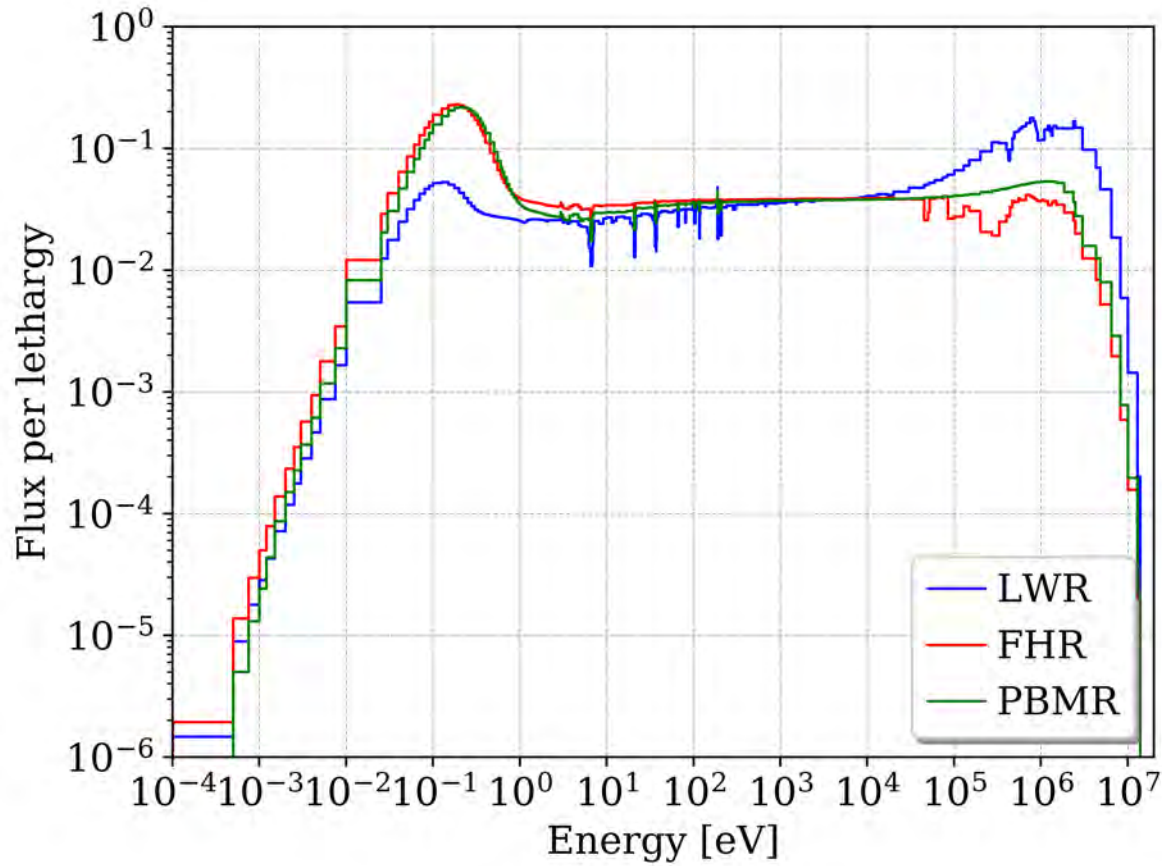


**Results:**

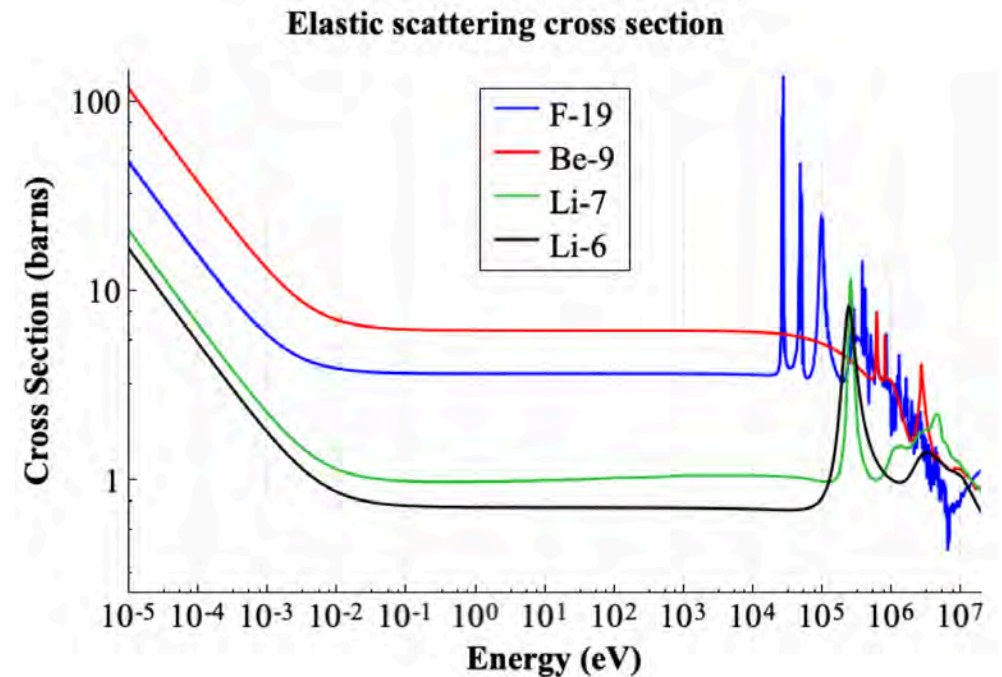
1. Power peak in the lower core region in eq. core due to increasing burnup with axial height
2. Difference between power profiles of the two outer iterations very small with max. 6% in the lowermost zone



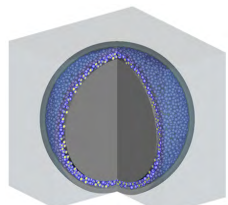
# 3. Example fuel cell flux spectrum comparison



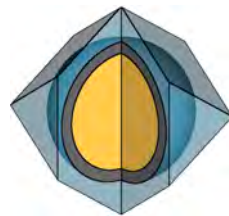
- UCB Mark 1 and PBMR show a larger thermal peak compared to LWR
- UCB Mark 1 shows smaller fast flux due to scattering with the salt



LWR pin

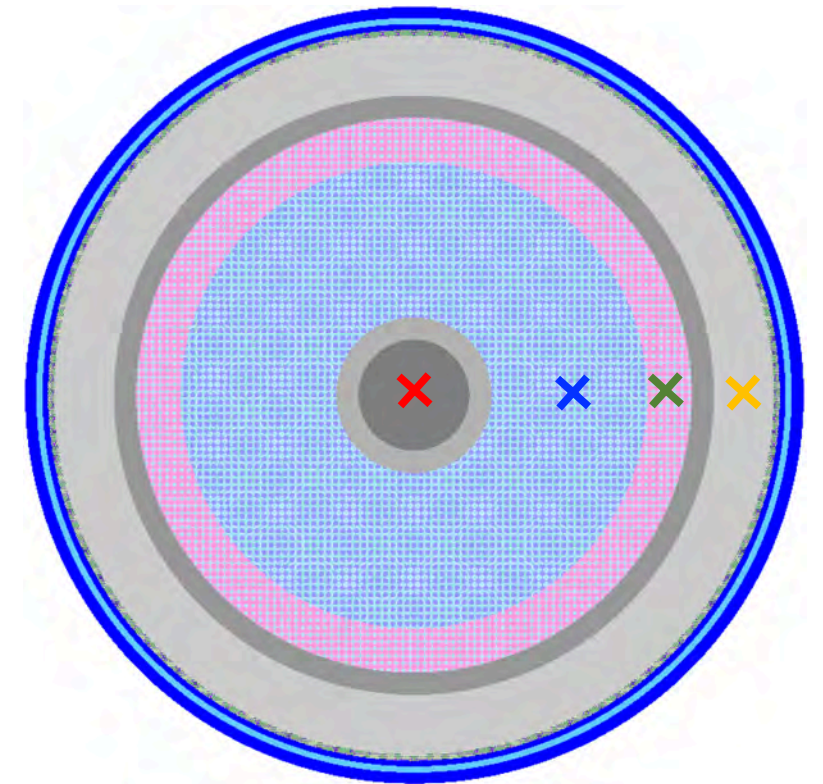
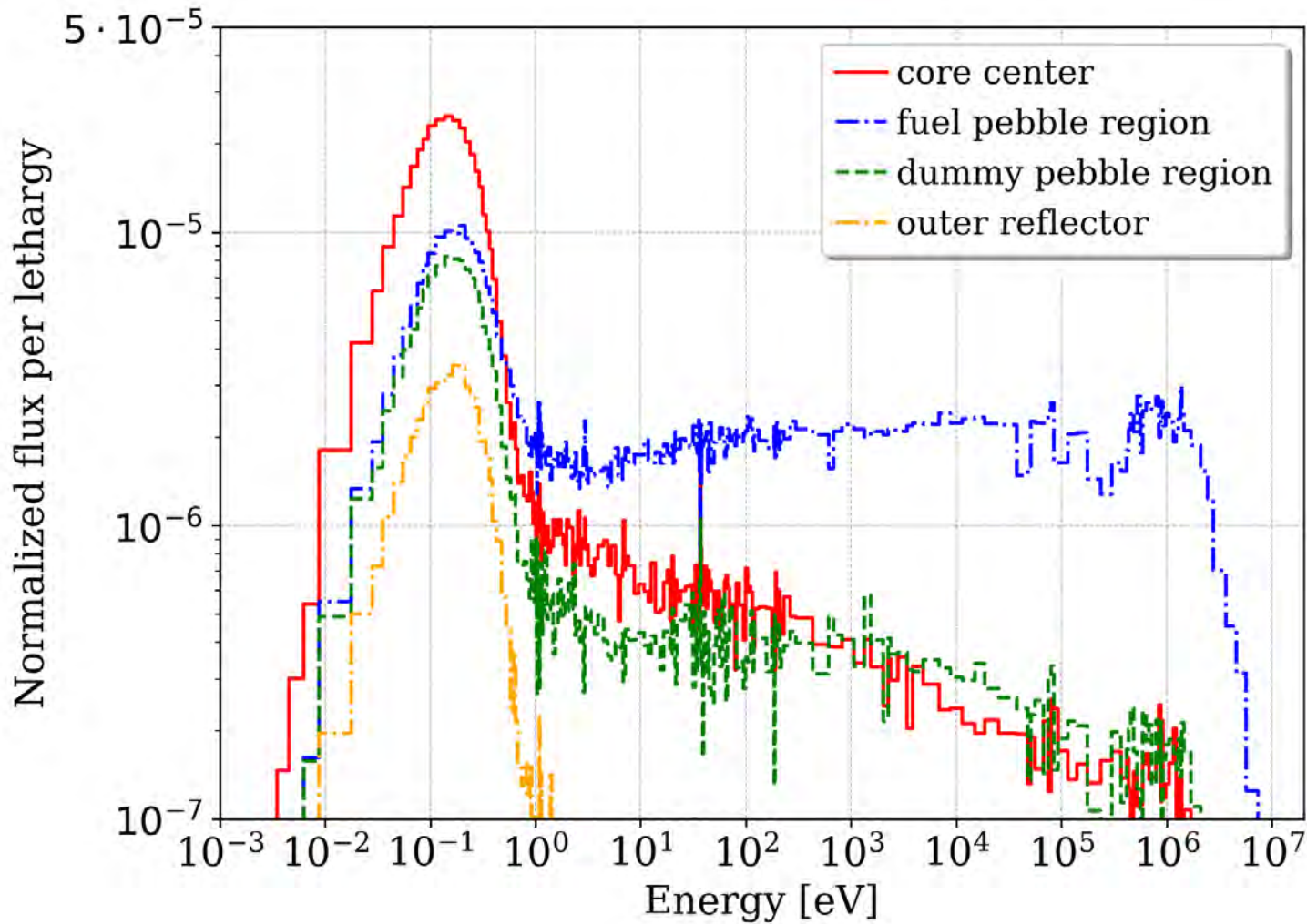


FHR pebble



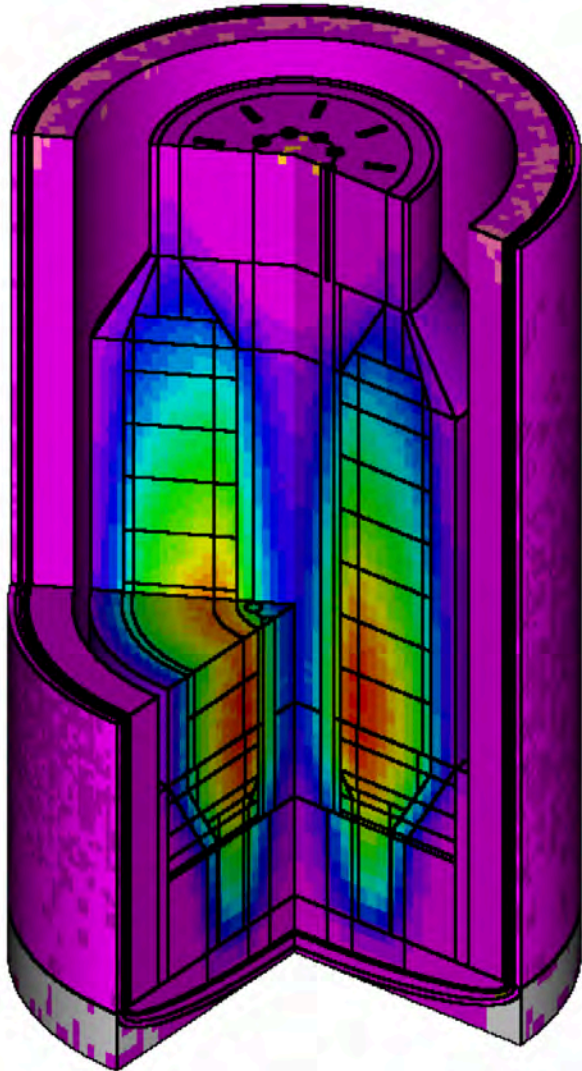
PBMR-400 pebble

### 3. Energy-dependent flux profile

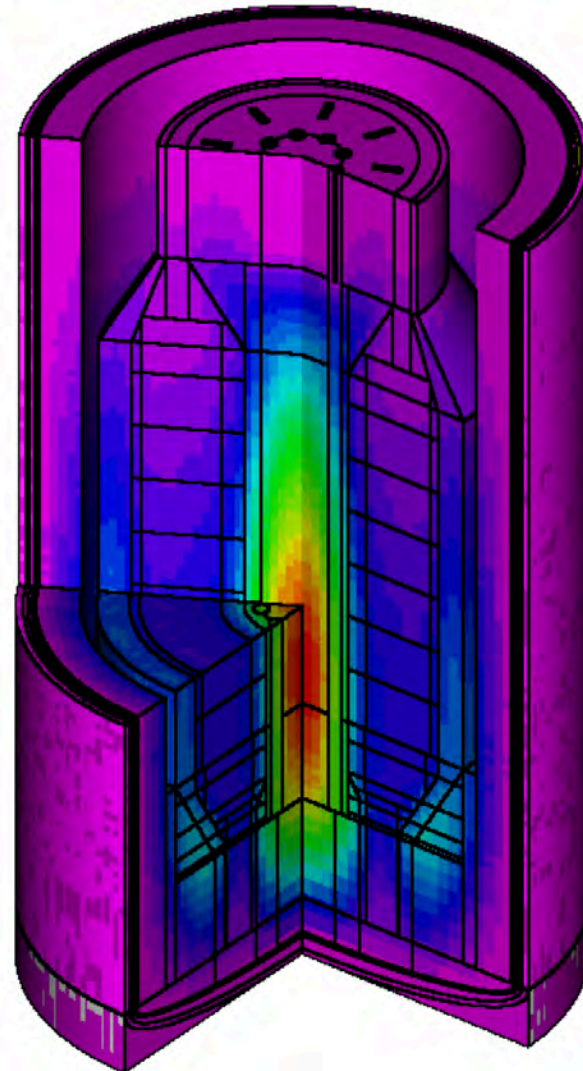




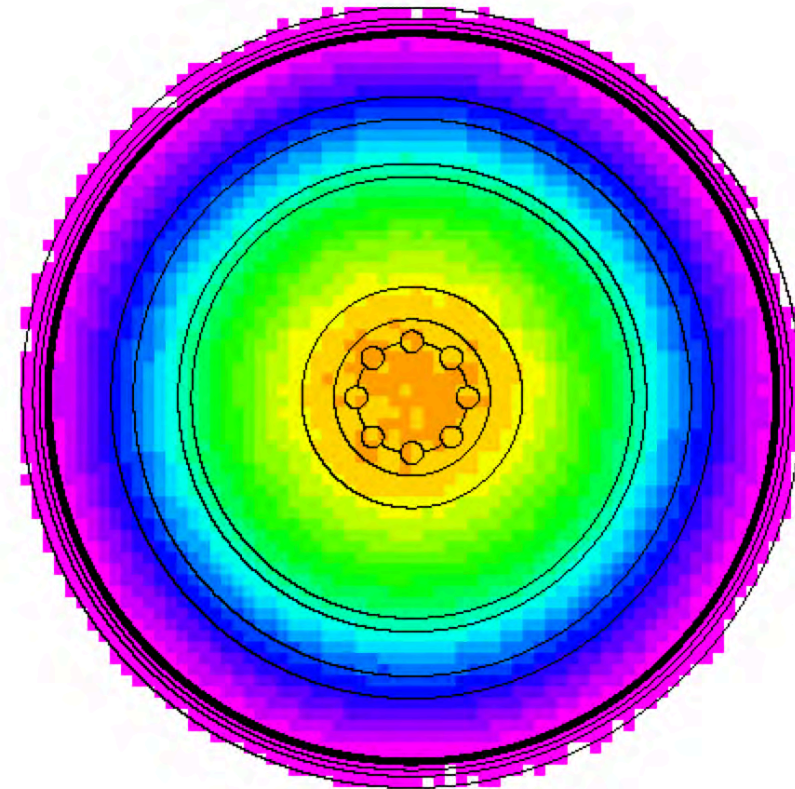
# 3. 3D full core flux visualizations



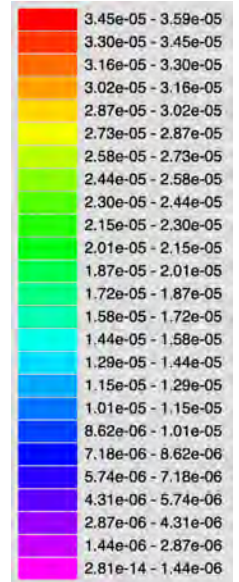
Fast flux,  $E > 0.625$  eV



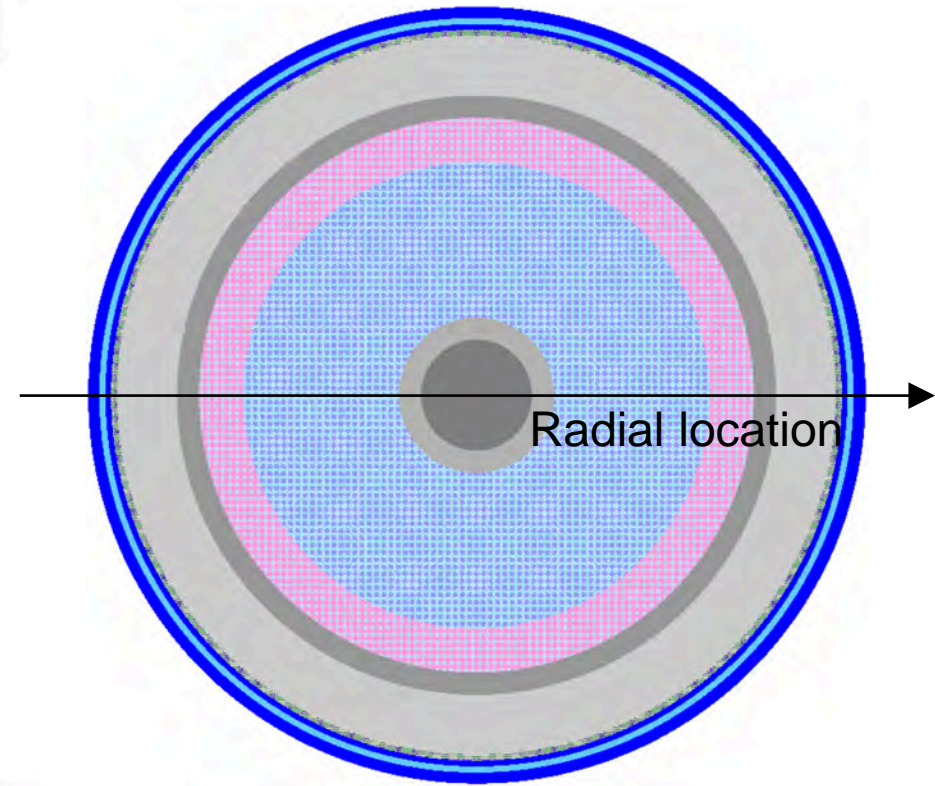
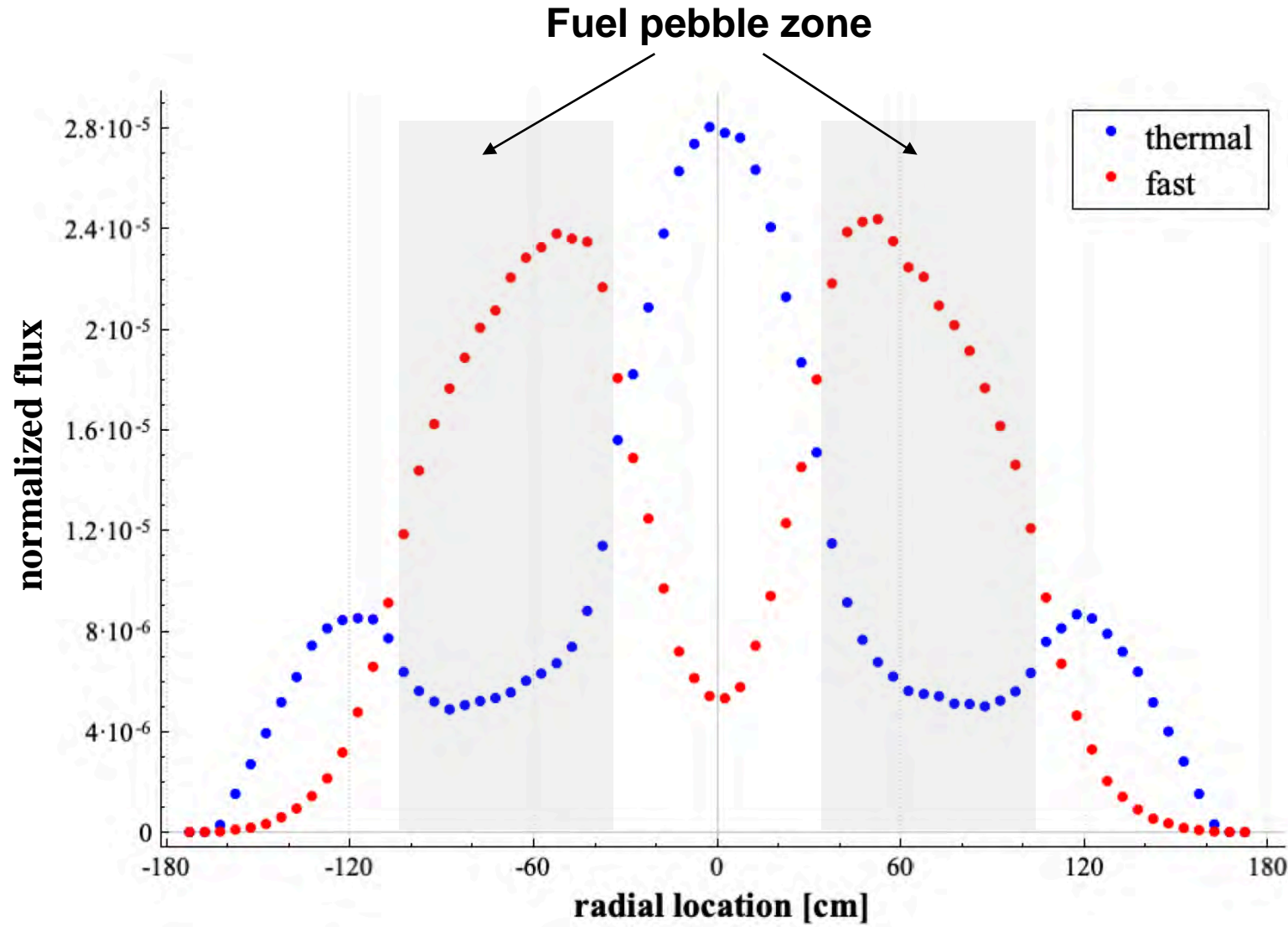
Thermal flux,  $E < 0.625$  eV



Total flux at the axial center of the core

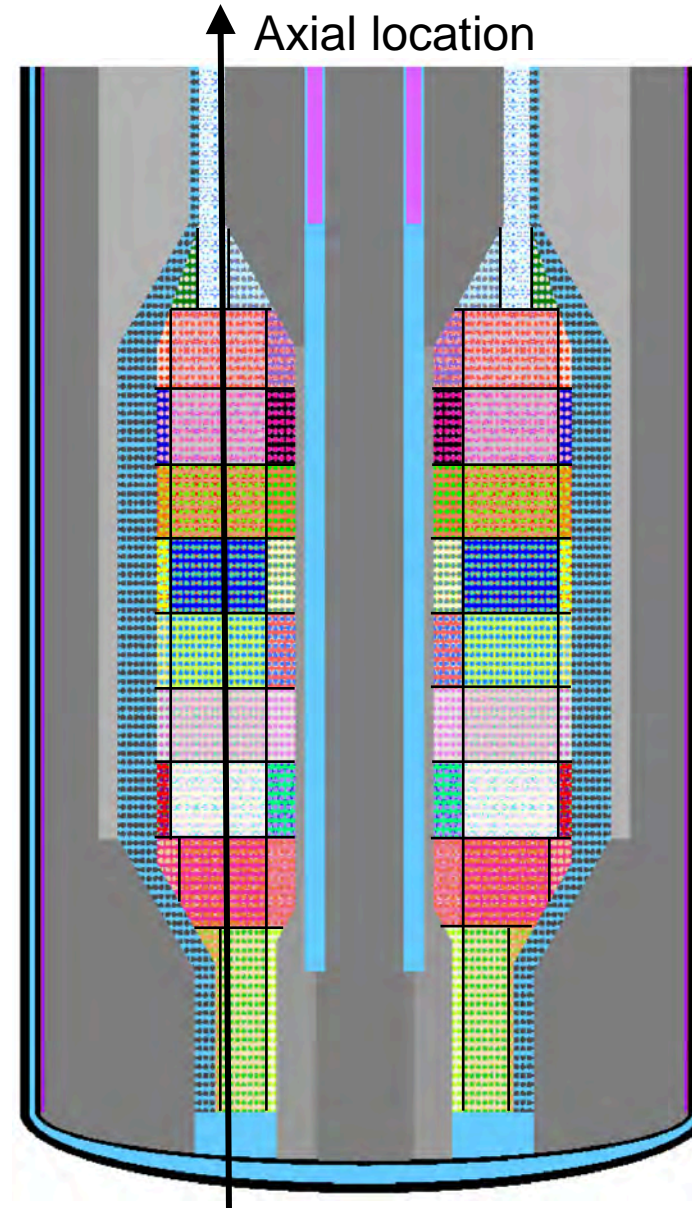
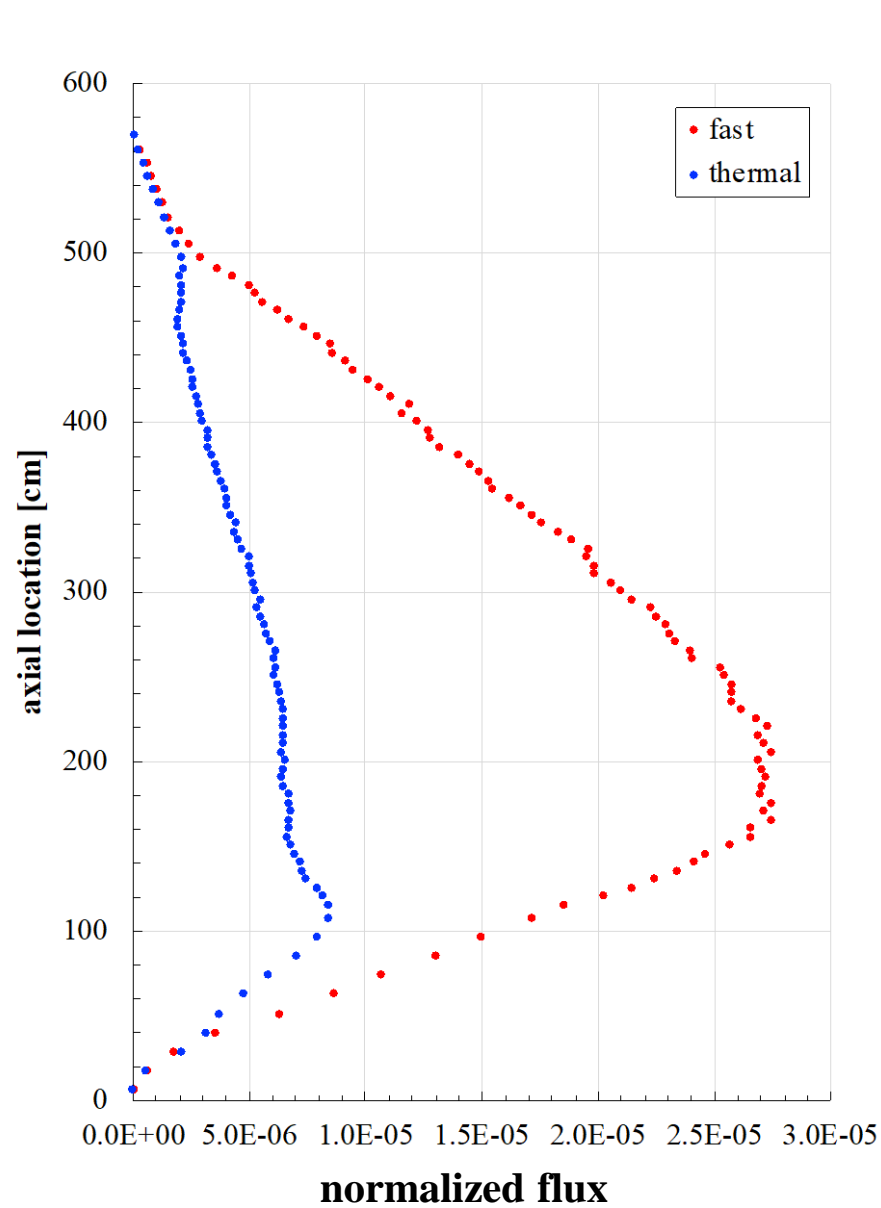


### 3. Radial flux distribution at axial core center (axial zone 5)





# 3. Axial flux distribution in the fuel region





# 4. Reactivity coefficients

- Isothermal temperature coefficient calculation:
  - $k_{eff}$  calculations with material temperatures varying over a range of several hundred K
  - Assuming constant temperature within material
  - Fitting of reactivity  $\rho$  to determine coefficient
- $\beta_{eff}$  and coolant void coefficient

**Nominal temperatures:**

- Fuel: 1003 K
- Salt coolant: 923 K
- Graphite moderator\*: 973/983 K
- Inner graphite reflector: 873 K
- Outer graphite reflector: 973 K

\*All carbonaceous materials in fuel pebbles

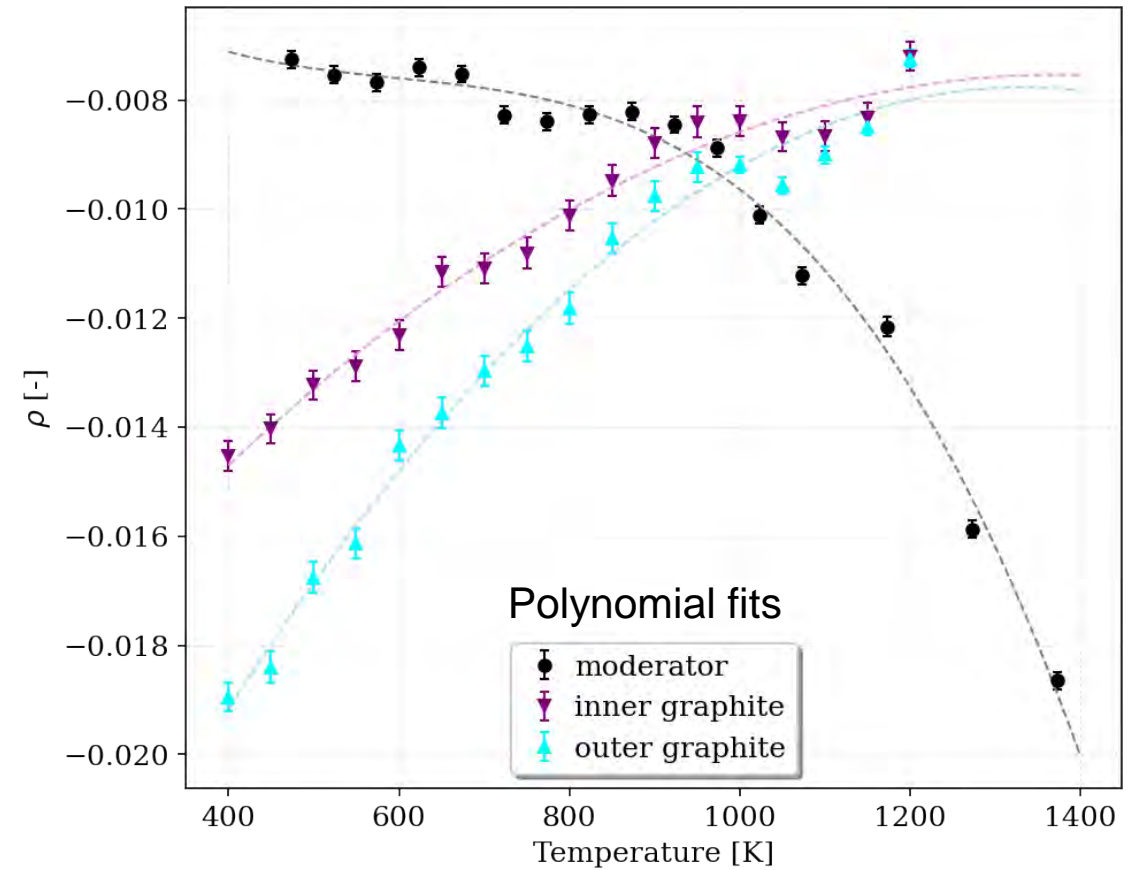
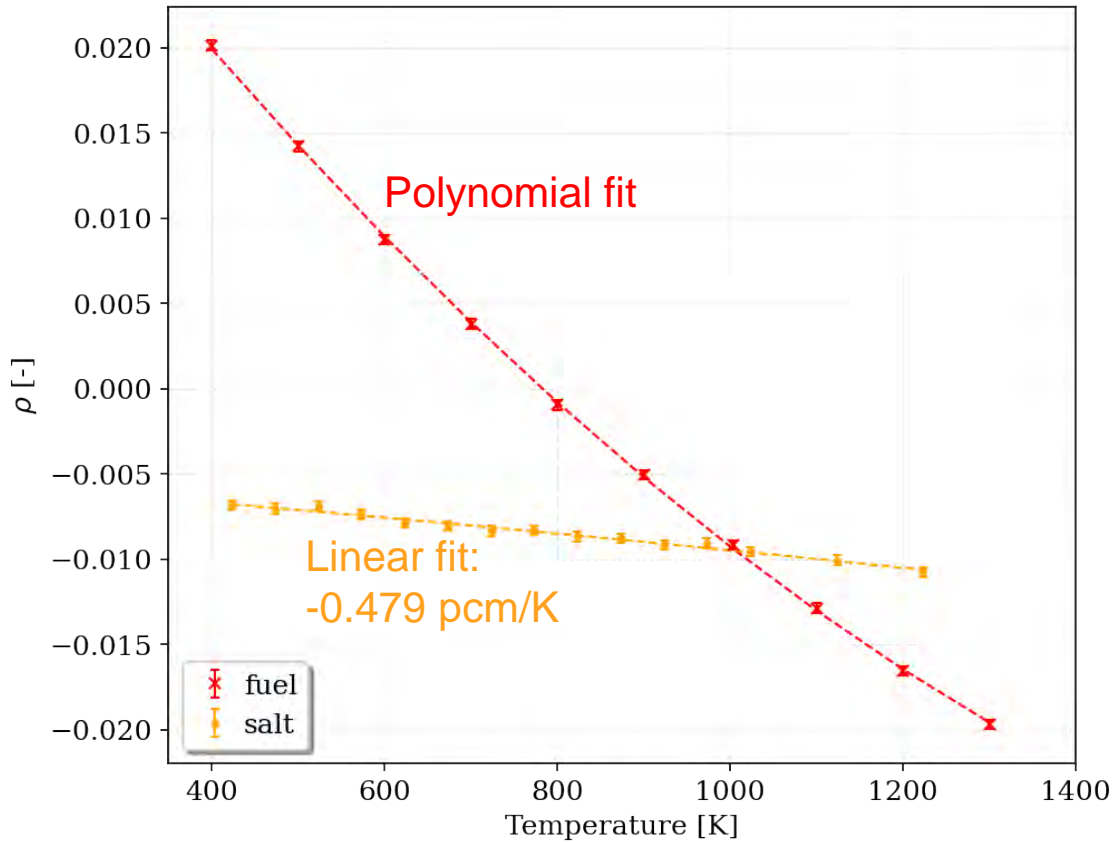
Quantity	Value [pcm]
$\beta_{eff}$	$541 \pm 20$
Coolant void	$-5094 \pm 21$

Component	Temperature Reactivity Coefficient at nominal temperature [pcm/K]
Salt coolant	-0.48
Fuel	-3.90
Graphite moderator	-1.10
Inner graphite reflector	+1.21
Outer graphite reflector	+0.61

} Linear fit

} Slope from polynomial fit

# 4. Isothermal temperature coefficients

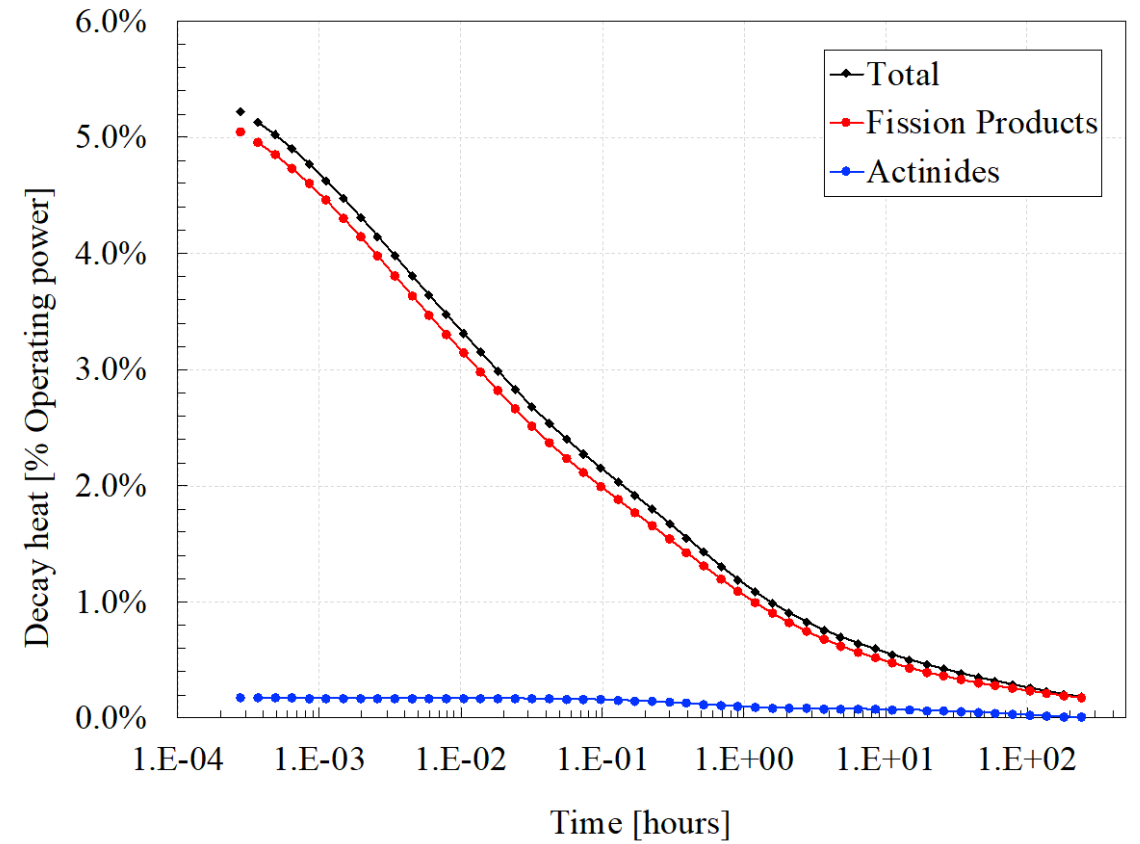
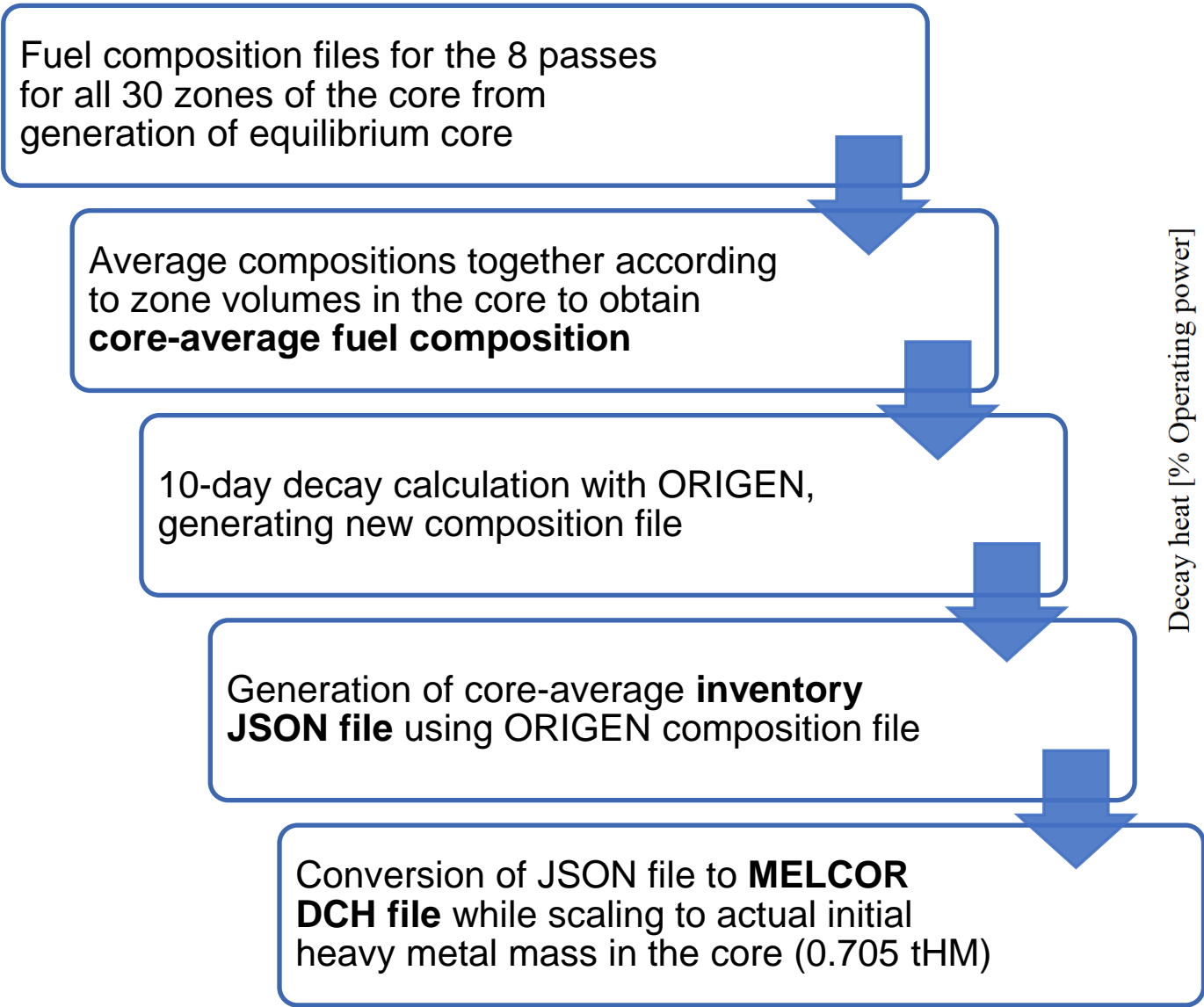


1. Linear fit for salt temperature coefficient
2. Polynomial fit or tabulated values for fuel, moderator, and graphite temperature coefficients

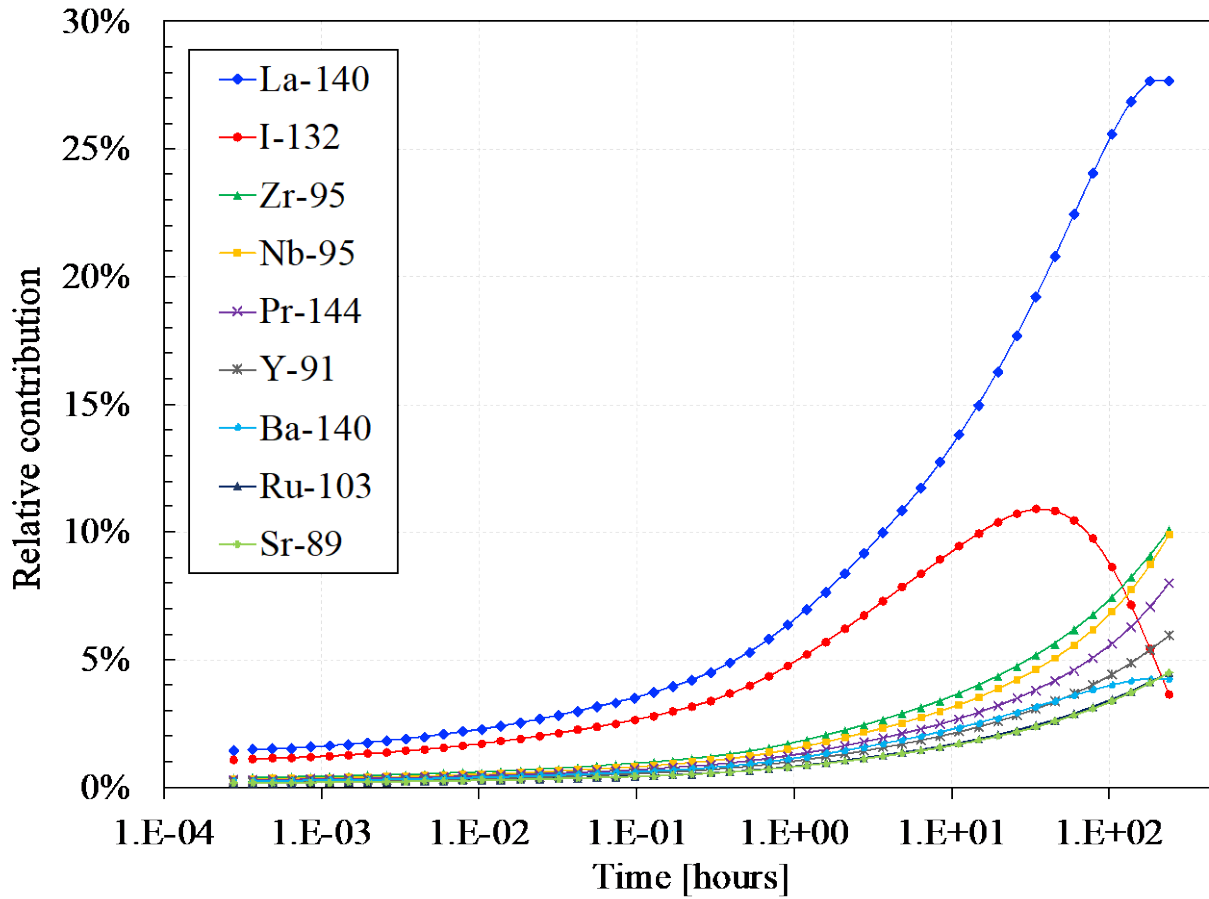
$$\rho = a + bT + cT^2 + dT^3$$

	a	b	c	d
Fuel	4.57E-02	-7.08E-05	1.59E-08	
Moderator	-2.02E-03	-2.48E-05	3.88E-08	-2.16E-11
Inner graphite	-2.18E-02	2.07E-05	-7.55E-09	
Outer graphite	-3.10E-02	3.49E-05	-1.31E-08	

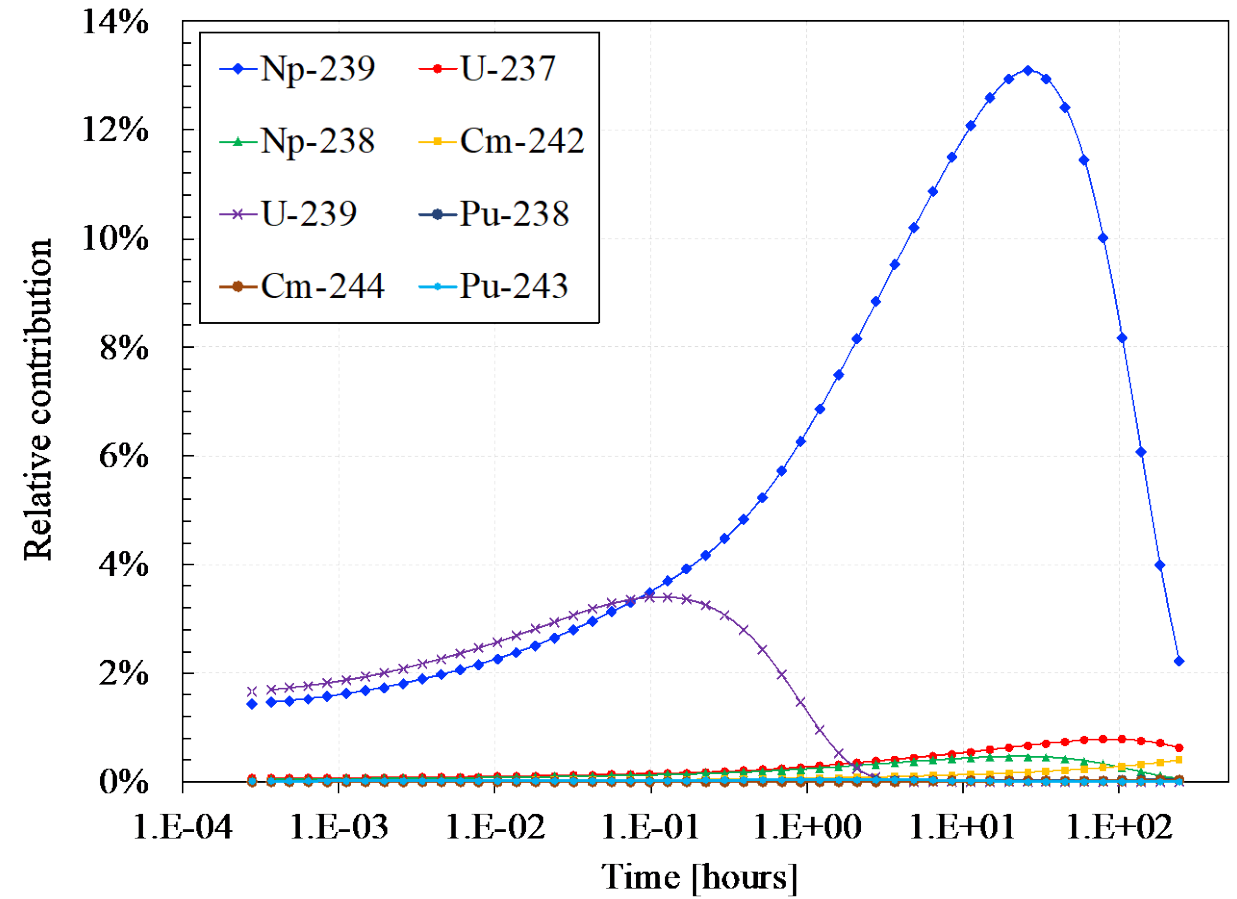
# 5. Generation of decay heat file for MELCOR



# 5. Generation of decay heat file for MELCOR

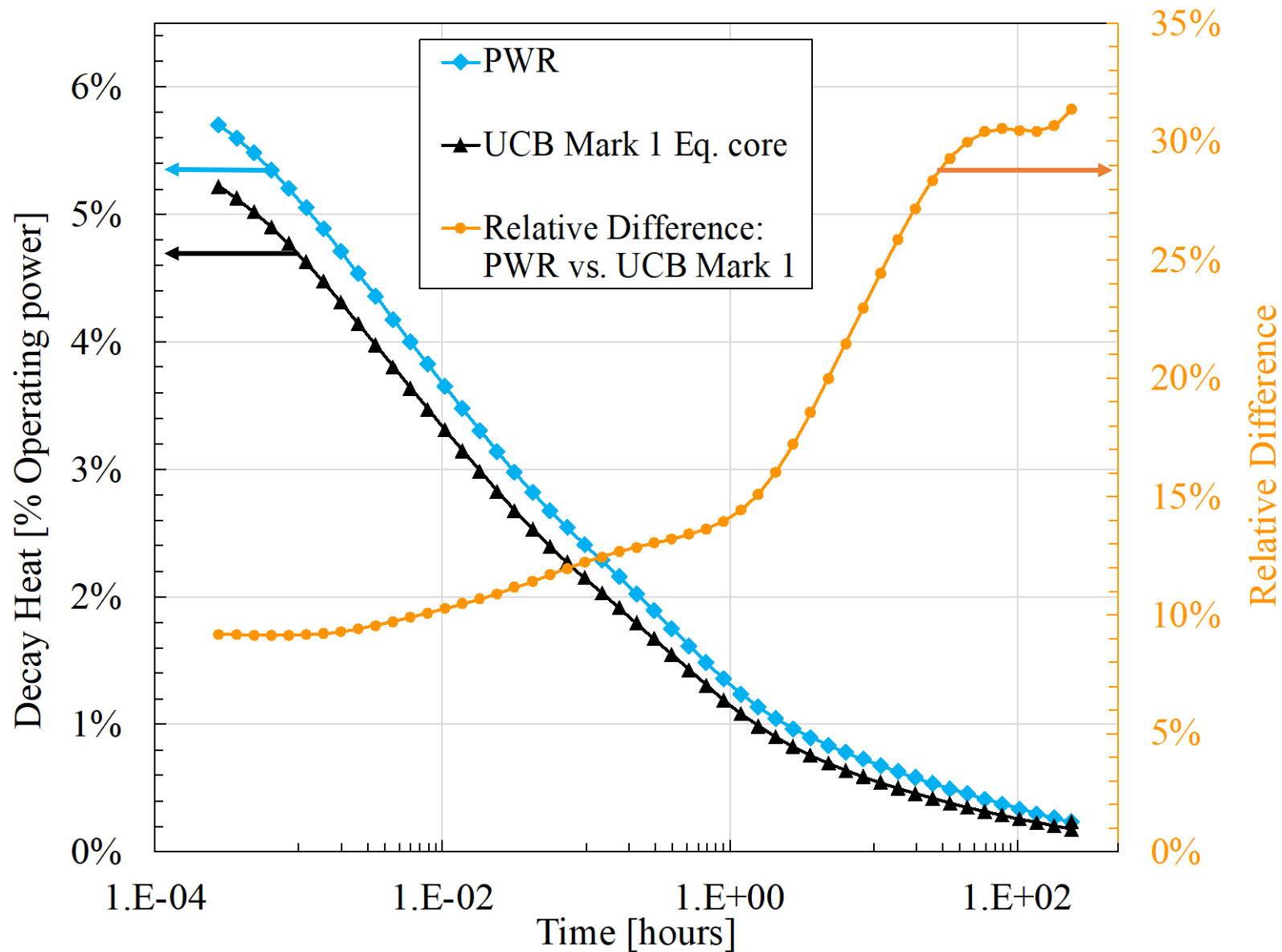


Relative contribution of top fission products



Relative contribution of top actinides

# 5. Decay heat comparisons

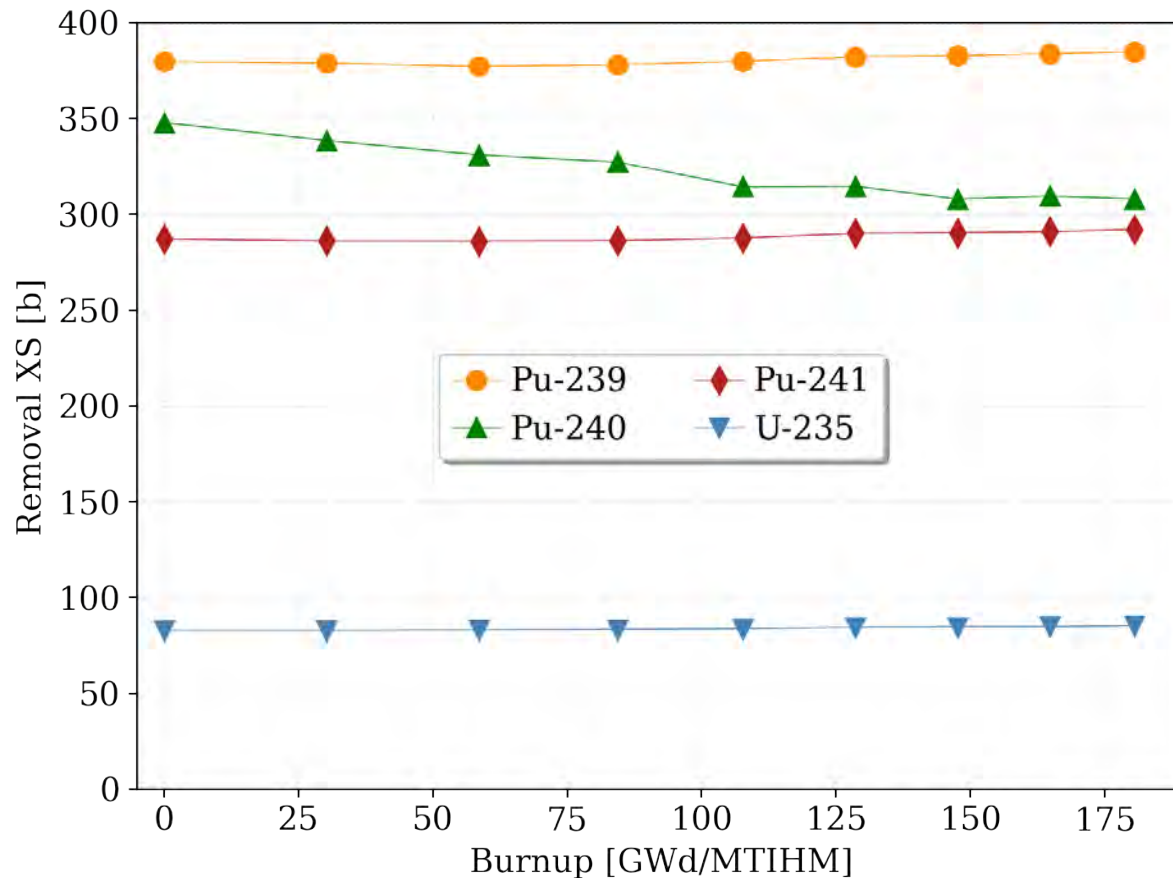


- UCB Mark 1: equilibrium core
- PWR: approximate end of cycle core (mixture of assemblies at burnup of 20, 40, 60 GWd/tHM)



## 6. Towards rapid inventory calculations with ORIGAMI

**Purpose of 1-group cross section analysis:** understand the spectral variations and their impact on 1-group cross sections which influence all inventory calculations

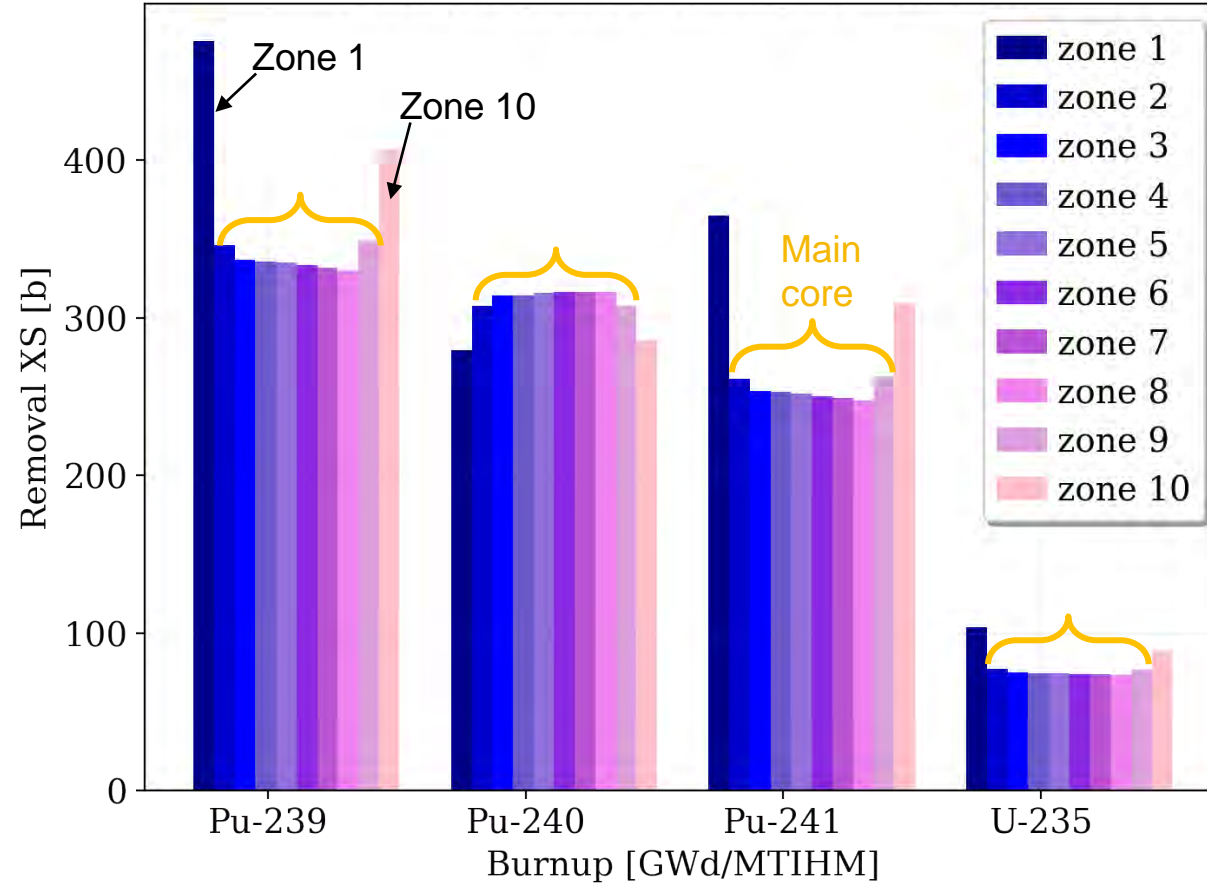
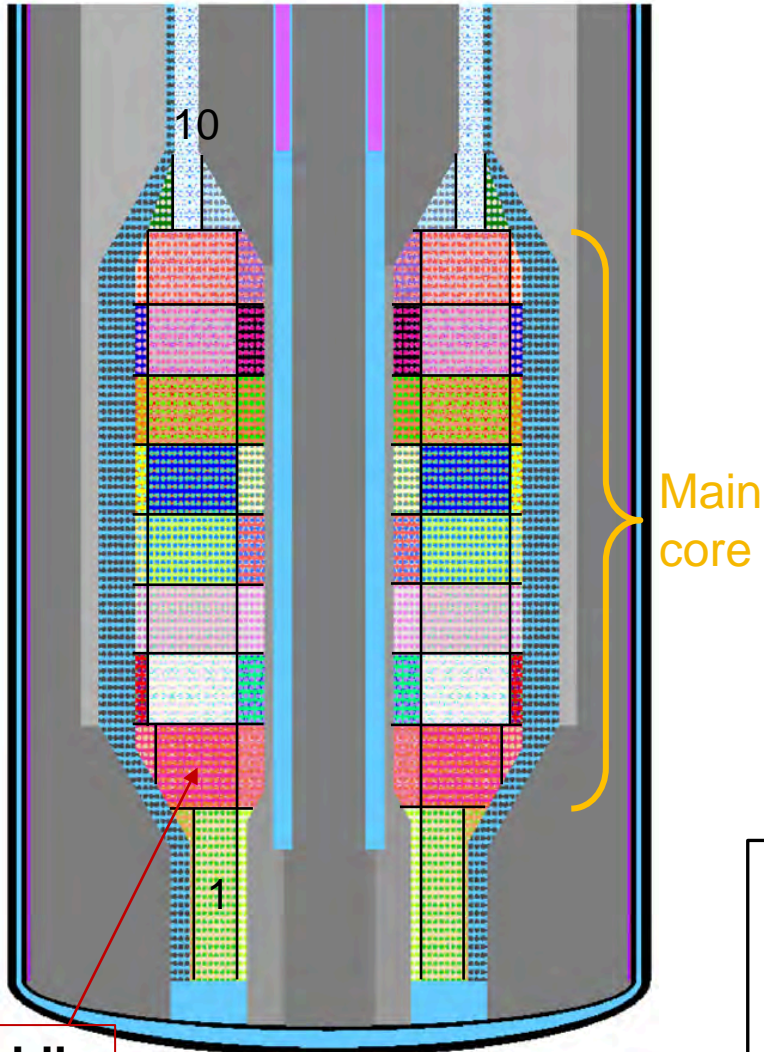


**UCB Mark 1 slice depletion (HFP)**

- Only small variation of 1-group removal cross section over depletion
- Small changes visible mainly in Pu-240

# 6. Axial variation of 1-group removal cross section

Axial variation, middle radial zone

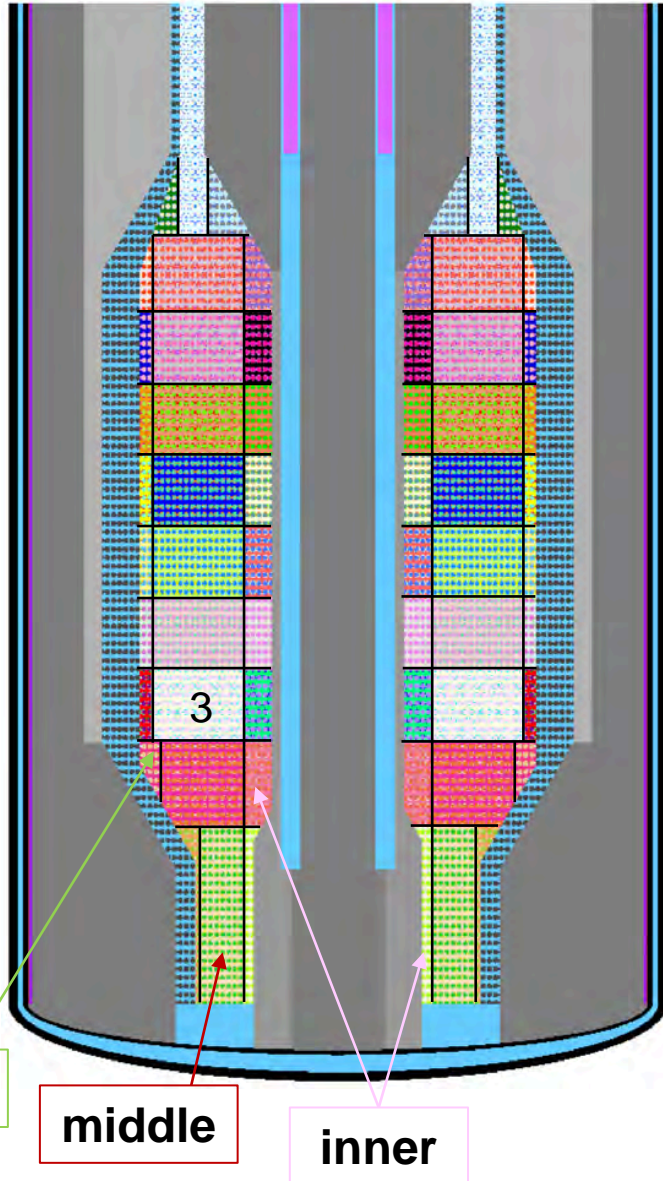


## Axial variation:

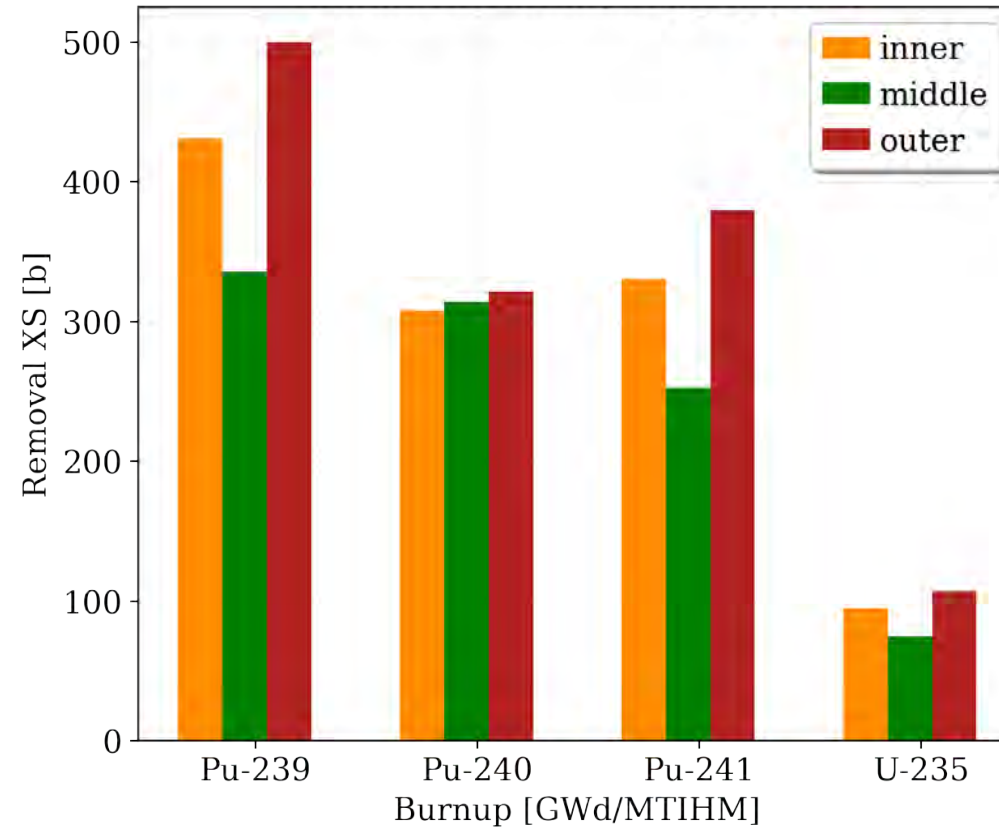
- Low variation within main core region
- Significant variation in inlet/outlet regions
- Opposing trends for certain nuclides, such as  $^{239}\text{Pu}$  vs.  $^{240}\text{Pu}$

middle

# 6. Radial variation of 1-group removal cross section



Radial variation, axial zone 3



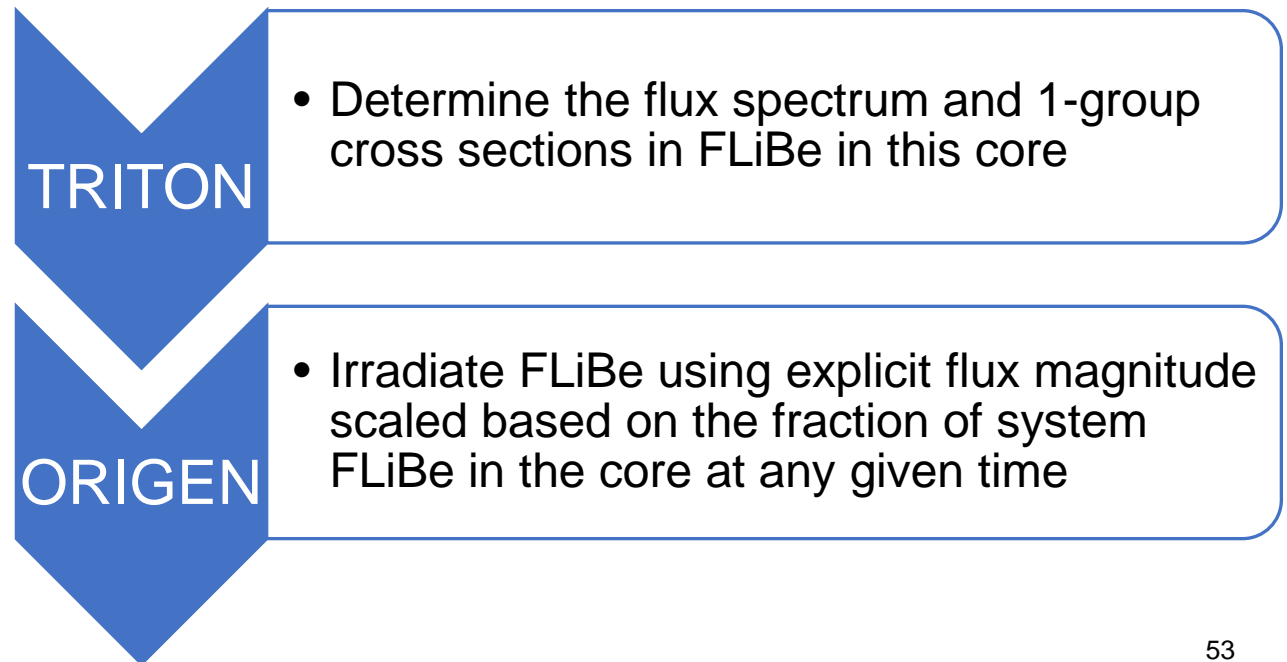
**Radial variation:**  
 Significant radial variation for various nuclides

# 7. Tritium production

## Tritium overview

- FHR uses FLiBe coolant
  - Lithium is enriched to >99.5% Li-7 because Li-6 is a neutron poison
- Li-6 and Li-7 react with neutrons to produce tritium
  - ${}^6\text{Li} + n \rightarrow {}^4\text{He} + {}^3\text{H}$
  - ${}^7\text{Li} + n \rightarrow {}^4\text{He} + {}^3\text{H} + n'$
- Tritium is a potential radiological dose hazard

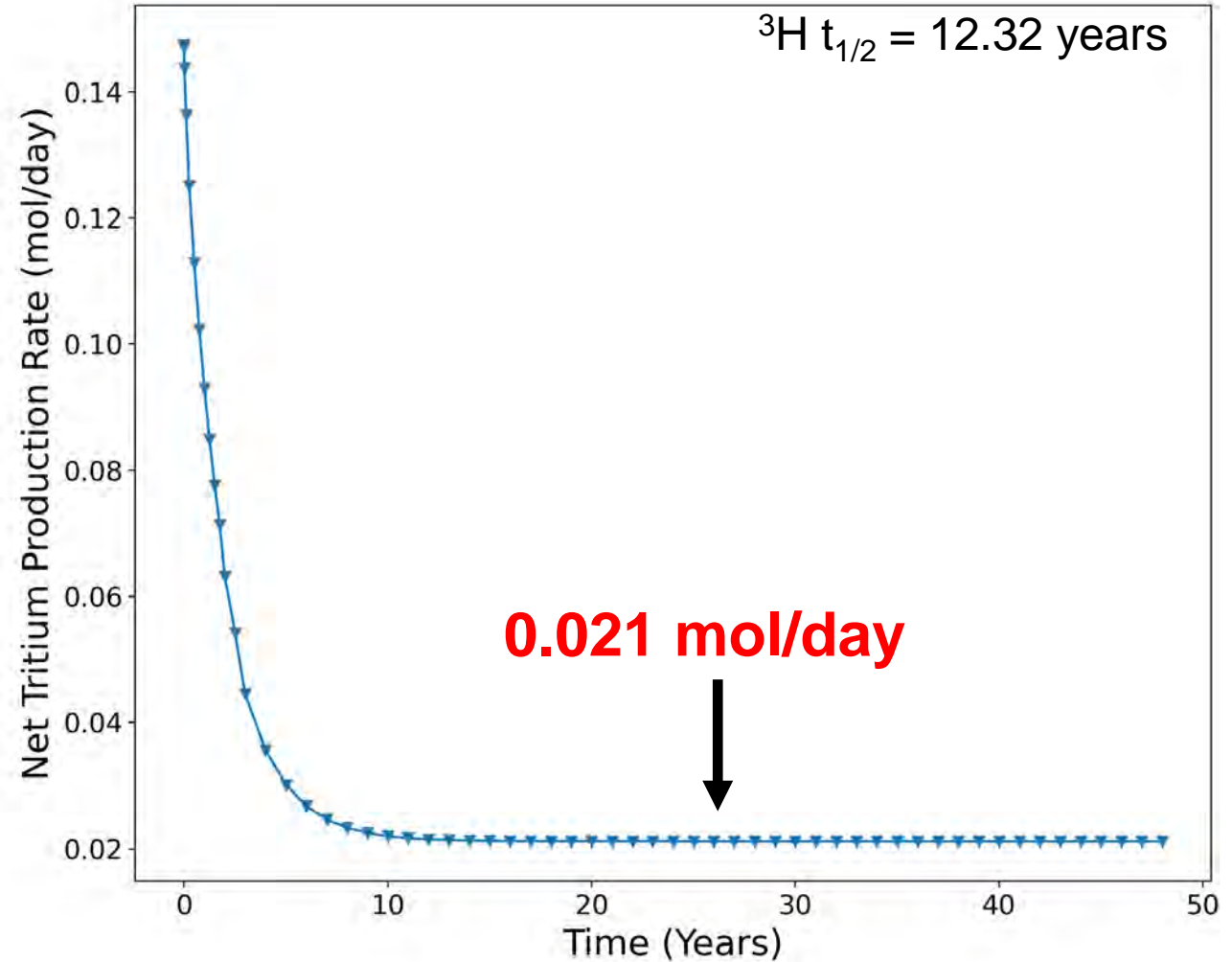
- Mass of FLiBe defined in the ORIGEN model is the total FLiBe mass in the entire system
  - To irradiate just the FLiBe in the core at a given time, we scale the flux in our ORIGEN model based on what volume fraction of FLiBe is in the core
- ORIGEN flux is equal to  $\phi \times \left(\frac{V_{core}}{V_{total}}\right)$





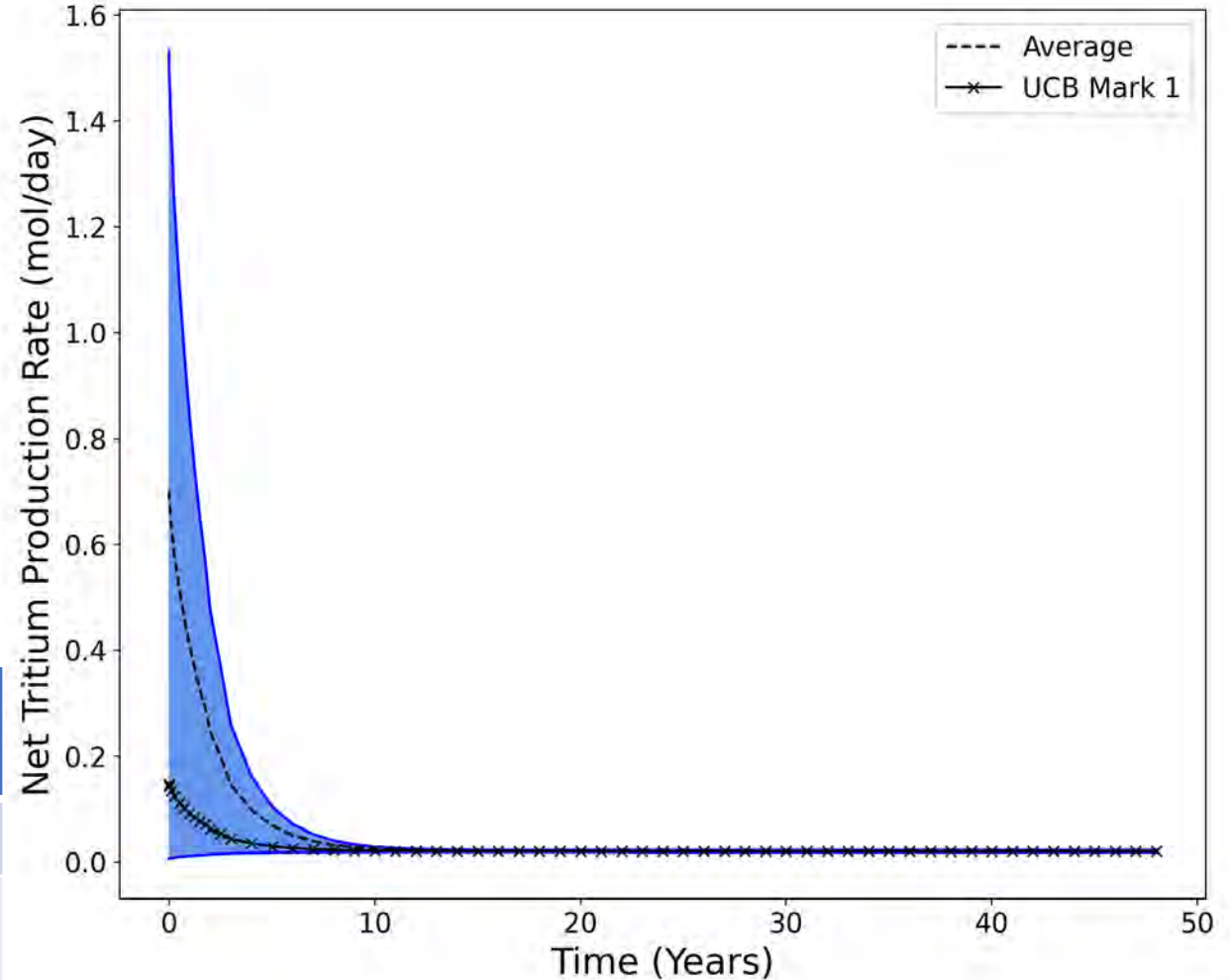
# 7. Equilibrium tritium production rate

- SCALE-predicted equilibrium value is 0.021 mol/day
  - Equilibrium value from Cisneros was 0.023 mol/day
- Equilibrium is a balance between Li-6 production and destruction
  - ${}^9\text{Be} + n \rightarrow {}^4\text{He} + {}^6\text{Li} + e^- + \bar{\nu}_e$
  - ${}^6\text{Li} + n \rightarrow {}^4\text{He} + {}^3\text{H}$
- The calculated behavior is consistent with established trends in the literature



# 7. Sensitivity analysis on tritium production

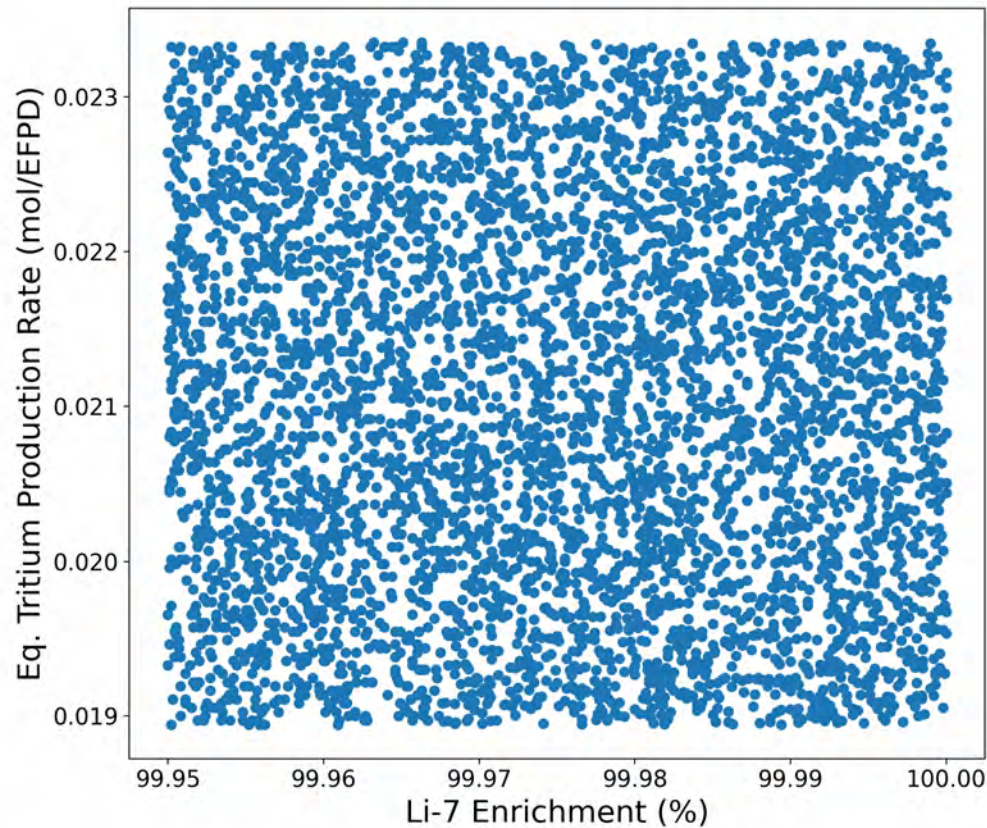
- We ran 5,000 combinations of initial Li-7 enrichment and flux using SAMPLER to determine their impact on equilibrium tritium production
- Variations in initial tritium production rate are quite large and depend on flux and initial Li-7 enrichment
  - Li-6 is a neutron poison, so FHR systems seek to enrich coolant in Li-7
  - Natural Li is 7.59% Li-6



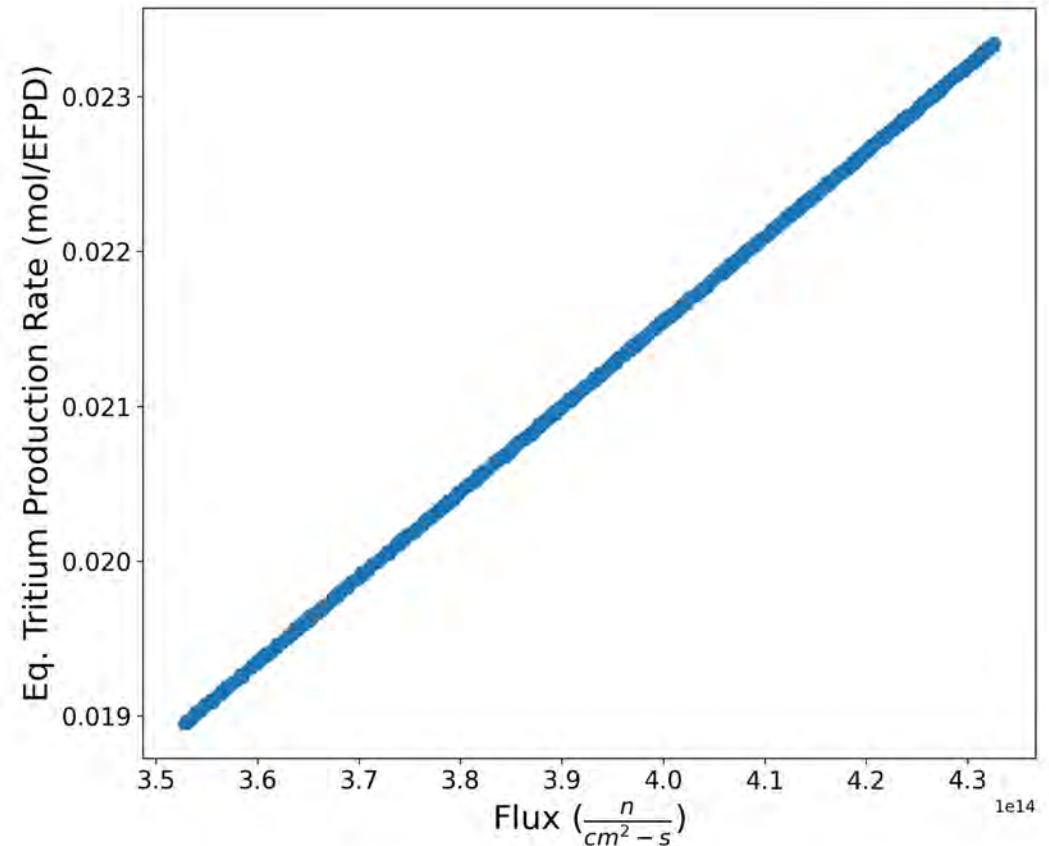
Property	Minimum Value	Maximum Value
Flux (n/cm <sup>2</sup> -s)	3.528x10 <sup>14</sup>	4.312x10 <sup>14</sup>
Initial Li-7 Enrichment (w/o)	99.95	100.0

# 7. Sensitivity analysis on tritium production

Initial Li-7 enrichment has no effect on *equilibrium tritium production rate*, while flux has a significant impact



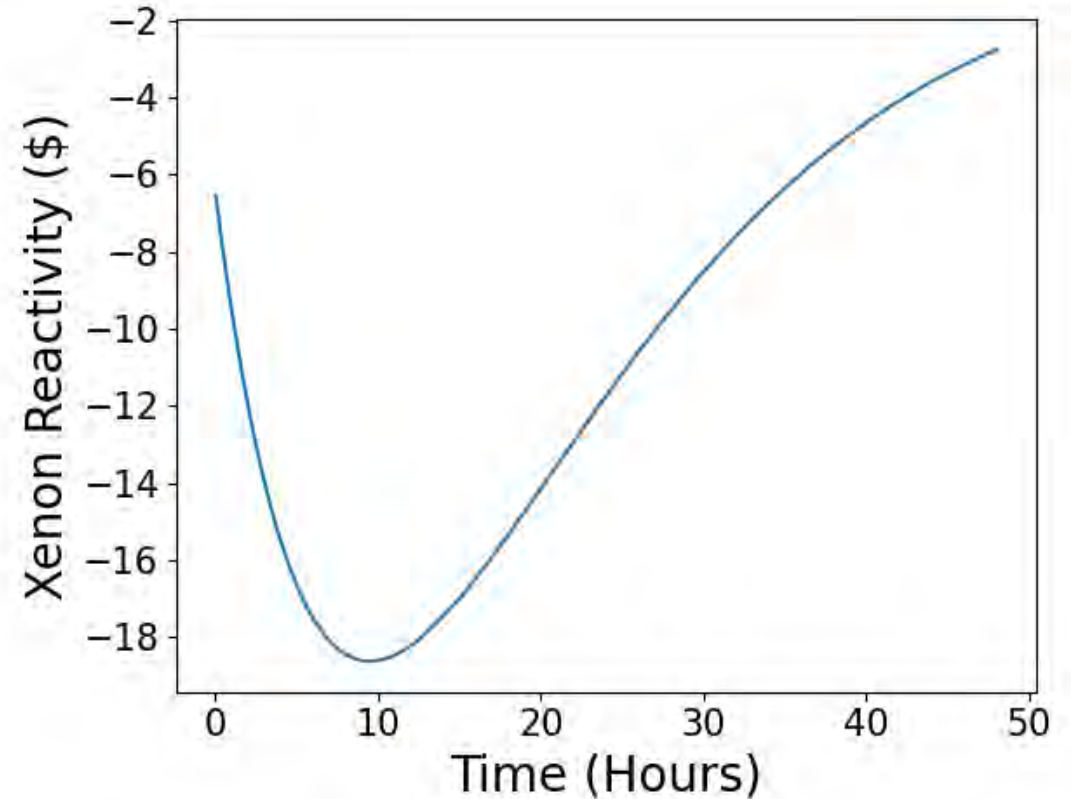
**No correlation for initial Li-7 enrichment**



**Strong correlation for neutron flux**

## 8. Transient xenon reactivity

- Steady-state Xe-135 reactivity worth is -6.48\$
- Using equilibrium I-135 and Xe-135 concentrations from UCB Mark 1 model, we can calculate time-dependent concentrations analytically
- When flux goes to zero, Xe-135 inventory is dictated only by decay of I-135 and Xe-135
- Peak Xe-135 reactivity is -18.6\$ and occurs at 9.49 hours
- Xe-135 reactivity drops below steady-state value after 34.67 hours



$$\frac{dI}{dt} = \gamma_I \Sigma_f \phi - \lambda_I I$$

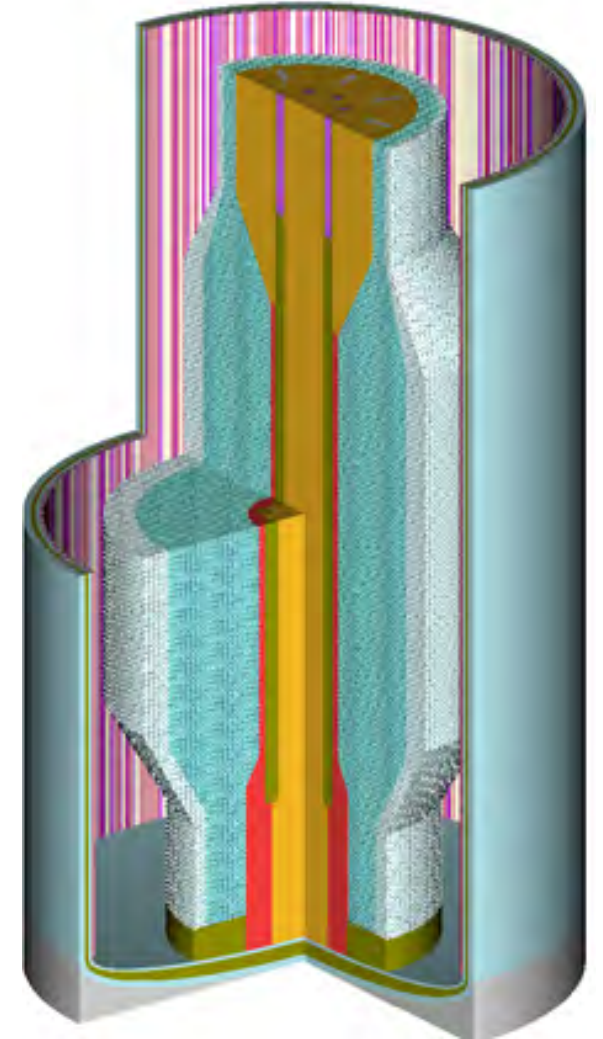
$$\frac{dX}{dt} = \gamma_X \Sigma_f \phi + \lambda_I I - \lambda_X X - \sigma_a X \phi$$



# Neutronics Summary

## Demonstrated SCALE's capabilities for FHR modeling

- SCALE's multigroup physics was confirmed adequate through FHR fuel pebble analysis:  $k_{\text{eff}}$  bias smaller than 260 pcm, while achieving 24 times faster runtime
- Fuel compositions for an equilibrium core were developed using an iterating scheme
- Power profiles and decay heat were determined for equilibrium core
- Temperature feedback: linear behavior found for salt, nonlinear trend for fuel and for materials containing graphite
- Strong radial variation for 1-group cross section was observed, while axial variation was limited to inlet/outlet regions
- Tritium production rate in coolant salt was estimated
- Preliminary results for time-dependent Xe-135 concentration



# MELCOR Molten Salt Models



**U.S. NRC**

 **OAK RIDGE**  
National Laboratory

 **Sandia**  
National  
Laboratories

# MELCOR Molten Salt Reactor Modeling

Added molten salt as working fluid

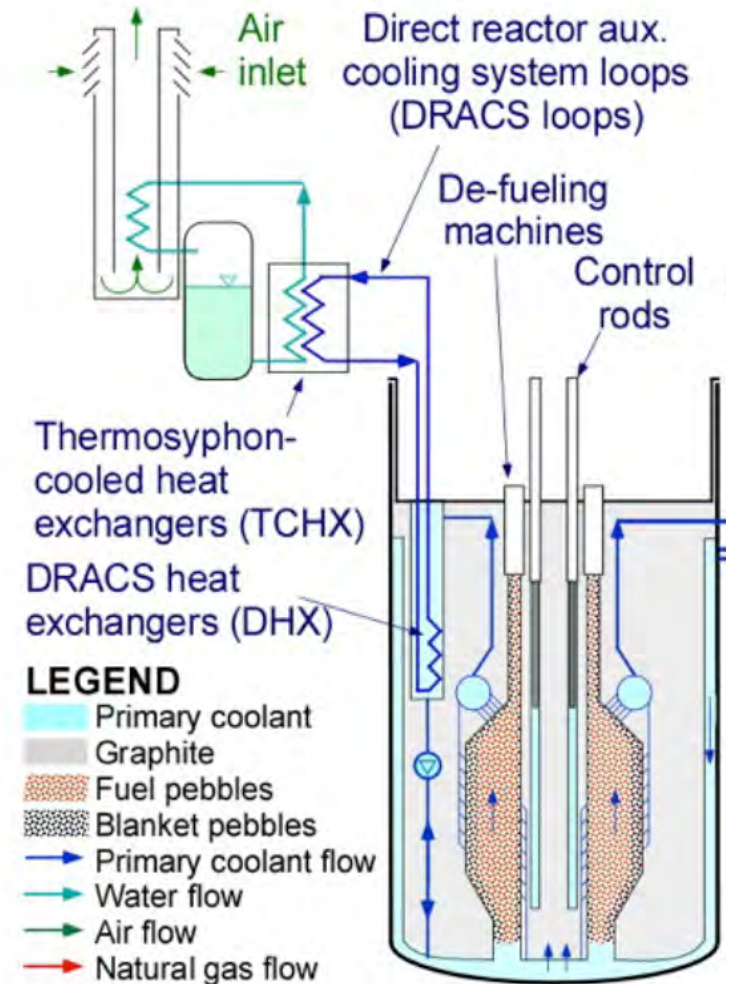
Fission product release

- Release from TRISO kernel
- Radionuclide distributions within the layers in the TRISO particle and compact
- Liquid-phase fission product chemistry and transport model

Additional core models

- Graphite oxidation
- Intercell and intracell conduction
- Convection & flow

Fluid point kinetics (liquid-fueled molten salt reactors)



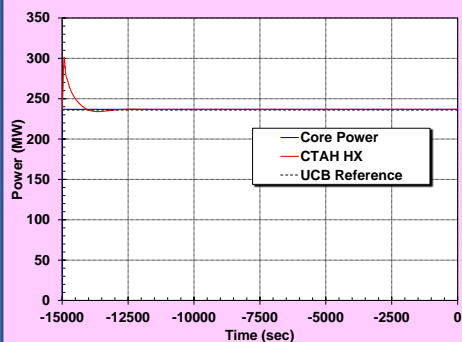
# Transient/Accident Solution Methodology

**Stage 0:**  
Normal Operation  
Establish thermal state

*Time constant in FHR graphite structures is very large*

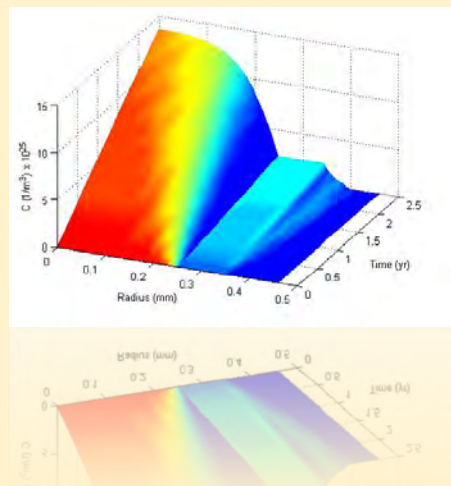
*Reduce heat capacities for structures to reach steady state thermal conditions.*

*Reset heat capacities after steady state is achieved.*



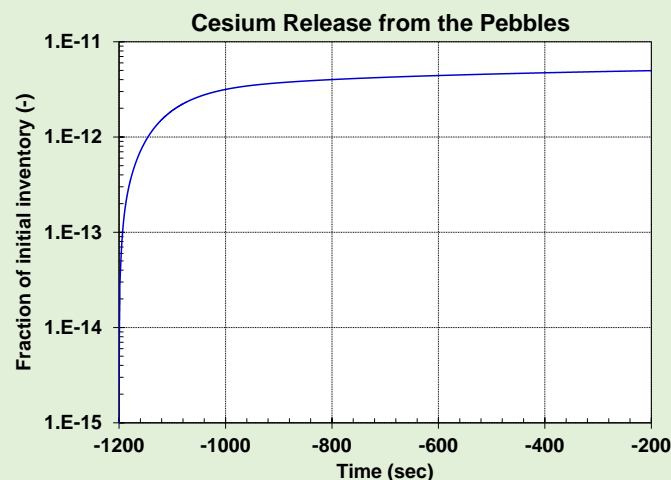
**Stage 1:**  
Normal Operation  
Diffusion Calculation

*Establish steady state distribution of radionuclides in TRISO particles, and matrix*



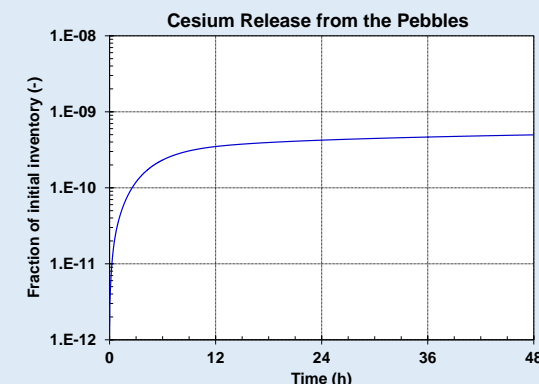
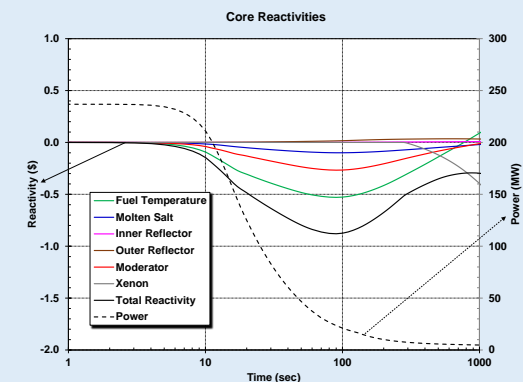
**Stage 2:**  
Normal Operation  
Transport Calculation

*Calculate steady state distribution of radionuclides into the molten salt (formation of soluble, colloidal fission products, deposition on surfaces, convection through flow paths)*



**Stage 3:**  
Accident  
Diffusion & Transport calculation

*Calculate accident progression and radionuclide release*



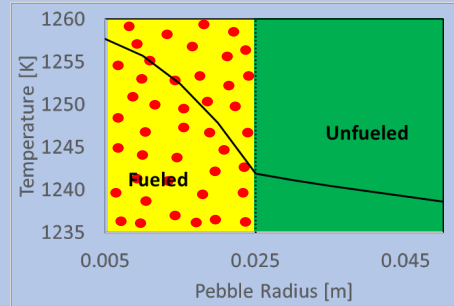
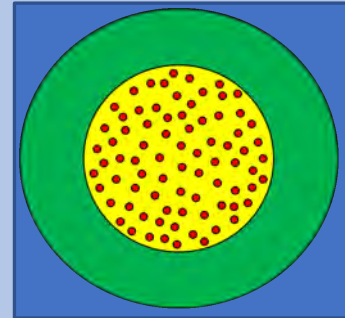


# Core components

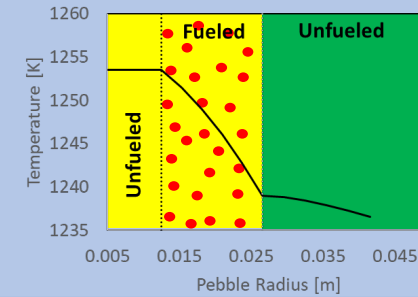
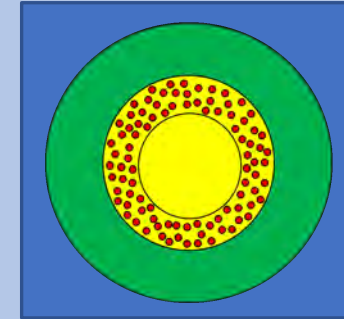
## • Pebble Bed Reactor Fuel/Matrix Components

- Fueled part of pebble
- Unfueled shell (matrix) is modeled as separate component
- Fuel radial temperature profile for sphere

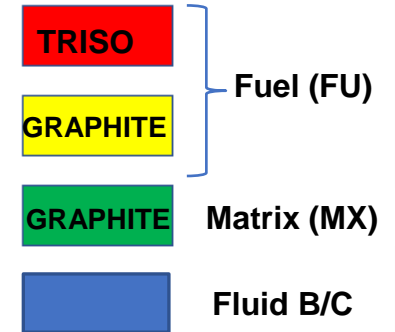
Fueled pebble core



Unfueled pebble core



## Legend

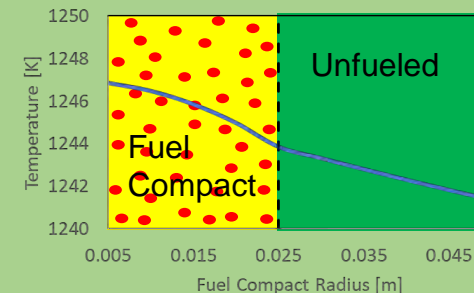
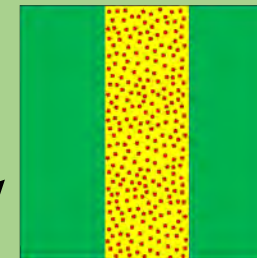
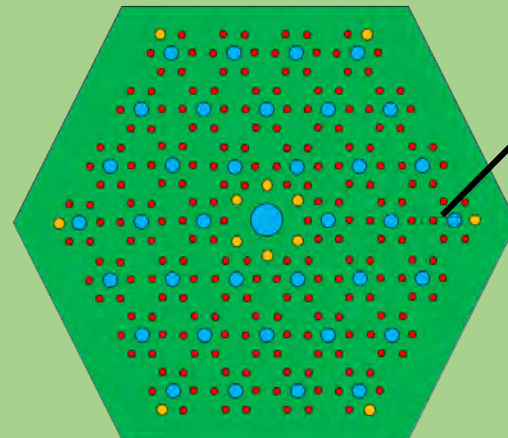


TRISO (FU)

*Sub-component model for zonal diffusion of radionuclides through TRISO particle*

## • Prismatic Modular Reactor Fuel/Matrix Components

- “Rod-like” geometry
- Part of hex block associated with a fuel channel is matrix component
- Fuel radial temperature profile for cylinder

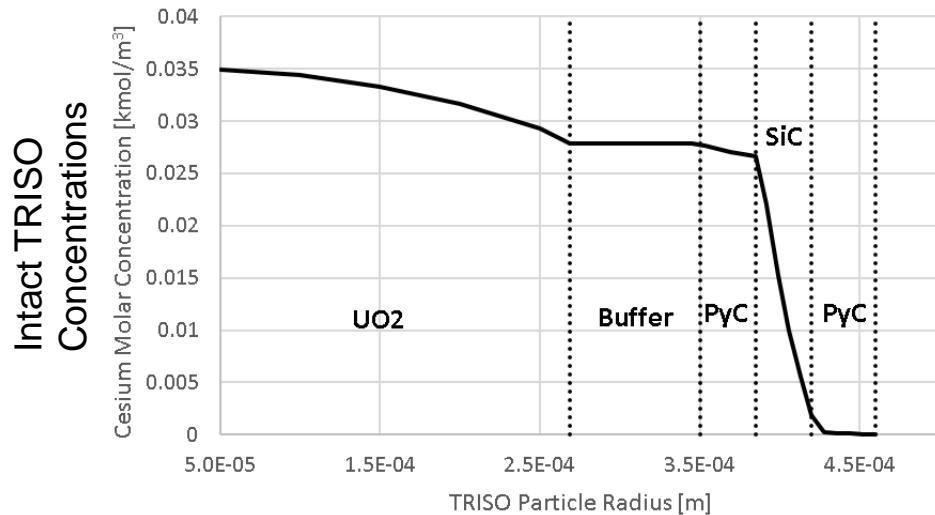
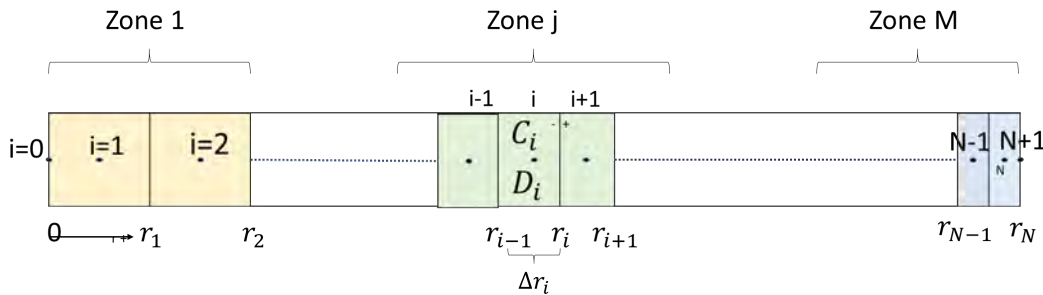


# Radionuclide Diffusion Release Model

## Intact TRISO Particles

- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

$$\frac{\partial C}{\partial t} = \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n D \frac{\partial C}{\partial r} \right) - \lambda C + \beta \quad D(T) = D_0 e^{-\frac{Q}{RT}}$$



## Diffusivity Data Availability

Radionuclide	UO <sub>2</sub>	UCO	PyC	Porous Carbon	SiC	Matrix Graphite	TRISO Overall	
Ag	Some	Not investigated	Some	Not found	Extensive	Some	Extensive	
Cs	Some		Some		Extensive	Some	Some	
I	Some		Some		Some	Not found	Not found	Not found
Kr	Some		Some		Not found	Some	Some	
Sr	Some		Some		Extensive	Some	Some	
Xe	Some		Some		Some	Some	Some	Not found

## Data used in the demo calculation [IAEA TECDOC-0978]

Layer	FP Species							
	Kr		Cs		Sr		Ag	
	D (m <sup>2</sup> /s)	Q (J/mole)	D (m <sup>2</sup> /s)	Q (J/mole)	D (m <sup>2</sup> /s)	Q (J/mole)	D (m <sup>2</sup> /s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6E-8	209000.0	2.2E-3	488000.0	6.75E-9	165000.0
Buffer	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0
PyC	2.9E-8	291000.0	6.3E-8	222000.0	2.3E-6	197000.0	5.3E-9	154000.0
SiC	3.7E+1	657000.0	7.2E-14	125000.0	1.25E-9	205000.0	3.6E-9	215000.0
Matrix Carbon	6.0E-6	0.0	3.6E-4	189000.0	1.0E-2	303000.0	1.6E00	258000.0
Str. Carbon	6.0E-6	0.0	1.7E-6	149000.0	1.7E-2	268000.0	1.6E00	258000.0

Iodine assumed to behave like Kr



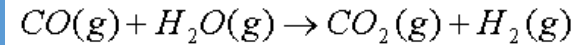
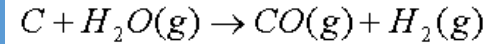
# Graphite Oxidation

Existing capability introduced with High-Temperature Gas-cooled Reactors (HTGRs)

## Steam oxidation

$$R_{OX,steam} = \frac{k_4 P_{H_2O}}{1 + k_5 P_{H_2}^{0.5} + k_6 P_{H_2O}}$$

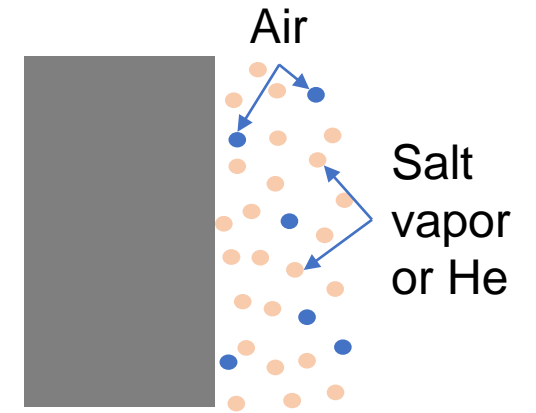
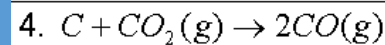
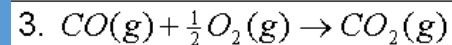
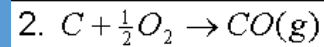
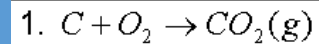
## Reactions



## Air oxidation

$$R_{OX} = 1.7804 \times 10^4 \exp\left(-\frac{20129}{T}\right) \left(\frac{P}{0.21228 \times 10^5}\right)^{0.5}$$

## Reactions

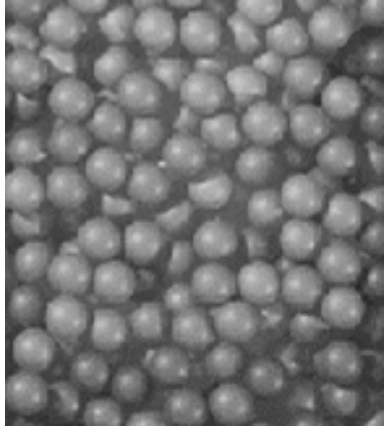


Air diffusion towards oxidation surface is rate limited due to mass transfer limitations in presence of salt vapor

$R_{OX}$  is the rate term in the parabolic oxidation equation [1/s]



# Energy Transport between Discrete Core Volumes



## Effective conductivity prescription for pebble bed (bed conductance)

- Zehner-Schlunder-Bauer, without radiation heat transfer

$$k_{eff} = (1 - \sqrt{1 - \epsilon})k_f + (\sqrt{1 - \epsilon})k_c(T, \epsilon, k_f, k_s)$$

where:

$\epsilon$  = Bed porosity [-]

$k_f$  = Fluid (FLiBe) conductivity [W/m/K]

$k_c$  = Effective bed conductivity [W/m/K], used with zero radiative conductivity

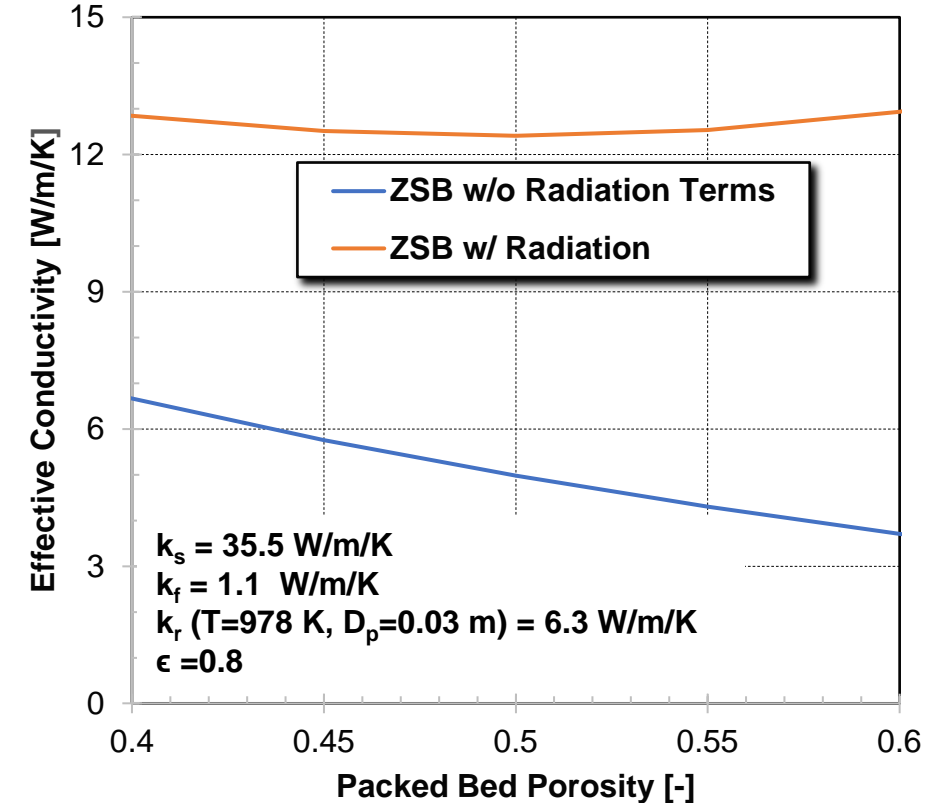
$k_s$  = Solid conductivity [W/m/K]

$T$  = Solid temperature [K]

- Effective fluid conductivity combines liquid and vapor contributions according to vapor fraction
- Radiative conductivity is combined by vapor fraction and used in ZSB model with radiation terms

$$k_{eff} = (1 - \sqrt{1 - \epsilon})k_r + (1 - \sqrt{1 - \epsilon})k_f + (\sqrt{1 - \epsilon})k_c(T, D_p, \epsilon, k_f, k_s, k_r(X_{Vapor}))$$

$$k_r = 4\epsilon\sigma T^3 D_p X_{Vapor}$$



# Interface Between Thermal Hydraulics and Reactor Core Structures

Heat transfer coefficient (Nusselt number) correlations for pebble bed convection:

- Isolated, spherical particles
- Use  $T_{film}$  to evaluate non-dimensional numbers, use maximum of forced and free Nu

$$Nu_{Free} = 2.0 + 0.6 Gr_f^{1/4} Pr_f^{1/3} \qquad Nu_{Forced} = 2.0 + 0.6 Re_f^{1/2} Pr_f^{1/3}$$

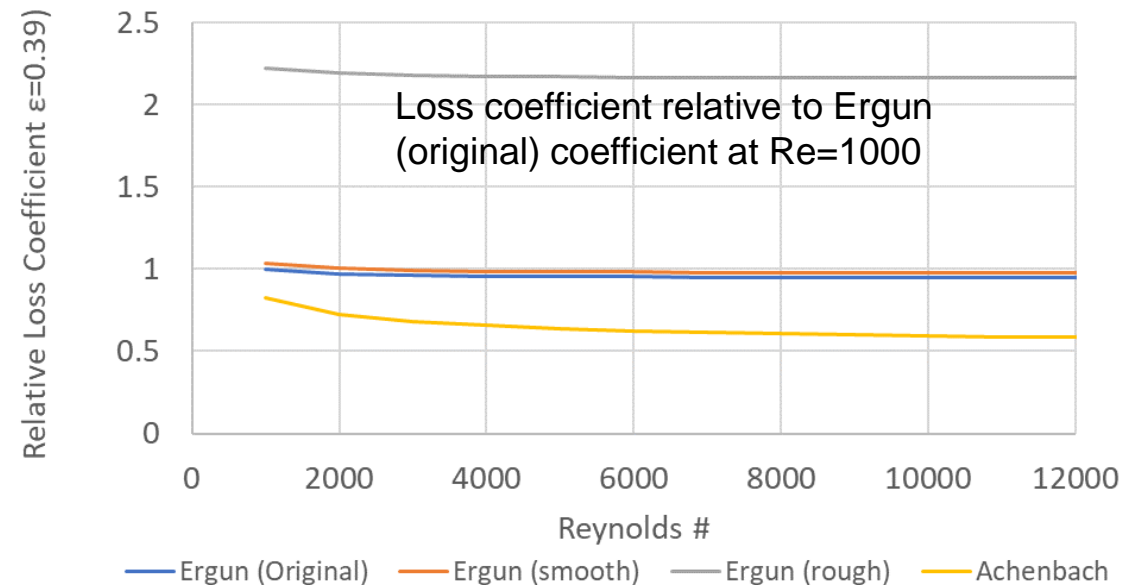
- Constants and exponents accessible by sensitivity coefficient

## Flow resistance

- Packed bed pressure drop

$$K_L(\epsilon, Re) = \left[ C_1 + C_2 \frac{1-\epsilon}{Re} + C_3 \left( \frac{1-\epsilon}{Re} \right)^{C_4} \right] \frac{(1-\epsilon)L}{\epsilon D_p}$$

Correlation	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>
Ergun (original)	3.5	300.	0.0	-
Modified Ergun (smooth)	3.6	360.	0.0	-
Modified Ergun (rough)	8.0	360.	0.0	-
Achenbach	1.75	320.	20.0	0.4



# Point Kinetics Modeling

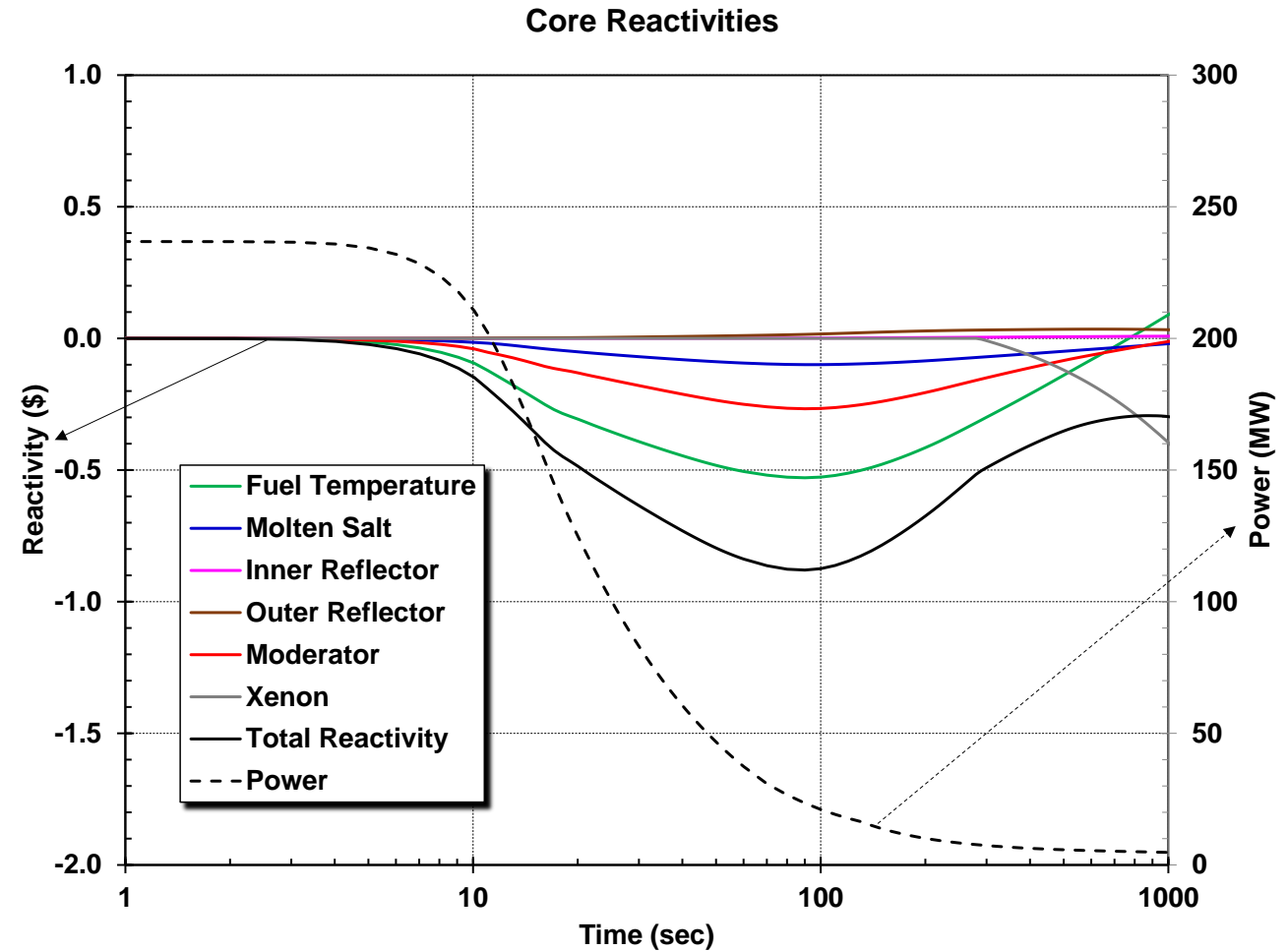
## Standard treatment

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

$$\frac{dY_i}{dt} = \left( \frac{\beta_i}{\Lambda} \right) P - \lambda_i C_i, \quad \text{for } i = 1 \dots 6$$

## Feedback models

- User-specified external input
- FHR example includes multiple feedbacks
  - Fuel
  - Molten salt around the fuel
  - Inner reflector
  - Outer reflector and unfueled pebbles
  - Moderator (matrix around fueled pebbles)



# Point Kinetics Modeling (MSR)

Derived from standard PRKEs and solved similarly

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

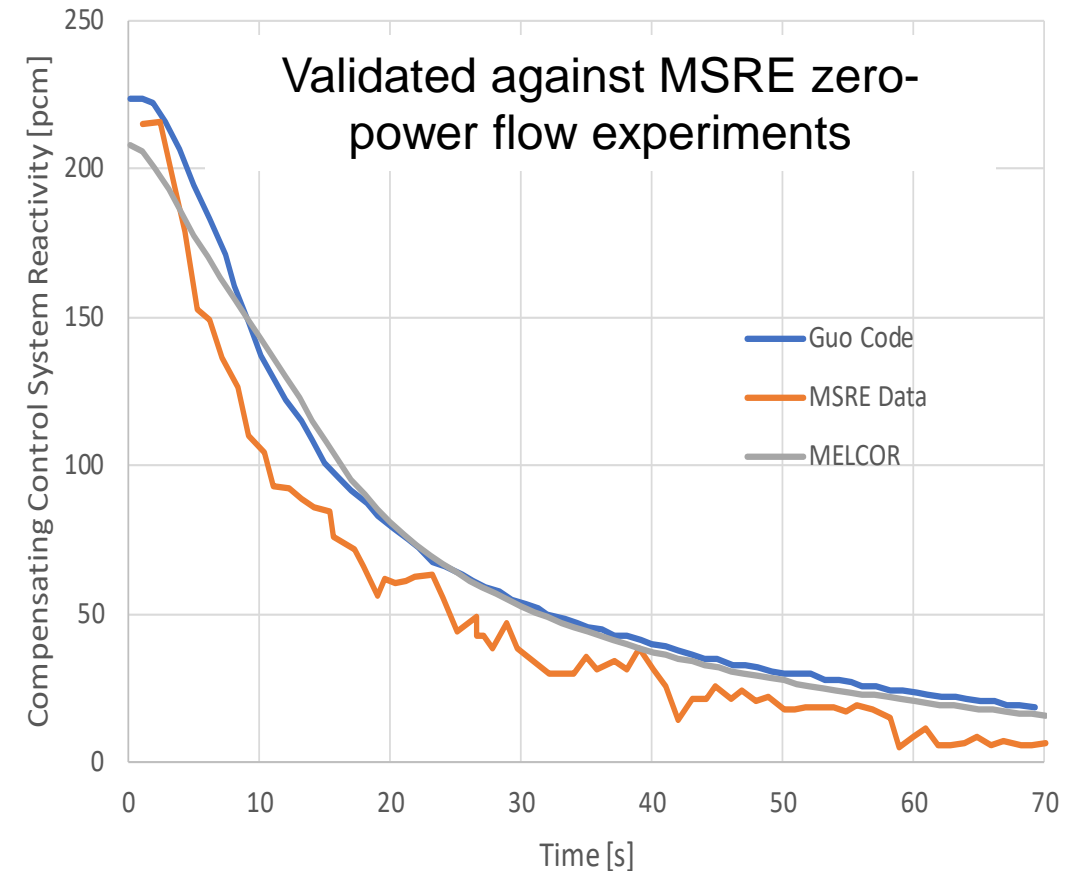
$$\frac{dC_i^C(t)}{dt} = \left( \frac{\beta_i}{\Lambda} \right) P(t) - \left( \lambda_i + 2/\tau_C \right) C_i^C(t) + \left( \frac{V_L}{V_C} \right) \left( \lambda_i + 2/\tau_L \right) C_i^L(t), \quad i = 1 \dots 6$$

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

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

## Feedback models

- User-specified external input
- Doppler
- Fuel and moderator density
- Flow reactivity feedback effects integrated into the equation set





# Molten Salt Chemistry and Radionuclide Release

Radionuclides grouped into forms found in the Molten Salt Reactor Experiment

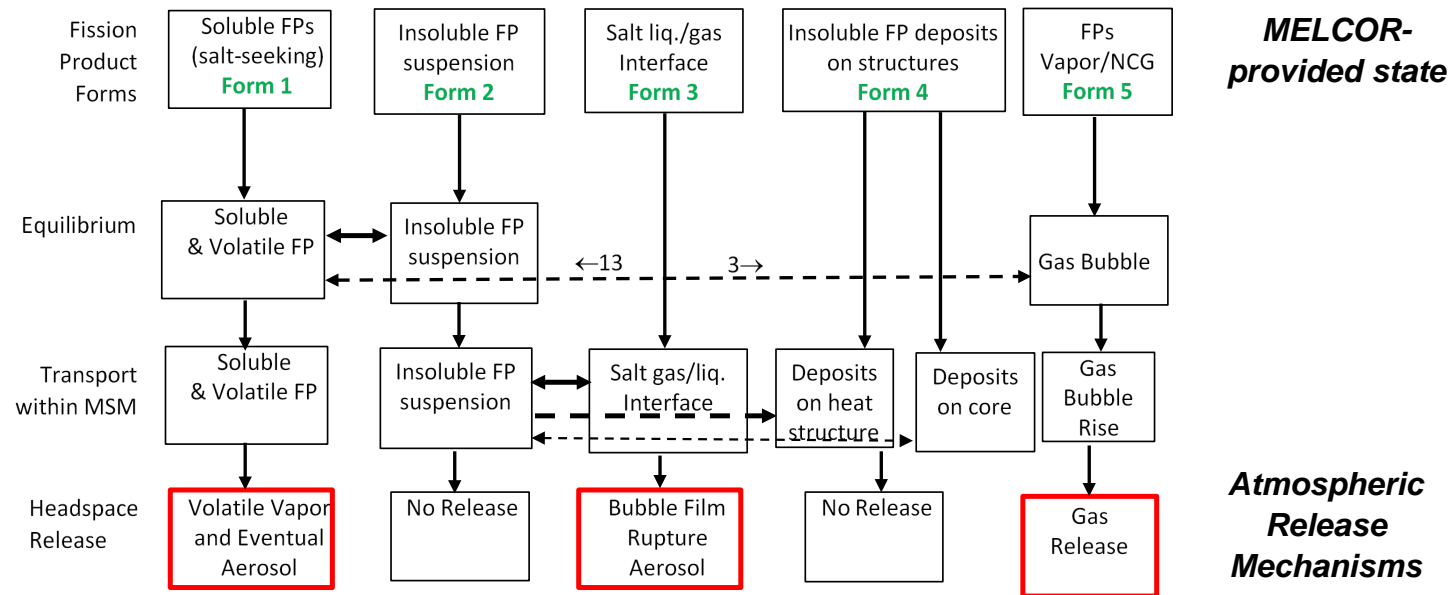
## Model Scope

### Evaluation of thermochemical state

- Gibbs Energy Minimization with Thermochemica
- Provides solubilities and vapor pressures

### Thermodynamic database

- Generalized approach to utilize any thermodynamic database
- An example is the Molten Salt Thermal Database
  - FLiBe-based systems
  - Chloride-based systems



## Initial Model Form

Solubility determined from empirical evidence (P. Britt ORNL 2017)

Solubilities mapped to 17 MELCOR fission product classes

Insoluble MELCOR classes are assigned to be colloidal

# Fluoride-salt-cooled High-Temperature Reactor Plant Model and Source Term Analysis



**U.S. NRC**



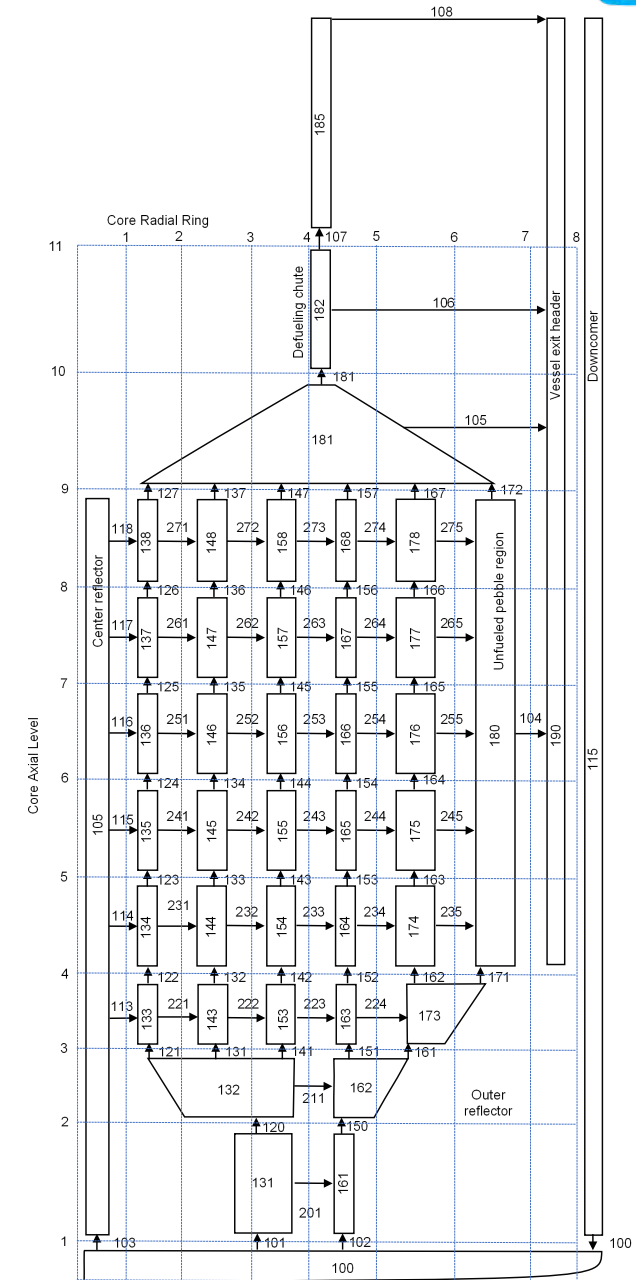
# Core and reactor vessel

## Core nodalization – light blue lines

- Assumes azimuthal symmetry
- Subdivided into 11 axial levels and 8 radial rings
- Core cells model molten salt fluid volume, reflector structures, the pebble-bed core, and the pebbles in the defueling chute

## Fluid flow nodalization – black boxes

- Molten salt enters through the downcomer and flows into the center reflector and into the bottom of the pebble bed
- Molten salt leaves through the periphery of the core and upwards through the refueling chute
- Unfueled graphite pebbles in box labeled “180”



# Recirculation loops

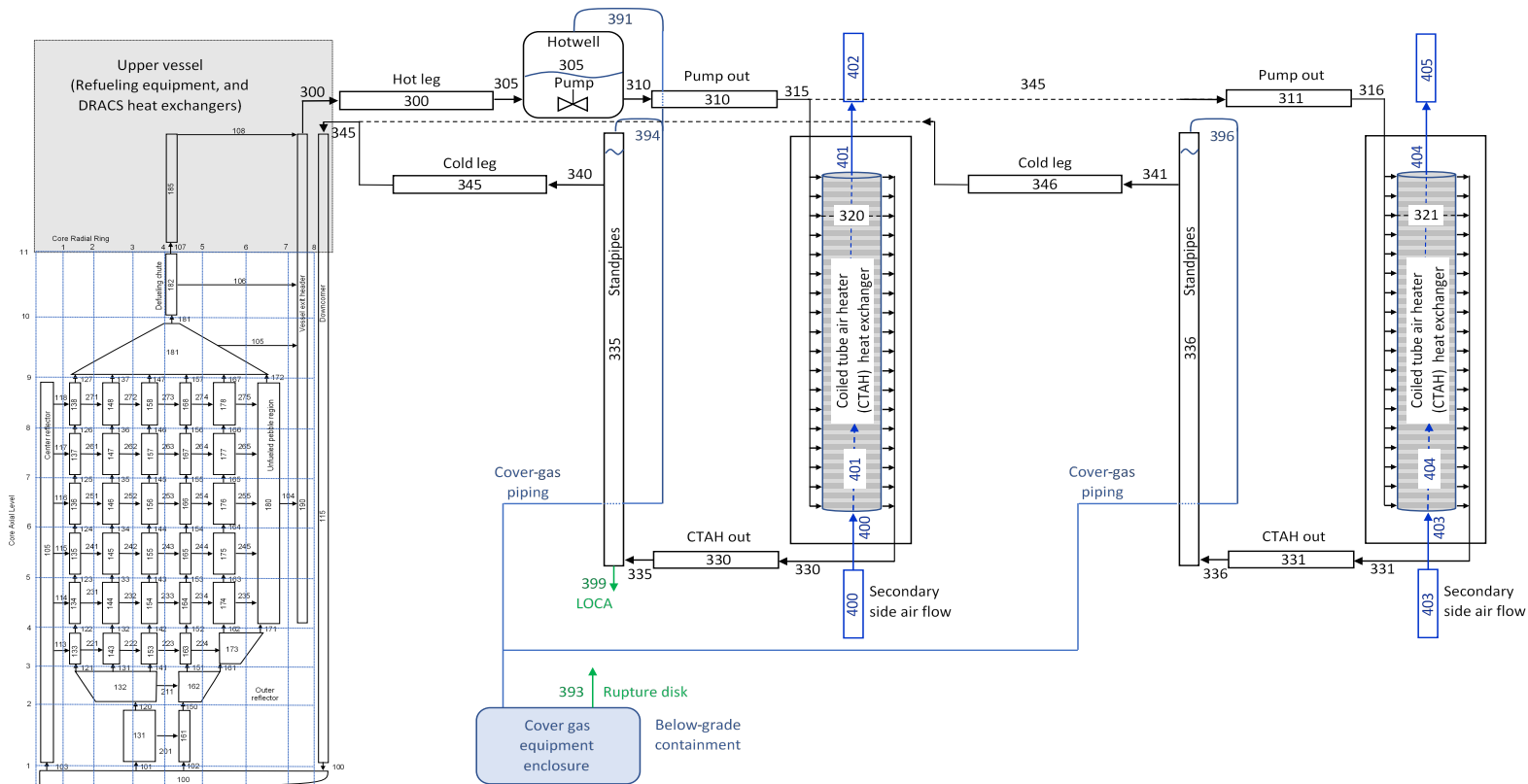
Each loop has a pump, a heat exchanger, and a standpipe

Molten salt has free surface in the hotwell and the standpipes

Argon gas above the free surfaces with connection to the cover-gas system

- Over-pressurization relief passes through the cover gas system
- Cover gas enclosure leaks into the containment when over-pressurized

Secondary-side air cools primary-side molten salt





# Direct Reactor Auxiliary Cooling System (DRACS)

3 trains – 2.36 MW/train

- 236 MWt reactor

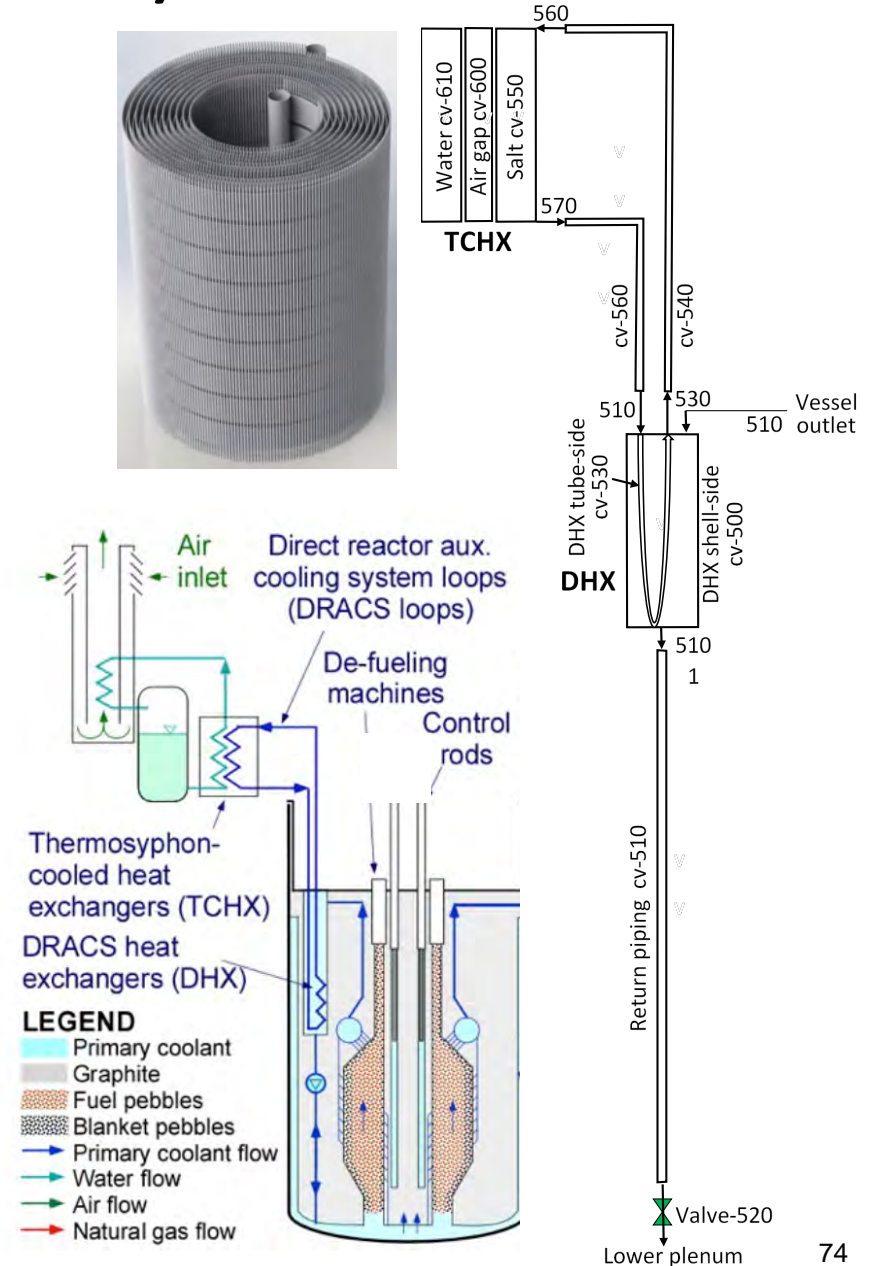
Each train has 4 loops in series

- Primary coolant circulates to DRACS heat exchanger
- Molten-salt loop circulates to the thermosyphon-cooled heat exchangers (TCHX)
- Water circulates adjacent to the secondary salt tube loop in the TCHX
- Natural circulation air circuit cools and condenses steam

Start-up: RCS-pump trip causes ball in valve to drop

Additional system information

- DHXs are in the reactor vessel
- TCHXs are in the shield building



# Containment

## Shield dome

- Protection against aircraft and natural gas detonations (co-fired turbine concept)
- Contains water for DRACS and RCCS
- DRACS air natural circulation chimneys connected to the shield dome

## Reactor cavity

- Fire-brick insulation
- Low free volume
- Low-leakage bellows between reactor cavity and adjacent cavities

## Separate compartments for the other RCS components

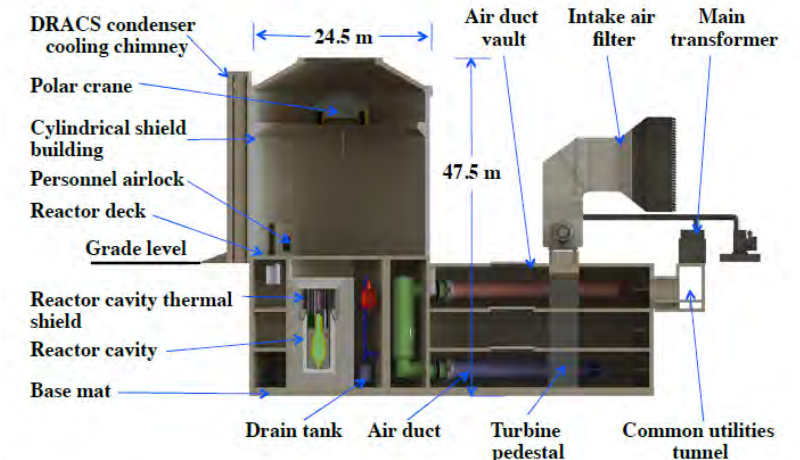
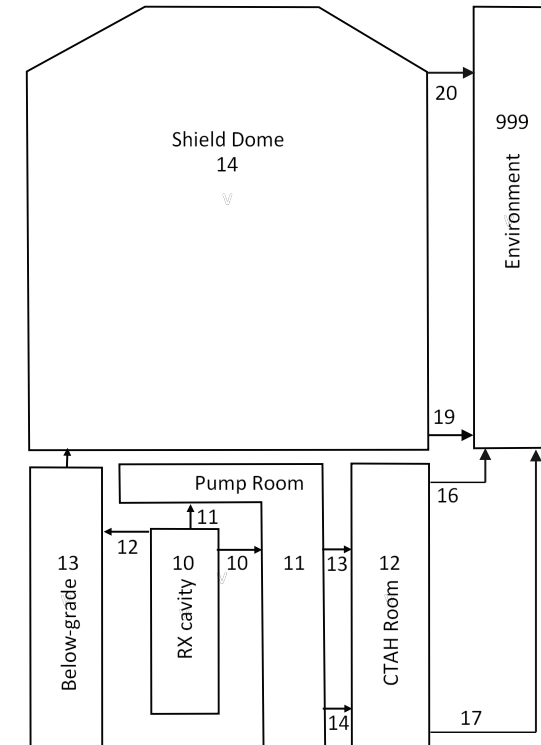
- Below-grade compartment includes the cover-gas enclosure for reactor cavity over-pressurization

## Reactor cavity cooling subsystem in reactor cavity wall

- Water circulation
- Cooling tubes affixed to reactor cavity steel liner
- Cools concrete during normal operation

## Leak rate assumed consistent with BWR Mark 1 reactor building

- 100% vol/day at 0.25 psig



# MELCOR model inputs (1/2)

Equilibrium inventory and decay heat from SCALE

Radial and axial power profiles from SCALE

Reactivity feedbacks from SCALE

Cell-to-cell radial and axial heat transfer in the pebble bed and to adjacent reflector structures

- Modified Zehner-Schlunder-Bauer model formulation
- Combined conductive and radiative (when core uncovered) heat transfer depends on the coolant and fuel conductivities, fuel (graphite) emissivity, pebble bed porosity

Pebble bed friction losses – Achenbach pressure drop formulation

$$K_{loss} = 2 + 320 \left( \frac{(1 - \epsilon)}{Re} \right) + 20 \left( \frac{(1 - \epsilon)}{Re} \right)^{0.4}$$

Pebble to fluid heat transfer within a cell

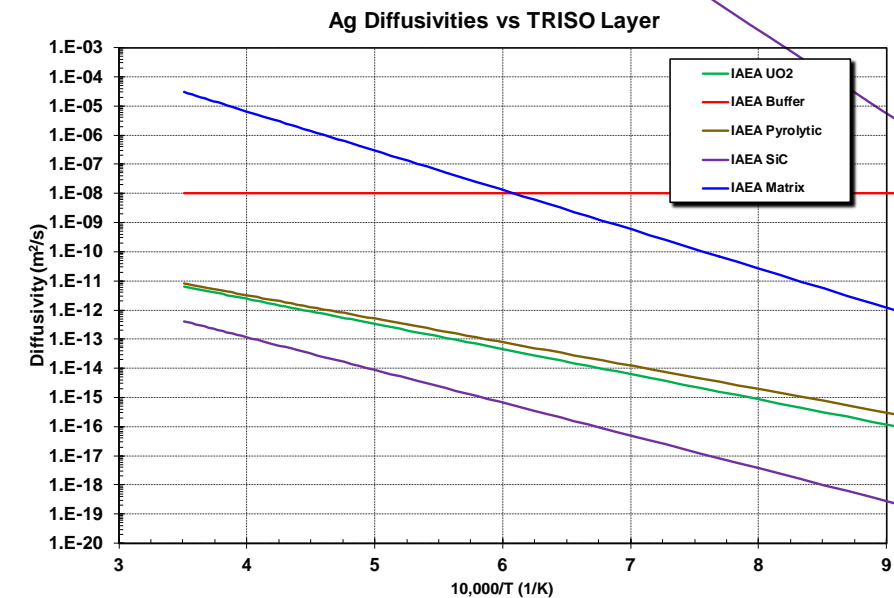
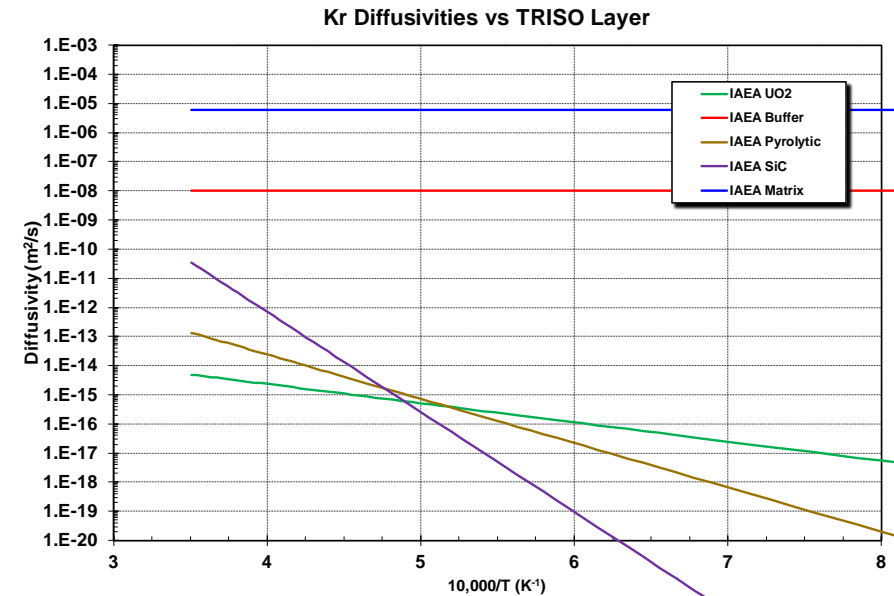
- Forced convection using Wakao correlation,  $Nu = 2 + 1.1 Re^{0.66} Pr^{0.33}$

# MELCOR model inputs (2/2)

Fission product diffusivities through the TRISO and the pebble matrix from IAEA-TECDOC-978, Appendix A

- Primarily based on values from German experiments with  $UO_2$  TRISO pebbles
  - $UO_2$  data can be easily updated to UCO data\*
- Limited data based on nuclides of Xe, Cs, Sr, and Ag
- Iodine assumed to behave like Kr

\* UCO TRISO thermal failure characteristics were not available, so  $UO_2$  TRISO diffusivity and  $UO_2$  failure data were used. Both are changeable through user input with design-specific data.





# Scenarios

Three scenarios with a loss of secondary heat removal

- ATWS – Anticipated transient without SCRAM
- SBO – Station blackout
- LOCA – Loss-of-coolant accident

Sensitivity calculations included

- DRACS performance
- Alternate cover-gas system interconnections (LOCA only)

## Loss-of-onsite power with failure to SCRAM

- Salt pumps shut off
- Reactor fails to SCRAM
- Secondary heat removal ends
- 0 to 3 trains of DRACS operating

## Includes preliminary analysis with xenon transient

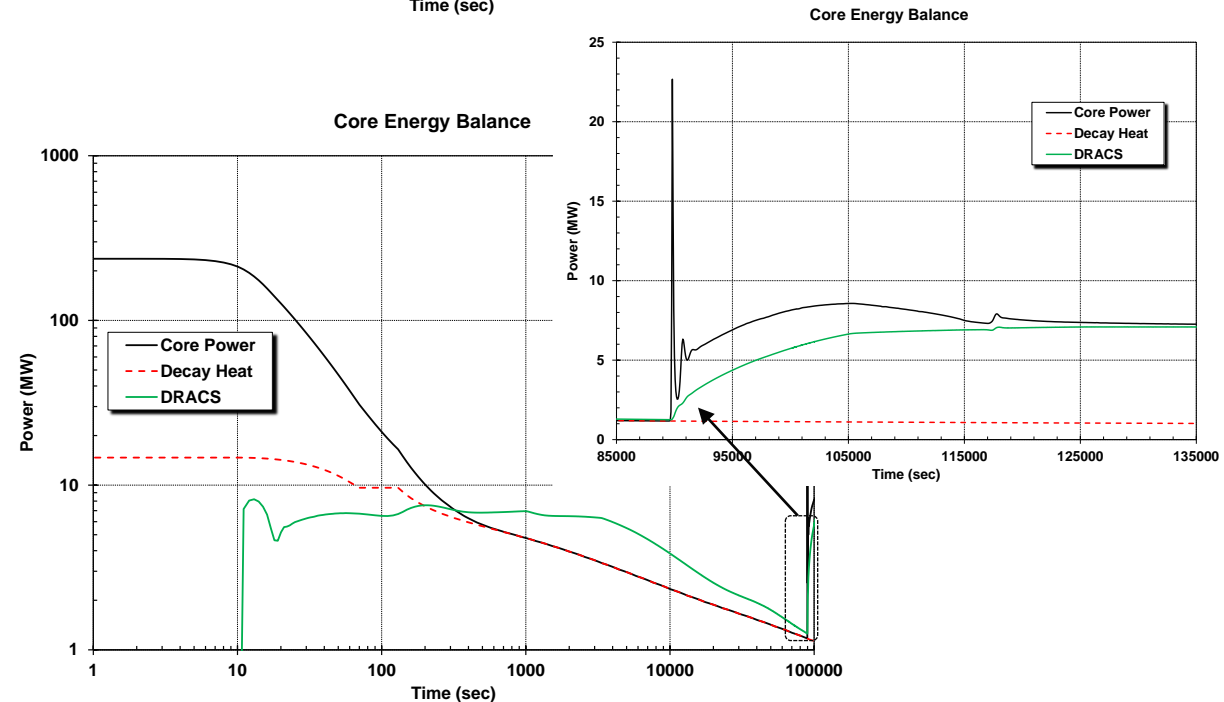
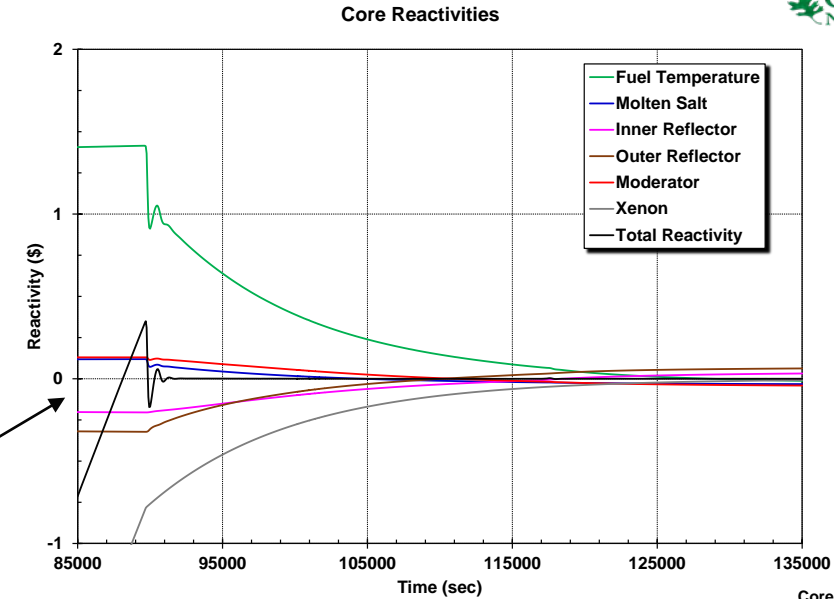
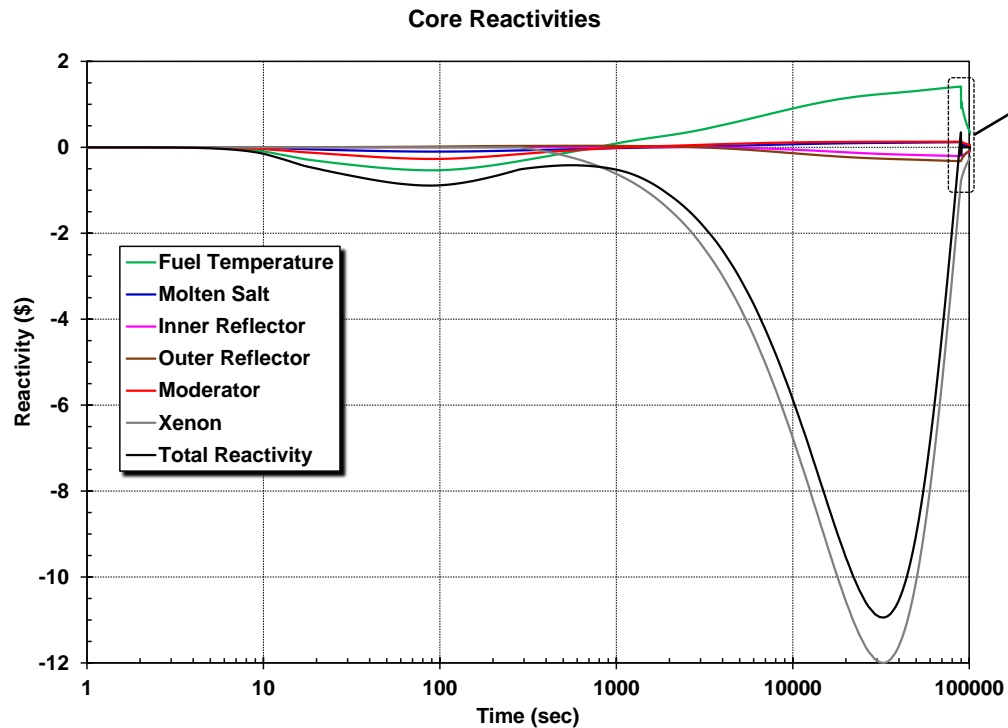
- Guided by ORNL calculations
- Xenon reactivity feedback model being implemented into MELCOR

# ATWS with 3xDRACS

Initial fuel heatup has strong negative fuel and moderator feedback that offsets positive reflector feedbacks

Strong negative xenon transient feedback \*

3xDRACS exceeds core power after 330 s



\* Xenon transient approximated.

# ATWS with variable DRACS (semi-log)

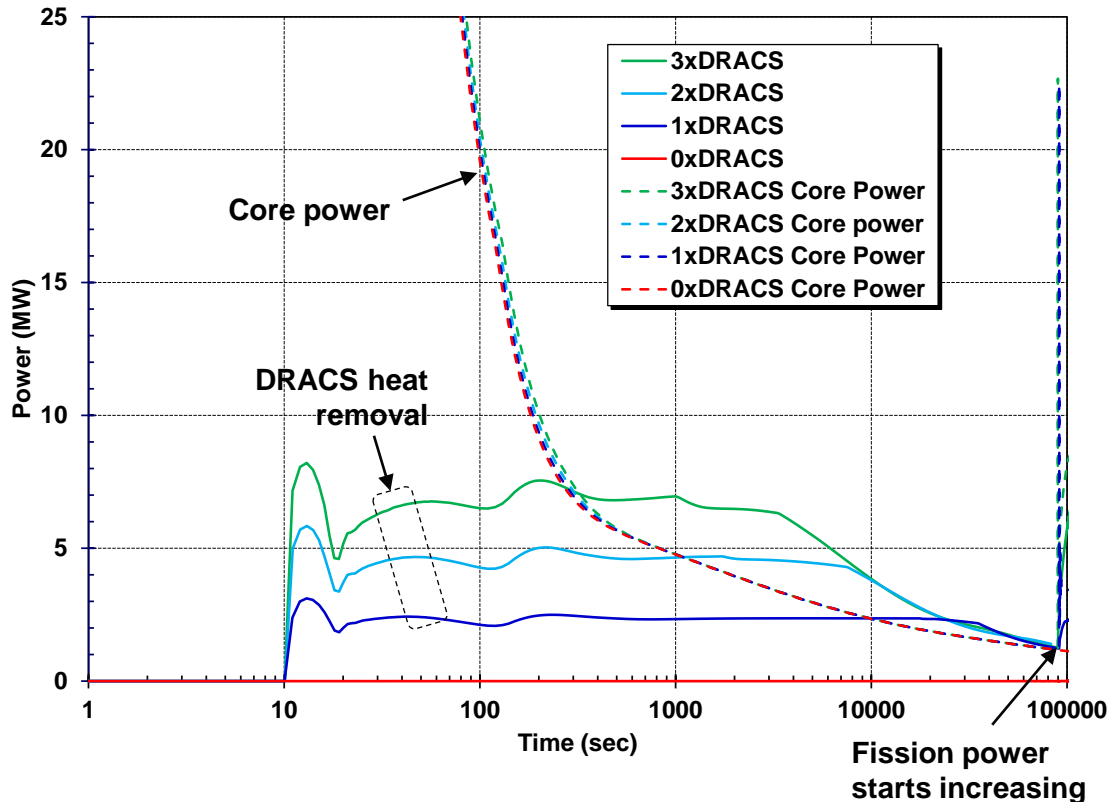
Early power decrease to decay heat level is similar for all cases

- 1xDRACS and 2xDRACS cases exceed decay heat later

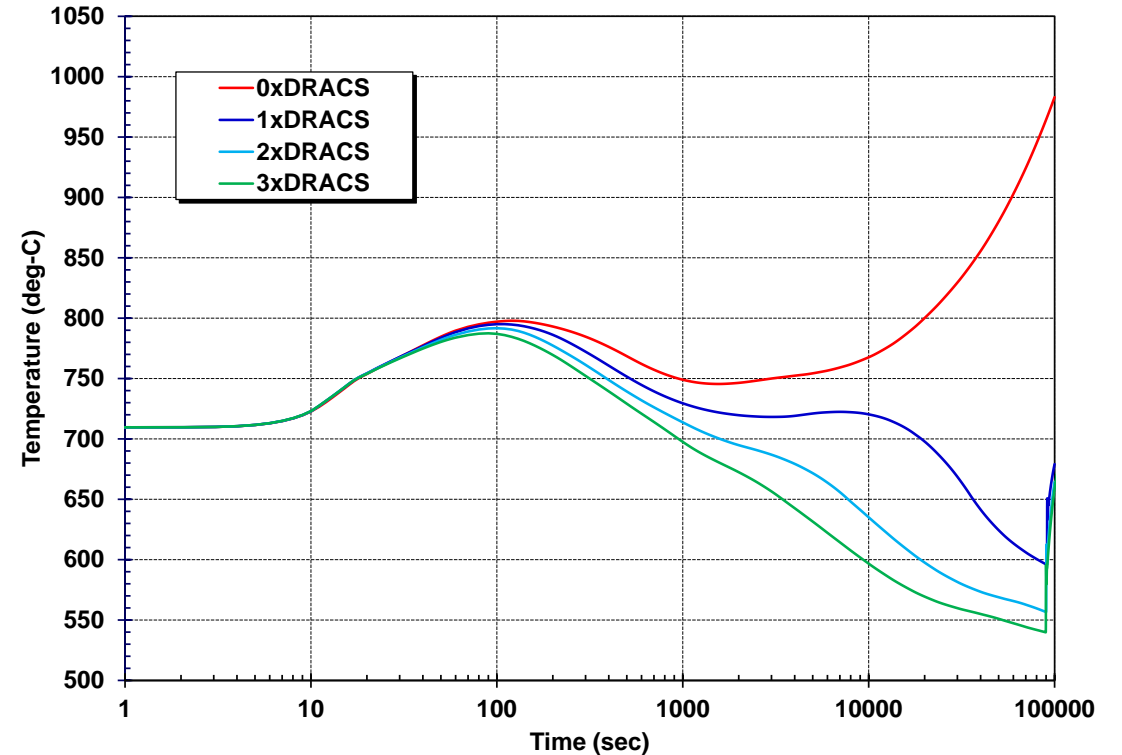
Fuel temperatures cool down according to DRACS heat removal rate

- 0xDRACS peak fuel temperature = 990 °C at  $10^5$  s ( $T_{sat} \sim 1350$  °C)

Core power and DRACS Heat Removal



Peak Fuel Temperatures



\* Xenon transient approximated.

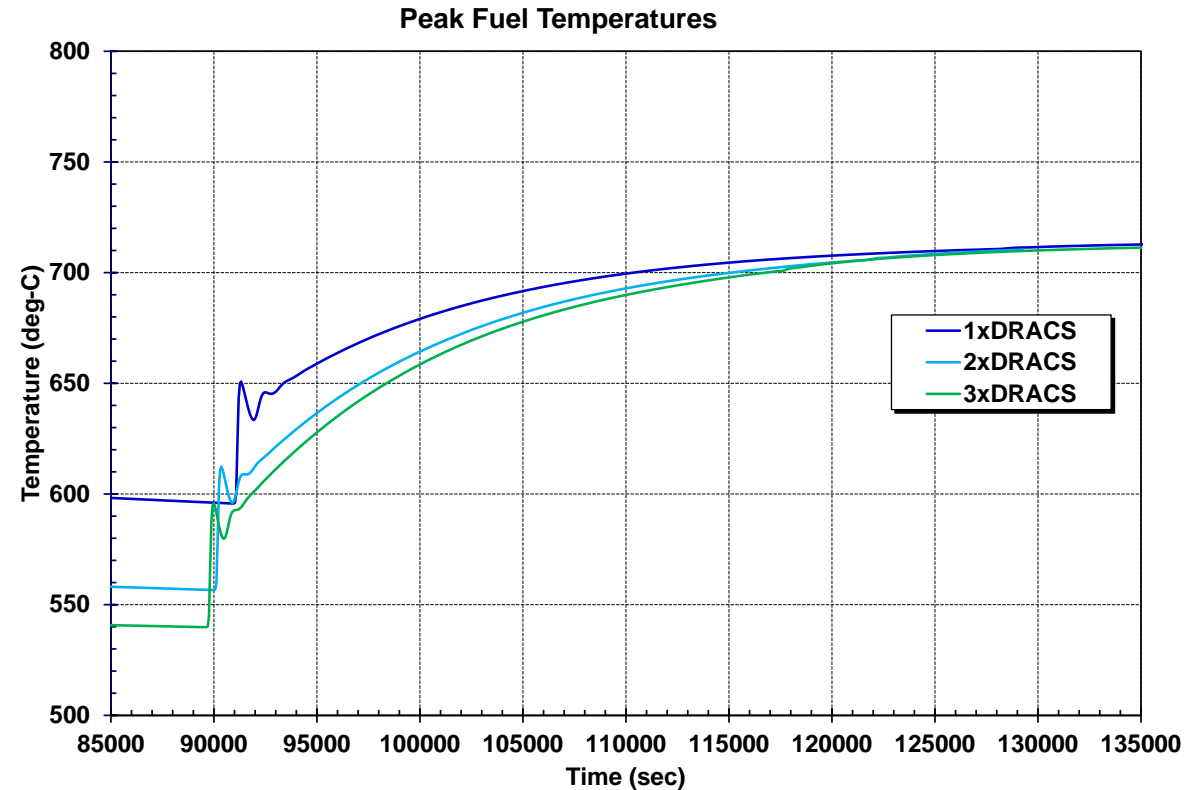
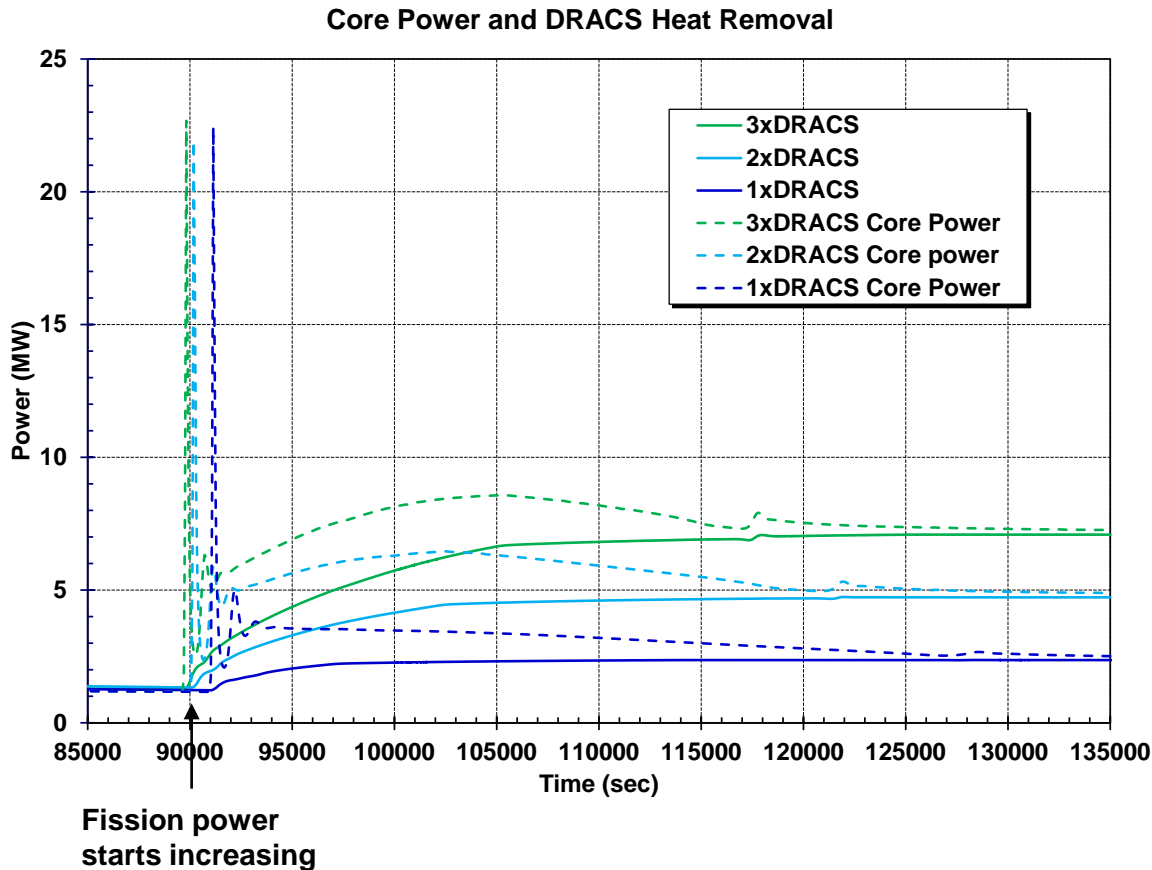


# ATWS with variable DRACS – (Linear scale)

When the total reactivity exceeds zero, the core power increases

- Increased power heats the fuel and reduces the positive fuel reactivity
- Core power eventually converges on the DRACS heat removal rate

The long-term fuel temperatures increase to offset changes in the xenon feedback



\* Xenon transient approximated.

# Station Blackout

## Loss-of-onsite power with SCRAM

- Salt pumps shut off
- Reactor scrams
- Secondary heat removal ends
- Variable DRACS operating (percentage of 1xDRACS)

## Unmitigated sensitivity case

- No DRACS and extended calculation to 7 days

# SBO results (1/3)

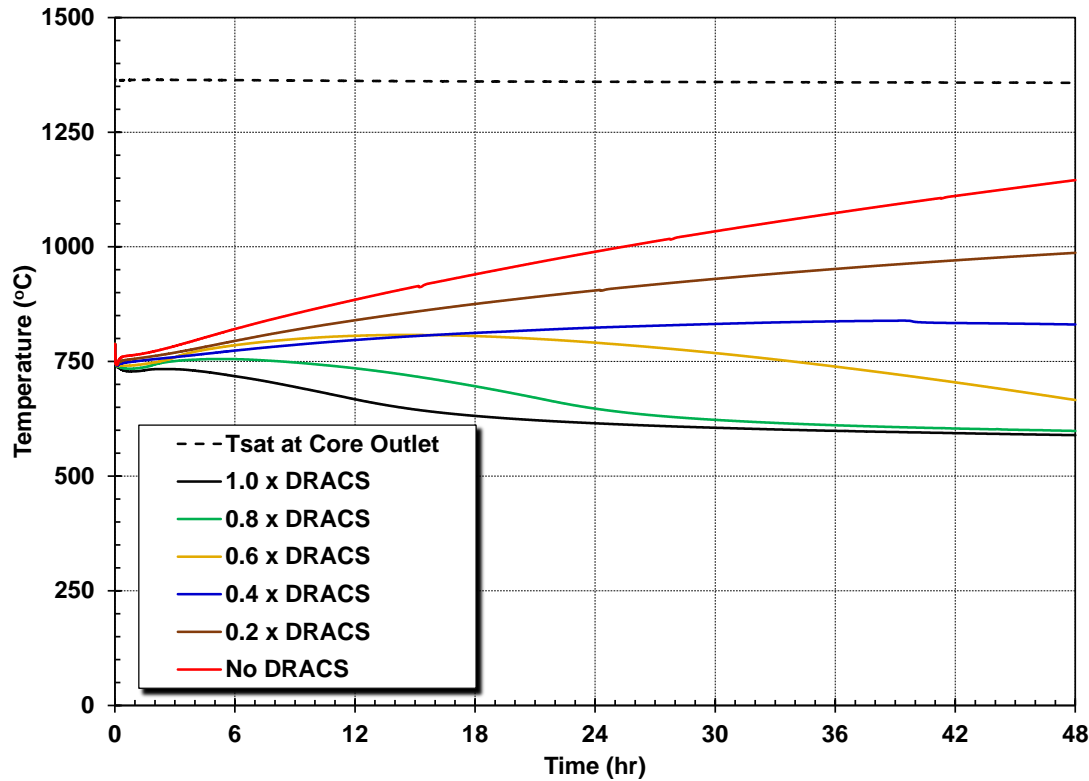
DRACS cases illustrate degraded response

- Results for fraction of 1xDRACS
- $\geq 40\%$  of one DRACS stops the temperature rise within 48 hr

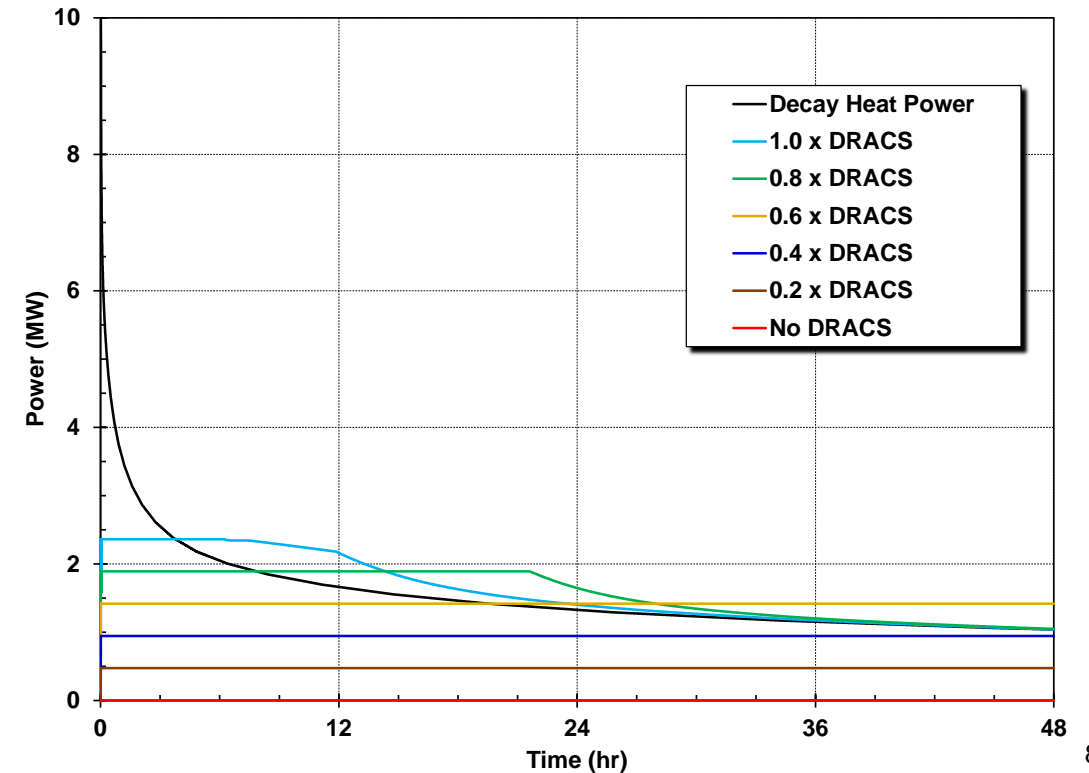
DRACS power follows heat removal requirements

- 1xDRACS exceeds decay heat within 3 hr

Peak Fuel Temperature



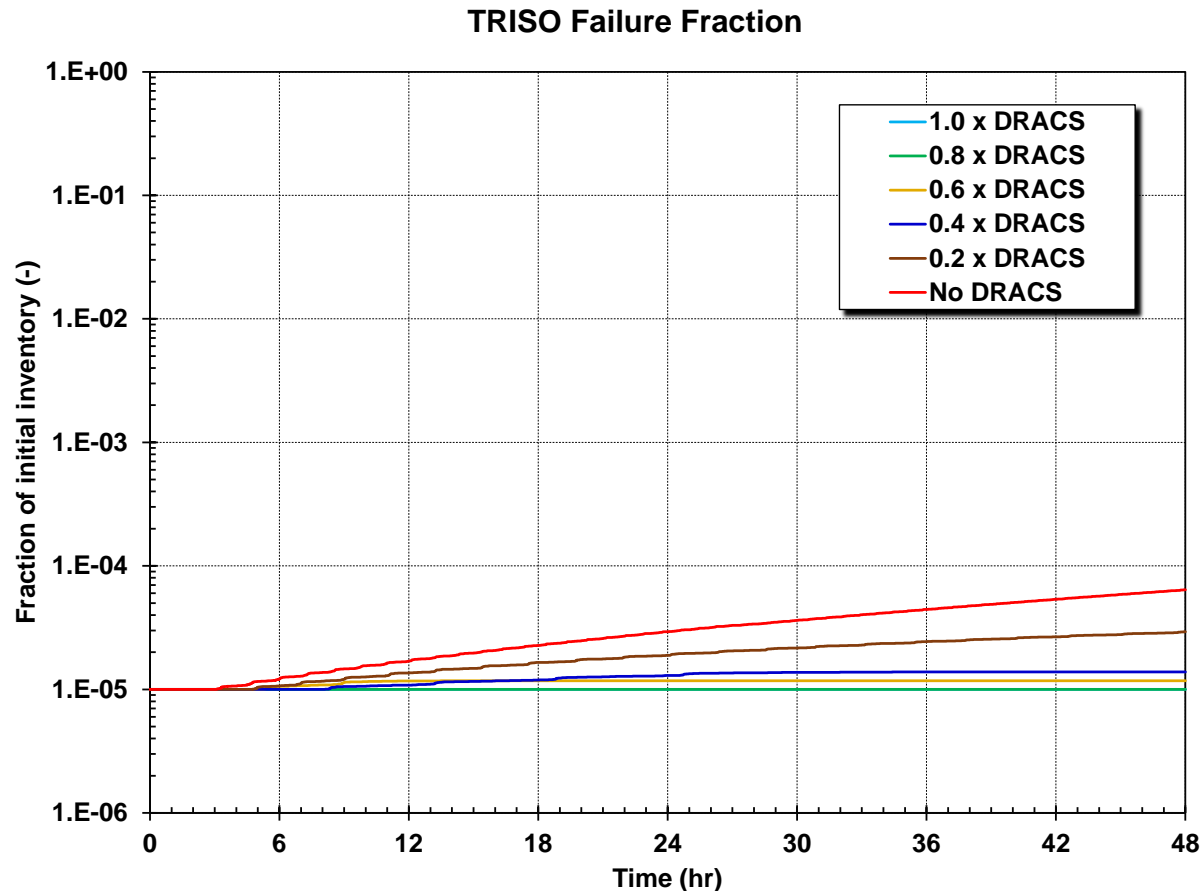
Decay Heat and DRACS Heat Rejection



# SBO results (2/3)

The TRISO failure fraction remains low ( $1 \times 10^{-5}$ ) in the SBO with one DRACS operating \*

- Higher TRISO failures were calculated as the DRACS degrades

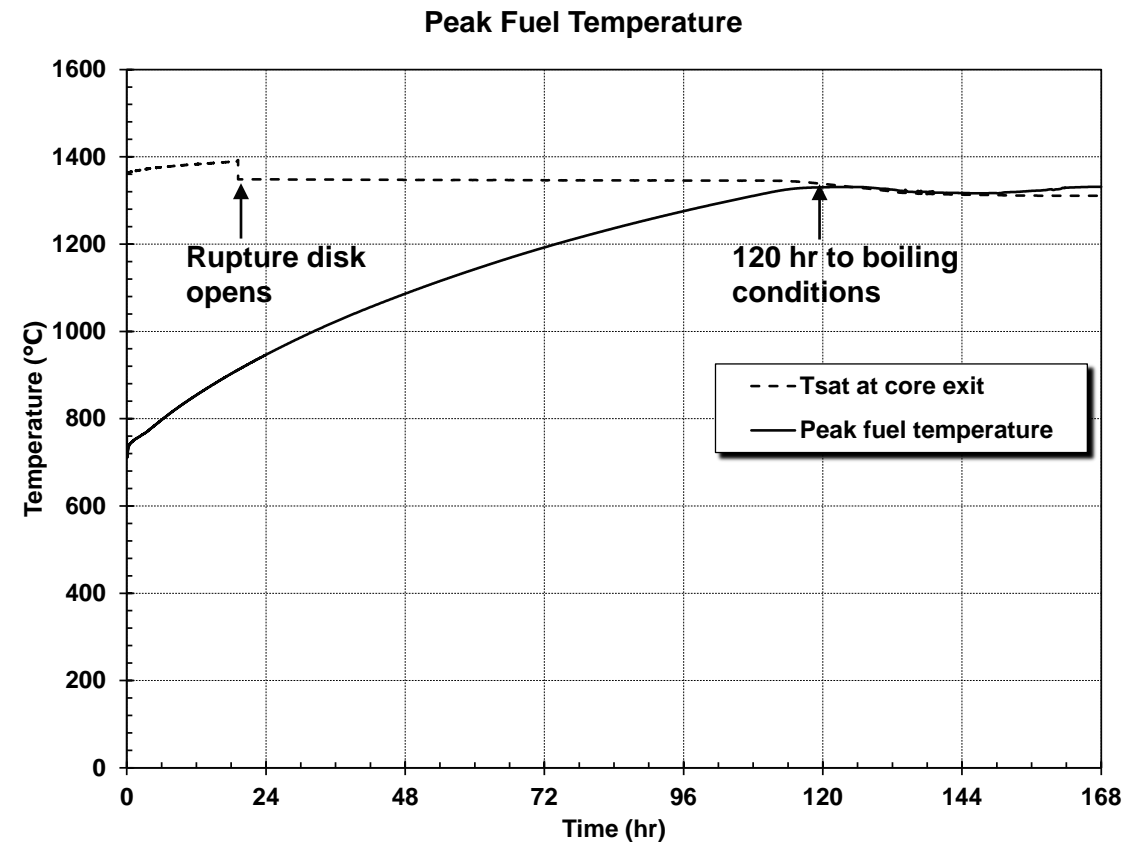
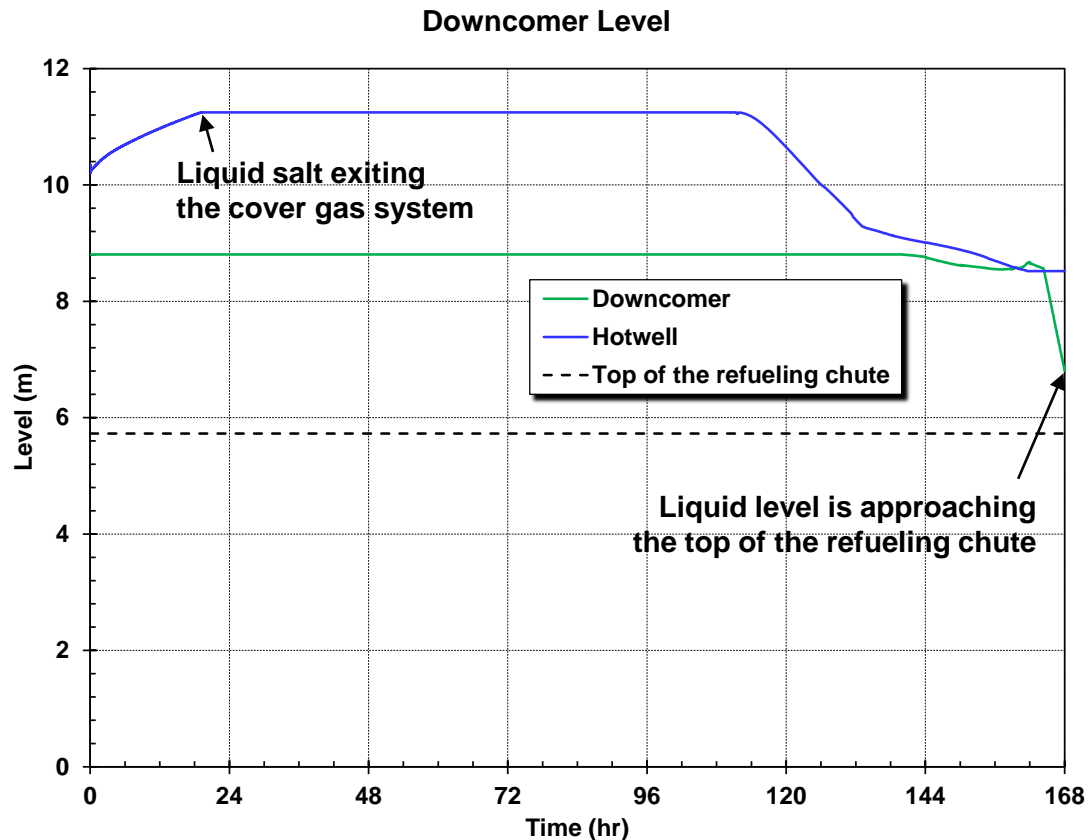


\* UCO TRISO thermal failure characteristics were not available, so  $UO_2$  TRISO diffusivity and  $UO_2$  failure data were used. Both are changeable through user input with design-specific data.

# SBO results (3/3)

The SBO with no DRACS was extended to 7 days

- No fuel uncover
- Peak fuel temperature approximately at  $T_{sat}$  (~1350 °C)





# LOCA

## Loss-of-onsite power with LOCA

- Variable size leaks of the 3" pipe of the drain tank line
- Salt pumps shut off
- Reactor scrams
- Secondary heat removal ends
- 1 or no trains of DRACS operating
- With or without a cover gas connection path between the hotwell and the standpipes

## Unmitigated sensitivity case

- No DRACS case extended to include fuel uncover

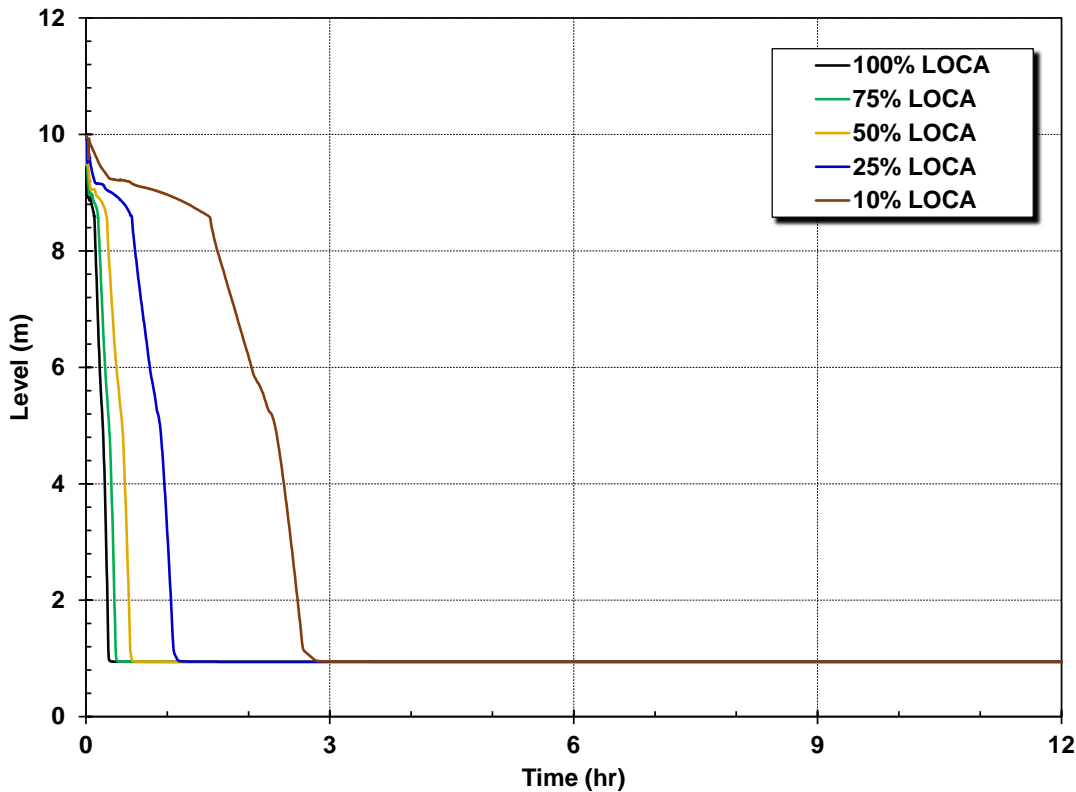
# LOCA results (1/6)

10% to 100% LOCA size did not significantly impact vessel boiloff timing

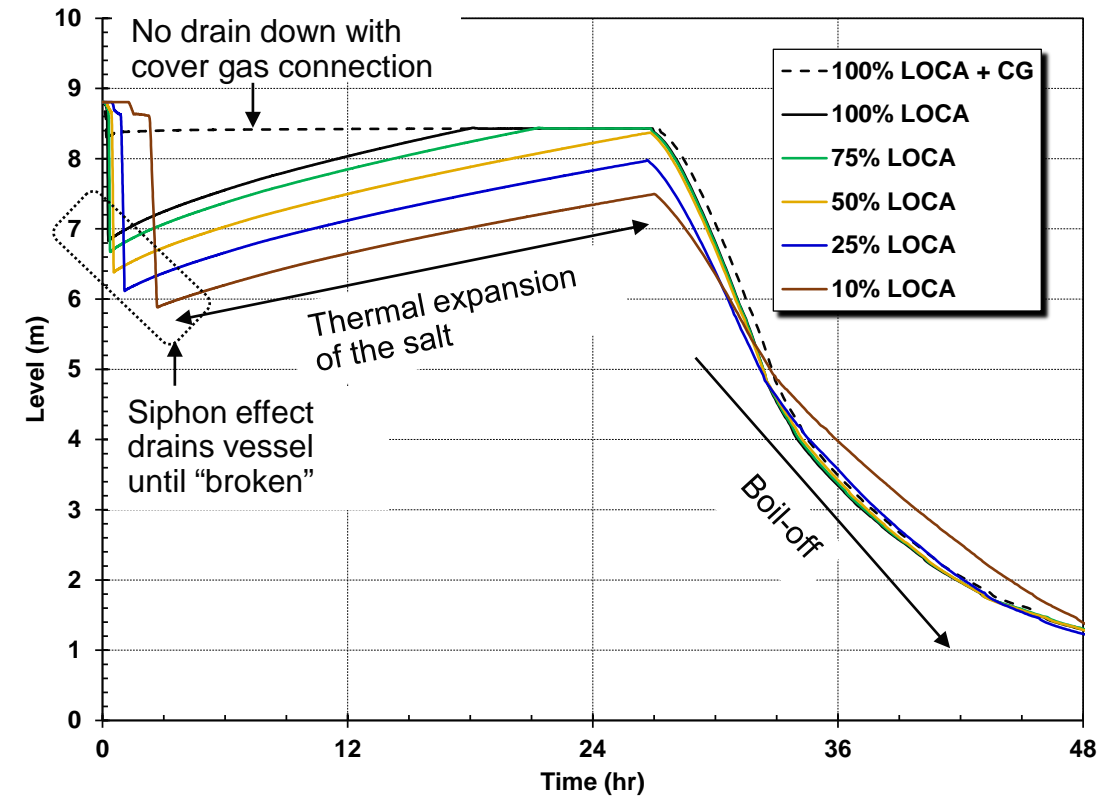
Cover gas connection (+ CG) between hotwell and standpipe prevents siphon

- Stops initial drain down of vessel fluid
- No significant impact on vessel boiloff timing

Standpipe Level



Downcomer Level



# LOCA results (2/6)

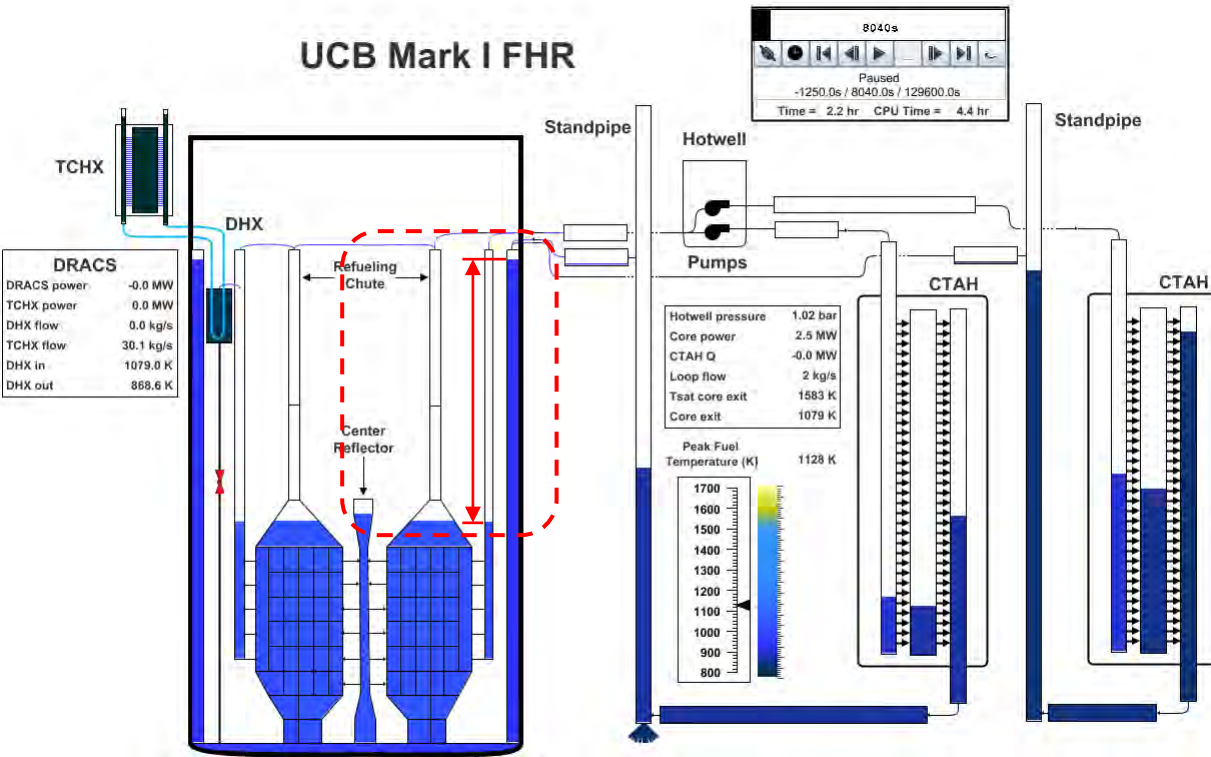
Liquid drain down initially creates siphon and then low pressure region

- Causes a level difference between the core and downcomer

Core and downcomer levels equilibrate once there is gas flow around the loop

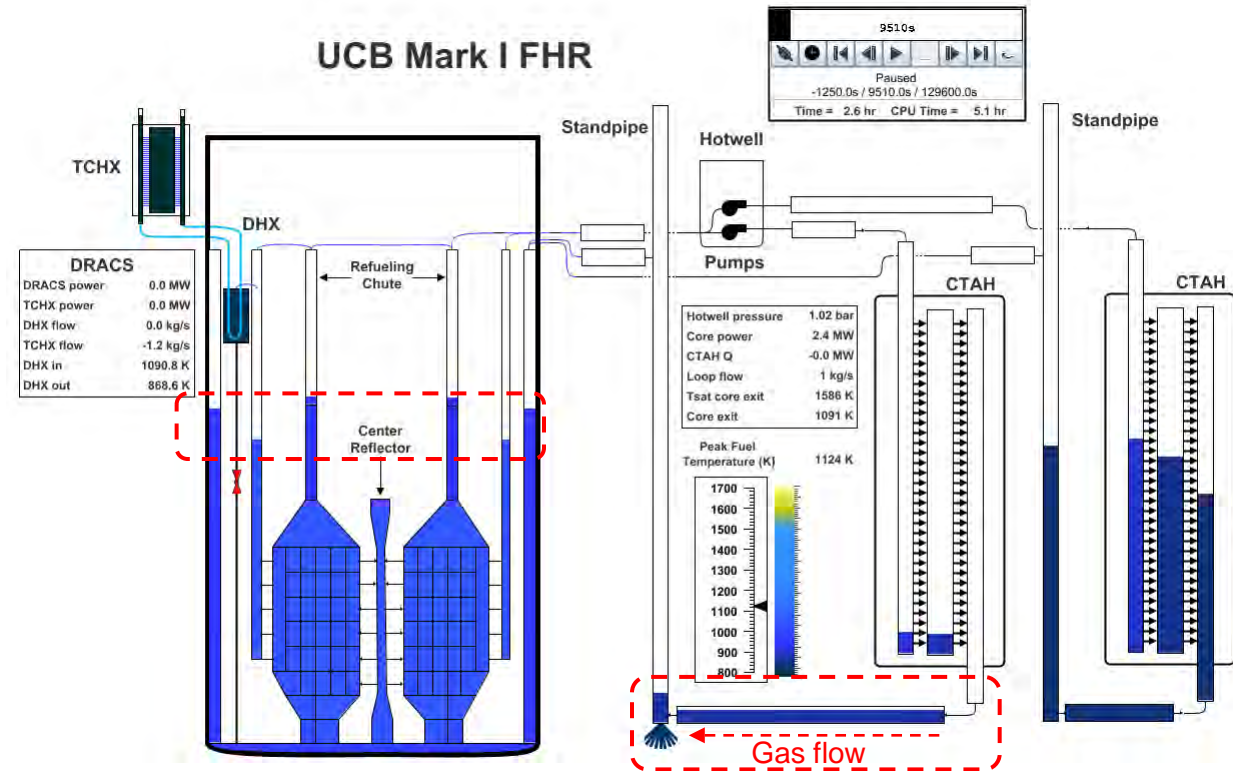
- Standpipe connections to the cover gas system are closed

UCB Mark I FHR



10% LOCA at maximum point in the "siphon"

UCB Mark I FHR



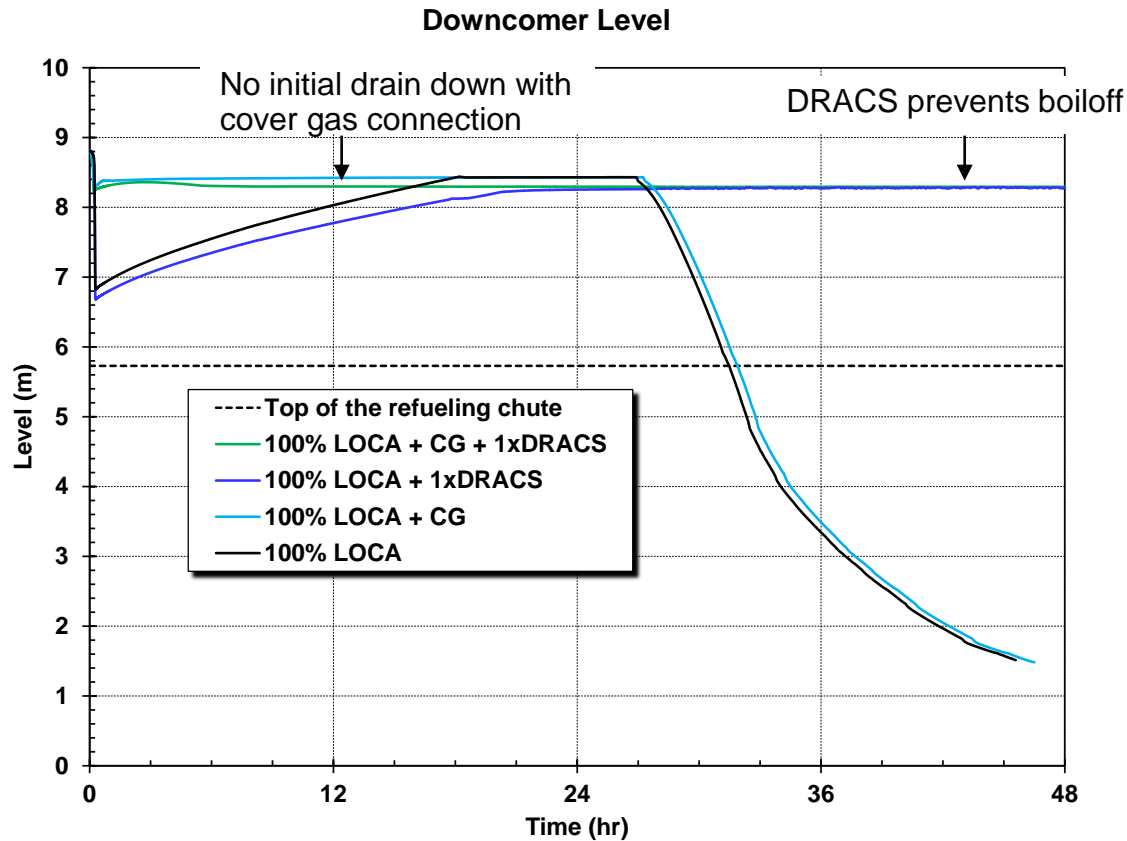
10% LOCA after equilibration

# LOCA results (3/6)

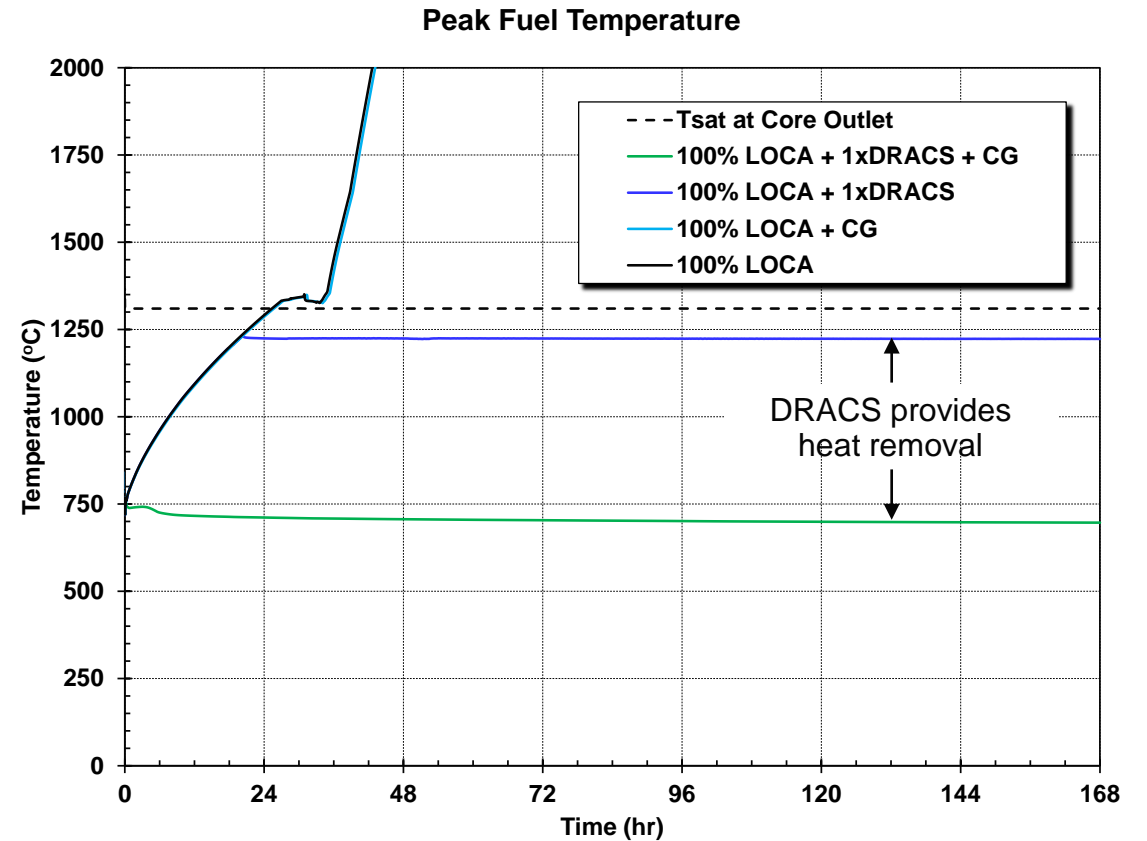
LOCA cases without DRACS proceed to fuel uncover at ~31 hr

Connection through the cover gas system keeps the DRACS active during the drain down

- Without the cover gas connection, the DRACS heat removal is delayed until the salt heats and expands



100% LOCA cases

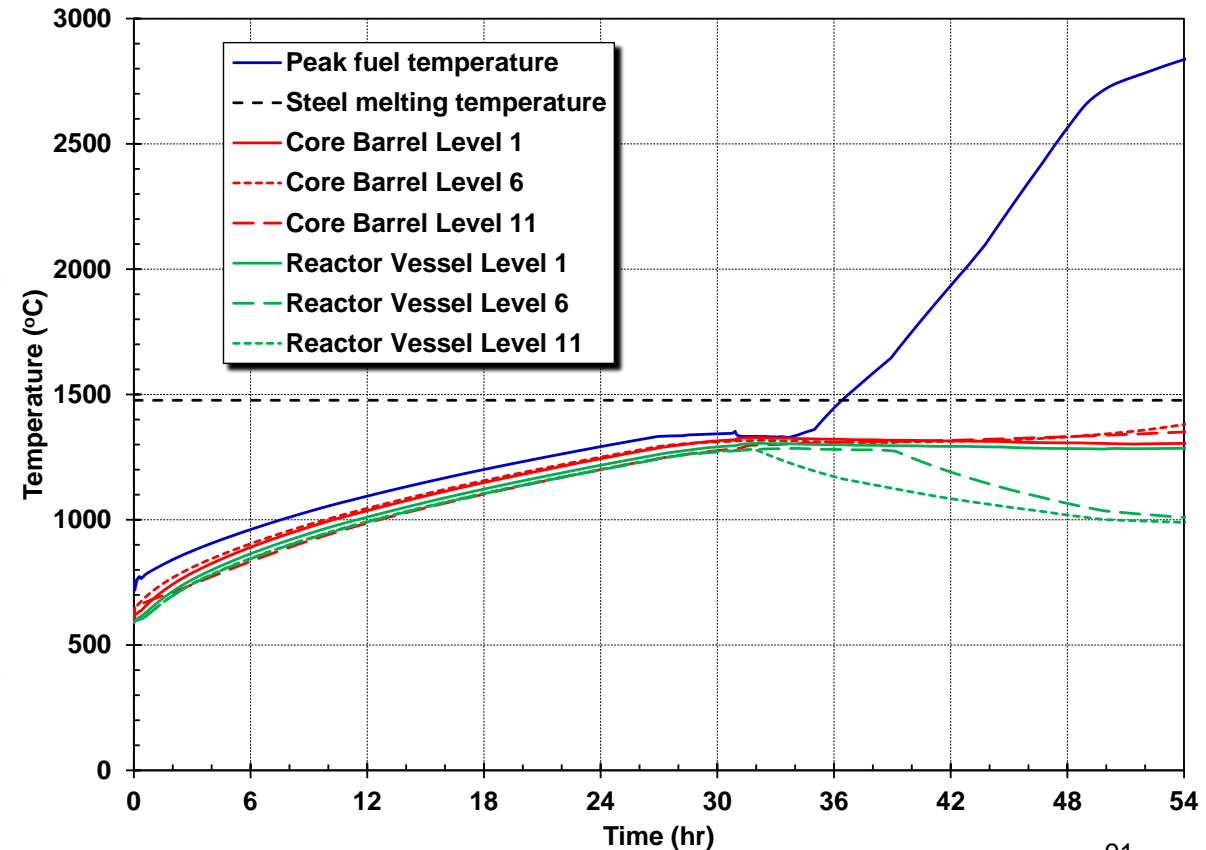
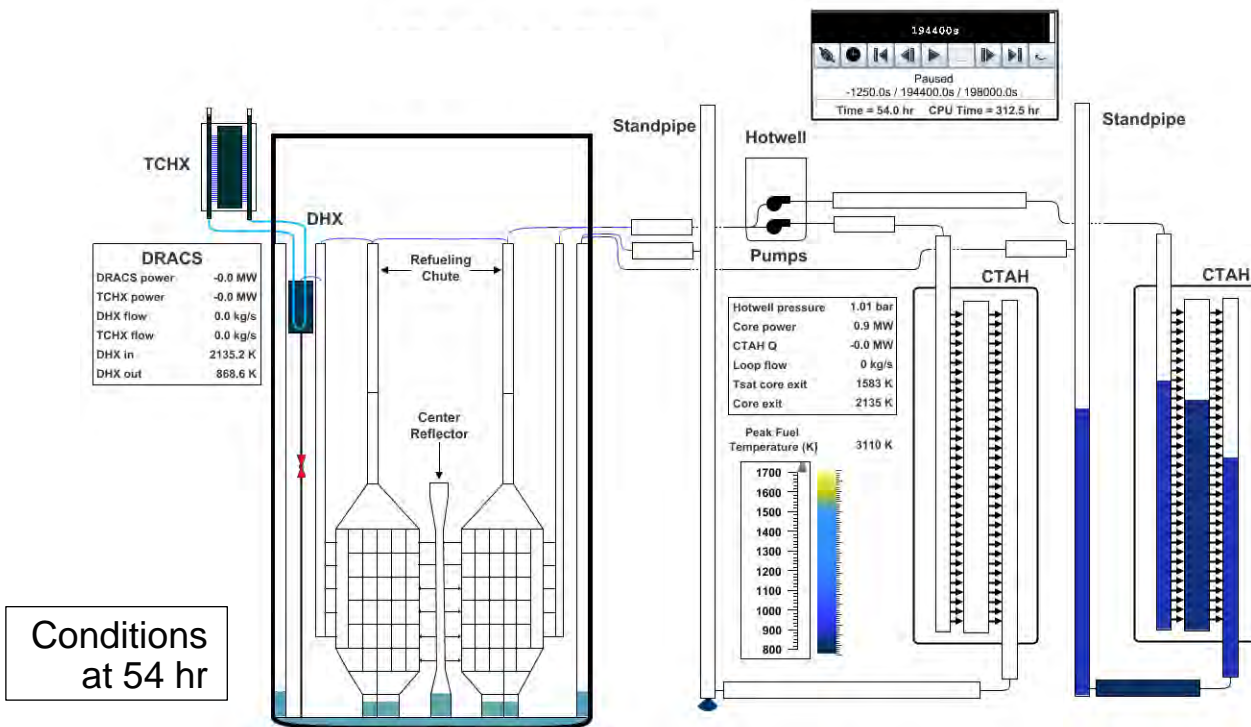


100% LOCA cases

# LOCA results (4/6)

We terminated the calculation at ~54 hr peak when the fuel kernel melting starts

- Reactor vessel wall and core barrel below the steel melting temperature
- Residual molten salt keeps the bottom level (level 1) at  $T_{sat}$
- Upper vessel wall cools after downcomer salt level drops
- Pebbles and reflectors below graphite sublimation temperature (3600°C)

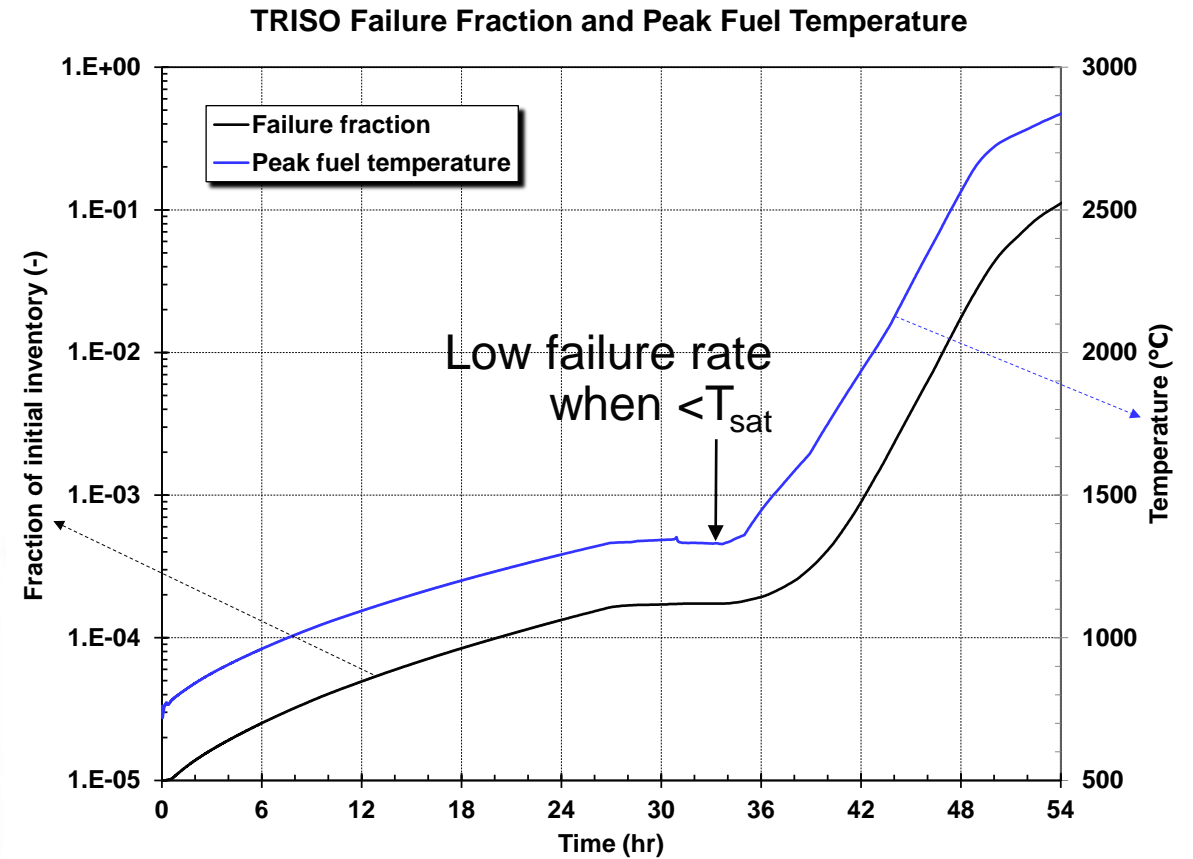
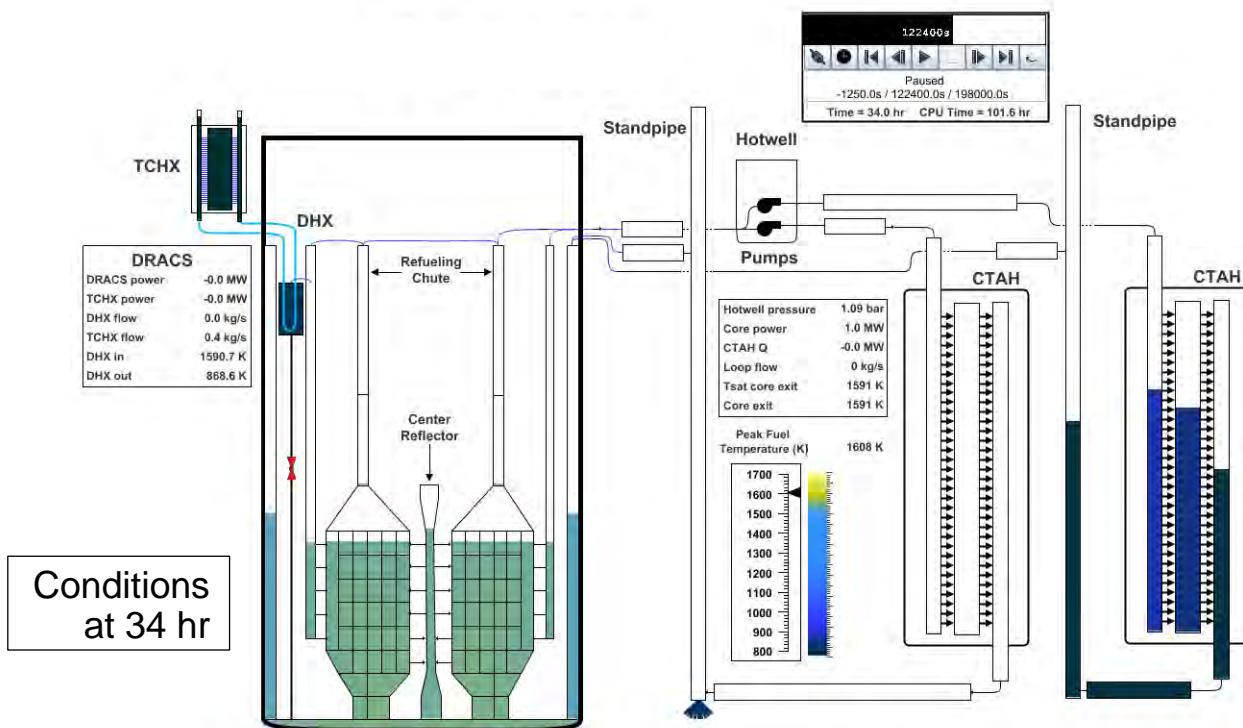




# LOCA results (5/6)

TRISO failure rate extrapolated from available  $UO_2$  TRISO data

- Correlation is based on data to 1800°C
- Initial failures set to  $10^{-5}$  (0.001%)
- 0.017% of the TRISOs failed at 34 hr
- 7.5% of the TRISOs failed at 54 hr



Note:  
 \*\* Fuel used thermal-physical properties of  $UO_2$ .

# LOCA results (6/6)

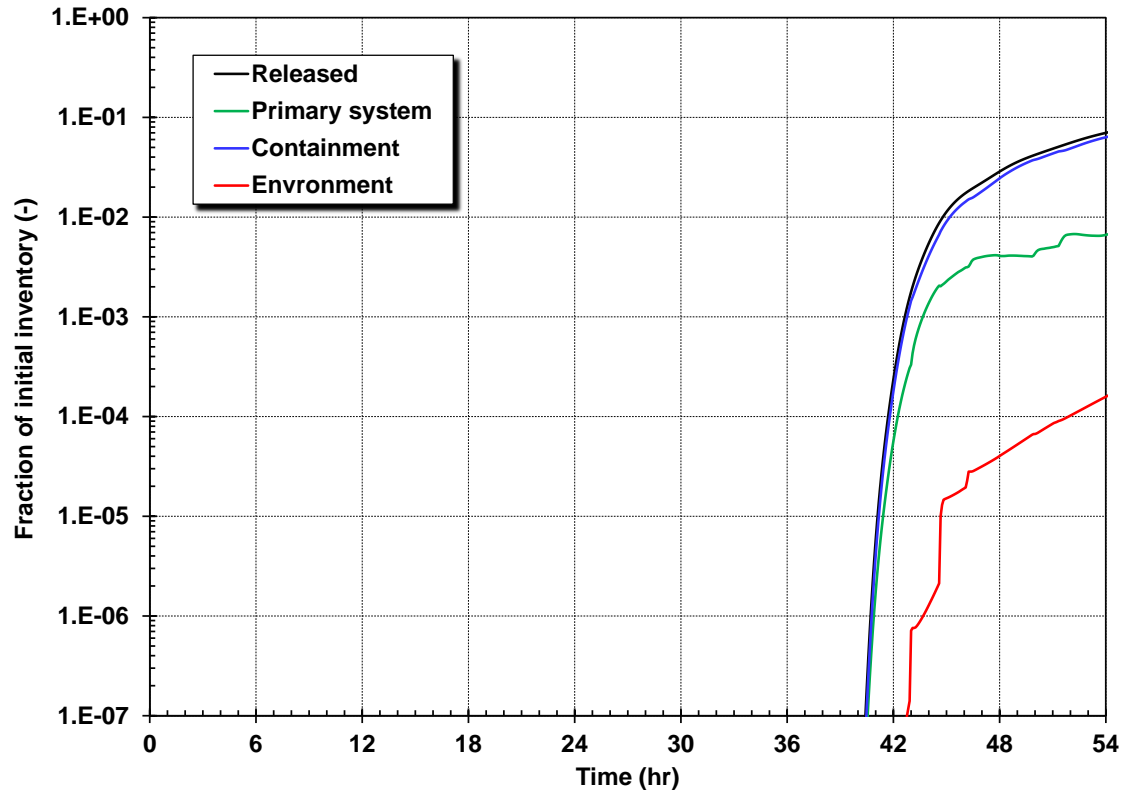
Most of the fission product release from fuel is retained in the containment

- Assumed hole size equivalent to 100% volume per day at 0.25 psig (8.7 in<sup>2</sup>)

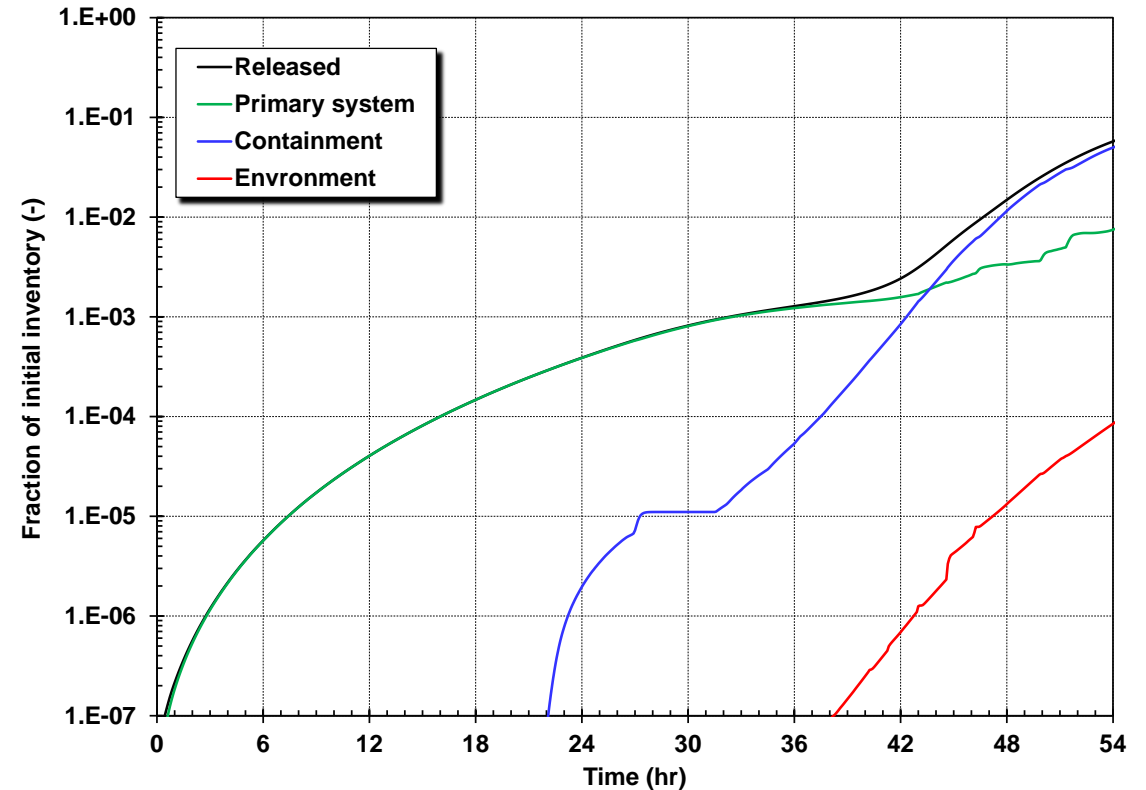
The radionuclide distribution is affected by the timing of the release from the TRISO

- Cesium release from the pebbles to the liquid molten salt starts earlier at lower fuel temperatures
- Most aerosols leaving the primary system settle in the containment

Iodine Release and Distribution



Cesium Release and Distribution



# Cesium vaporization from the molten salt

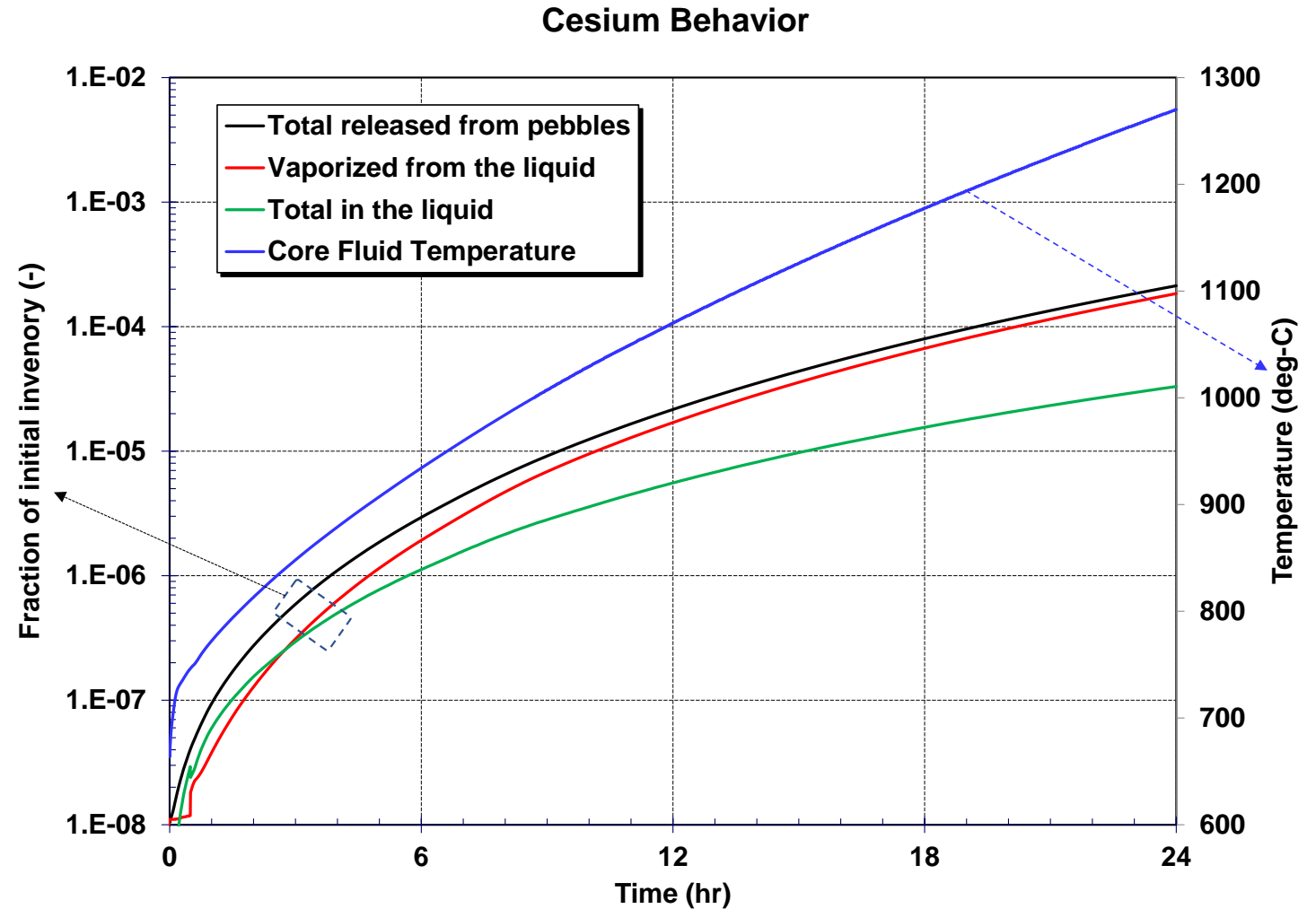
Molten salt chemistry and radionuclide release model calculates cesium and cesium fluoride release to the gas spaces

- Results use OECD/NEA JRC database for Thermochemica \*
- Includes vapor phase data for CsF

## LOCA sequence

- No accelerated steady state
- No core uncover through 24 hr
  - Cesium releases are from pebbles → liquid → gas

Model shows Cs/CsF vaporization to gas spaces at higher temperatures



\* With modifications by Ontario Tech.

# Summary



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# Conclusions

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



# Background Slides



**U.S. NRC**

 **OAK RIDGE**  
National Laboratory



**Sandia**  
National  
Laboratories

# Further SCALE analysis details



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# Comparison of the FHR with other concepts

	Mk1 PB-FHR	ORNL 2012 AHTR	Westing- house 4-loop PWR	PBMR	S- PRISM
Coolant	flibe	flibe	water	helium	sodium
Core inlet/outlet temperatures (°C)	600-700	650-700	292/326	500/900	355/510
Reactor thermal power (MWt)	236	3400	3411	400	1000
Reactor electrical power (MWe)	100	1530	1092	175	380
Fuel enrichment †	19.90%	9.00%	4.50%	9.60%	8.93%
Fuel discharge burn up (MWt-d/kg)	180	71	48	92	106
Fuel full-power residence time in core (yr)	1.38	1.00	3.15	2.50	7.59
Power conversion efficiency	42.4%	45.0%	32.0%	43.8%	38.0%
Core power density (MWt/m <sup>3</sup> )	22.7	12.9	105.2	4.8	321.1
Fuel average surface heat flux (MWt/m <sup>2</sup> )	0.189	0.285	0.637	0.080	1.13
Fuel specific surface area (area/volume) (1/m)	120	45	165	60	285
Reactor vessel diameter (m)	3.5	10.5	6.0	6.2	9.2
Reactor vessel height (m)	12.0	19.1	13.6	24.0	19.6
Reactor vessel specific power (MWe/m <sup>3</sup> )	0.866	0.925	2.839	0.242	0.292
Start-up fissile inventory (kg-U235/MWe) ††	0.79	0.62	2.02	1.30	6.15
EOC Cs-137 inventory in core (g/MWe) *	30.8	26.1	104.8	53.8	269.5
EOC Cs-137 inventory in core (Ci/MWe) *	2672	2260	9083	4667	23359
Spent fuel dry storage density (MWe-d/m <sup>3</sup> )	4855	2120	15413	1922	-
Natural uranium (MWe-d/kg-NU) **	1.56	1.47	1.46	1.73	-
Separative work (MWe-d/kg-SWU) **	1.98	2.08	2.43	2.42	-

† For S-PRISM, effective enrichment is the Beginning of Cycle weight fraction of fissile Pu in fuel

†† Assume start-up U-235 enrichment is 60% of equilibrium enrichment; for S-PRISM startup uses fissile Pu

\* End of Cycle (EOC) life value (fixed fuel) or equilibrium value (pebble fuel)

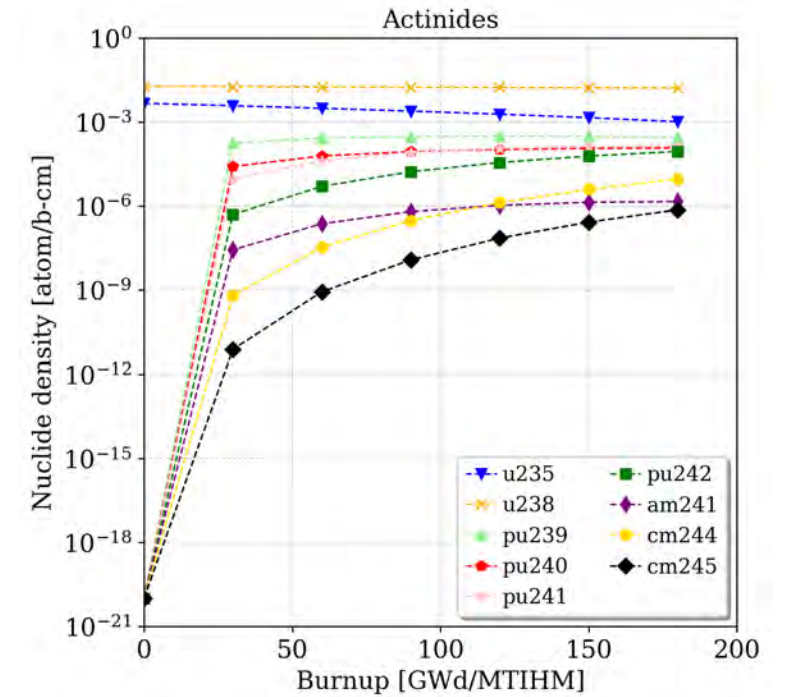
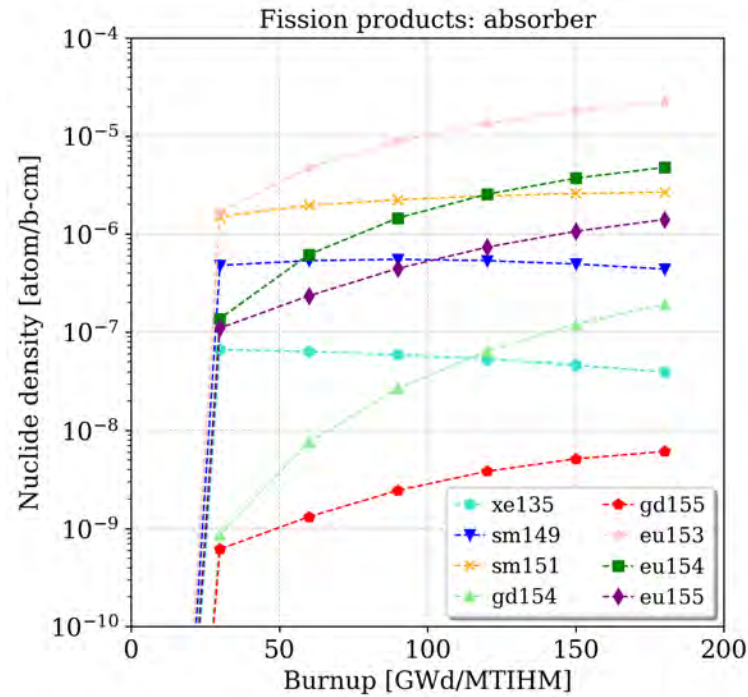
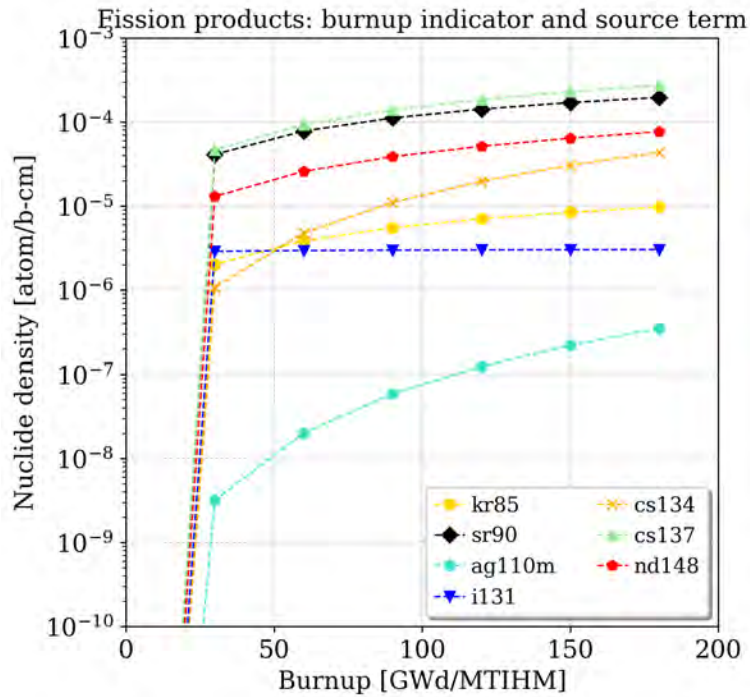
\*\* Assumes a uranium tails assay of 0.003.

C. Andreades et al., "Technical Description of the "Mark 1" Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant," Berkeley, CA, UCBTH-14-002, 2014.



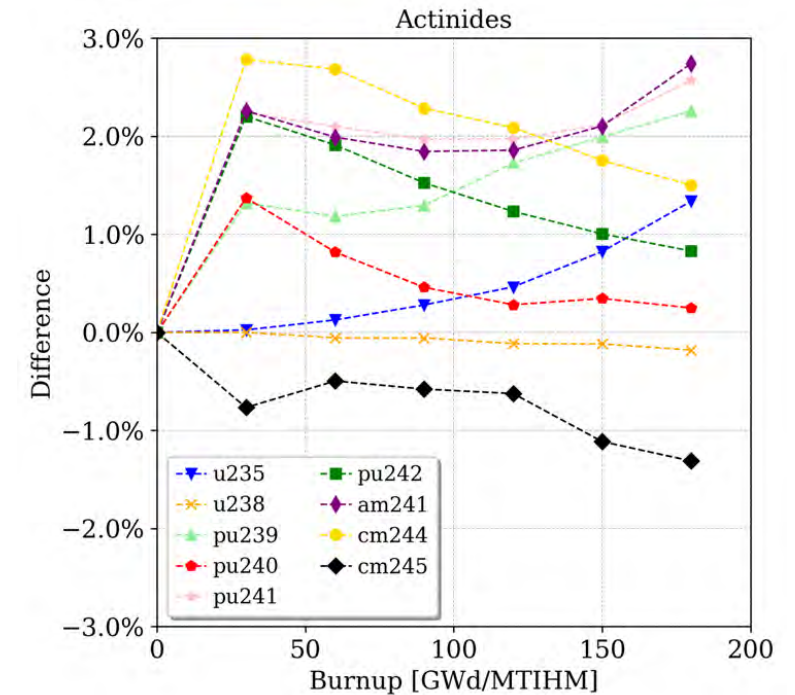
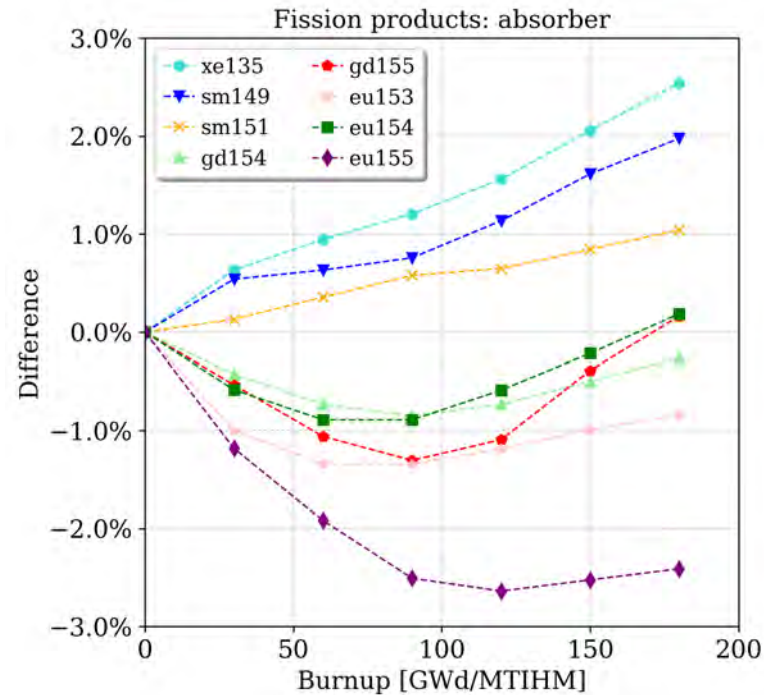
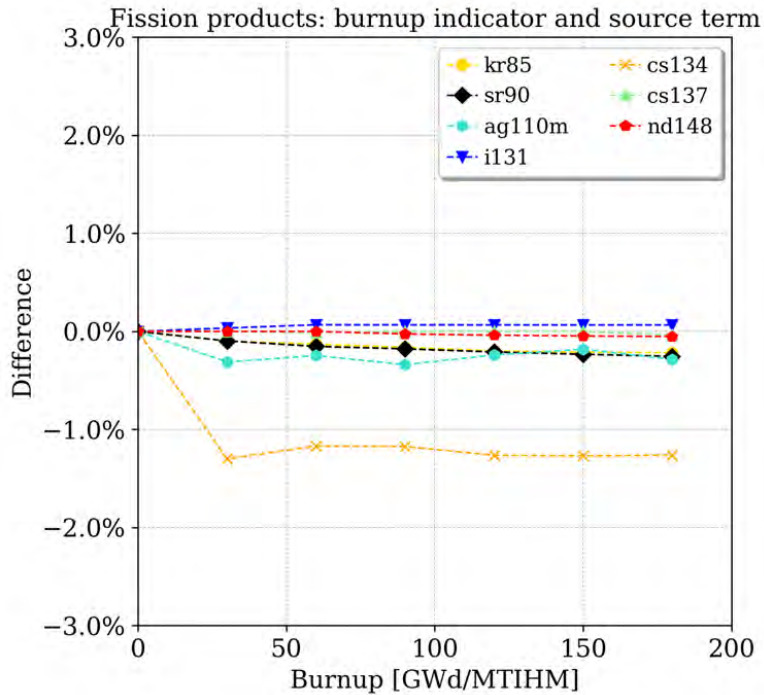
# 1. Single pebble nuclide density over depletion

## CE random results:



# 1. Single pebble nuclide density comparison over depletion

## Comparison of MG against CE random:

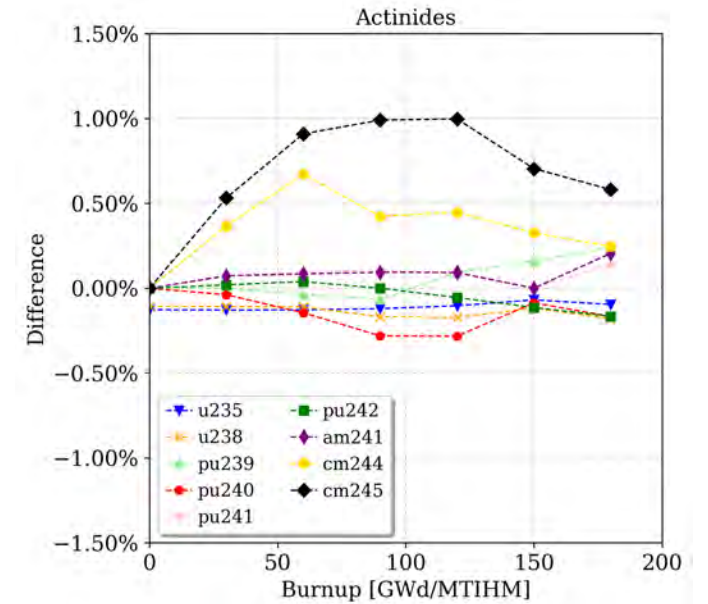
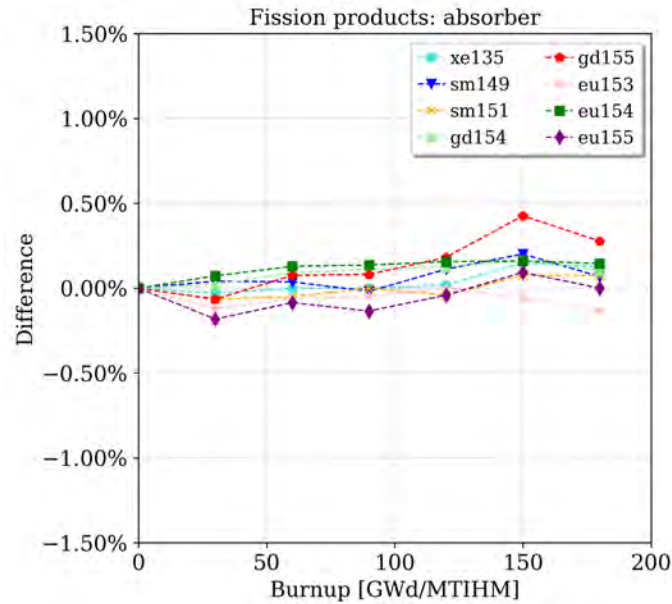
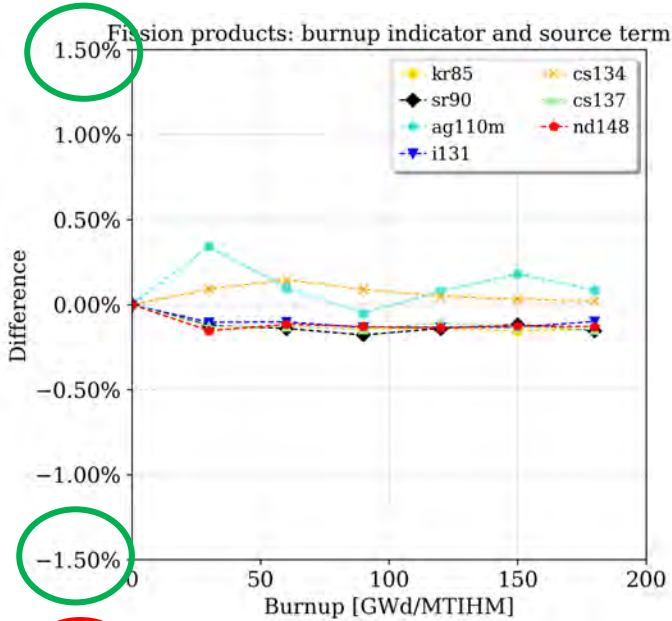


**Result:** MG bias remains below 3% for relevant nuclide densities over depletion

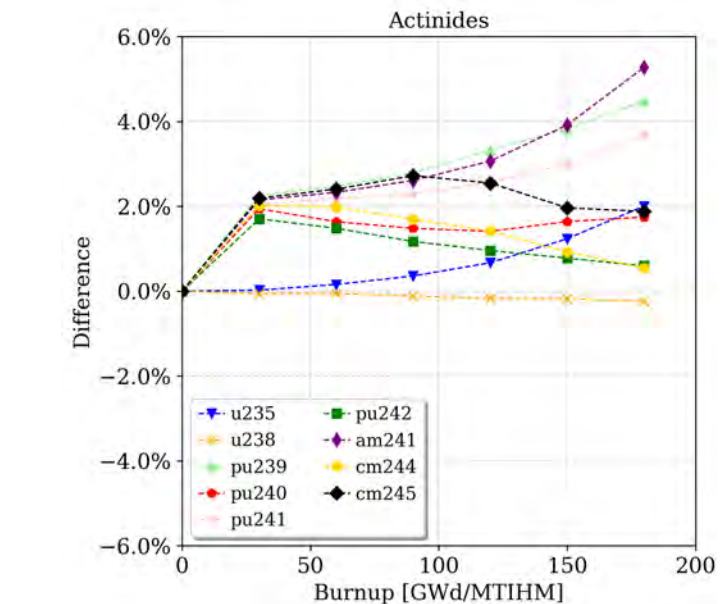
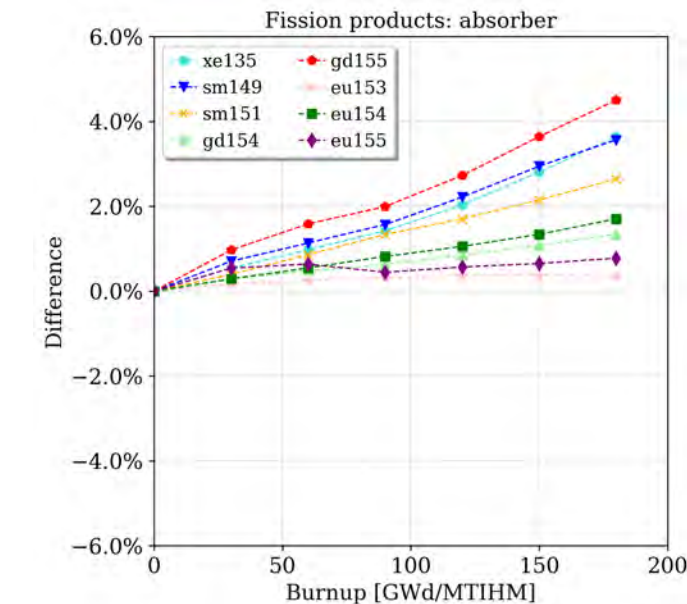
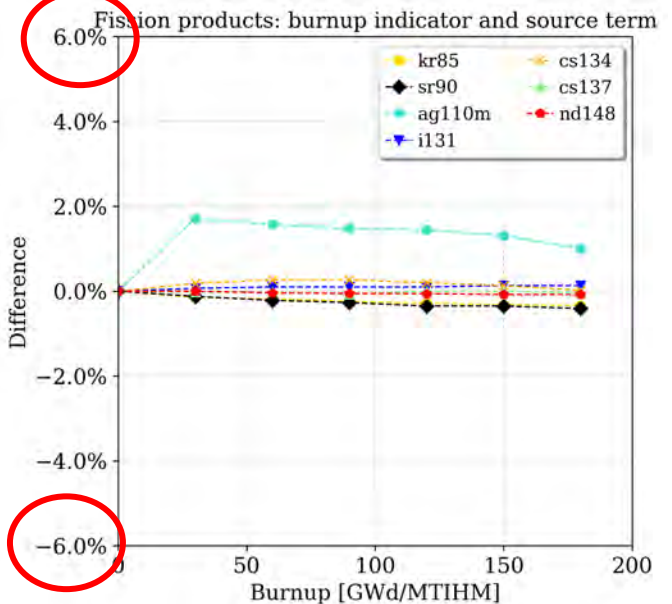


# 1. Single pebble nuclide density comparison of against reference CE random results

CE, lattice, unclipped



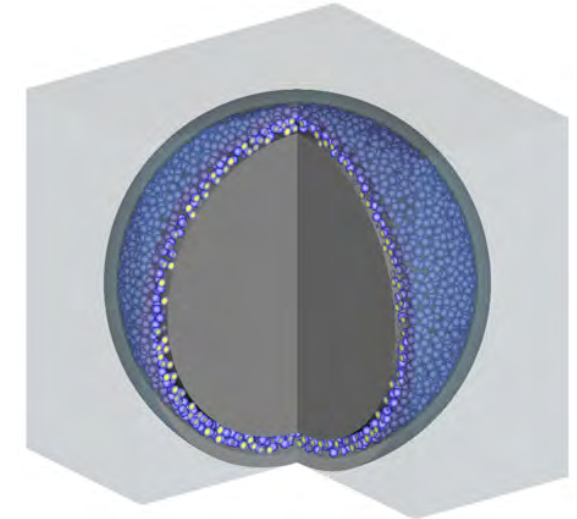
CE, lattice, clipped



# 1. Single pebble runtime comparison

## Monte Carlo calculation settings:

- 25,000 neutrons per cycle in 500 active and 100 inactive generations
- 1 node with 32 processors

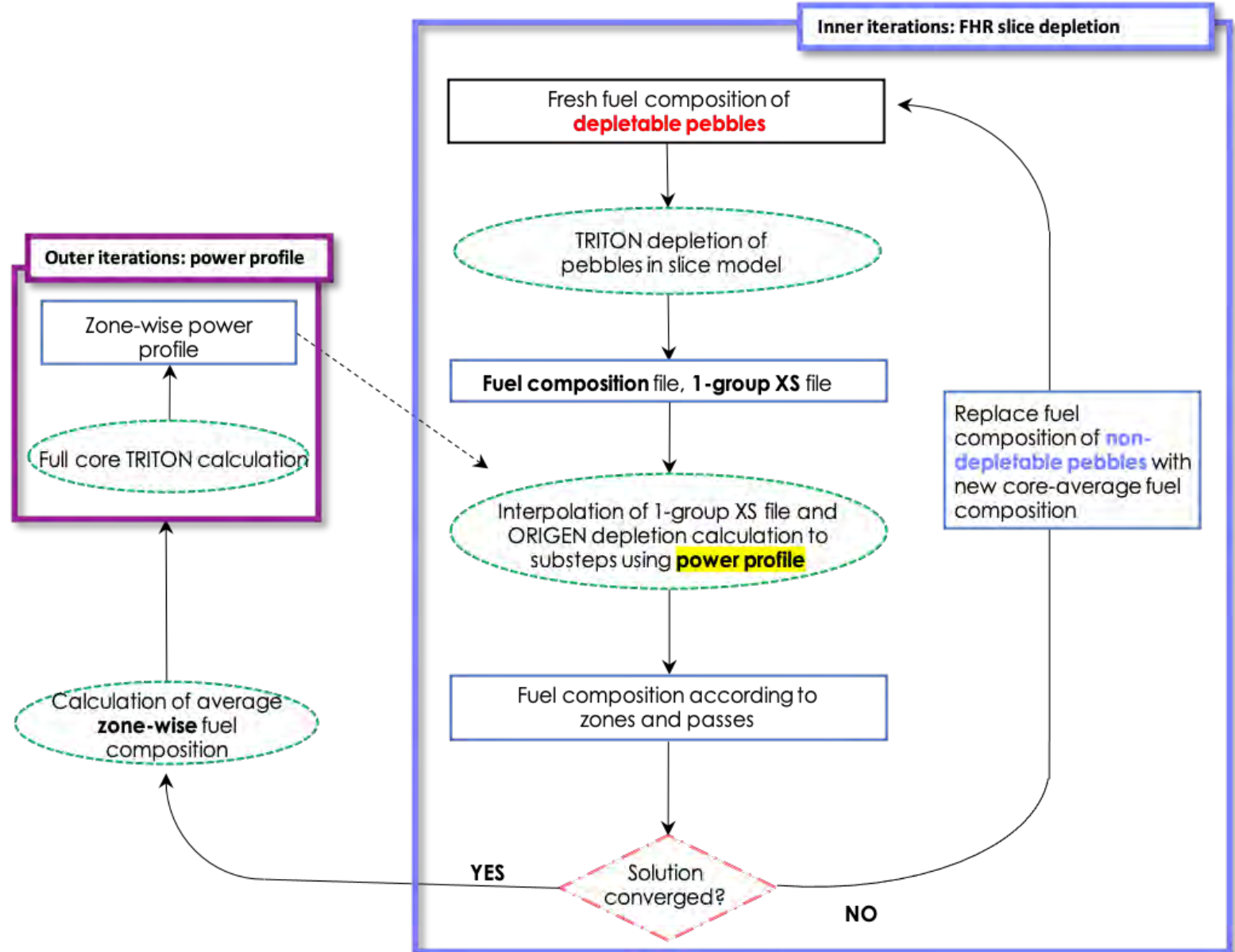


SCALE model a UCB Mark 1 pebble in a cube surrounded by FLiBe

Model		Runtime [min]
CE, random	no clipping	~79 (per realization)
CE, lattice	no clipping	15.28
CE, lattice	clipping	15.78
MG		3.25

# 2. Generation of isotopics for an equilibrium state

- **Outer iteration 1:**
  - Flat axial power profile
  - Consider only axial zones
  - No radial zones or radial power distribution
- **Outer iteration 2:**
  - Use axial and radial power profile from outer iteration 1
  - Consider axial and radial zones
  - Additional assumption: homogenization of compositions of all radial zones after each pass → initial composition for next pass



## 2. Convergence of results during iterations

**Table 4. Slice depletion calculation iterations of outer iteration 1 (constant power).**

$i$	$t_{final}$ (days)	$bu_{final}$ ( $GWd/tHM$ )	$\frac{bu_{final}}{180 GWd/tHM} - 1$	$k_{eff}$	$k_i - k_{i-1}$ (pcm)	$N_D^{235U}$ ( $atoms/b-cm$ )	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$	$N_D^{239Pu}$ ( $atoms/b-cm$ )	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$
0	540.54	144.56	-19.69%	1.32689	–	2.454E-03	–	2.063E-04	–
1	673.08	194.90	8.28%	1.03112	-29577	2.257E-03	-8.00%	2.147E-04	4.10%
2	621.63	187.44	4.13%	1.00464	-2648	2.273E-03	0.71%	2.104E-04	-2.02%
3	596.95	182.68	1.49%	1.00680	216	2.294E-03	0.91%	2.098E-04	-0.27%
4	588.21	180.39	0.22%	1.00954	274	2.304E-03	0.44%	2.102E-04	0.16%
5	586.94	180.15	0.08%	1.01046	92	2.307E-03	0.14%	2.114E-04	0.59%
6	586.45	180.01	0.00%	1.01120	74	2.314E-03	0.27%	2.123E-04	0.40%
7	586.43	179.84	-0.09%	1.01128	8	2.315E-03	0.04%	2.126E-04	0.18%
8	586.95	179.95	-0.03%	1.01126	-2	2.316E-03	0.06%	2.127E-04	0.05%

**Table 5. Slice depletion calculation iterations using outer iteration 2 (axial/radial power profile).**

$i$	$t_{final}$ (days)	$bu_{final}$ ( $GWd/tHM$ )	$\frac{bu_{final}}{180 GWd/tHM} - 1$	$k_{eff}$	$k_i - k_{i-1}$ (pcm)	$N_D^{235U}$ ( $atoms/b-cm$ )	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$	$N_D^{239Pu}$ ( $atoms/b-cm$ )	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$
0	540.54	144.56	-19.69%	1.32689	–	2.454E-03	–	2.0881E-04	–
1	673.08	194.18	7.88%	1.03206	-29483	2.257E-03	-8.20%	2.1643E-04	3.65%
2	623.93	187.83	4.35%	1.00585	-2621	2.273E-03	0.93%	2.1384E-04	-1.20%
3	597.91	182.83	1.57%	1.00772	187	2.294E-03	0.96%	2.1432E-04	0.22%
4	588.67	180.46	0.26%	1.00991	219	2.304E-03	0.61%	2.1516E-04	0.39%
5	587.16	179.74	-0.14%	1.01122	131	2.307E-03	0.06%	2.1491E-04	-0.11%
6	588.01	179.62	-0.21%	1.01218	96	2.314E-03	0.03%	2.1403E-04	-0.41%
7	589.24	180.11	0.06%	1.01256	38	2.315E-03	-0.06%	2.1468E-04	0.31%
8	588.87	179.76	-0.13%	1.01178	-78	2.316E-03	-0.10%	2.1390E-04	-0.36%
9	589.66	180.40	0.22%	1.01168	-10	2.316E-03	0.01%	2.1432E-04	0.20%

### Convergence after 8 or 9 iterations:

- $k_{eff}$  converged
- Nominal discharge burnup achieved
- Nuclide densities converged



## 2. Comparison of final core average fuel compositions

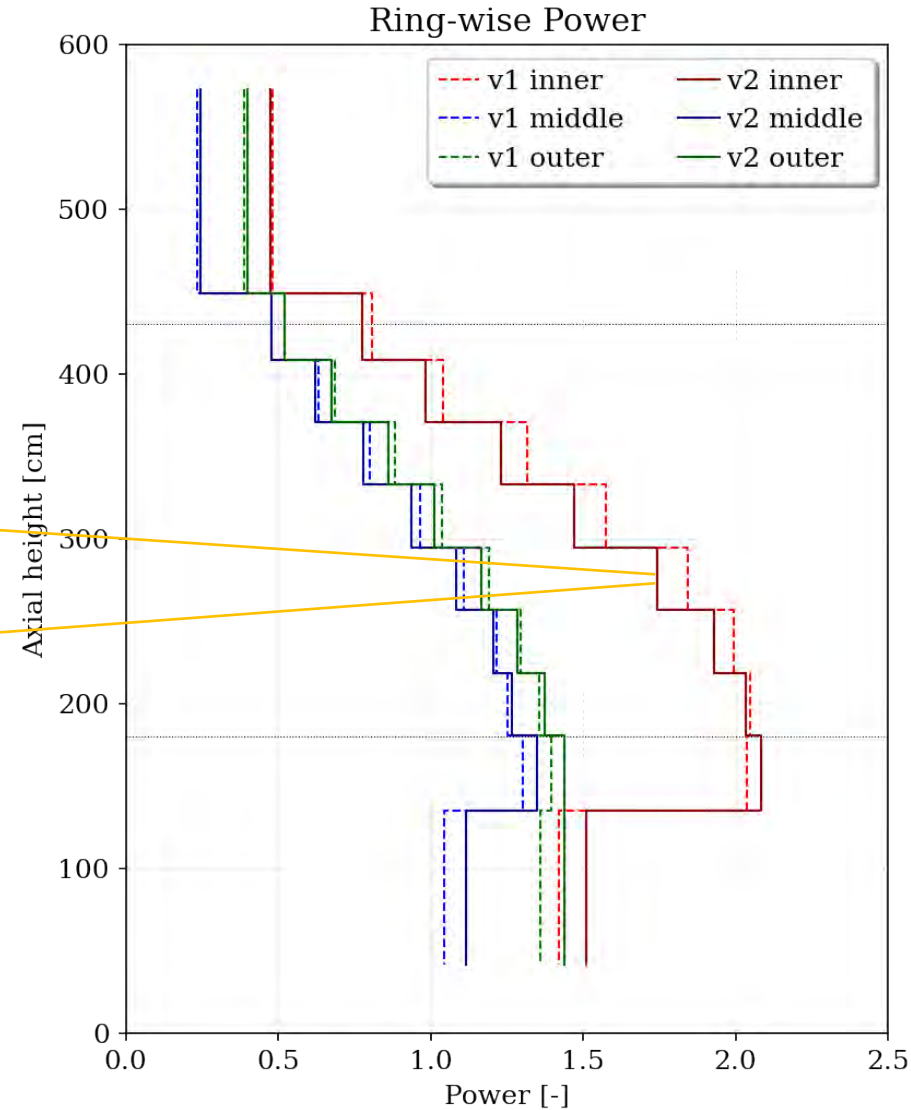
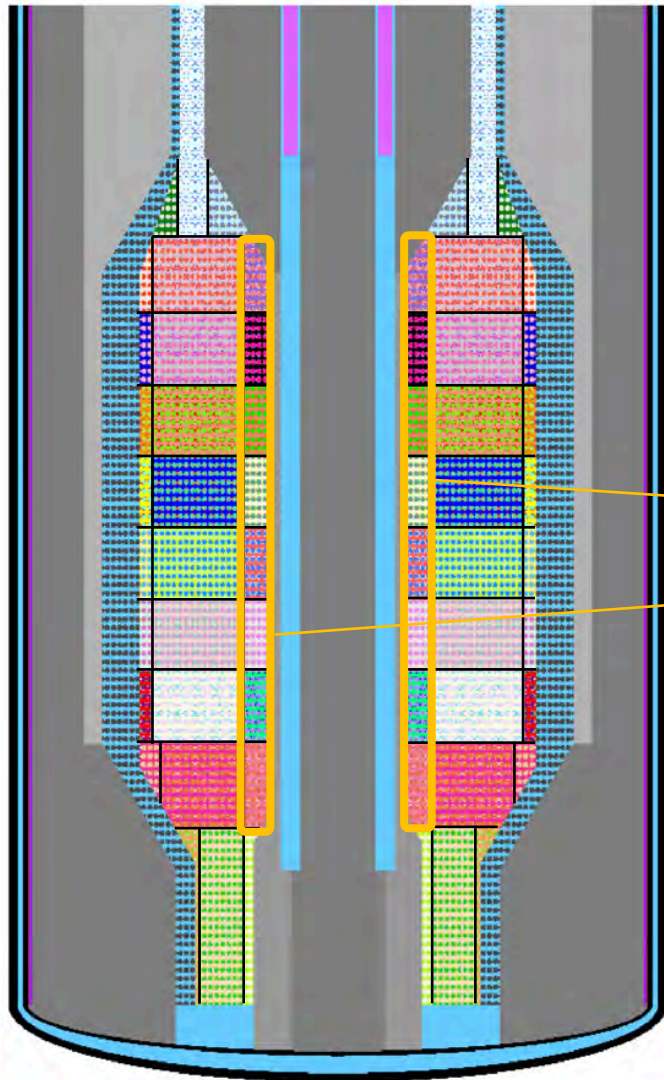
Nuclide	Density [at/b-cm]		Relative difference
	Outer iteration 1	Outer iteration 2	
xe-135	4.587E-08	4.422E-08	-3.6%
cs-134	1.542E-05	1.509E-05	-2.2%
cs-137	1.570E-04	1.568E-04	-0.1%
nd-148	4.405E-05	4.414E-05	0.2%
sm-149	4.019E-07	4.122E-07	2.6%
sm-151	1.856E-06	1.861E-06	0.3%
gd-154	6.098E-08	6.104E-08	0.1%
gd-155	2.865E-09	3.137E-09	9.5%
eu-153	1.077E-05	1.065E-05	-1.1%
eu-154	1.788E-06	1.759E-06	-1.6%
eu-155	5.965E-07	5.876E-07	-1.5%

Nuclide	Density [at/b-cm]		Relative difference
	Outer iteration 1	Outer iteration 2	
u-235	2.316E-03	2.306E-03	-0.4%
u-238	1.786E-02	1.788E-02	0.1%
pu-239	2.127E-04	2.143E-04	0.7%
pu-240	8.041E-05	8.033E-05	-0.1%
pu-241	6.724E-05	6.662E-05	-0.9%
pu-242	2.980E-05	2.910E-05	-2.3%
am-241	6.746E-07	6.873E-07	1.9%
cm-242	4.772E-07	4.672E-07	-2.1%
cm-244	1.467E-06	1.420E-06	-3.2%

Relative difference of core-average fuel composition is negligible besides very few exceptions in case of small nuclide densities.



# 3. Full core power profile



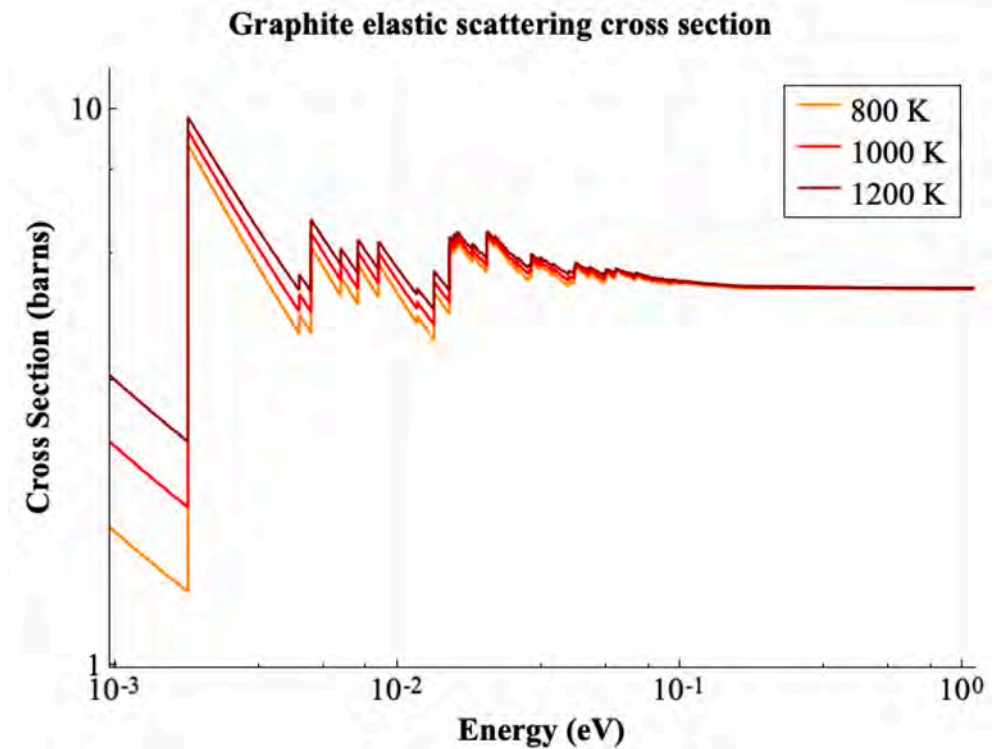
## Results:

- Power is peaking in the inner fuel region
- Consideration of axial/radial power profile in the iterations to obtain the equilibrium core compositions has minor effect.

# 4. Comparison of isothermal temperature coefficients

- Reactivity coefficient calculation:
  - $k_{eff}$  calculations with material temperatures varying over a range of several hundred K
  - Assuming constant temperature within material
  - Fitting of  $\rho$  to determine coefficient

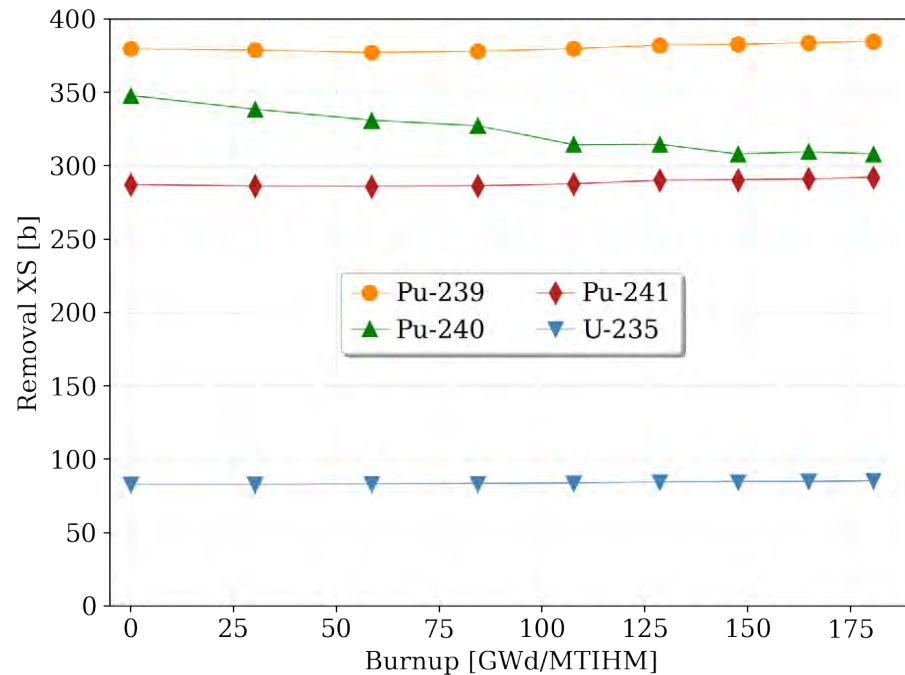
Component	Temperature Reactivity Coefficient at HFP [pcm/K]	
	Cisneros [1]	ORNL
Fuel	-3.8	-3.90
Salt coolant	-1.8	-0.48
Graphite moderator	-0.7	-1.10
Inner graphite reflector	+0.9	+1.21
Outer graphite reflector	+0.9	+0.61



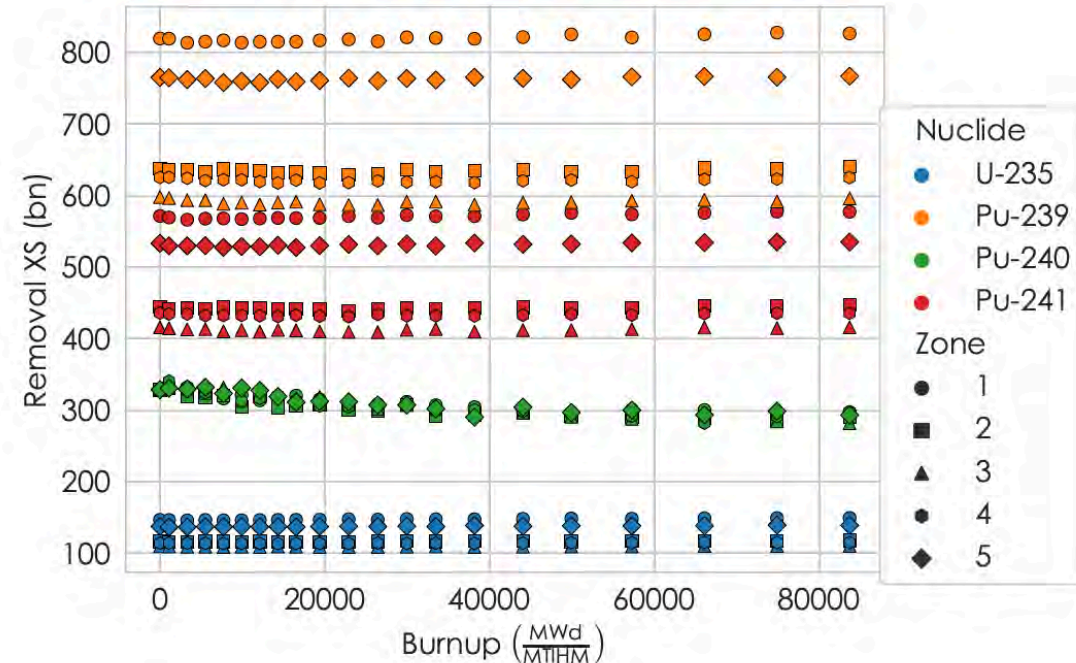
[1] A. T. Cisneros, "Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)," University of California, Berkeley, 2013.

# 6. Towards rapid inventory calculations with ORIGAMI

**Purpose of 1-group cross section analysis:** understand the spectral variations and their impact on 1-group cross sections which influence all inventory calculations



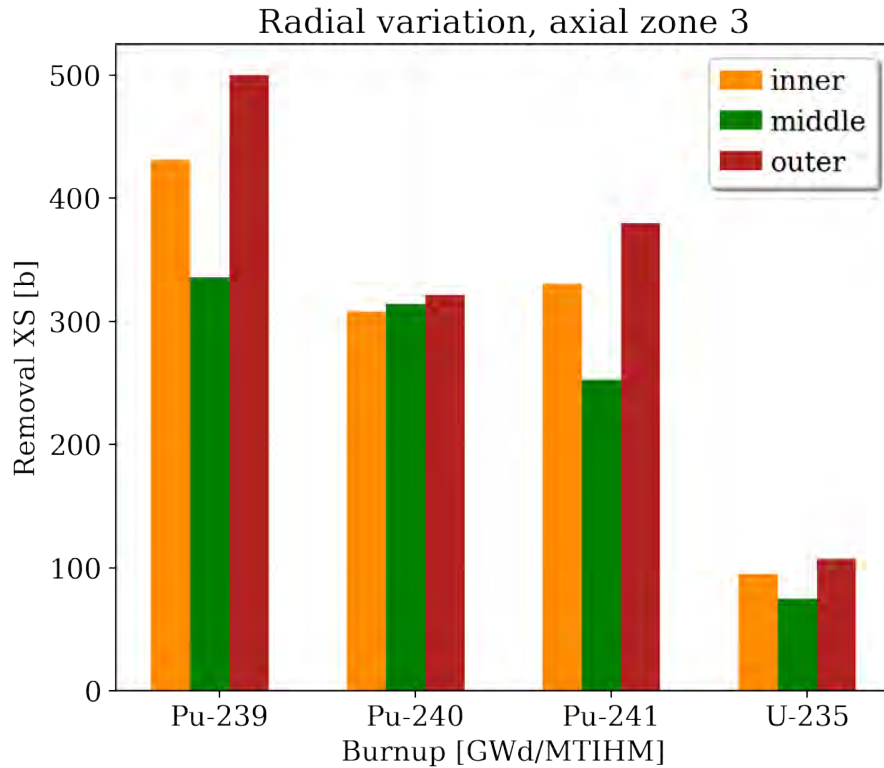
**UCB Mark 1 slice depletion (HFP)**



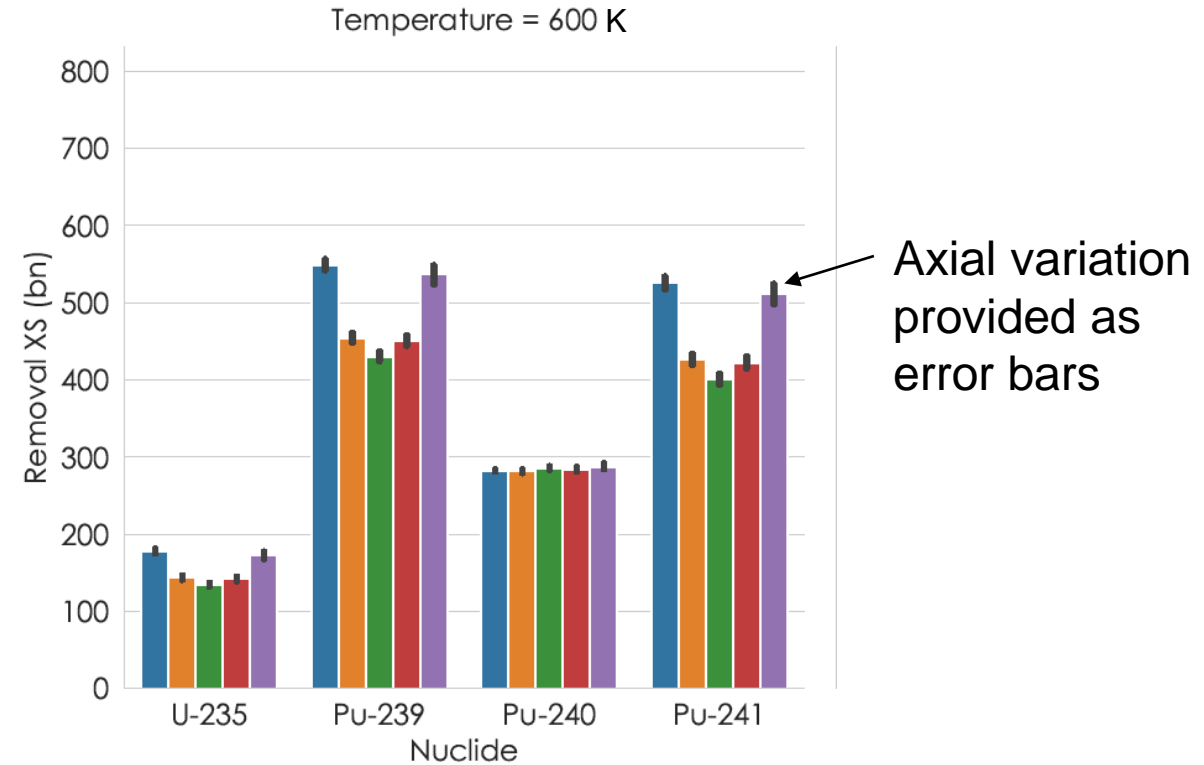
**PBMR-400 slice depletion\***

- Only small variation of 1-group removal cross section over depletion
- Small changes visible mainly in Pu-240

# 6. Comparison between UCB Mark 1 and PBMR-400



**UCB Mark 1**



**PBMR-400\***

- Both cores showed significant radial variation for various nuclides
- Only UCB Mark 1 showed axial variation due to inlet/outlet geometry

\*S. Skutnik, W. Wieselquist, ORNL/TM-2020/1886, 2021. <https://www.osti.gov/servlets/purl/1807271>

## 7. Analytical model to calculate tritium production

- A simplified analytical model was developed by Cisneros et al\*. using a flux and one-group cross sections to allow estimation of tritium generation rates for an arbitrary initial Li-7 enrichment

$$\dot{T}(t) = \phi \sigma_{Li-7}^T N_{Li-7} + \phi \sigma_{Li-6}^T \left( N_{Li-6}^0 e^{-\frac{V_{core}}{V_{Loop}} \phi \sigma_{Li-6}^{abs} t} + \frac{\phi \sigma_{Be-9}^{\alpha} N_{Be-9}}{\phi \sigma_{Li-6}^{abs}} \left( 1 - e^{-\frac{V_{core}}{V_{Loop}} \phi \sigma_{Li-6}^{abs} t} \right) \right)$$

- SCALE results using TRITON/ORIGEN: **0.021 mol/day**
- Equilibrium value from Cisneros analytical approach: **0.023 mol/day**

\*Cisneros, A. T., 2013. *Pebble Bed Reactors Design and Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)* (PhD). University of California Berkeley.



# MELCOR for Accident Progression and Source Term Analysis

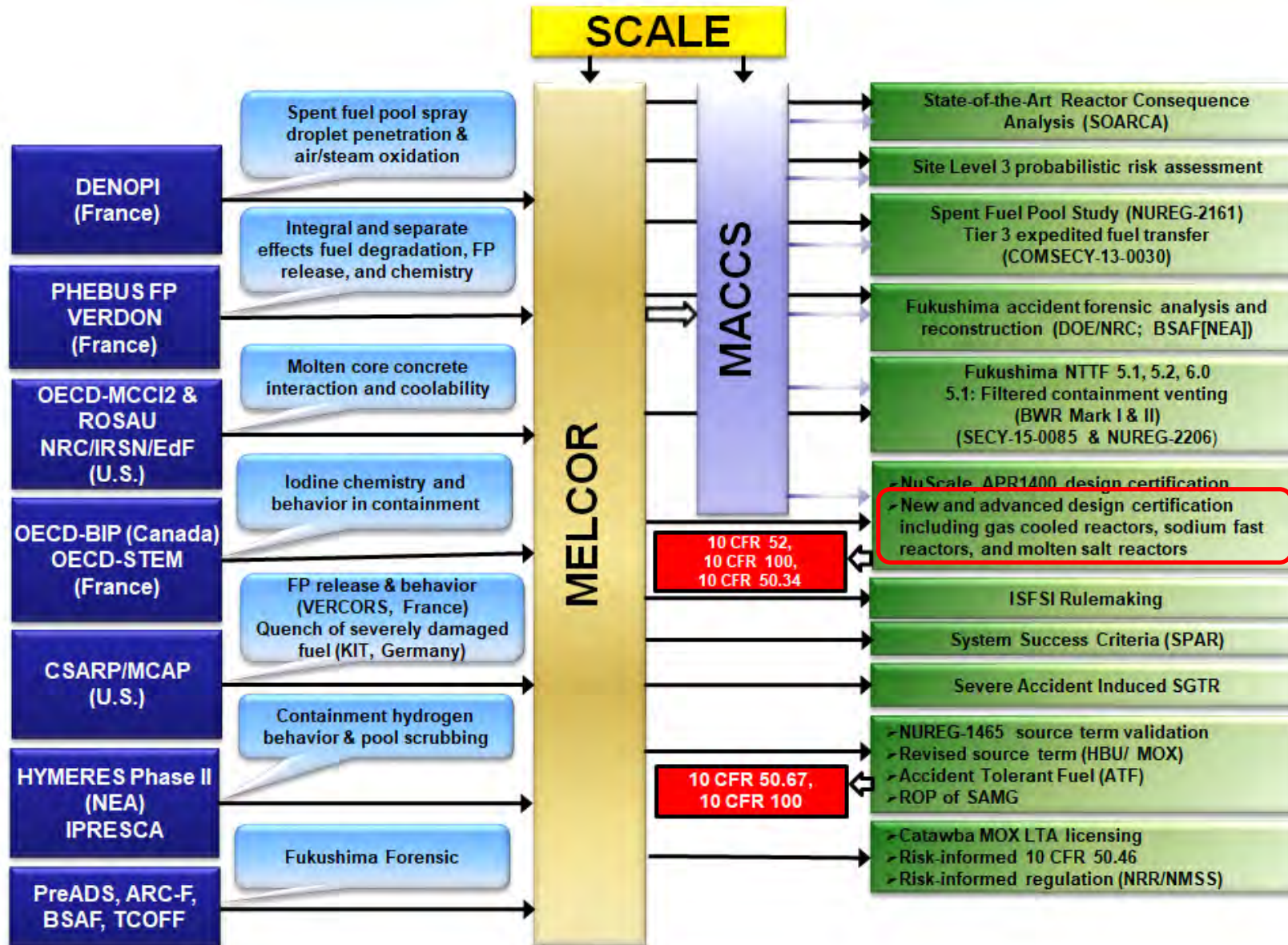


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# MELCOR Development for Regulatory Applications



## 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?

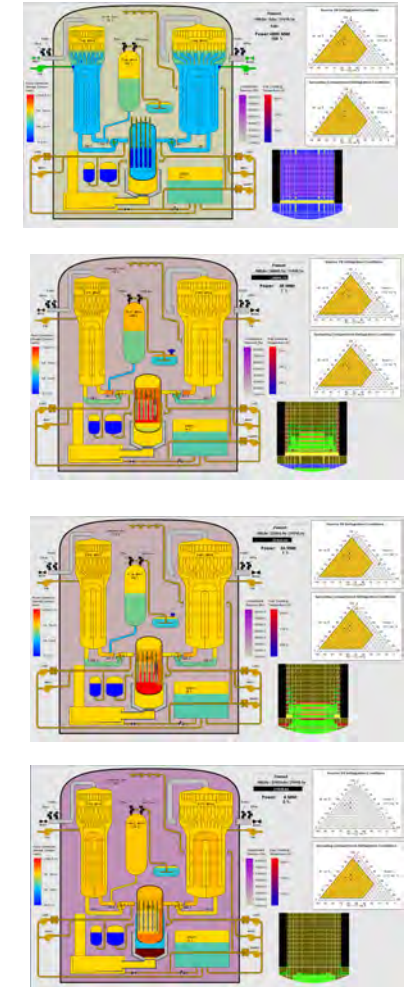
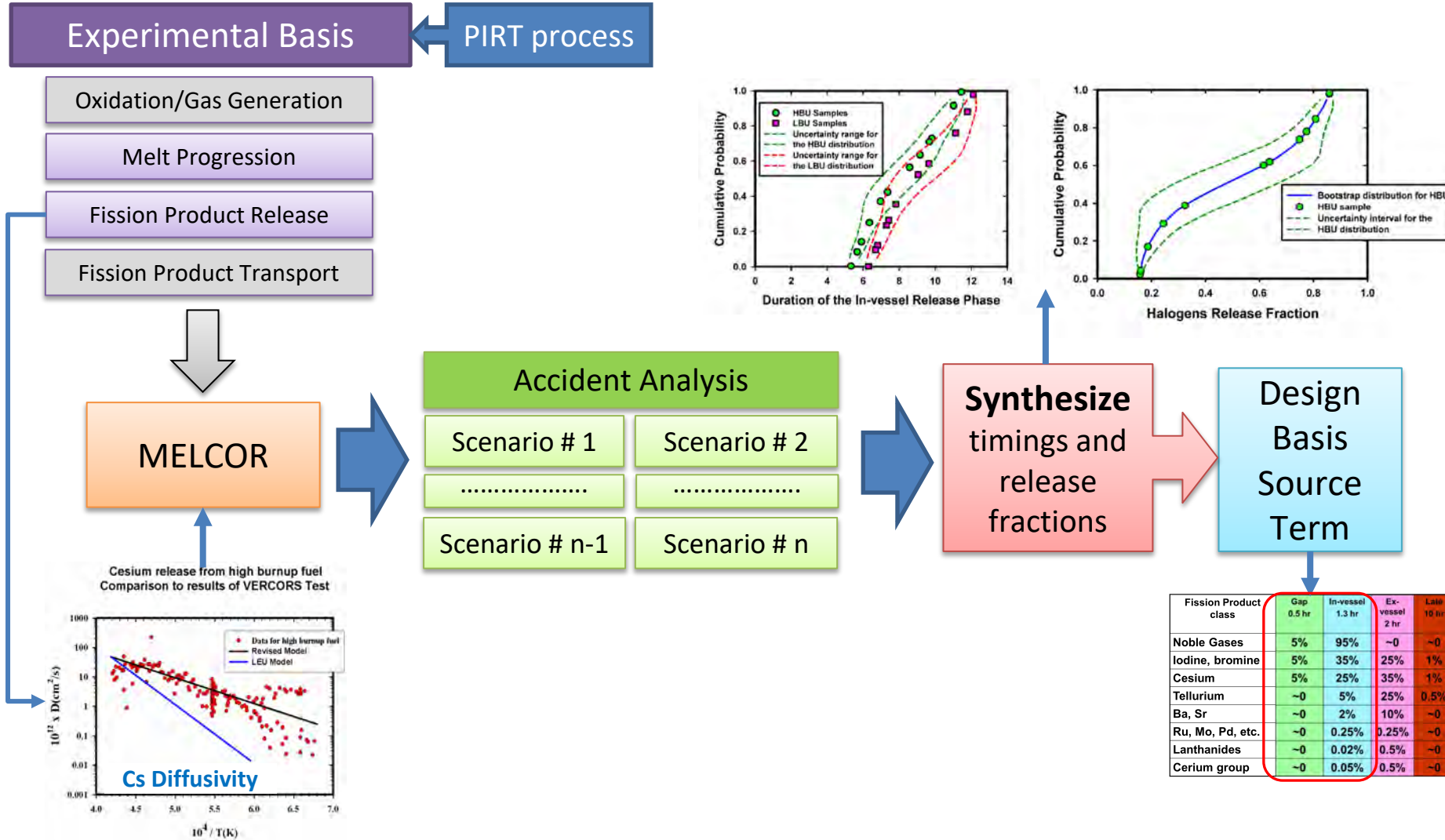
MELCOR is used to support severe accident and source term activities at NRC, including the development of regulatory source terms for LWRs, analysis of success criteria for probabilistic risk assessment models, site risk studies, and forensic analysis of the Fukushima accident.

## 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



# 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

## Non-Reactor 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

### 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

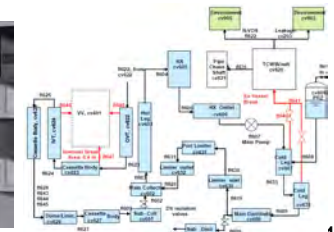
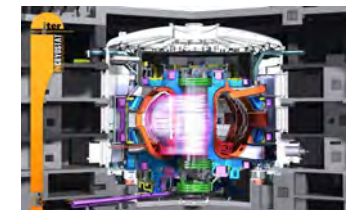
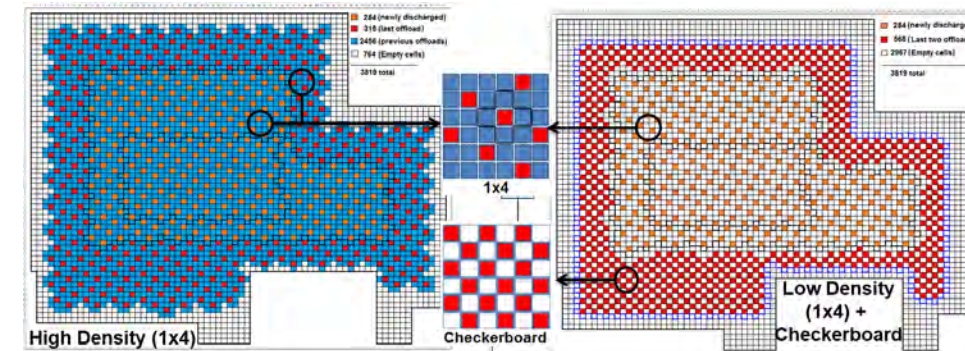
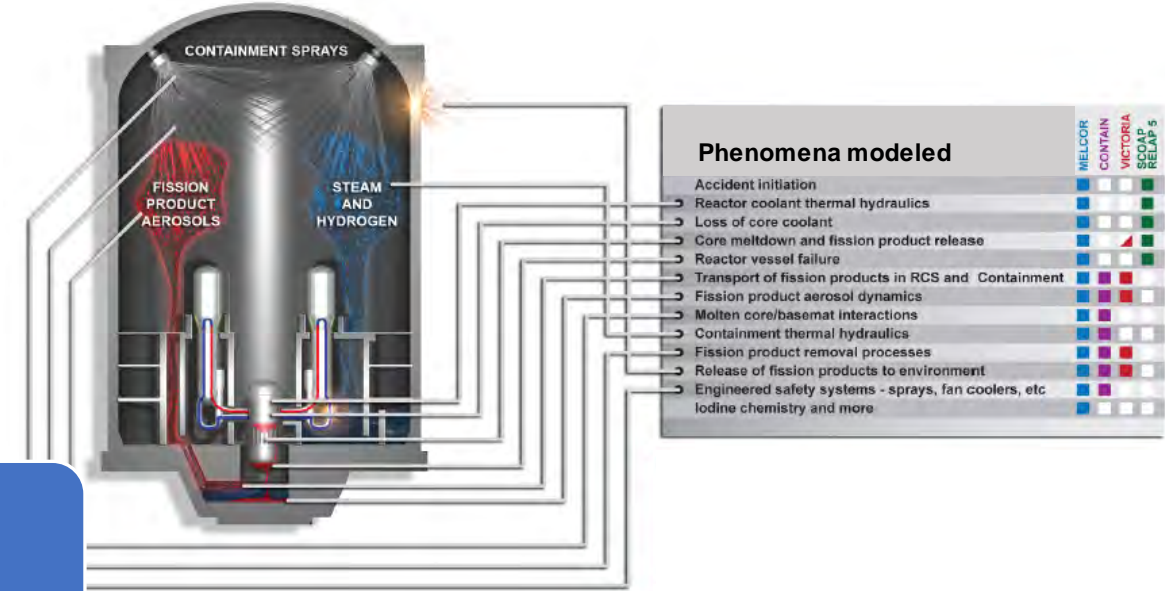
- Thermal-hydraulic response of reactor coolant system, reactor cavity, reactor enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

### 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

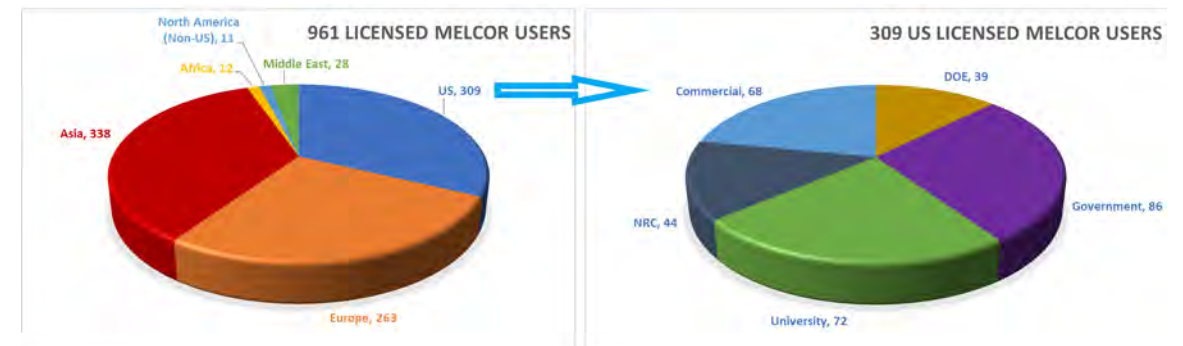
International LWR fleet relies on safety assessments performed with the MELCOR code

### International Collaboration

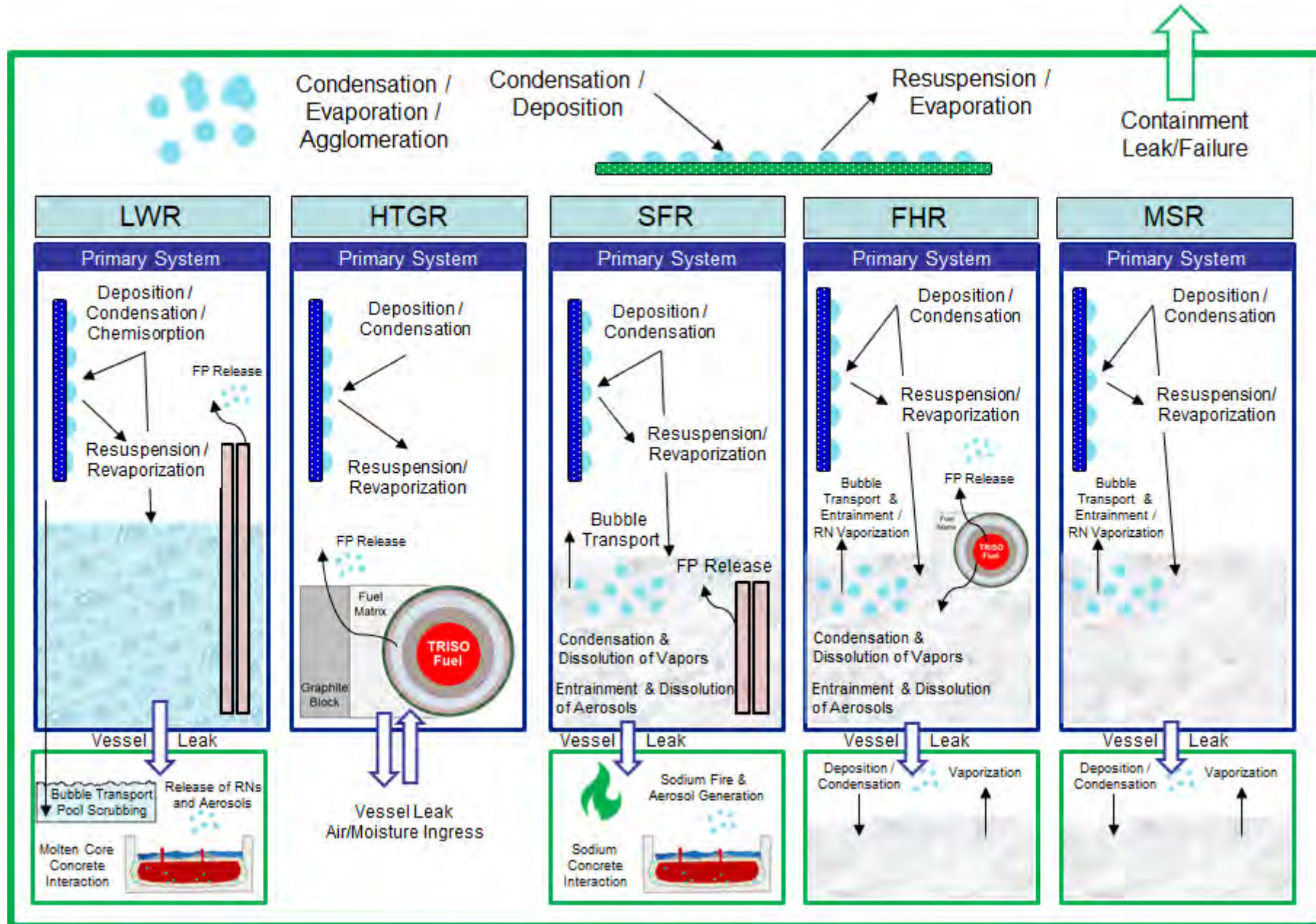
Cooperative Severe Accident Research Program (CSARP) – June/U.S.A  
 MELCOR Code Assessment Program (MCAP) – June/U.S.A  
 European MELCOR User Group (EMUG) Meeting – Spring/Europe  
 European MELCOR User Group (EMUG) Meeting – Fall/Asia







# Common Phenomenology











# MELCOR Software Quality Assurance – Best Practices

**MELCOR SQA Standards**  
 SNL Corporate procedure IM100.3.5  
 CMMI-4+  
 NRC NUREG/BR-0167

## 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

**Emphasis is on Automation**  
**Affordable solutions**  
**Consistent solutions**



## Bug tracking and reporting

- Bugzilla online

## Code Validation

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

## Documentation

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

## Project Management

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

## Sharing of information with users

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

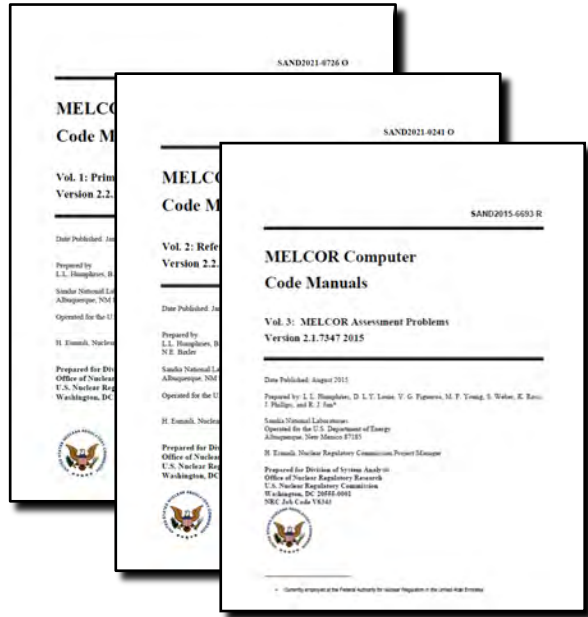


Case	BUR	CAV	CF	COR	CVH	DCH	FCL	FDI	FL	HS	NCG	PAR	RN	SPR
M-8-1 NoMix			X		X				X	X	X			
M-8-1 SYM			X		X				X	X	X			
Lace7			X		X	X			X	X	X		X	
Lace8			X		X	X			X	X	X		X	
Vanam-M3			X		X				X	X	X		X	
Molten Salt			X	X	X				X	X	X			
PHEBUS-B9			X	X	X				X	X	X			
FPT1			X	X	X	X			X	X	X		X	
LOFT			X	X	X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

Table 1-1: Physics Package Coverage



# MELCOR Verification & Validation Basis



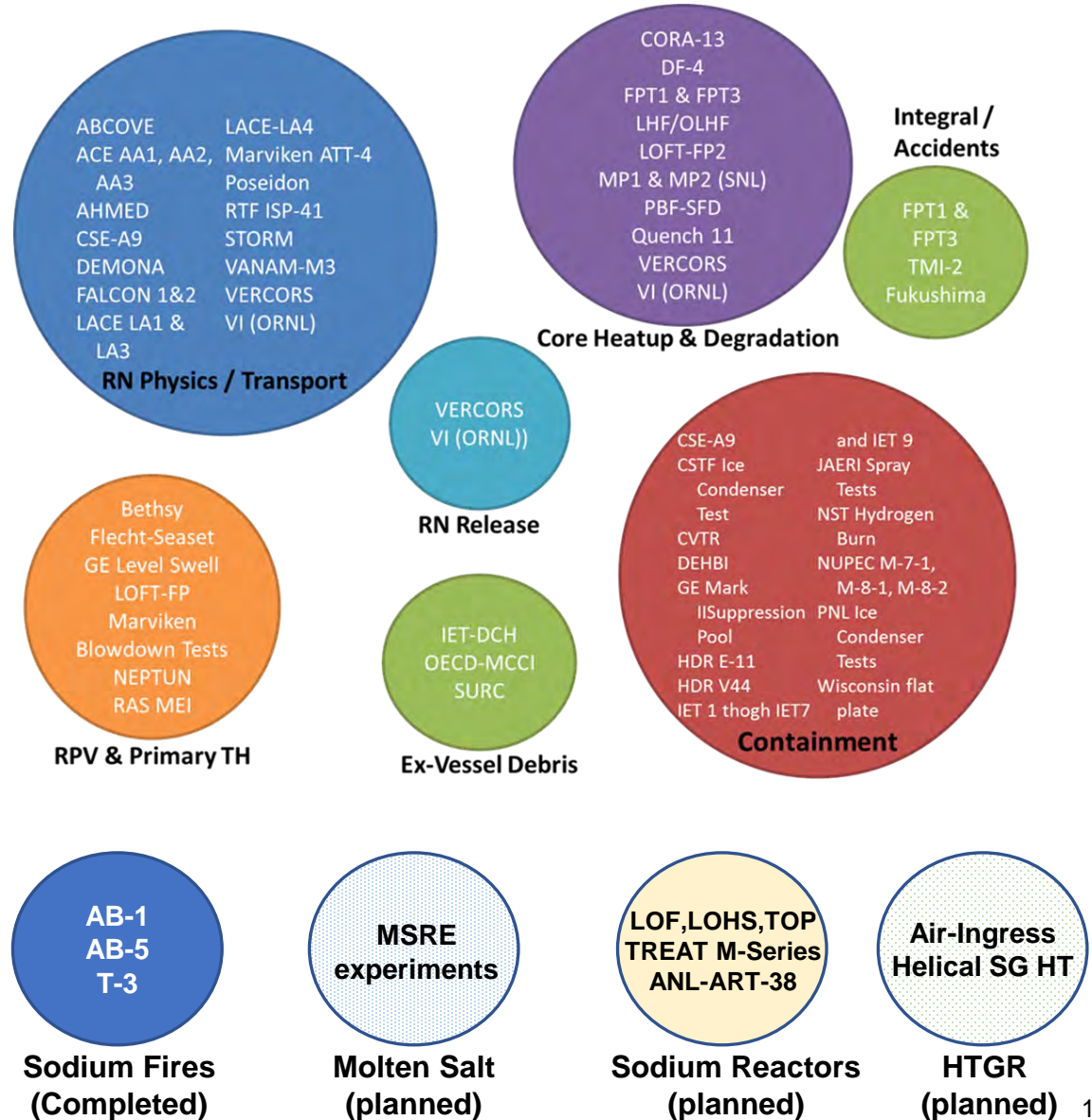
**Volume 1: Primer & User Guide**  
**Volume 2: Reference Manual**  
**Volume 3: MELCOR Assessment Problems**  
 [SAND2015-6693 R]

## 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

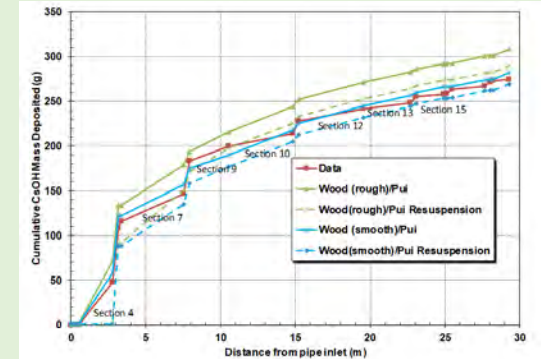
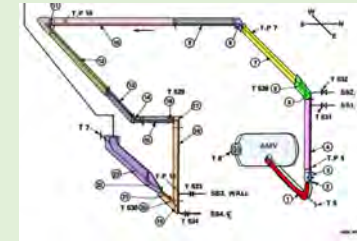
Case	1a	1b	2a	2b	3a	3b
US/INL	0.467	1.0	0.026	0.996	1.32E-4	0.208
US/GA	0.453	0.97	0.006	0.968	7.33E-3	1.00
<b>US/SNL</b>	<b>0.465</b>	<b>1.0</b>	<b>0.026</b>	<b>0.995</b>	<b>1.00E-4</b>	<b>0.208</b>
US/NRC	0.463	1.0	0.026	0.989	1.25E-4	0.207
France	0.472	1.0	0.028	0.995	6.59E-5	0.207
Korea	0.473	1.0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

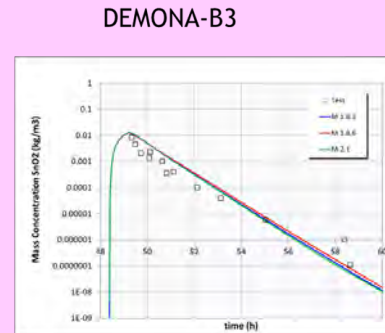
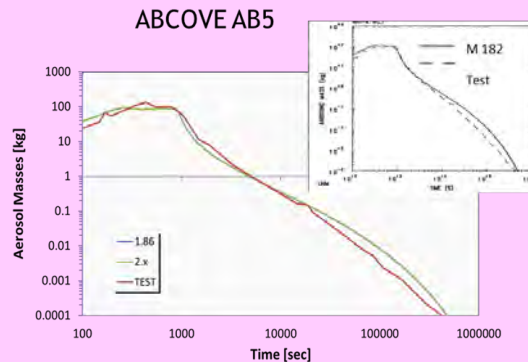


## Aerosol Physics

- Agglomeration
- Deposition
- Condensation and Evaporation at surfaces

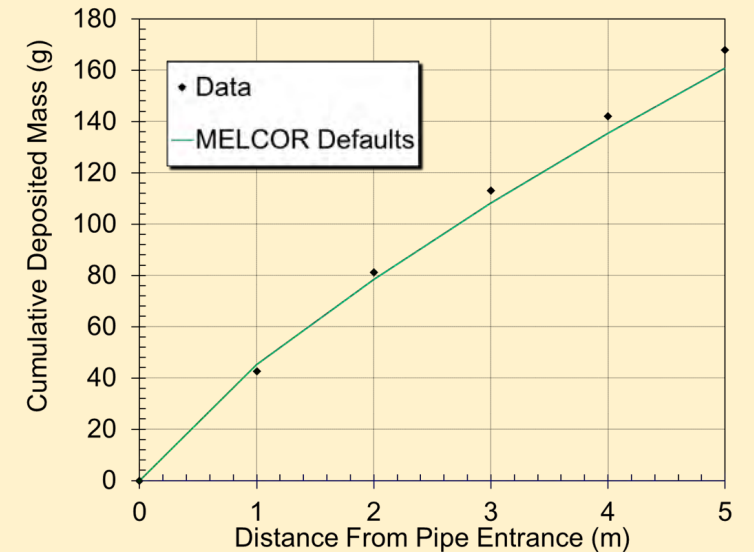
### Validation Cases

- 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

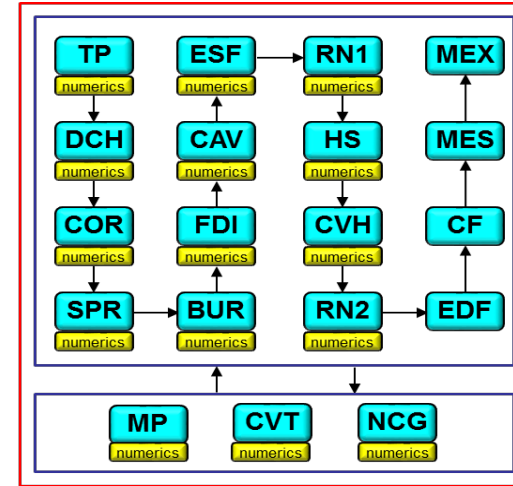
Generalized numerical solution engine

Hydrodynamics

In-vessel damage progression

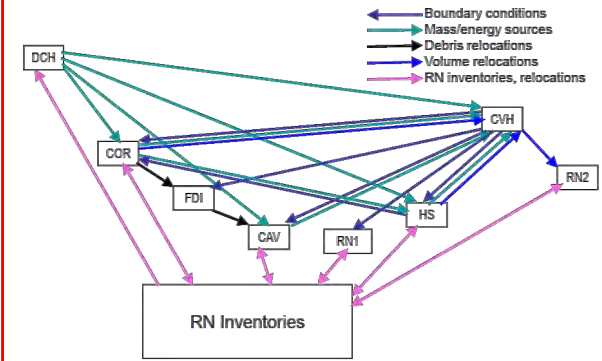
Ex-vessel damage progression

Fission product release and transport

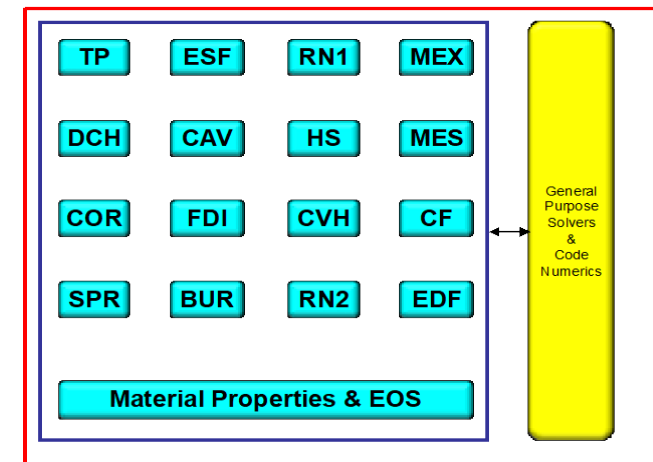
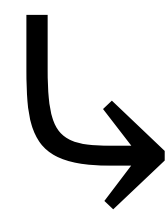


TP = Transfer Process  
 DCH = Decay Heat  
 COR = Core  
 SPR = Containment Spray  
 BUR = Gas Combustion  
 FDI = Fuel Dispersal Interaction  
 CAV = Cavity (MCCI)  
 ESF = Engineered Safety Features  
 MP = Material Properties

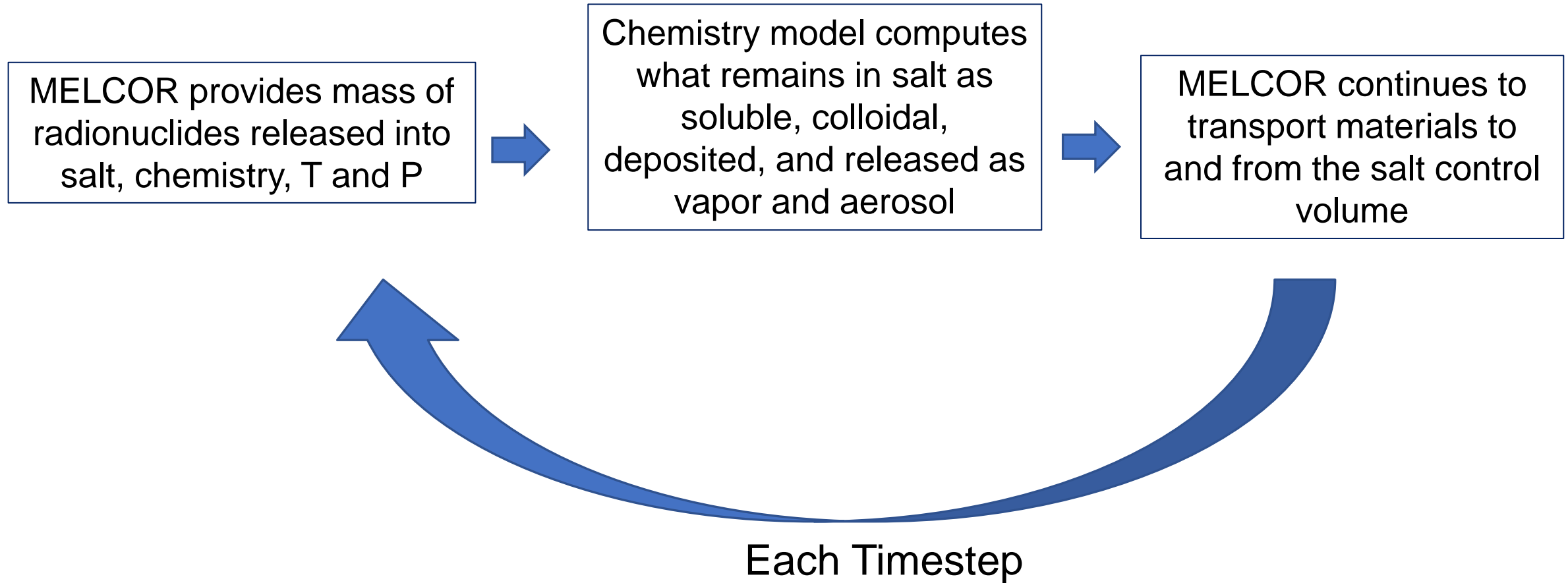
RN = Radionuclide  
 HS = Heat Structure  
 CVH = CV Hydrodynamics  
 EDF = External Data File  
 CF = Control Function  
 MES = Special Messages  
 MEX = Executive  
 CVT = CV Thermodynamics  
 NCG = Non Condensable Gas



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



# Molten Salt Chemistry and Radionuclide Release – Integration into MELCOR





# Cs vapor pressures in MSM calculations

