

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

September 14, 2021



U.S. NRC



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Outline

NRC strategy for non-LWR source term analysis

Project scope

Overview of fluoride-salt-cooled High-Temperature Reactor (FHR)

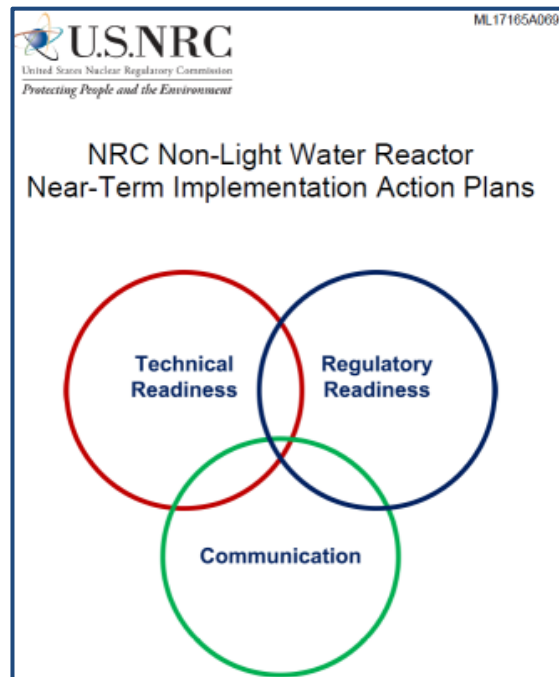
FHR reactor fission product inventory/decay heat methods & results

MELCOR molten salt models

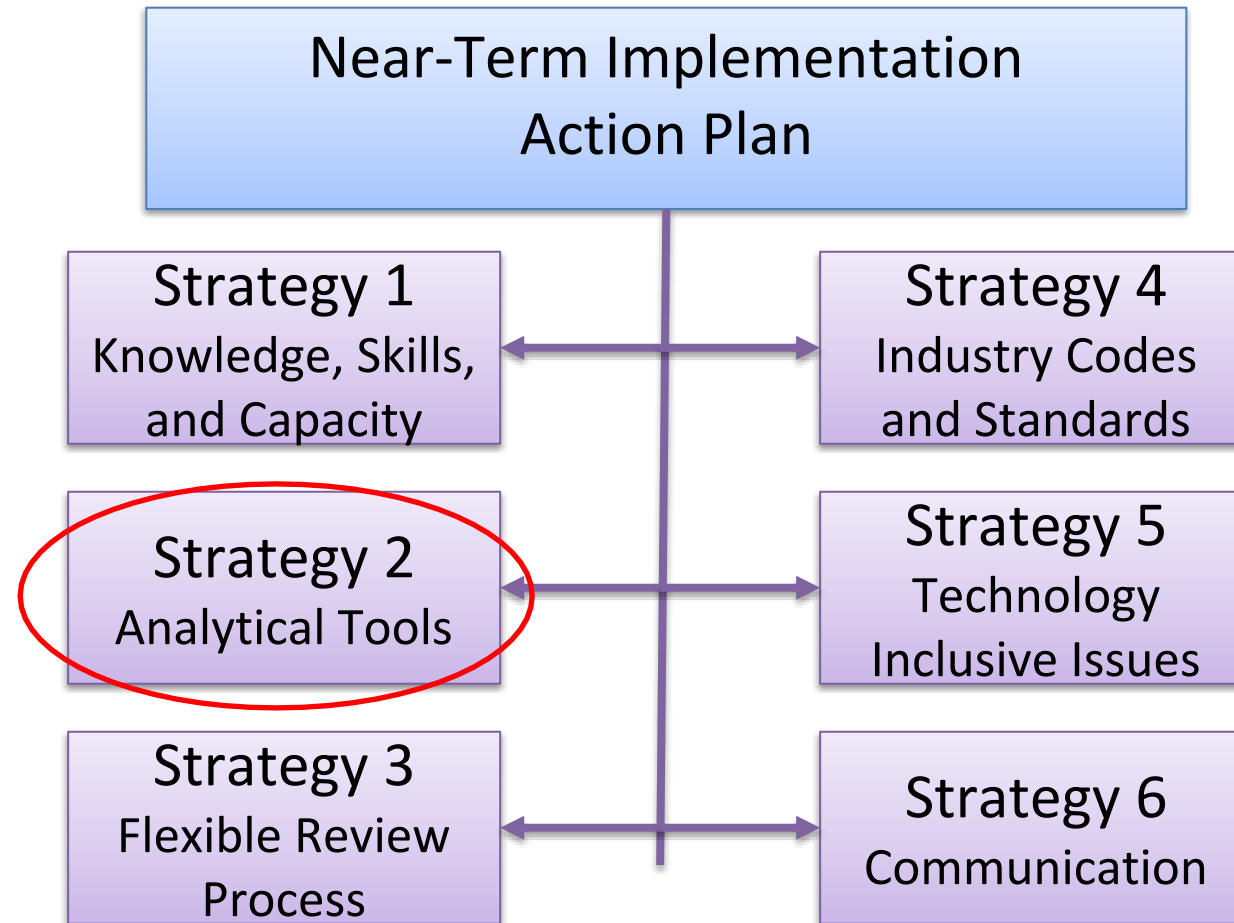
FHR plant model and source term analysis

Summary

Integrated Action Plan (IAP) for Advanced Reactors



[ML17165A069](#)



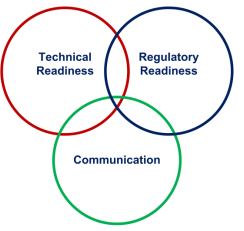
IAP Strategy 2 Volumes

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

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Protecting People and the Environment

Revision 1
January 31, 2020

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

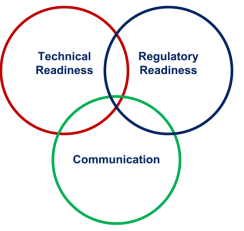


Introduction
[ML20030A174](#)

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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*

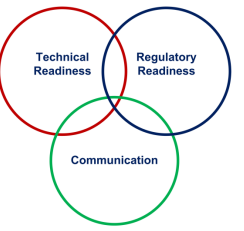


Volume 1
[ML20030A176](#)

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



Volume 2
[ML20030A177](#)

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Revision 1
March 31, 2021

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

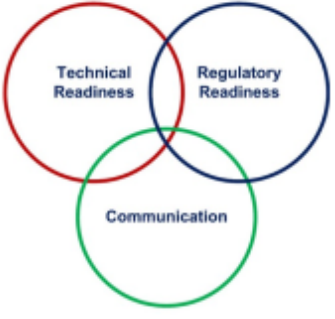


Volume 4
[ML21085A484](#)

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Revision 1
MARCH 31, 2021

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

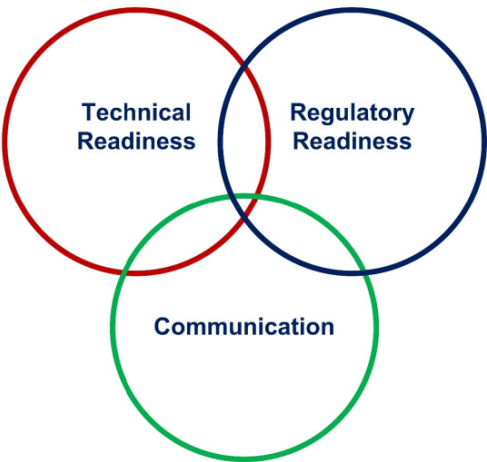


Volume 5
[ML21088A047](#)

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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*



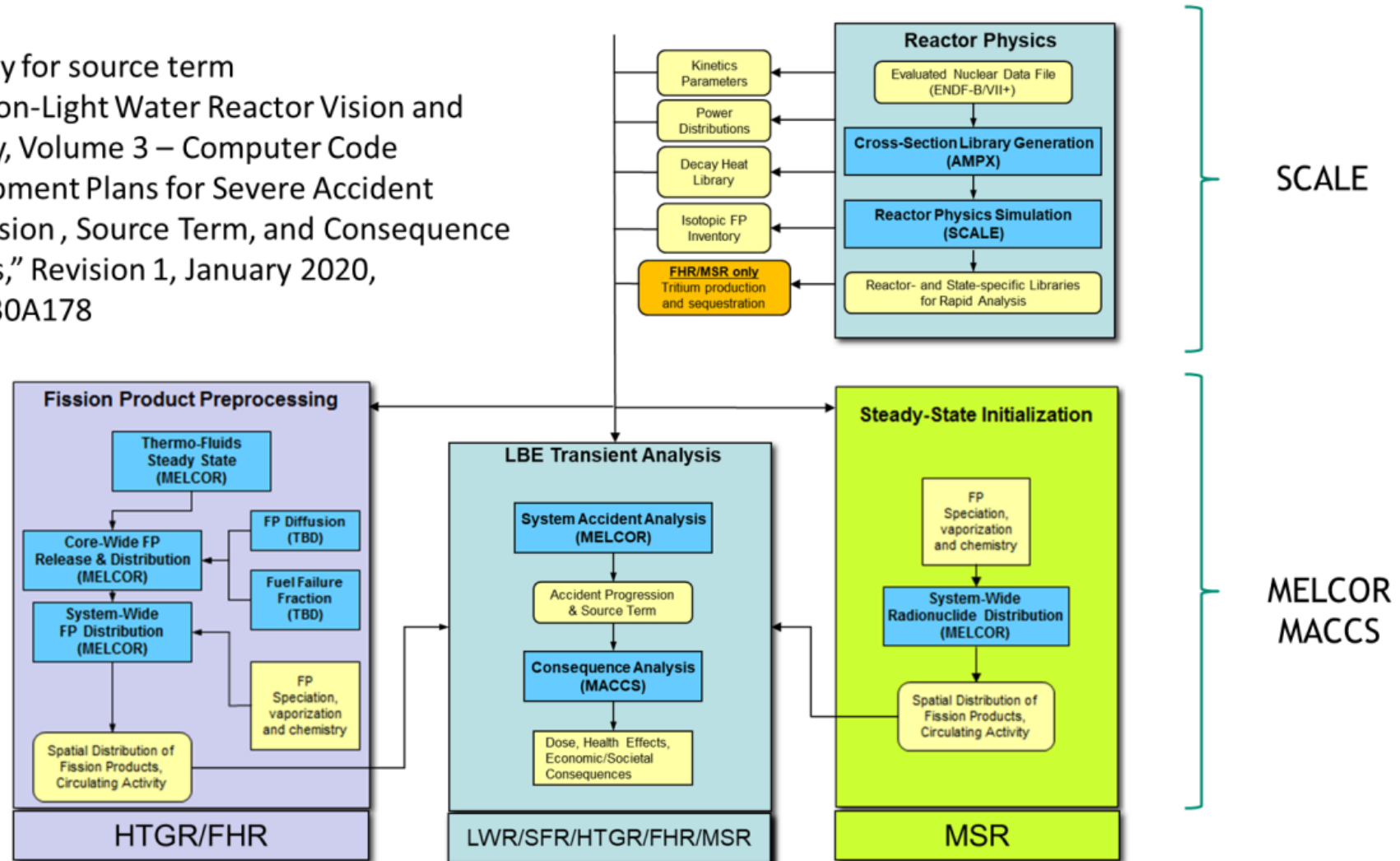
Volume 3
[ML20030A178](#)

NRC strategy for non-LWR analysis (Volume 3)

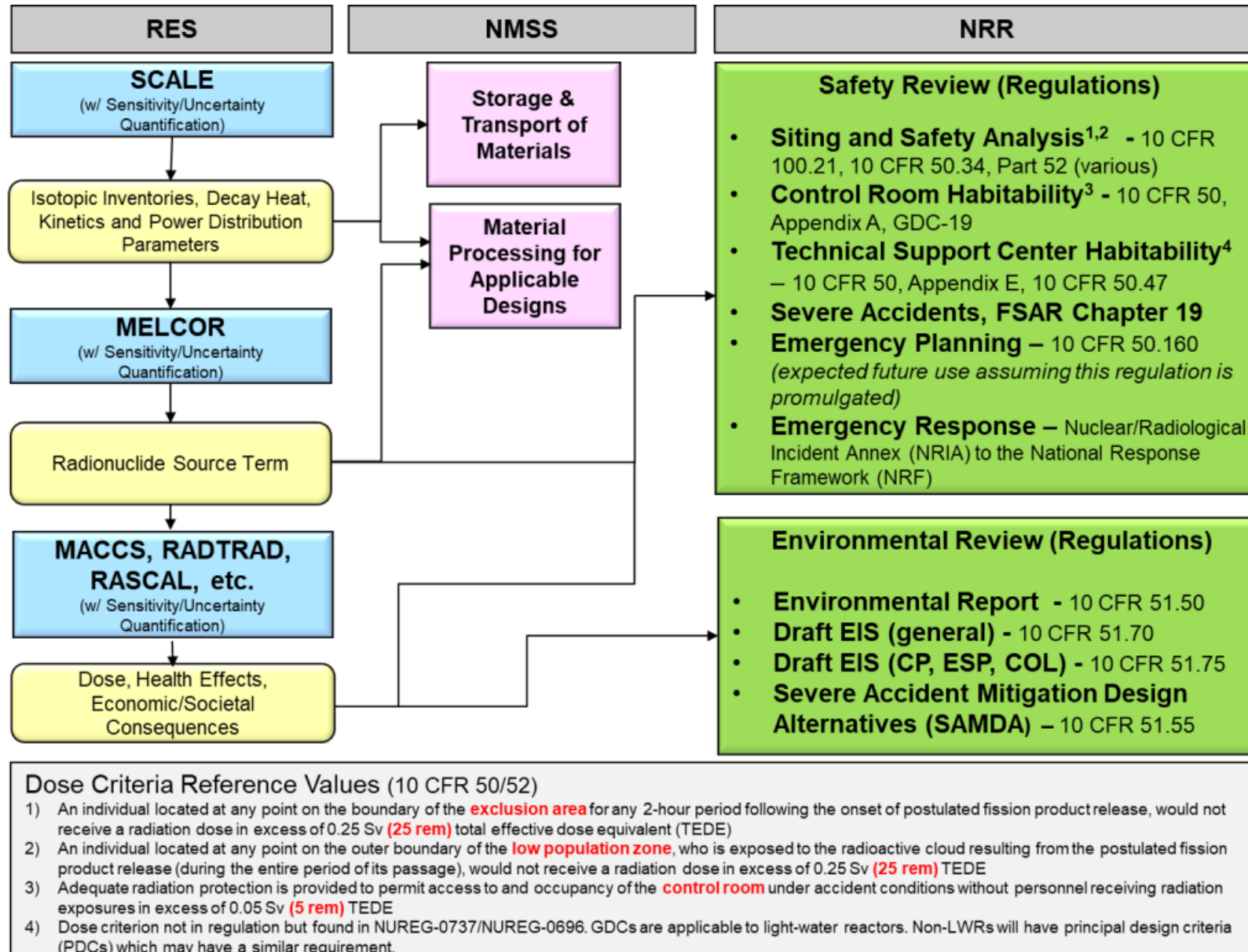
Evaluation Model and Suite of Codes

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

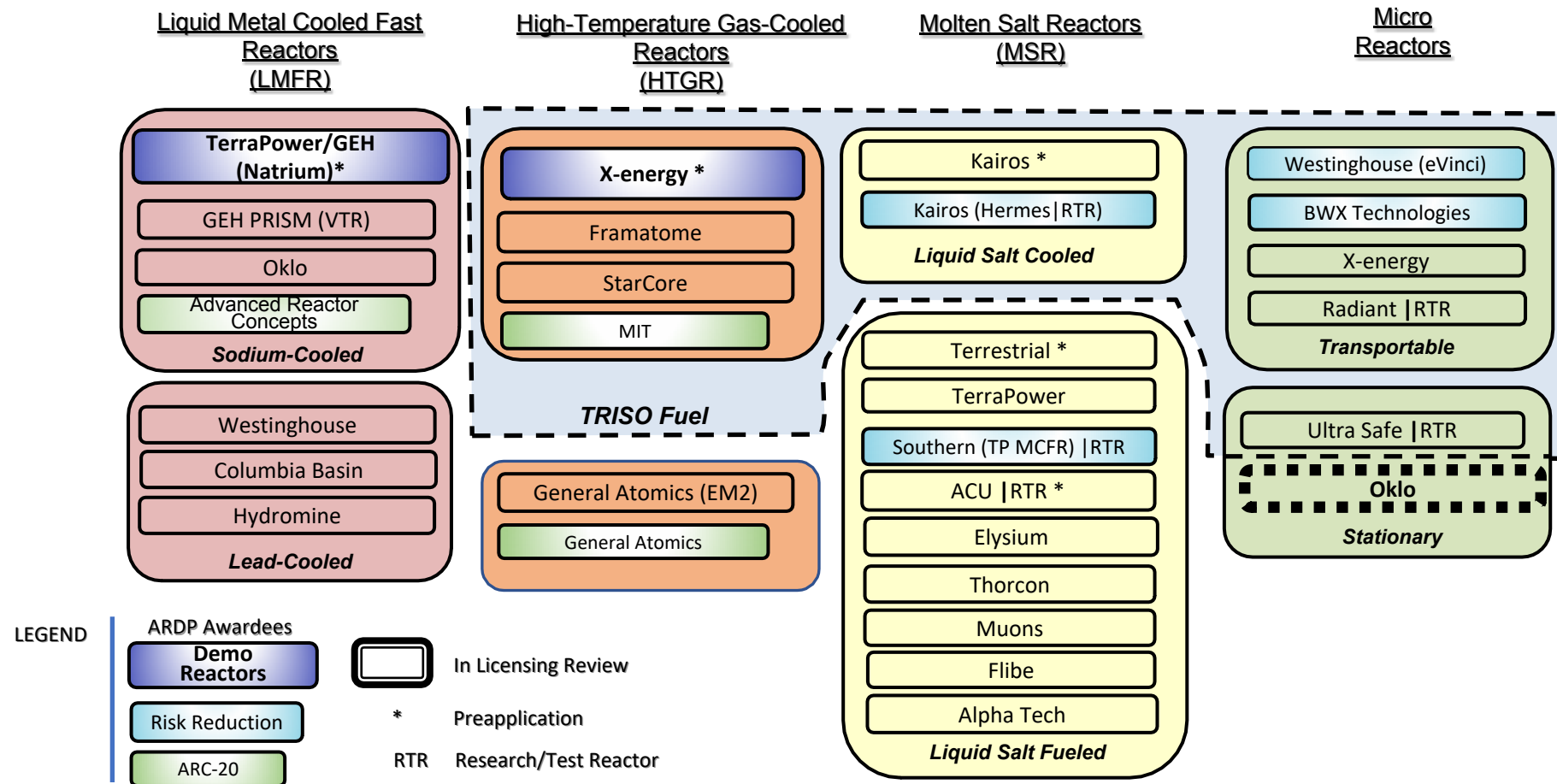
FY22

- 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)



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Molten-salt reactors (1/3)

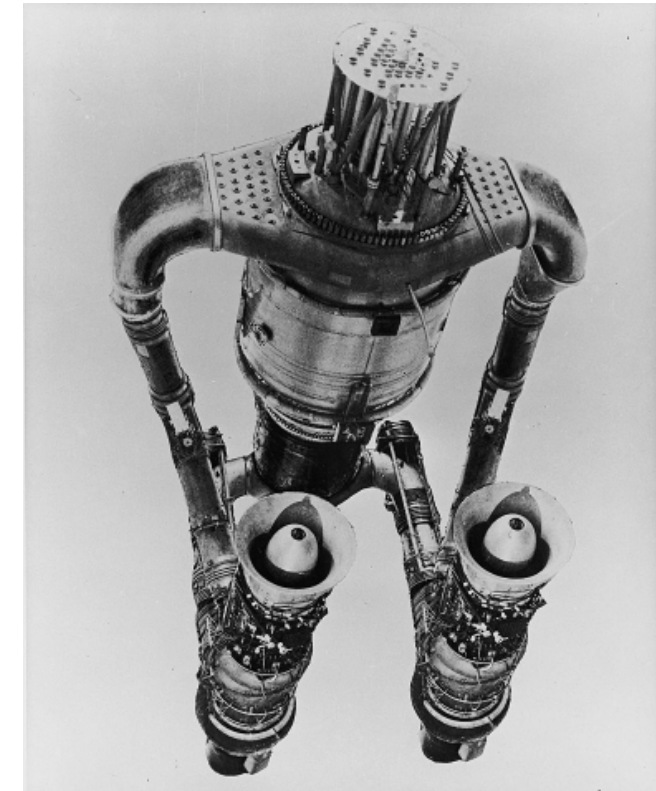
Aircraft Nuclear Propulsion Program (ANP) – 1946-1961

- 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]



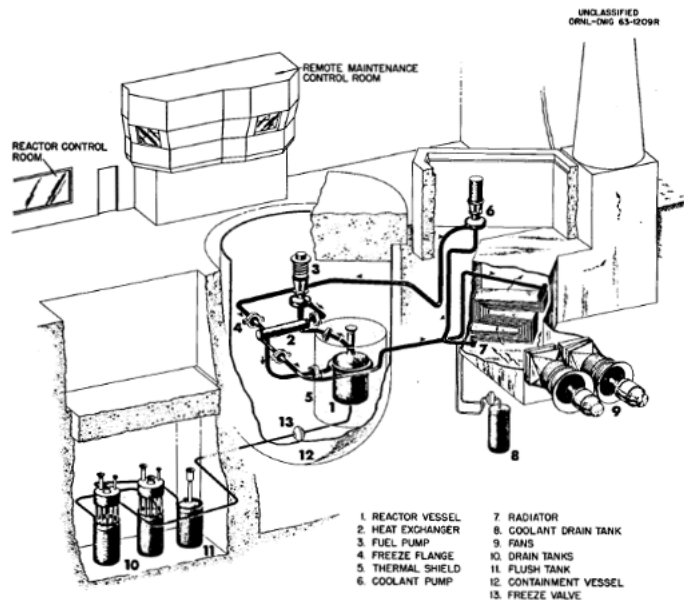
Heat Transfer Reactor Experiment #3

[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]

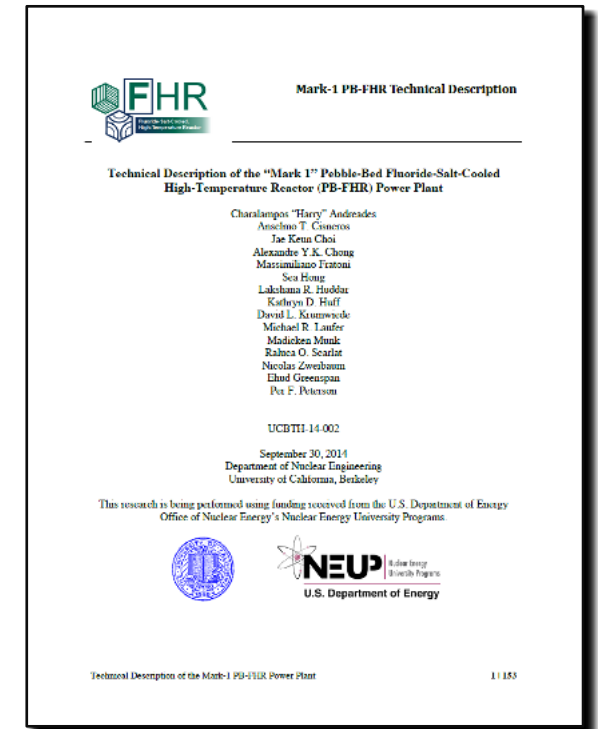


MSRE Graphite Core Structure
[https://en.wikipedia.org/wiki/Molten-Salt_Reactor_Experiment]

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)

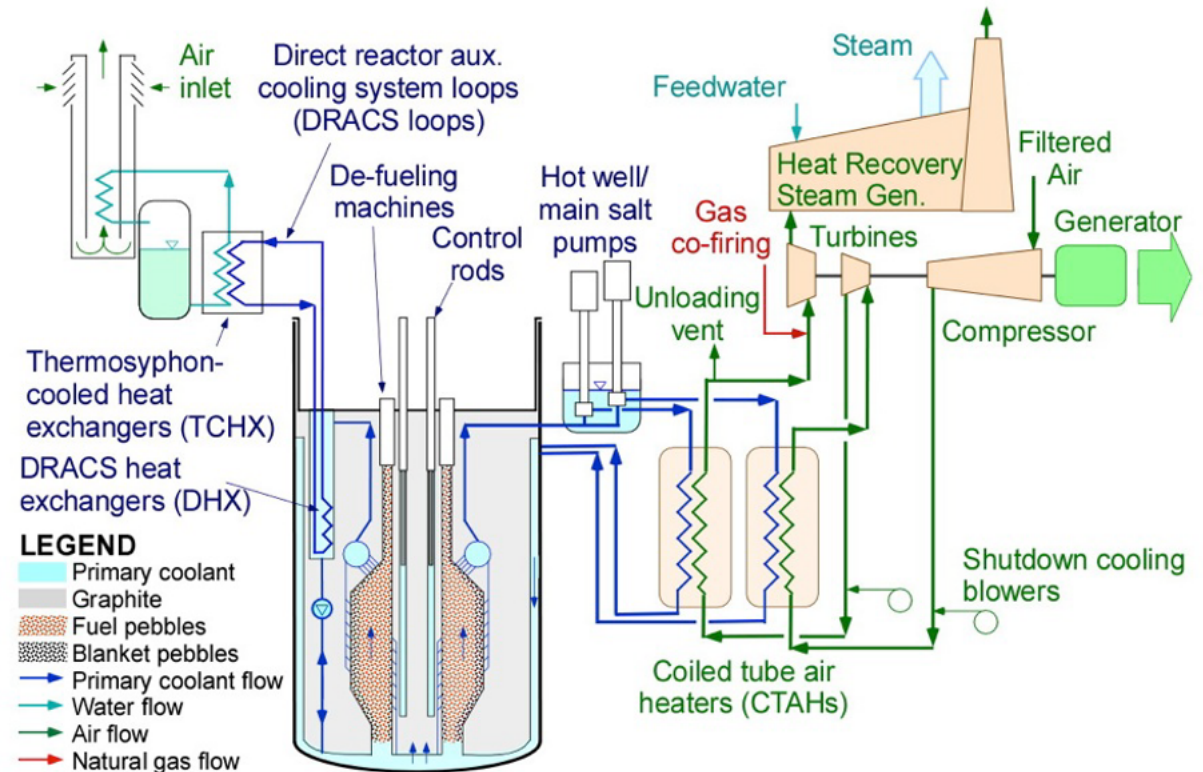
Reactor

- 236 MW_{th} / 100 MW_e
- Atmospheric pressure
- 500°C core inlet temperature
- 900°C core inlet temperature
- 976 kg/s core flowrate
- FLiBe molten salt coolant

Core

- 470,00 fueled pebbles + 218,000 unfueled pebbles in core and defueling chute
- 180 MWd/kgHM discharge burnup
- 19.9% enrichment
- Online refueling

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

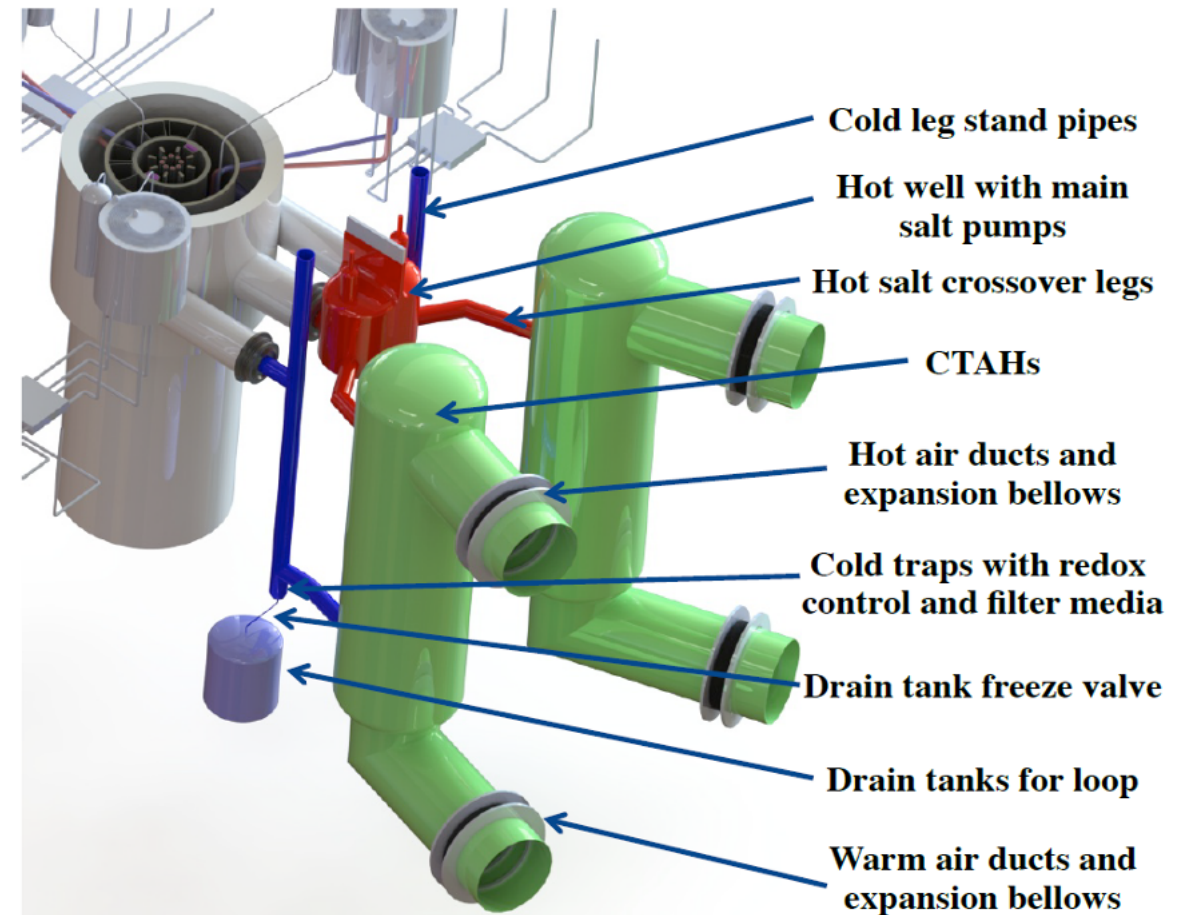


UCB Mark 1 schematic
[UCBTH-14-002]

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

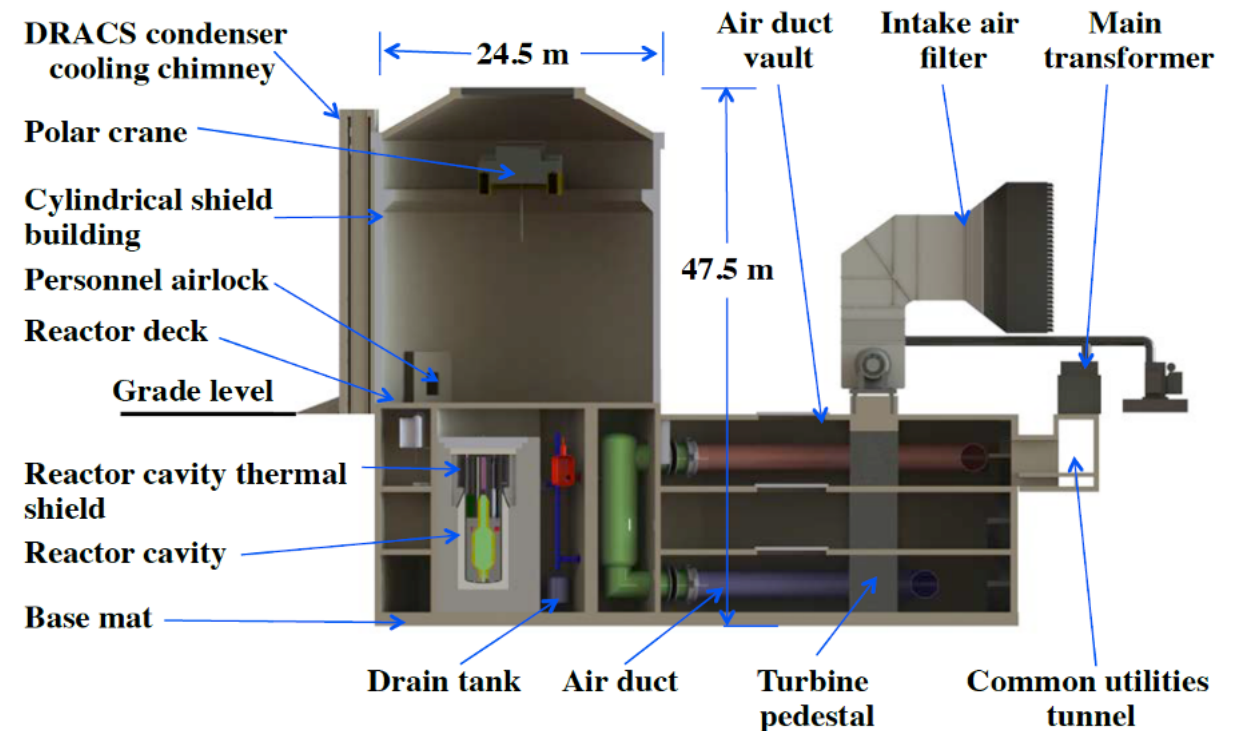


UCB Mark 1 schematic
[UCBTH-14-002]

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]

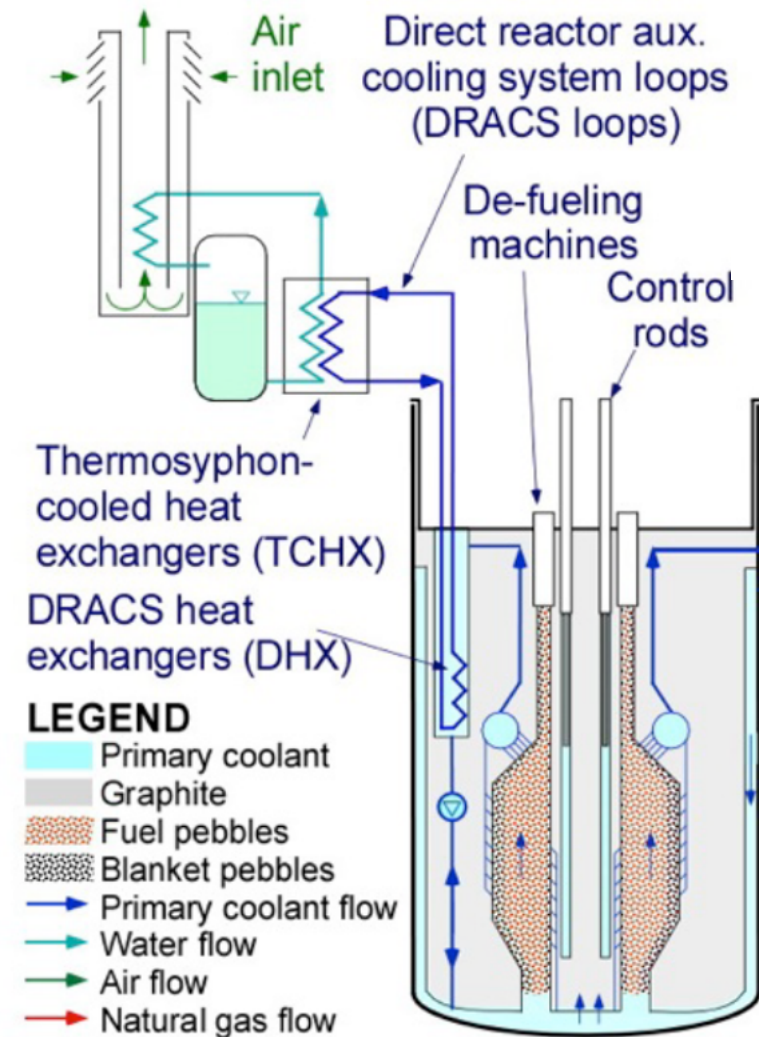
UCB Mark 1 (4/4)

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: RCS-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]

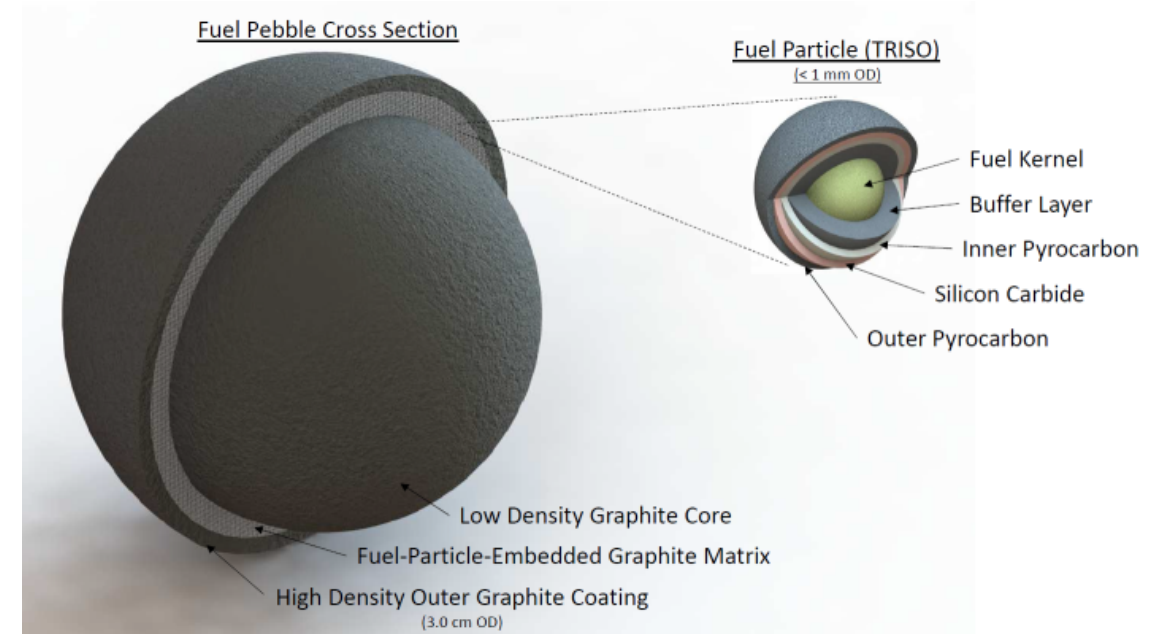
UCB Mark 1 fuel

TRISO particle

- TRISO is a portmanteau of **tr**istructural **is**otropic
- Kernel – 1.5 g of UCO, 200 μm 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



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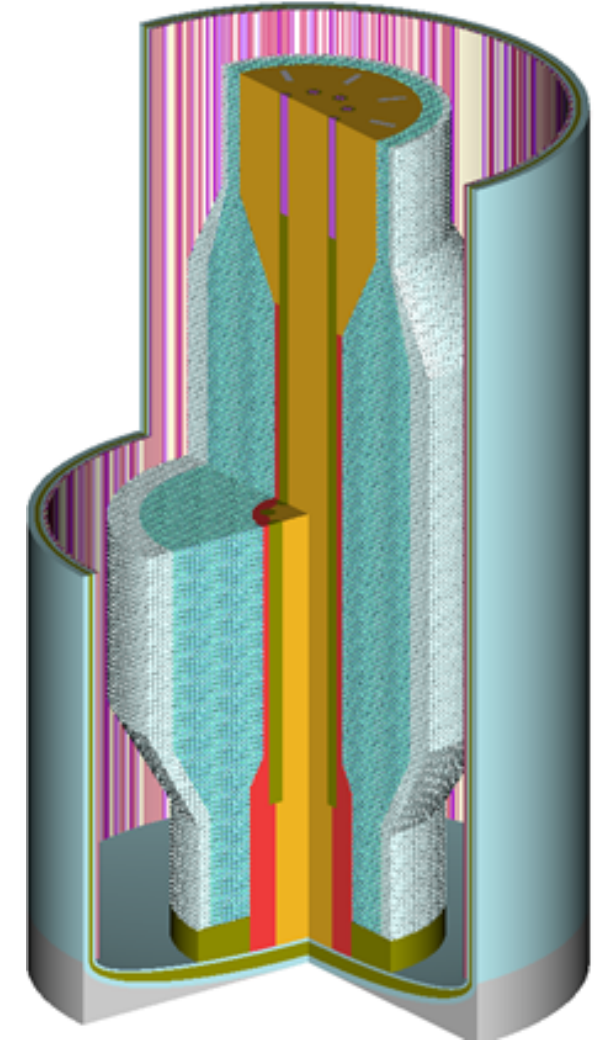
FHR analysis with SCALE: Overview

- **Key assumptions**

- License applications will specify strategy for pebble circulation and generation of equilibrium core
- Analyzing the equilibrium core is the limiting case from an inventory/decay heat standpoint

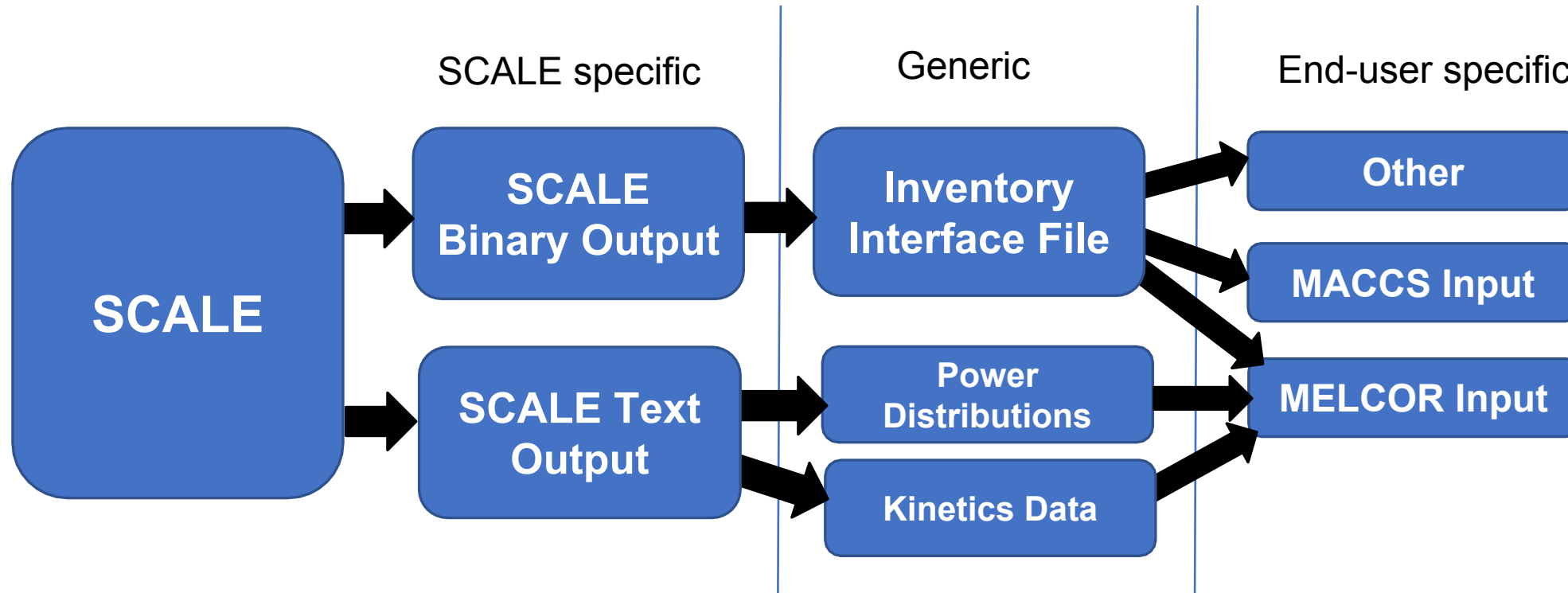
- **Main goals**

- Generate fuel composition in different zones for an equilibrium core using an approach that may differ from how applications determine their equilibrium core isotopics
- Evaluate neutronic characteristics
- **Generate core-average inventory and decay heat for MELCOR**



**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*

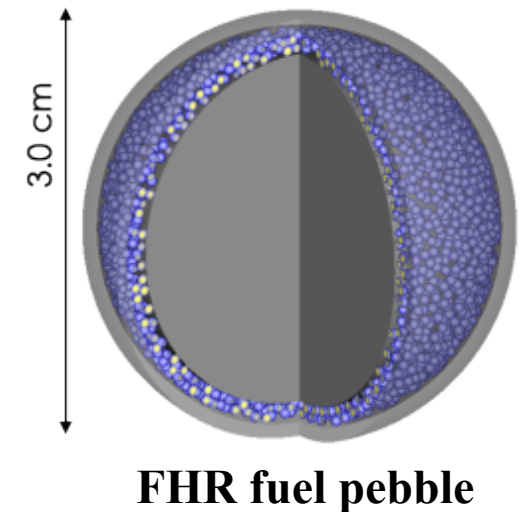
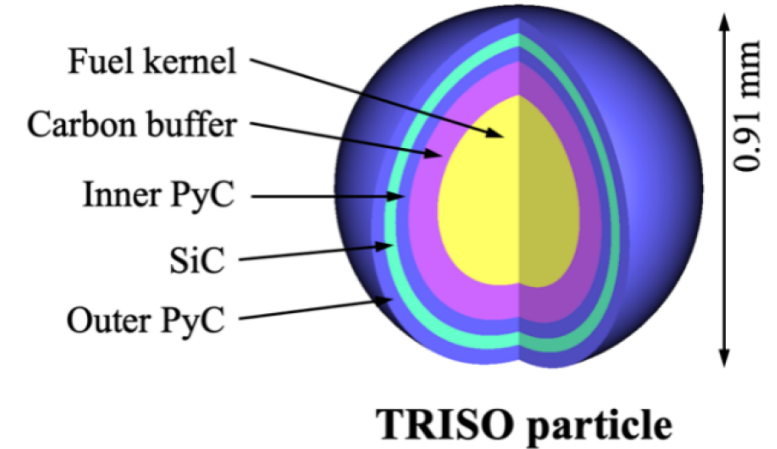
- Sequences:

- 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.

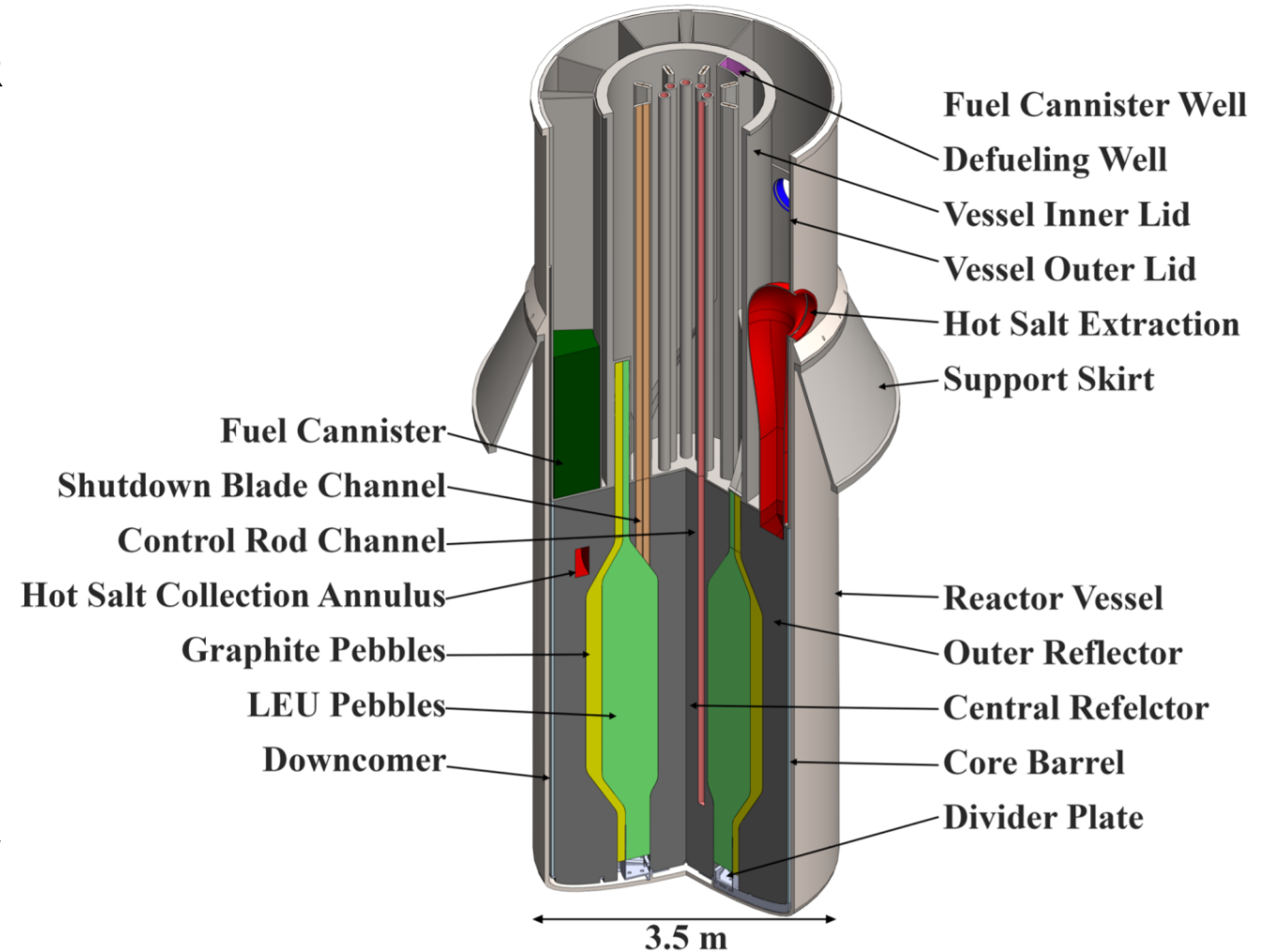
Neutronics overview

- Relevant characteristics and differences to HTGR
 - 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

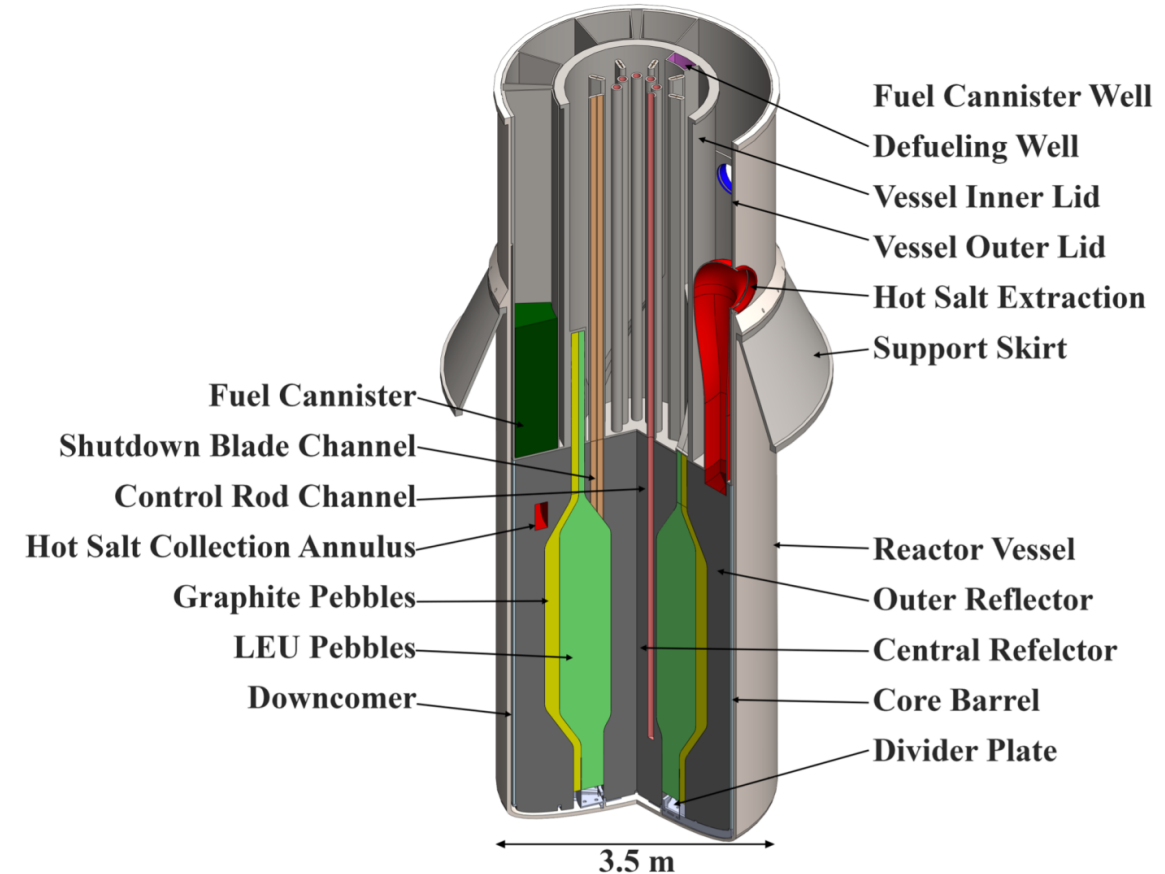
- Relevant characteristics and differences to HTGR
 - Fuel: UCO fuel in TRISO particles in fuel pebbles
 - TRISO particles located in shell instead of sphere
 - Coolant: FLiBe salt instead of helium
 - Moderator: graphite
- Challenges for modeling:
 - Tritium production in FLiBe
 - TRISO particles with 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	19.9 wt.%
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	40%
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	60%
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 ³
Average pebble thermal power	500 W
Average pebble discharge burnup	180 GWd/MTIHM
Average pebble full-power lifetime	1.40 years

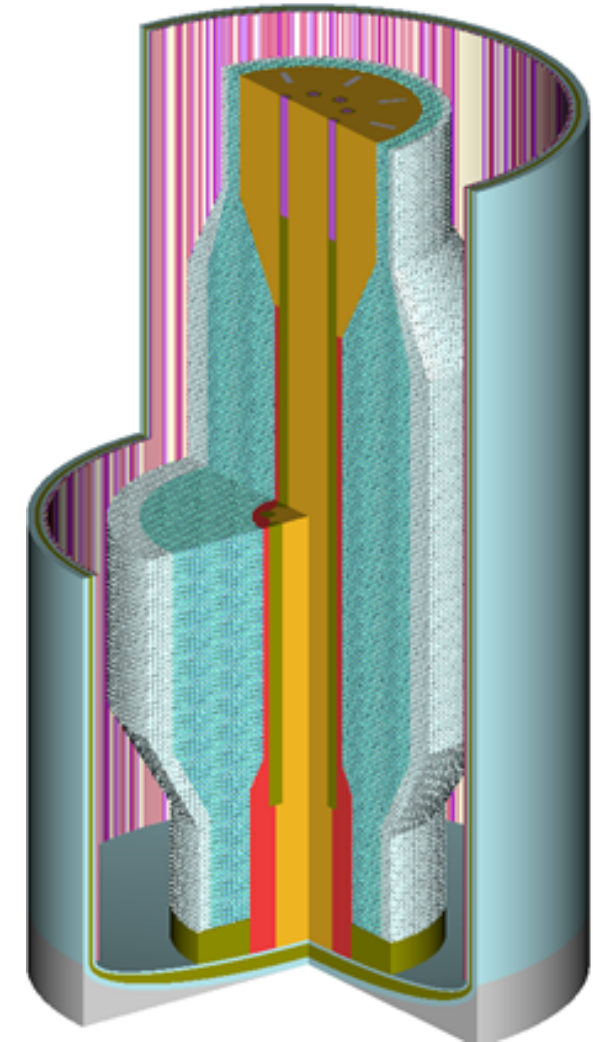


SCALE model developed based on:

- [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

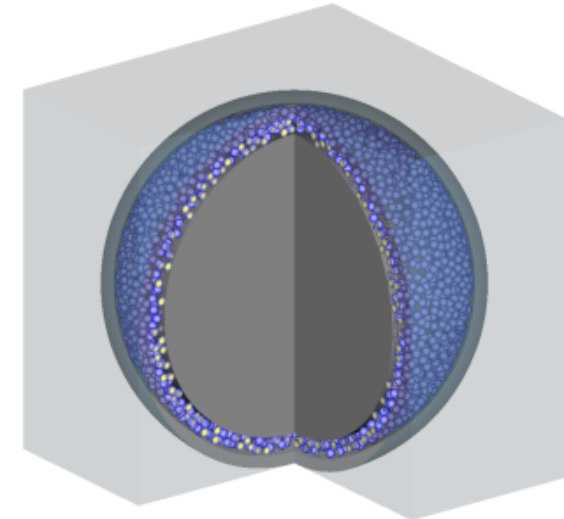
1. Verification of multigroup physics
2. Generation of equilibrium core
3. Power profile and neutron spectrum
4. Temperature feedback
5. Decay heat
6. 1-group cross sections
7. Tritium production



**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?**
 - Modeling time can be significant to realize random distributions or particle arrays without permitting particle clipping
 - Computation time can be significant for models with many cells/surfaces (consider thousands of particles)
- **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



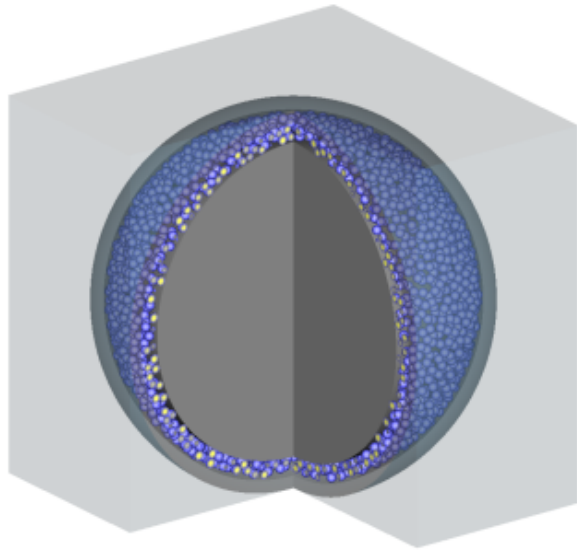
SCALE model a UCB Mark 1 pebble in a cube surrounded by FLiBe

Calculation:

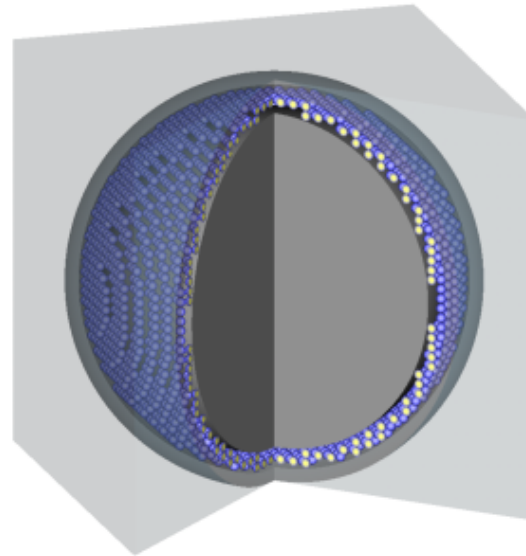
- TRITON/KENO-VI CE and MG
- Depletion calculation to reach discharge burnup of 180 GWd/tHM
- Comparison between calculations: k-eff, nuclide densities, runtime

CE, random	~79 minutes	
CE, lattice	15.28 minutes	×4.7
MG	3.25 minutes	×24

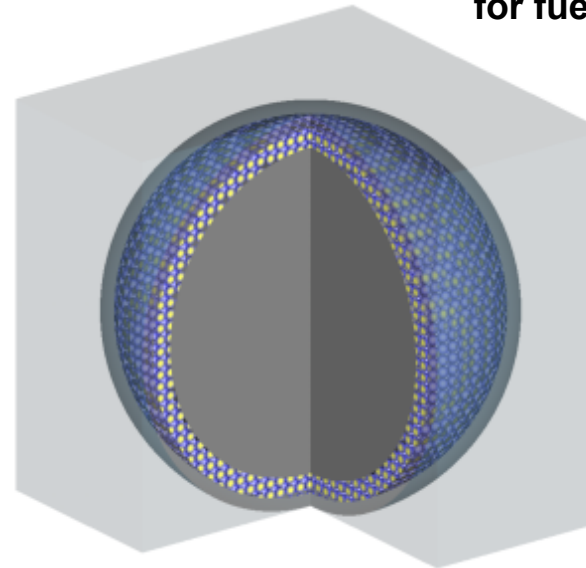
1. Single pebble models



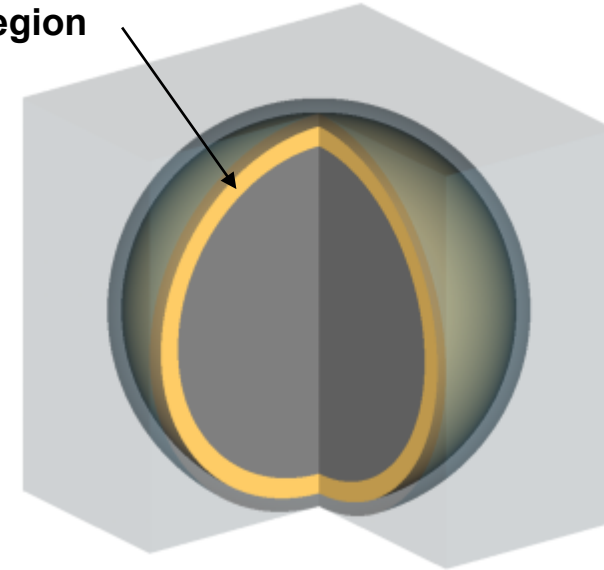
1. CE model: Random particle distribution



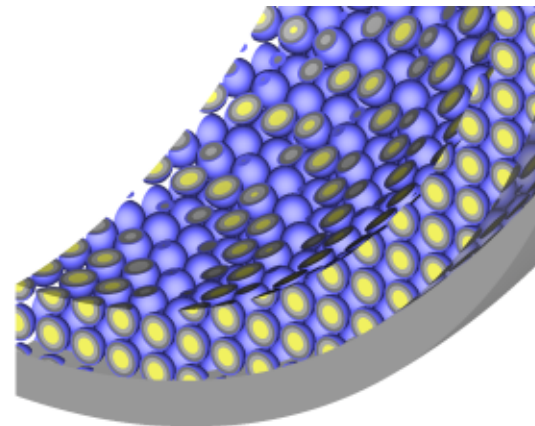
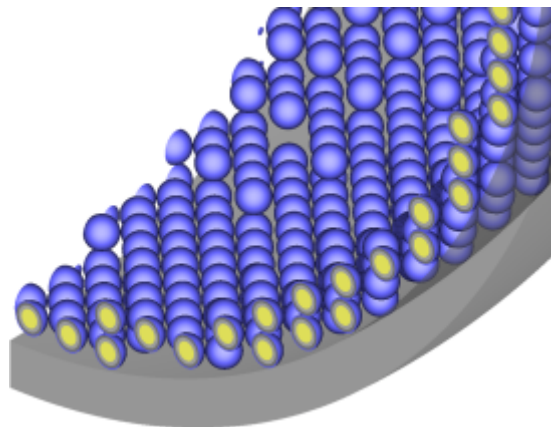
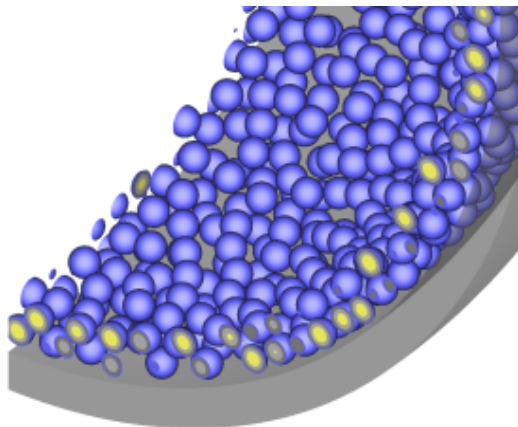
2. CE model: particle lattice (no clipping)



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

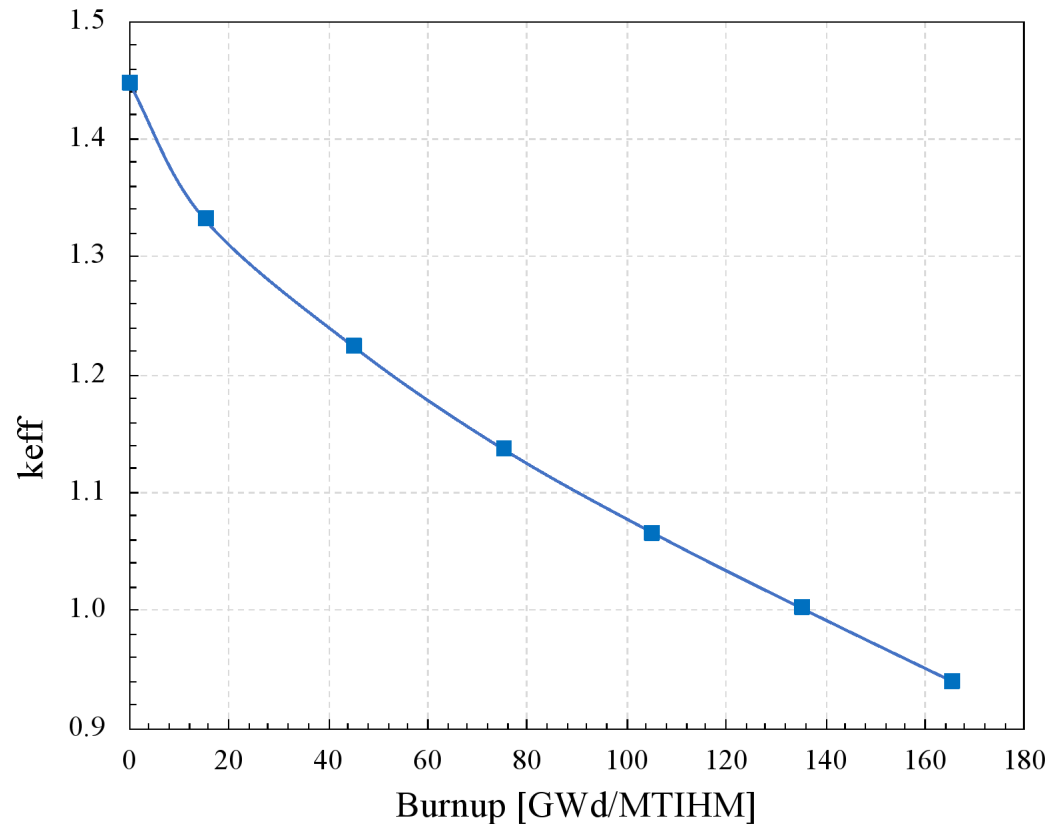
1. Single pebble initial criticality

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

- **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**

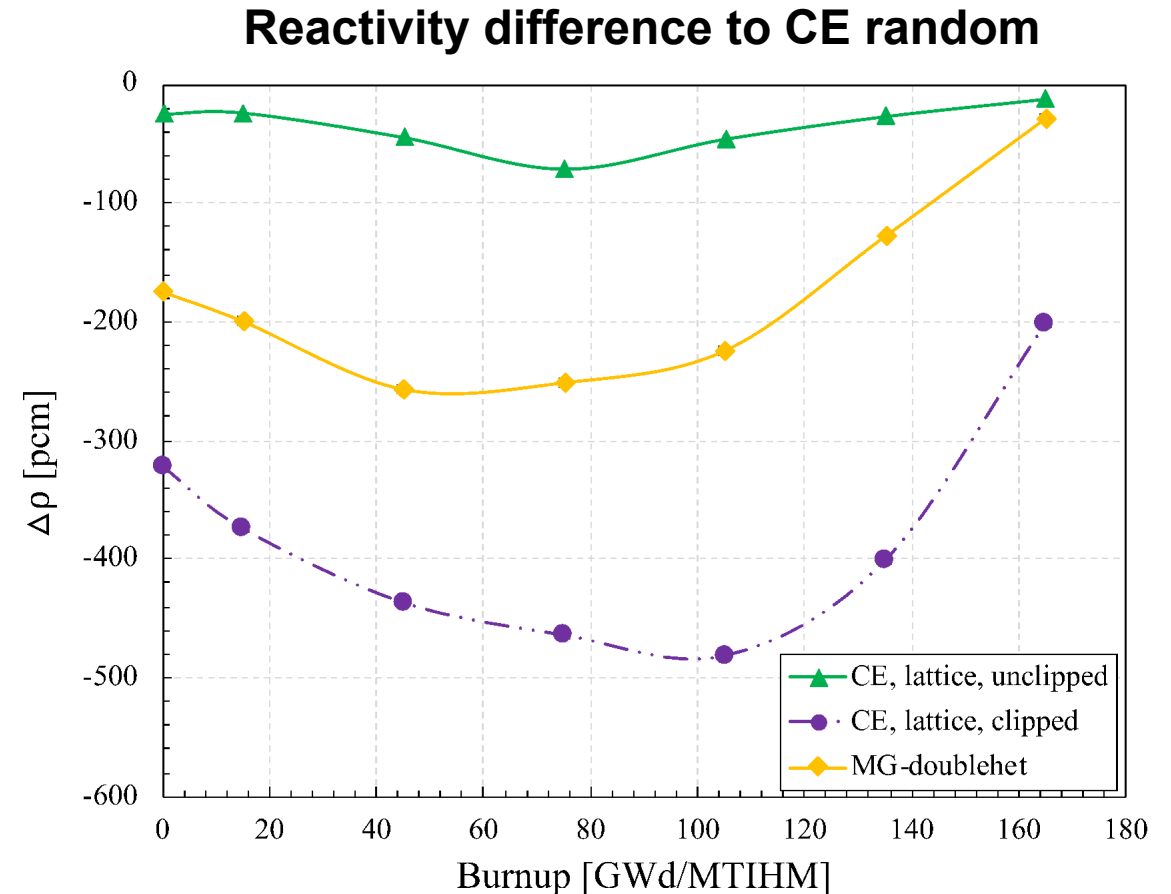
Result: MG k_{eff} calculations show good agreement with reference CE result independent of the temperature

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



Calculation details:

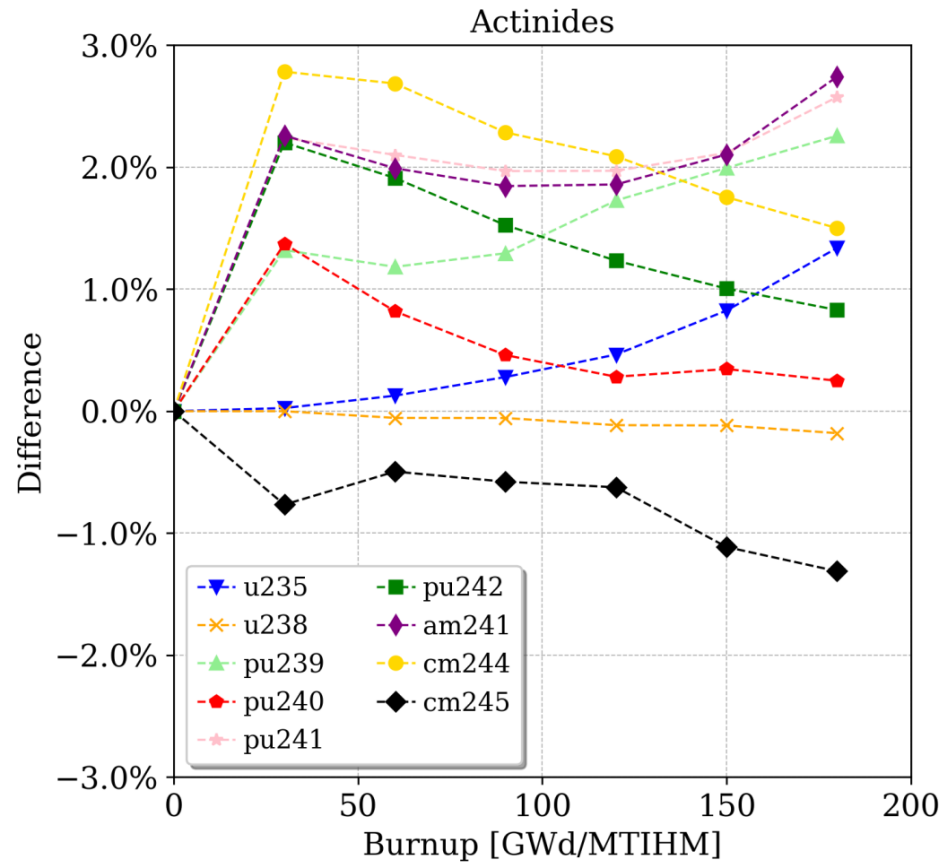
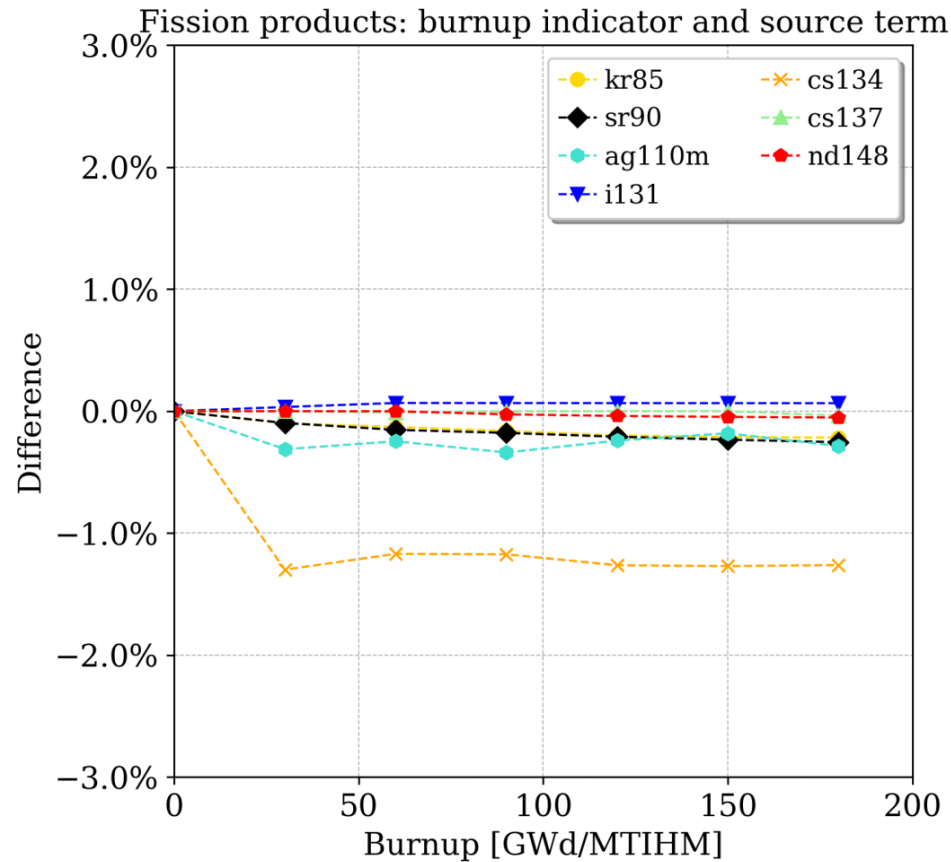
- TRITON-KENO depletion of the **HFP case**
- 540.54 days at 333 MW/MTIHM



Result: MG bias remains below 260 pcm over depletion

1. Single pebble nuclide density comparison over depletion

Comparison of MG against CE random:

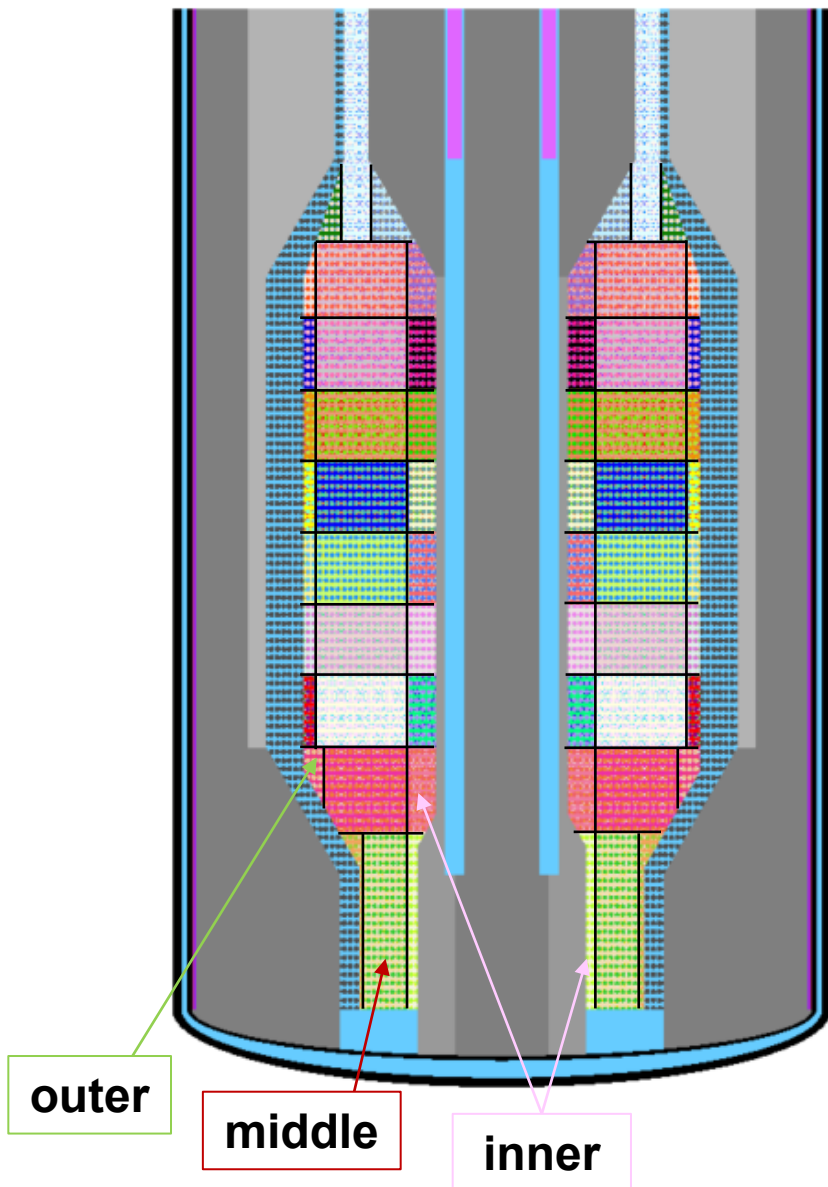


Result: MG bias remains below 3% for relevant nuclide densities over depletion

1. MG performance summary for UCB Mark 1

- Excellent performance of SCALE's MG capability for double-heterogeneous systems has previously been demonstrated for spheres
- We confirmed the performance in terms of k_{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 equilibrium full core



Goal: Determine fuel composition of pebbles in a full core corresponding to an equilibrium state

Boundary conditions:

- Pebble final discharge burnup: 180 GWd/tHM
- Average number of passes per pebble: 8
- Average power: 333 MW/tHM

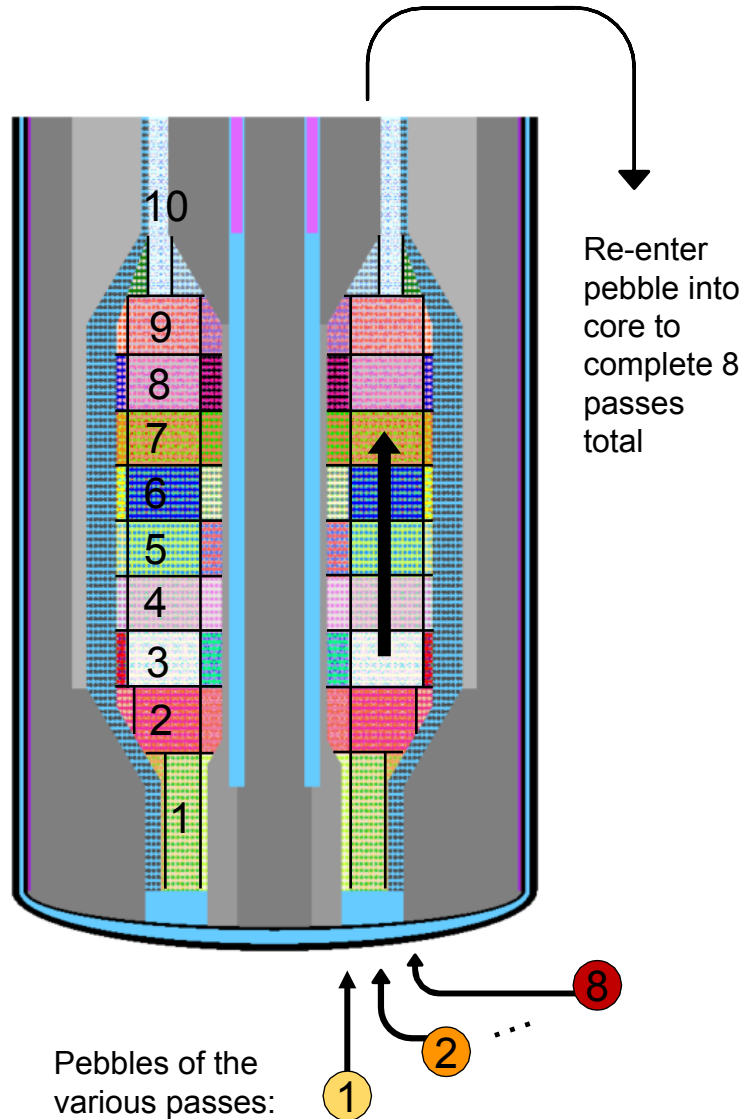
Full core model discretization:

- 10 axial zones of equal volume
- 3 radial zones with $1/8^{\text{th}}$, $6/8^{\text{th}}$, $1/8^{\text{th}}$ fractional volumes

Assumptions:

- All pebbles within a zone contain the same fuel composition
- Fuel composition within a zone represents average of individual pebbles of different passes/burnups in this zone

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 spectral effects in equilibrium environment

2.

Depletion of every pebble according to its detailed **power** and spectral history (pass and zone in 3D core)

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

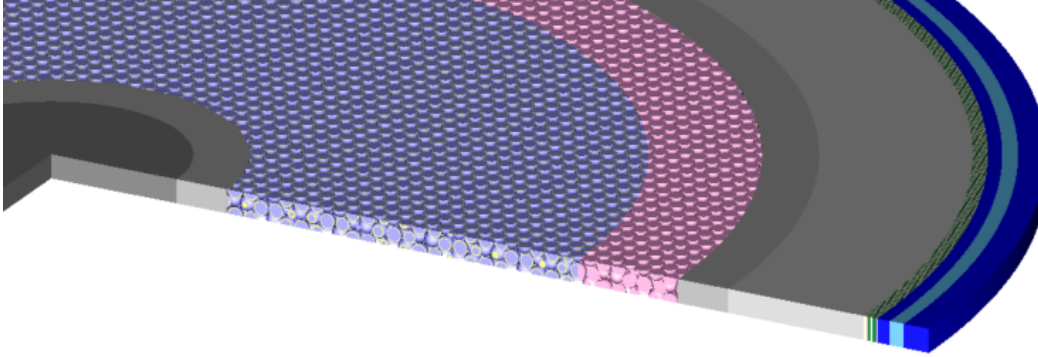
3.

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

4.

Check convergence for k_{eff} and core-average fuel composition: stop or return to step 1 with new core-average fuel composition

2. Slice depletion model



Why a slice and not a single pebble:

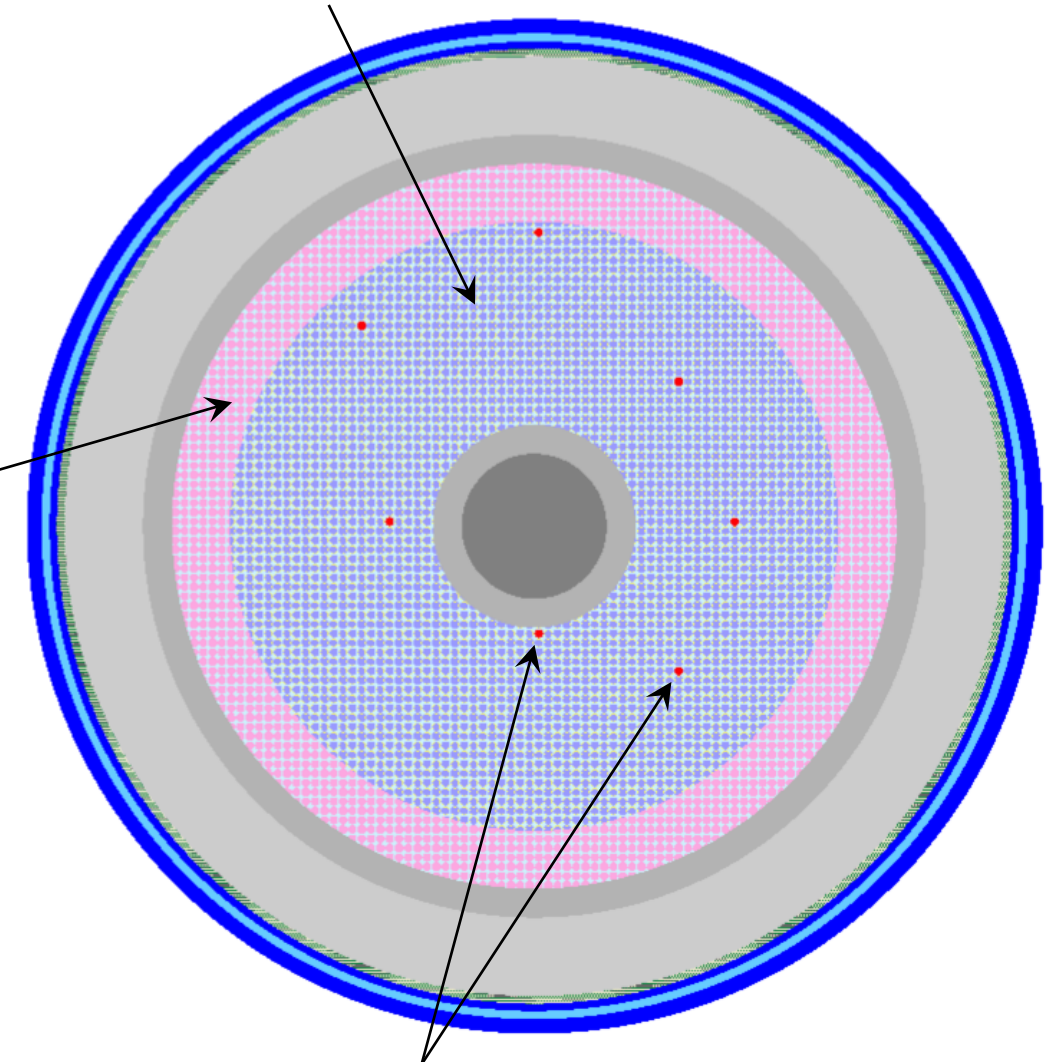
- Representative moderator/fuel ratio
- Representative neighboring conditions (spectral effects)

Depletion model:

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

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

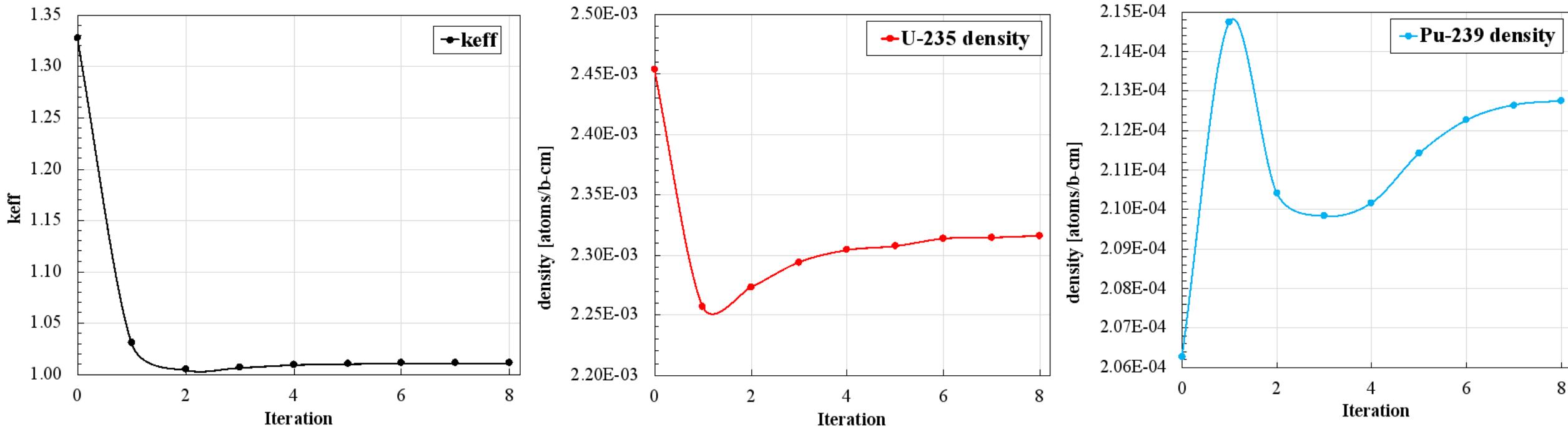
Graphite pebbles



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

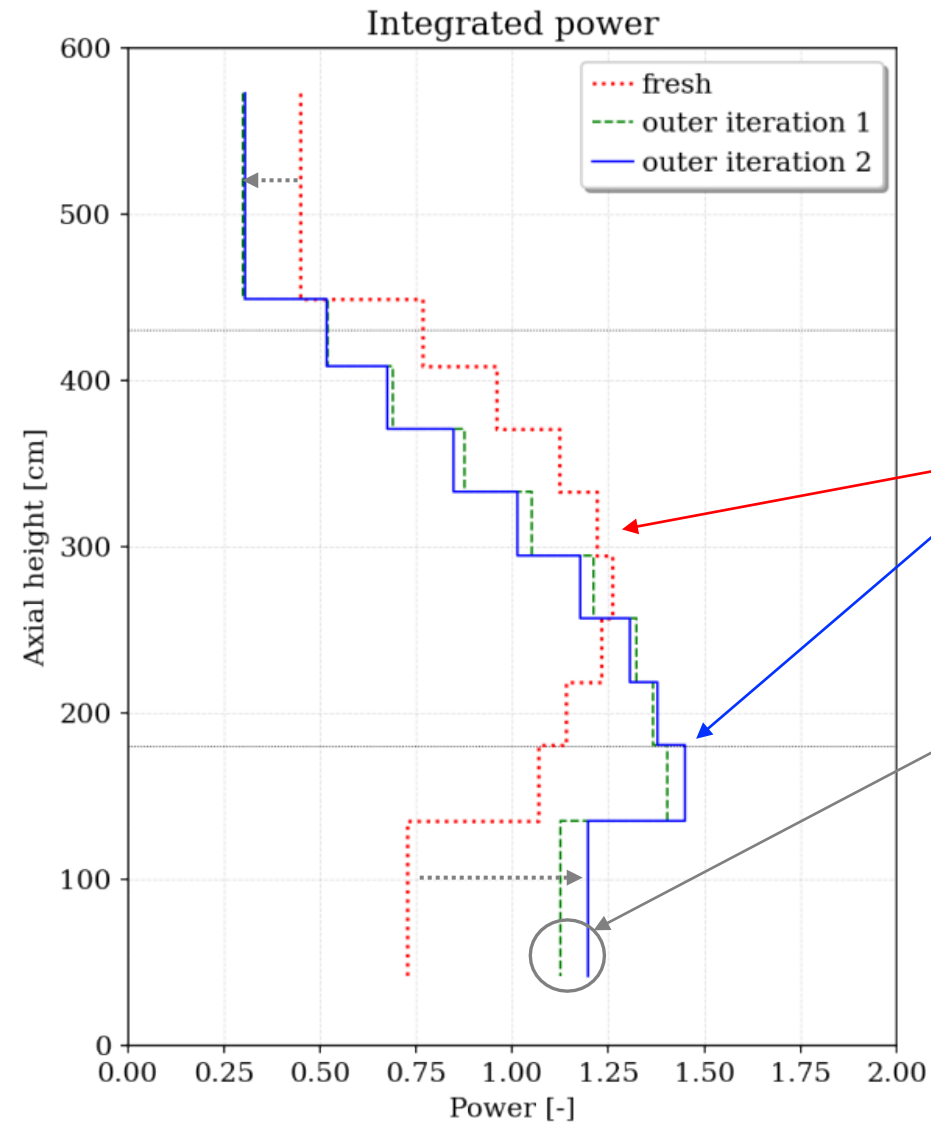
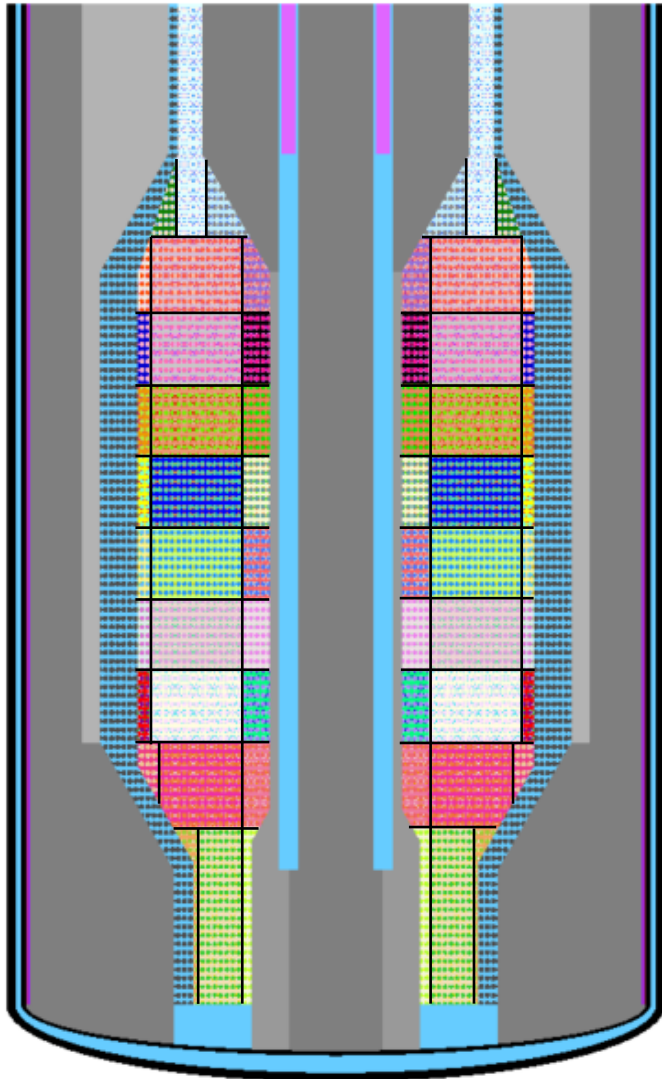
2. K_{eff} and nuclide density convergence

Outer iteration 1 using constant core power



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

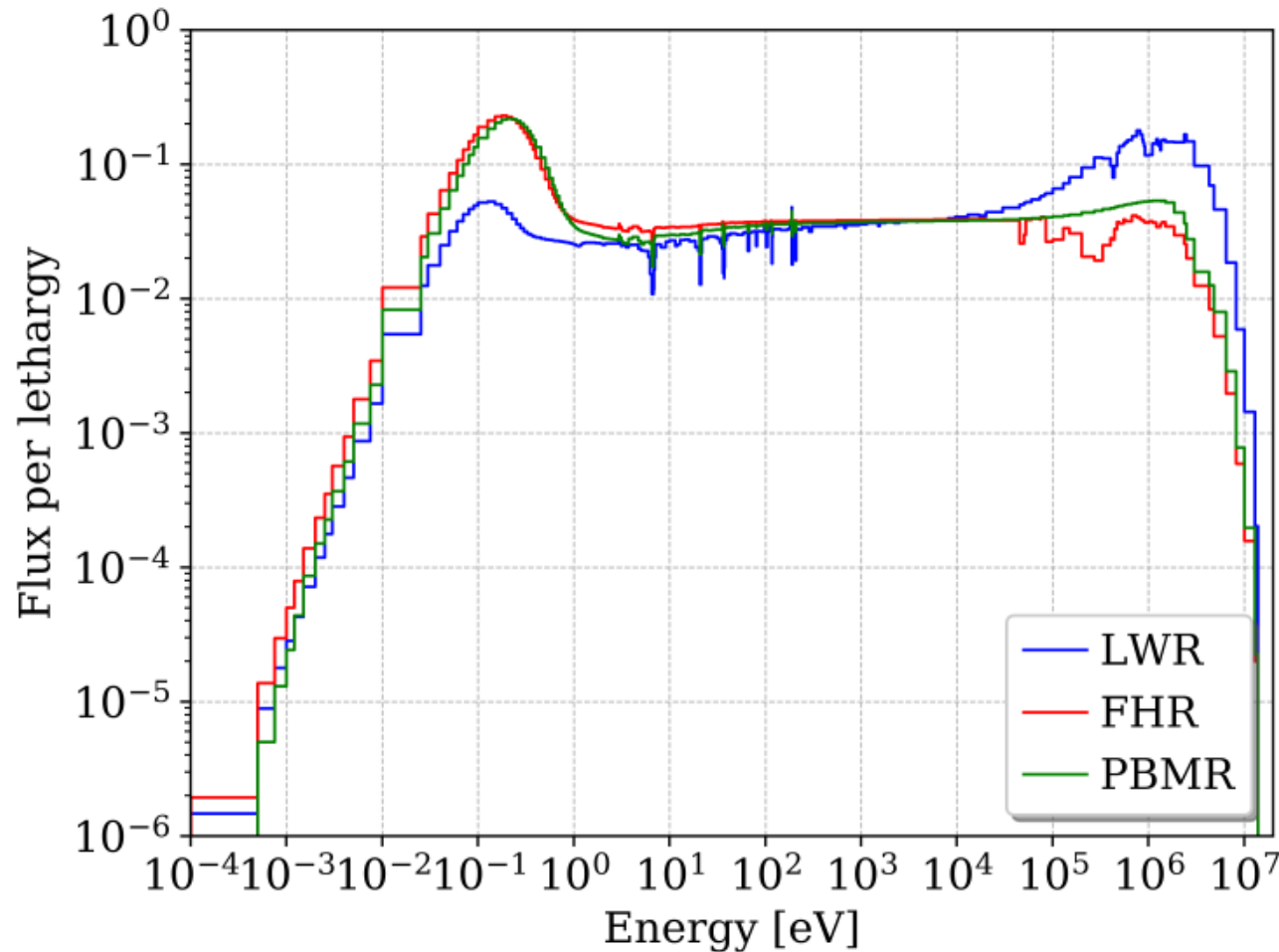
3. Full core power profile



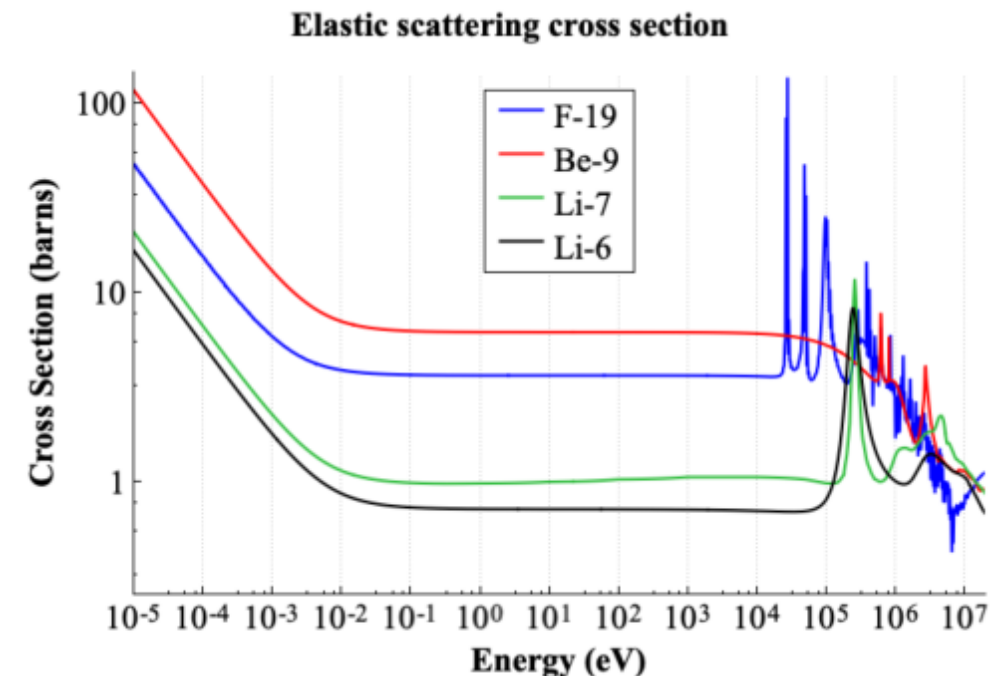
Results:

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

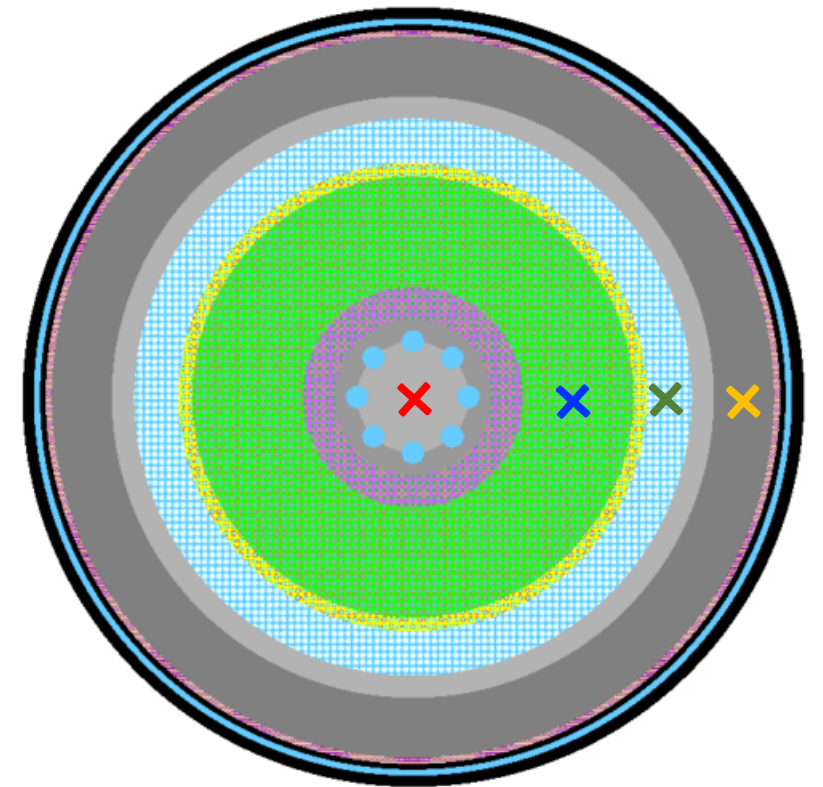
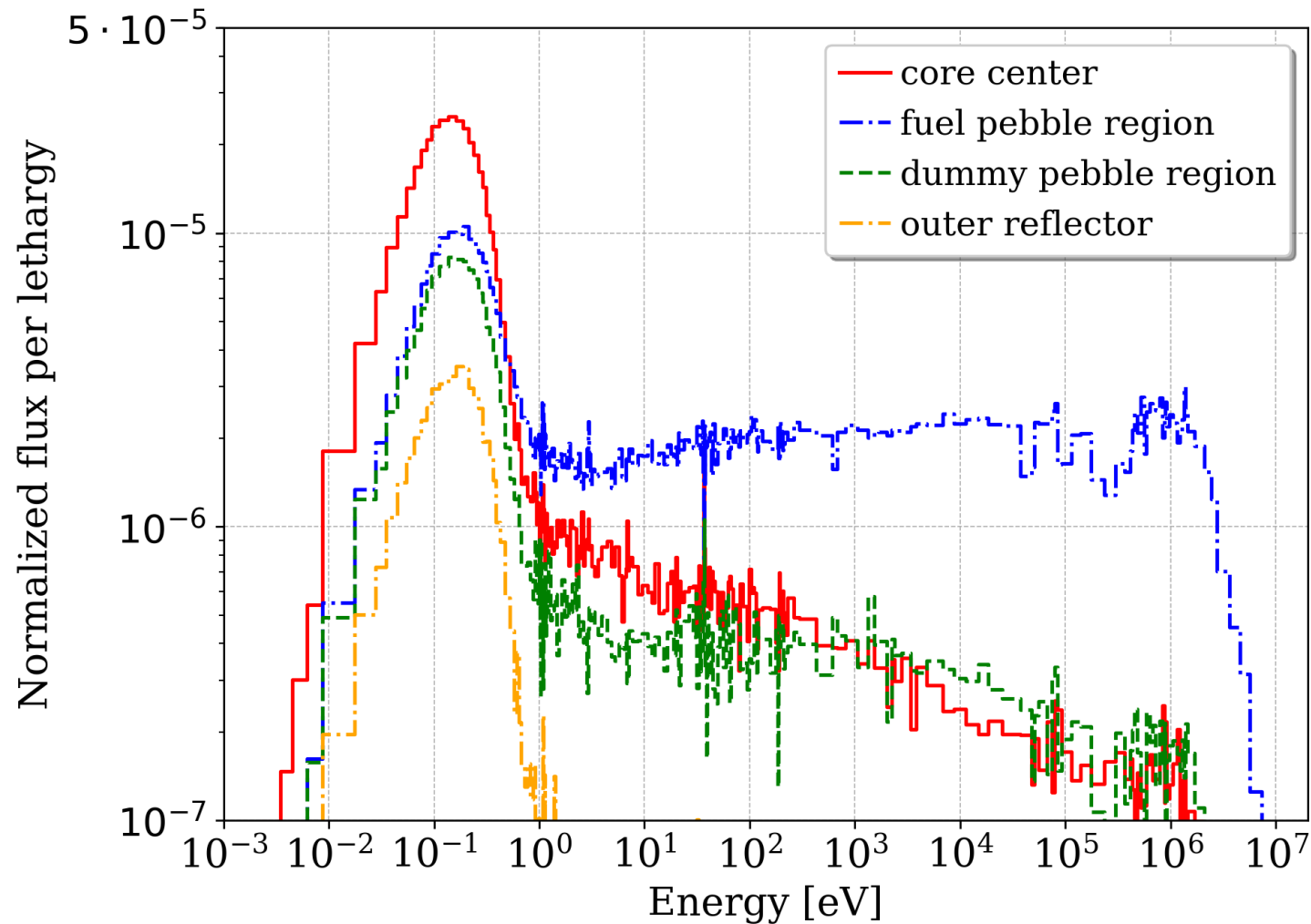
3. Example fuel cell flux spectrum comparison



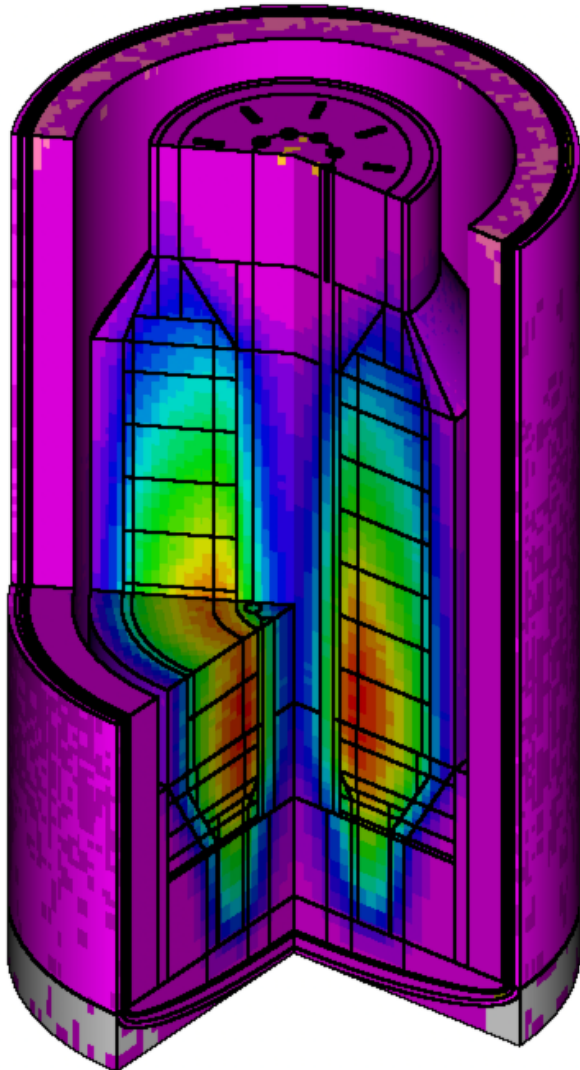
- UCB Mark 1 and PBMR show a larger thermal peak compared to LWR
- UCB Mark 1 shows smaller fast flux due to scattering with the salt



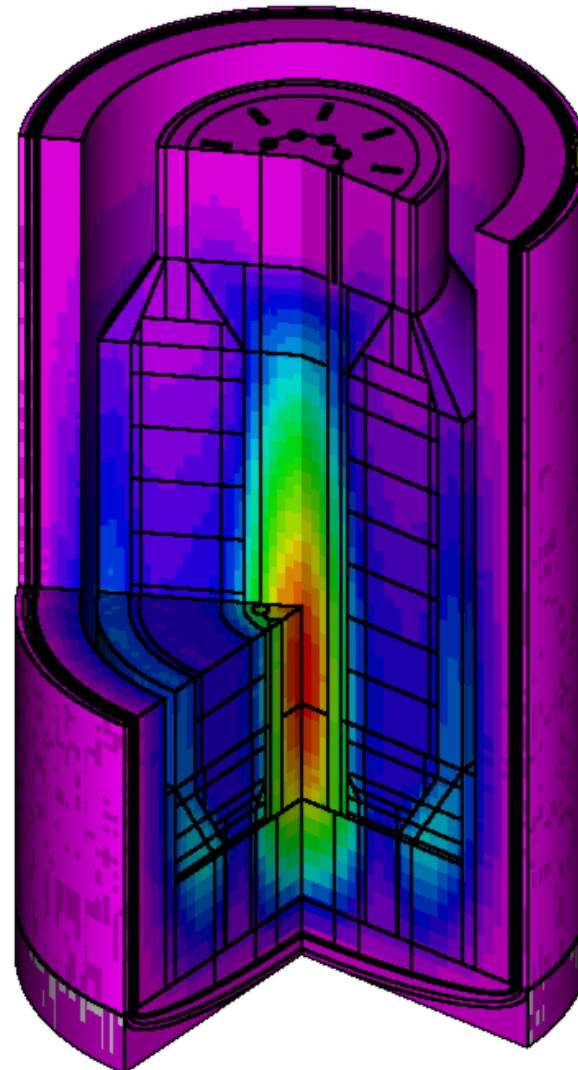
3. Energy-dependent flux profile



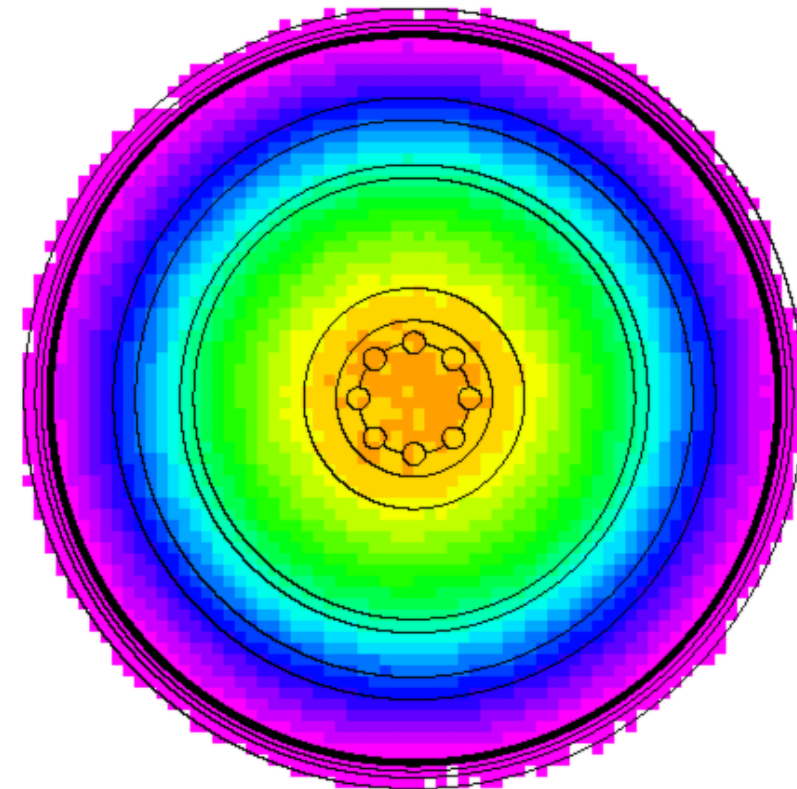
3. 3D full core flux visualizations



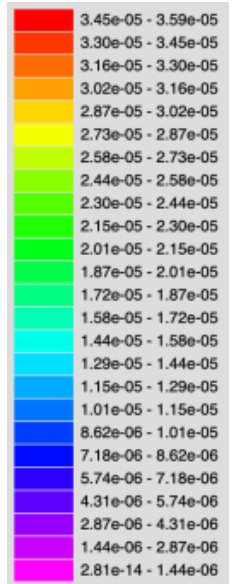
Fast flux, $E > 0.625$ eV



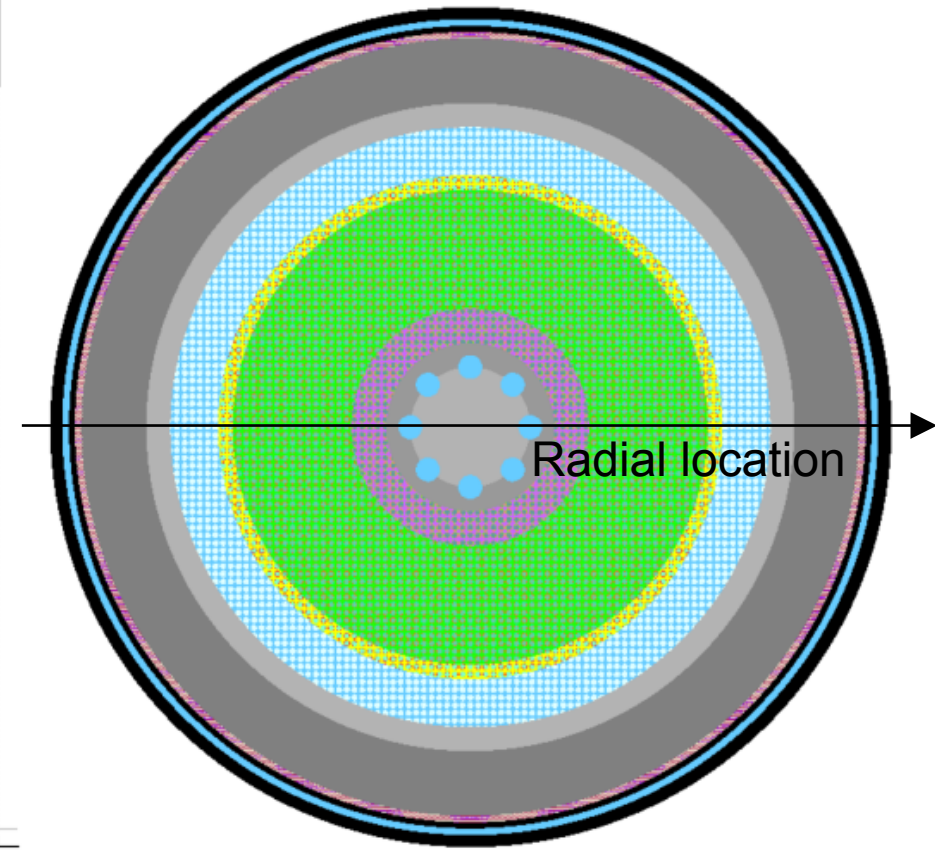
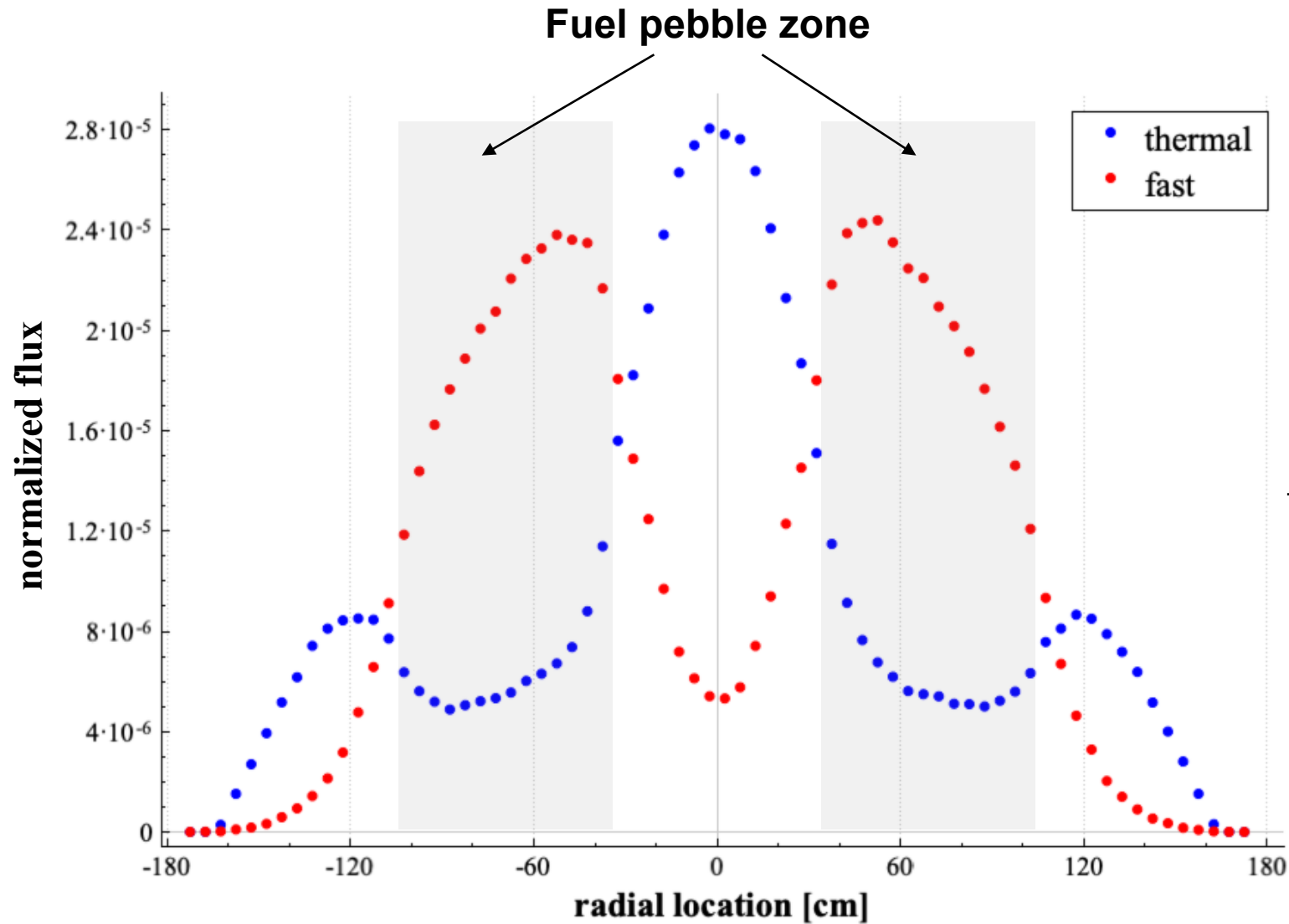
Thermal flux, $E < 0.625$ eV



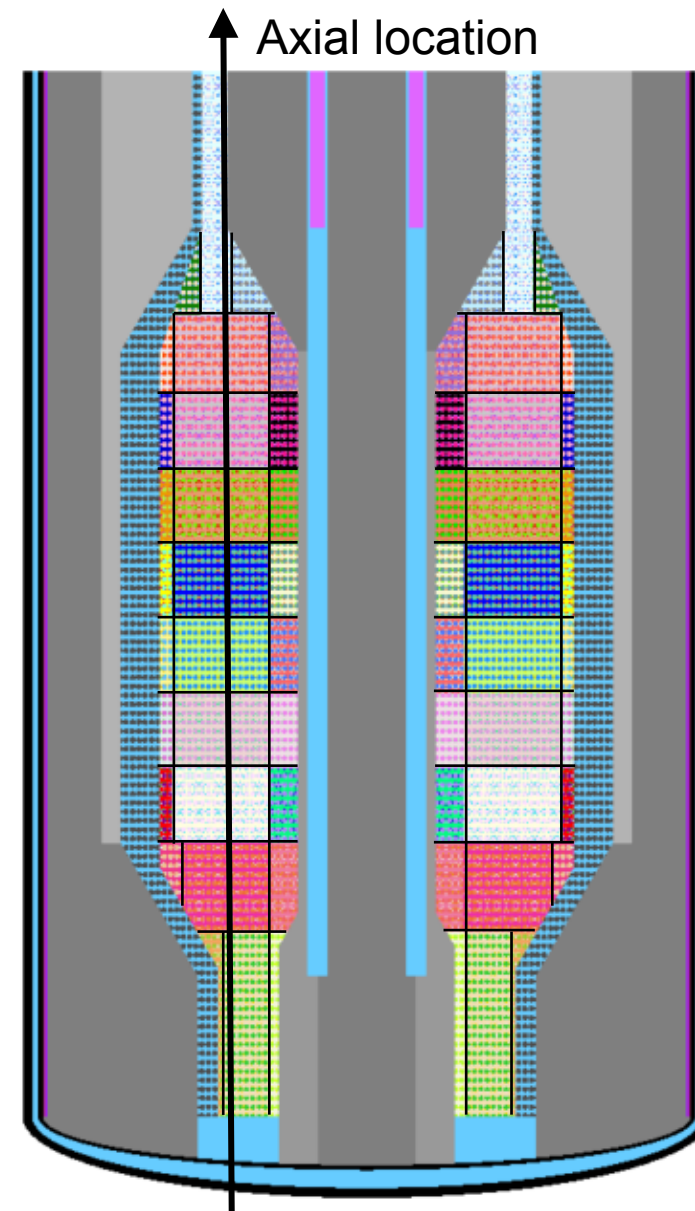
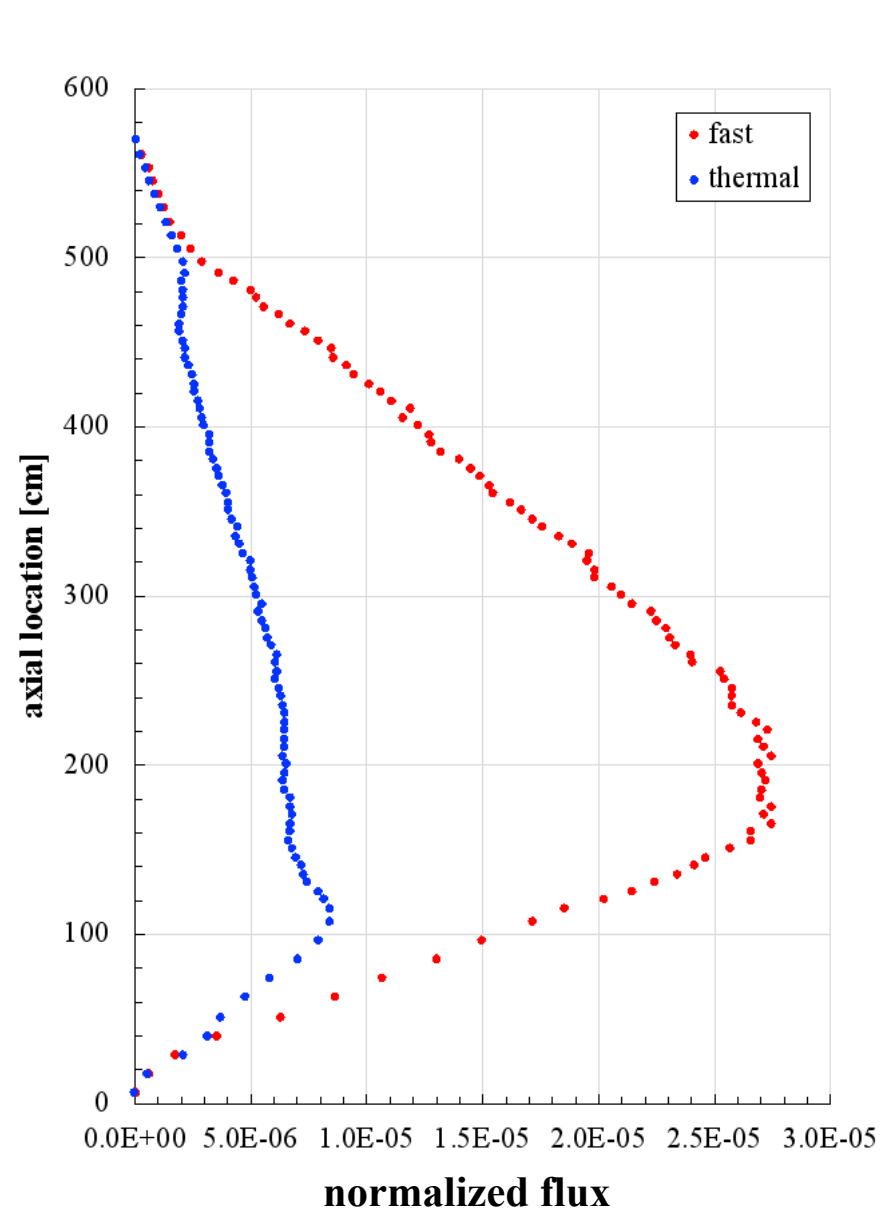
Total flux at the axial center of the core



3. Radial flux distribution at axial core center



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 ρ to determine coefficient
- β_{eff} and coolant void coefficient

Nominal temperatures:

- Fuel: 1003 K
- Salt coolant: 923.15 K
- Graphite moderator: 973.15/983.15 K
- Inner graphite reflector: 873.15 K
- Outer graphite reflector: 973.15 K

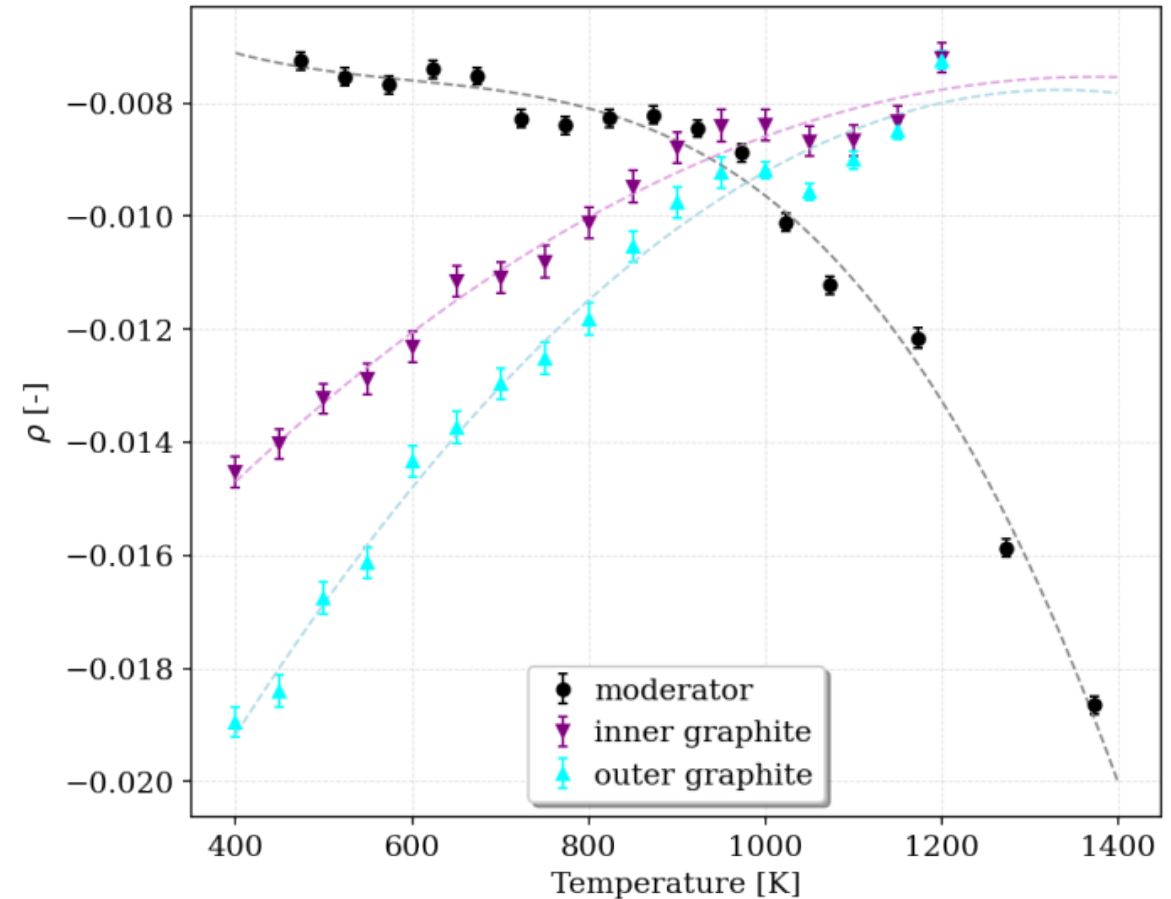
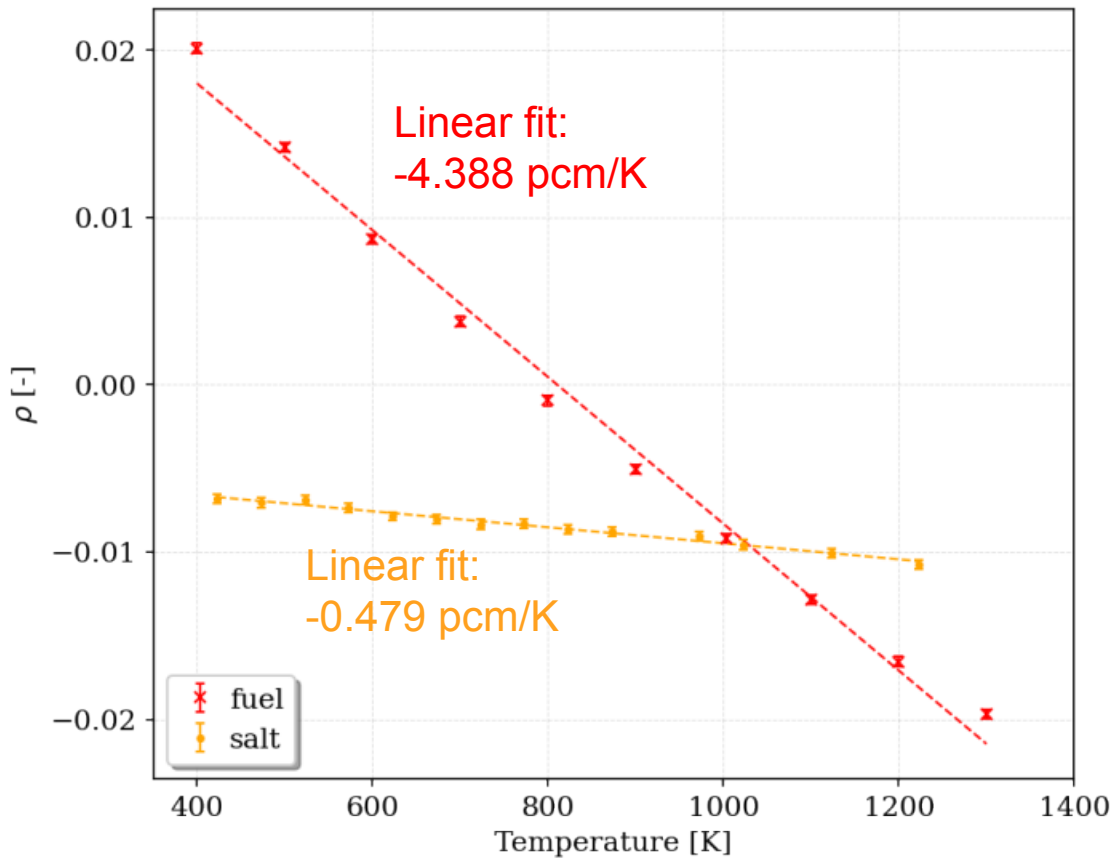
Quantity	Value [pcm]
β_{eff}	541 ± 20
Coolant void	-5094 ± 21

Component	Temperature Reactivity Coefficient at nominal temperature [pcm/K]
Fuel	-4.388
Salt coolant	-0.479
Graphite moderator	-1.095
Inner graphite reflector	1.205
Outer graphite reflector	0.605

Linear fit

Slope from polynomial fit

4. Isothermal temperature coefficients



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

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

	a	b	c	d
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

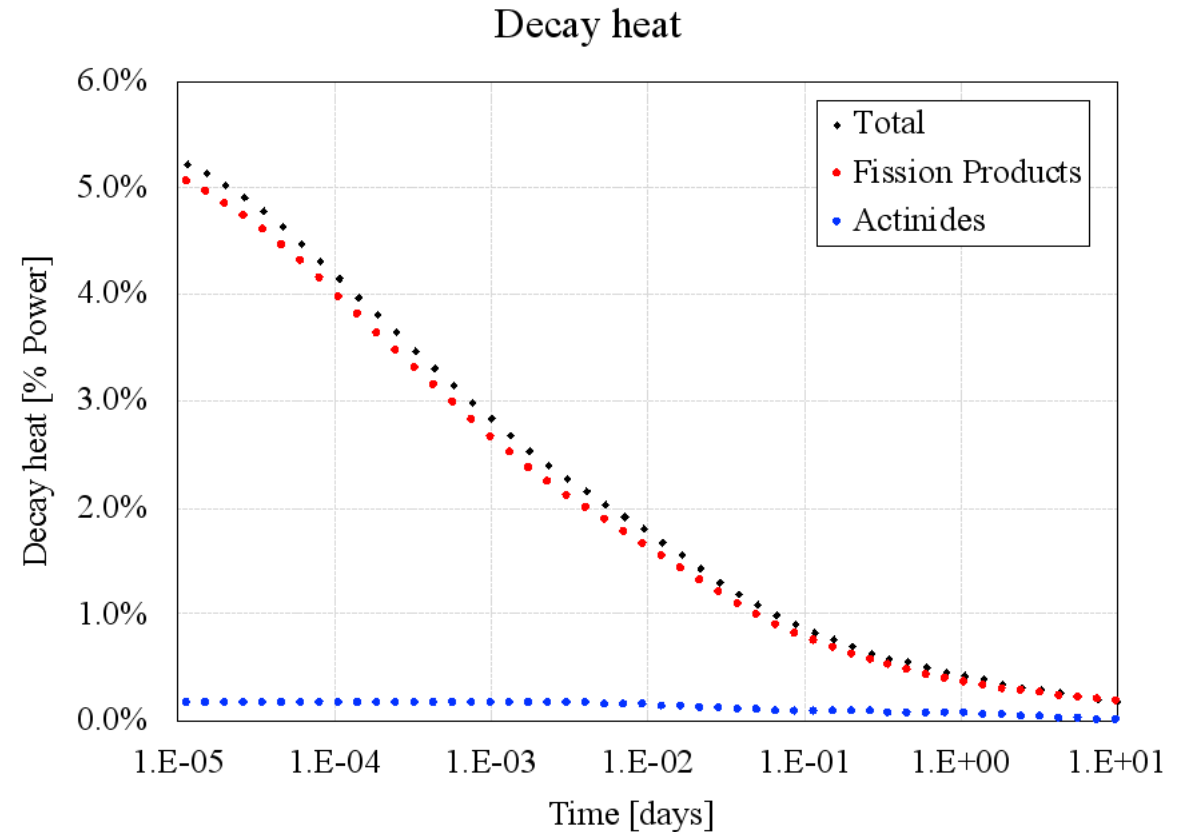
Fuel composition files for the 8 passes for all 30 zones of the core from generation of equilibrium core

Average compositions together according to zone volumes in the core to obtain **core-average fuel composition**

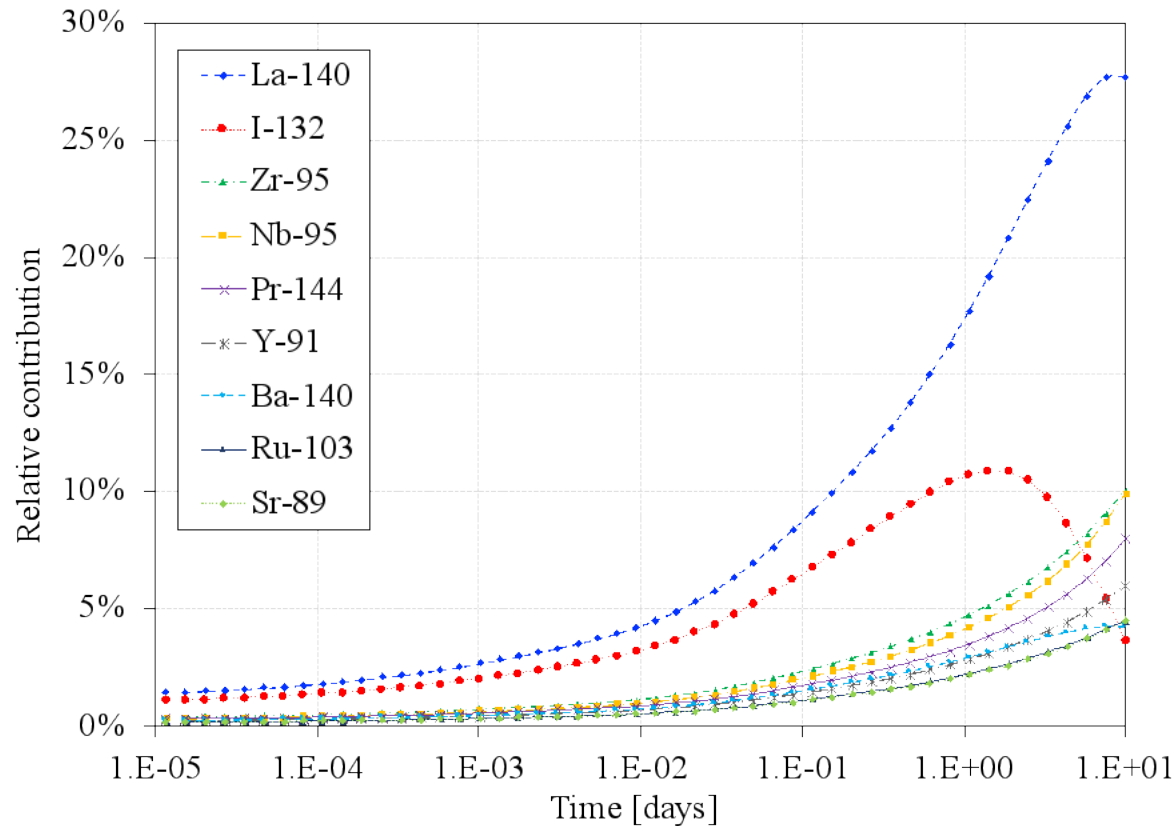
10-day decay calculation with ORIGEN, generating new composition file

Generation of core-average **inventory JSON file** using ORIGEN composition file

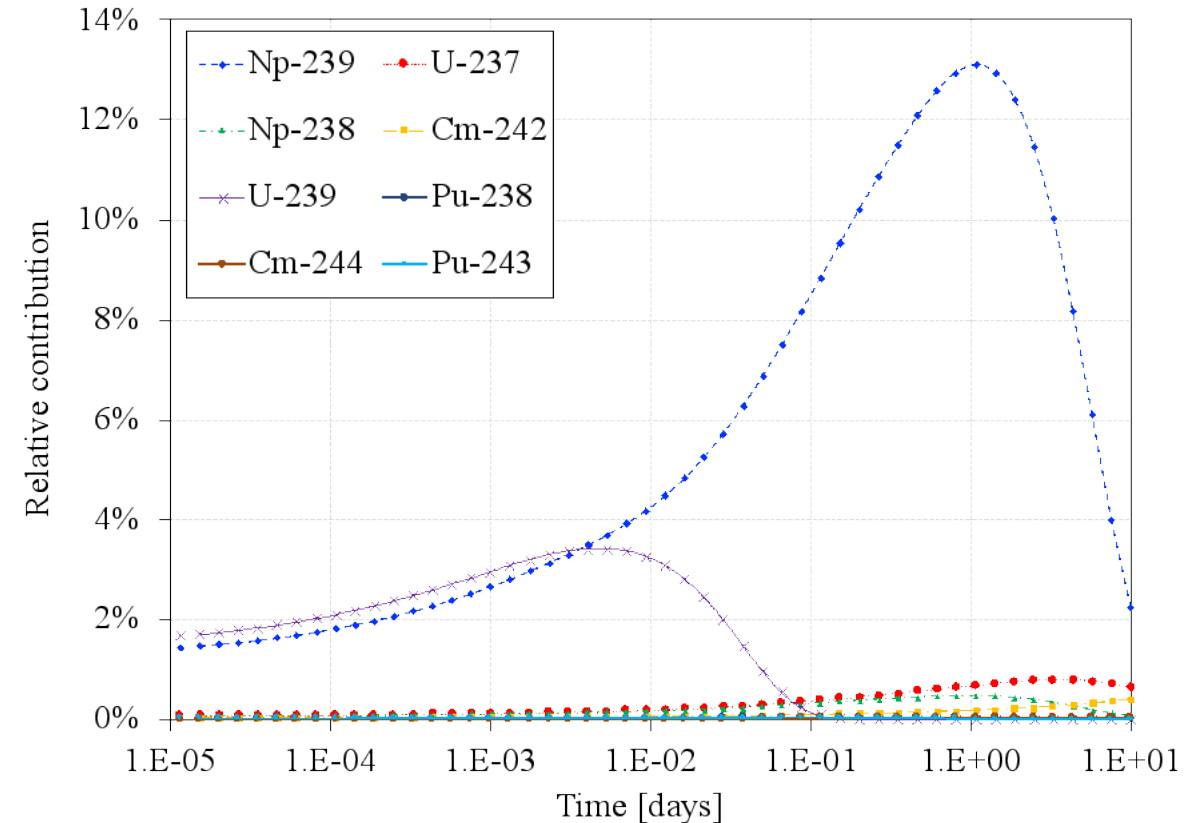
Conversion of JSON file to **MELCOR DCH file** while scaling to actual initial heavy metal mass in the core (0.705 tHM)



5. Generation of decay heat file for MELCOR

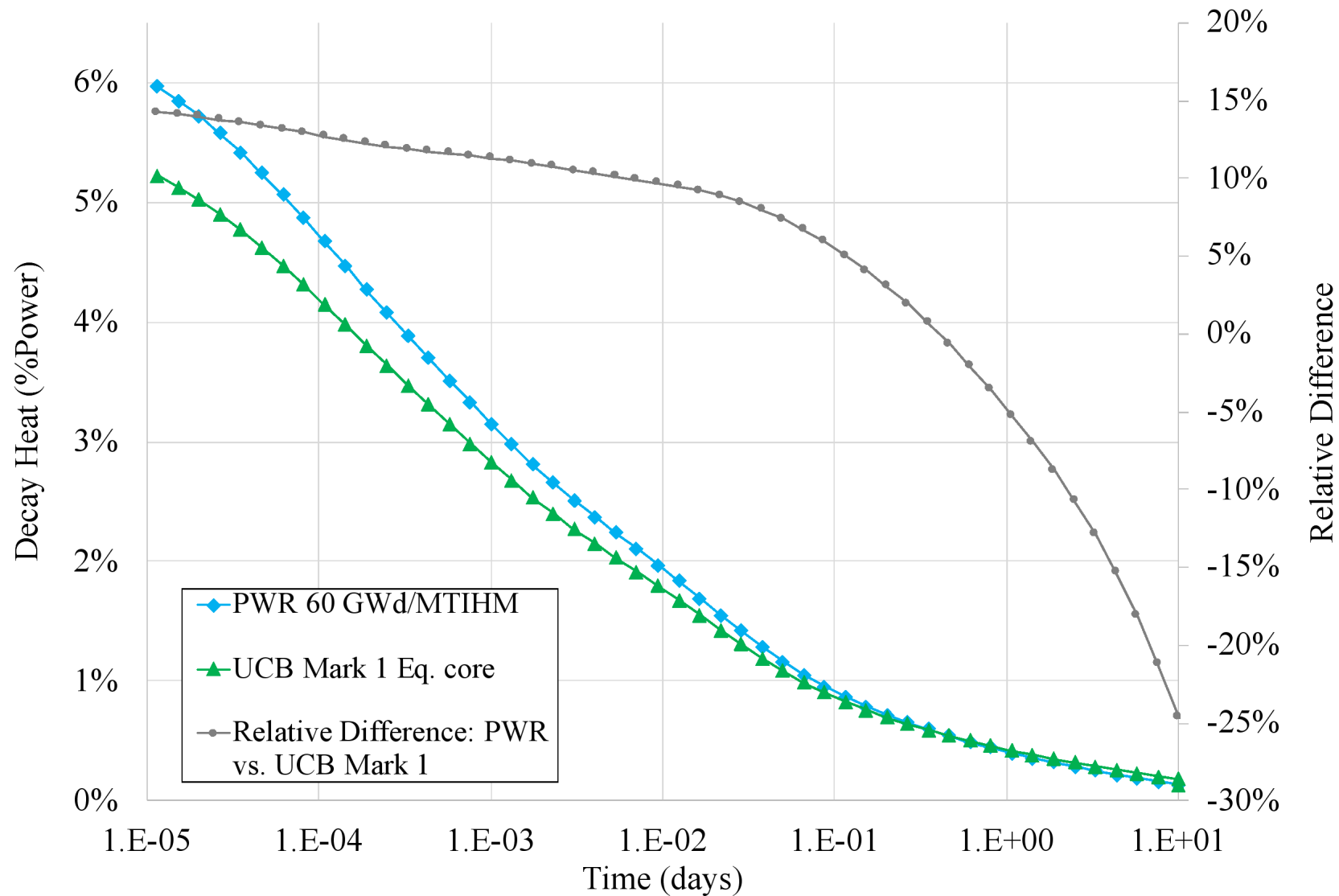


Relative contribution of top fission products



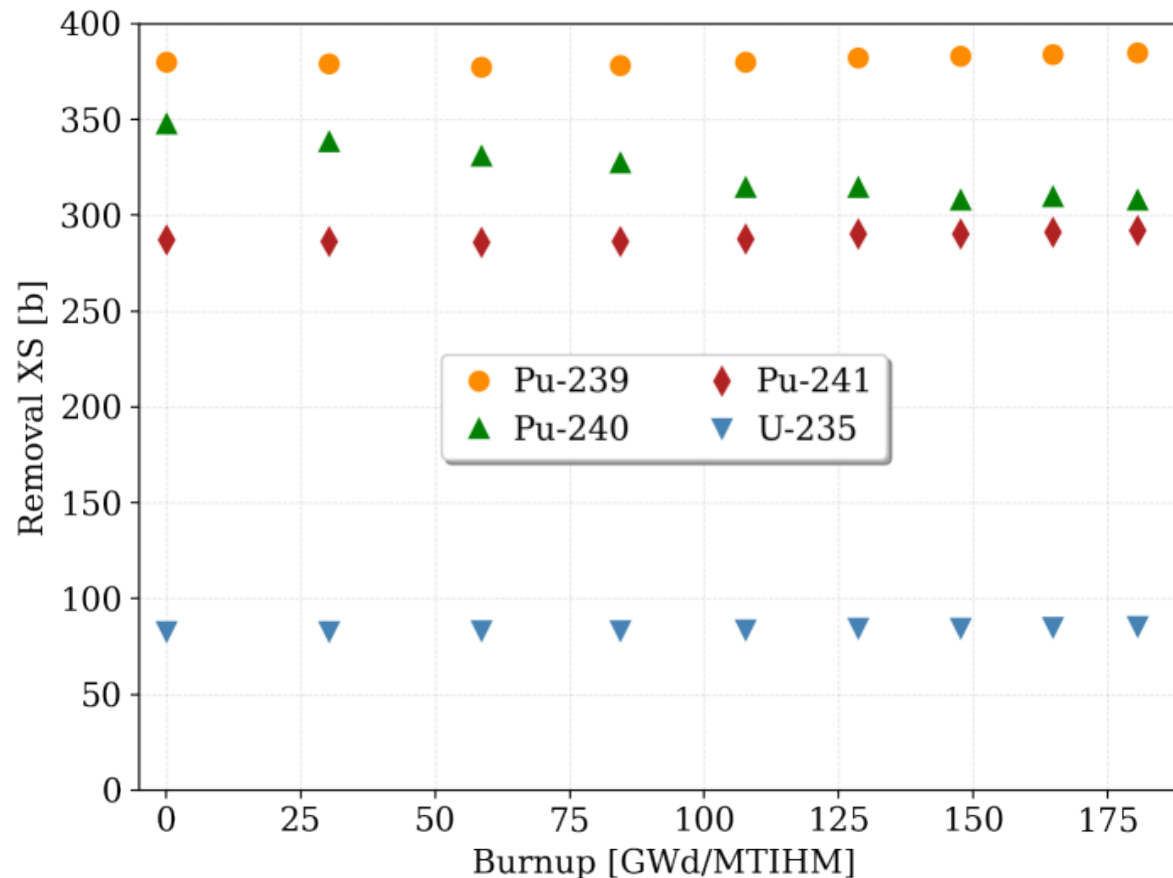
Relative contribution of top actinides

5. Decay heat comparisons



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

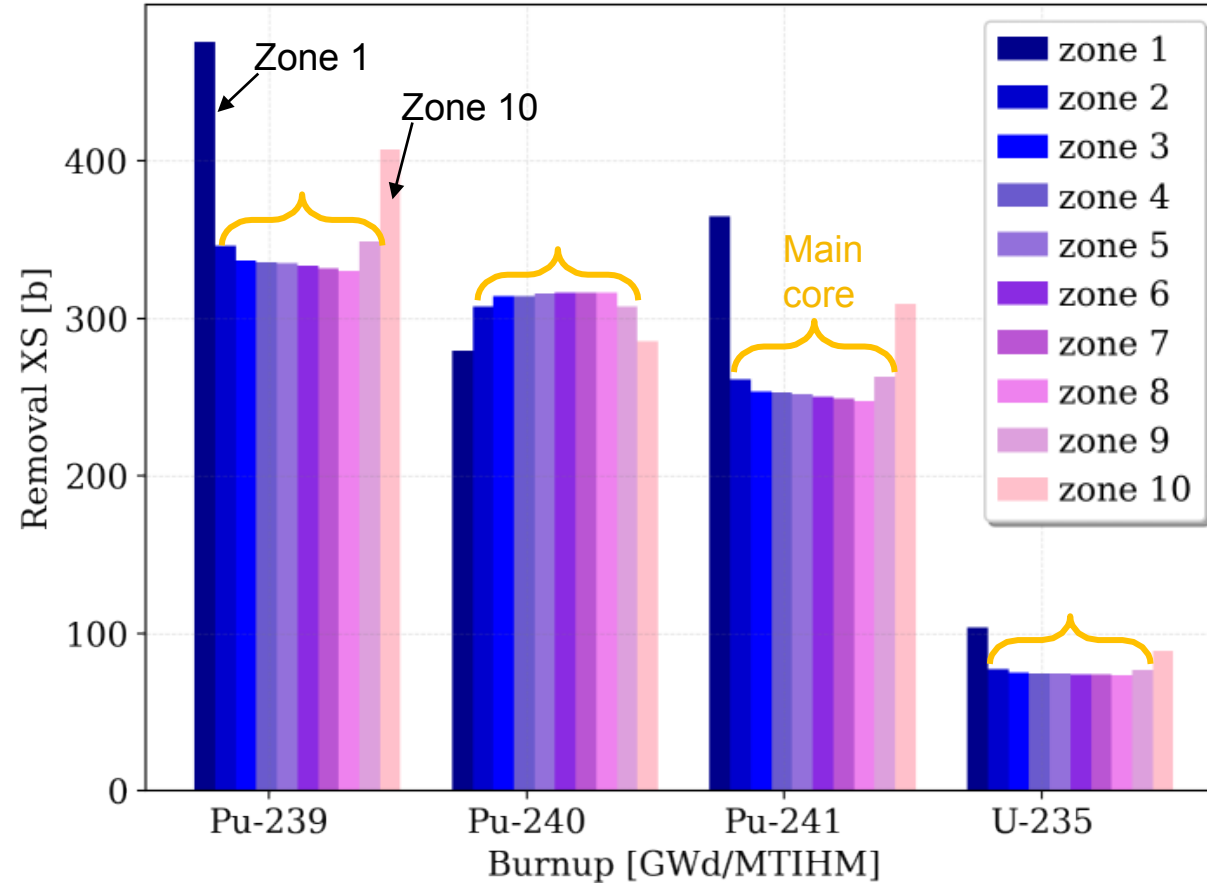
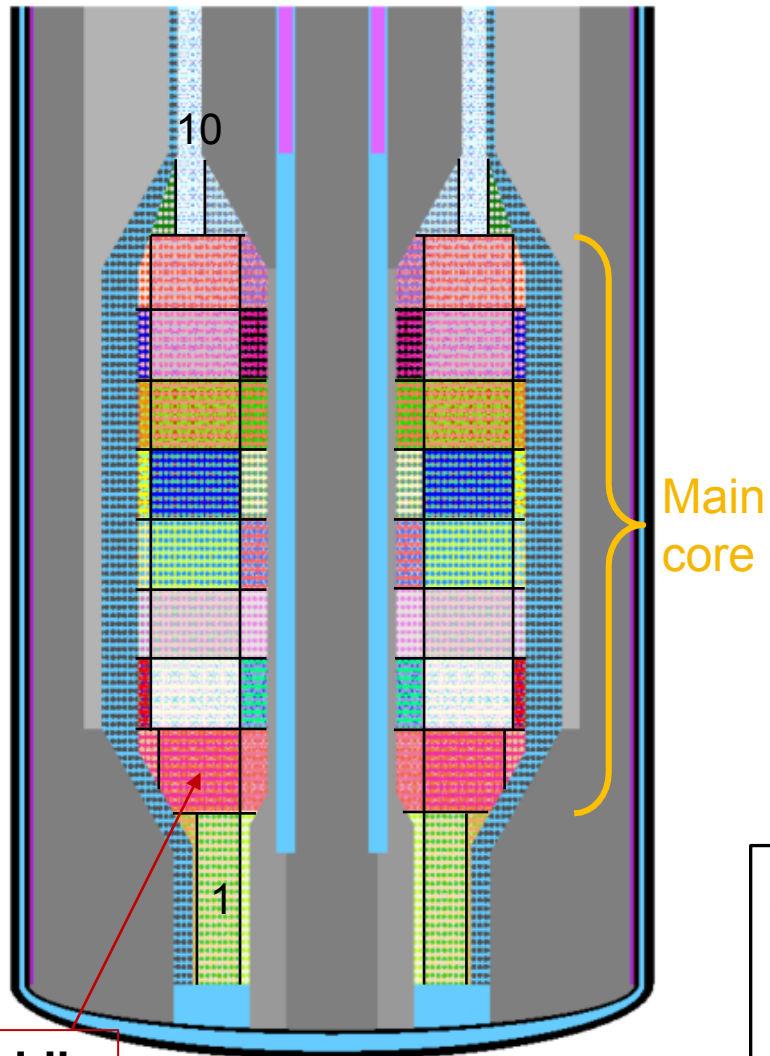


UCB Mark 1 slice depletion (HFP)

- 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

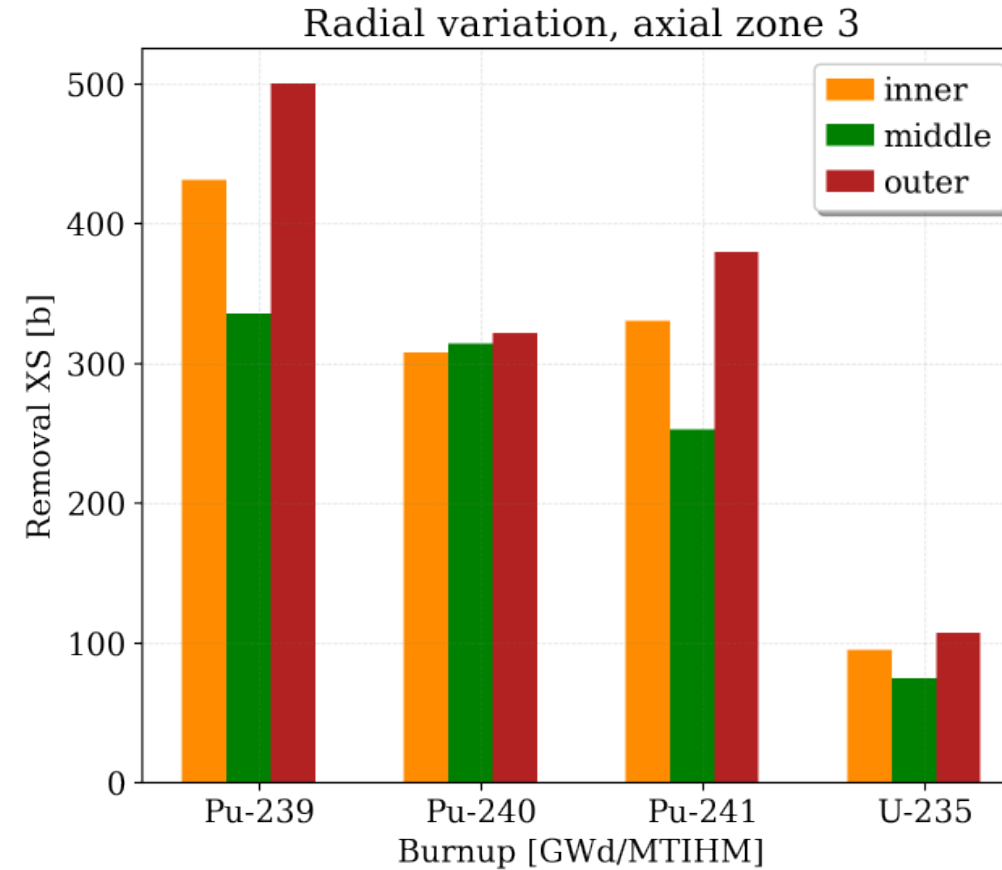
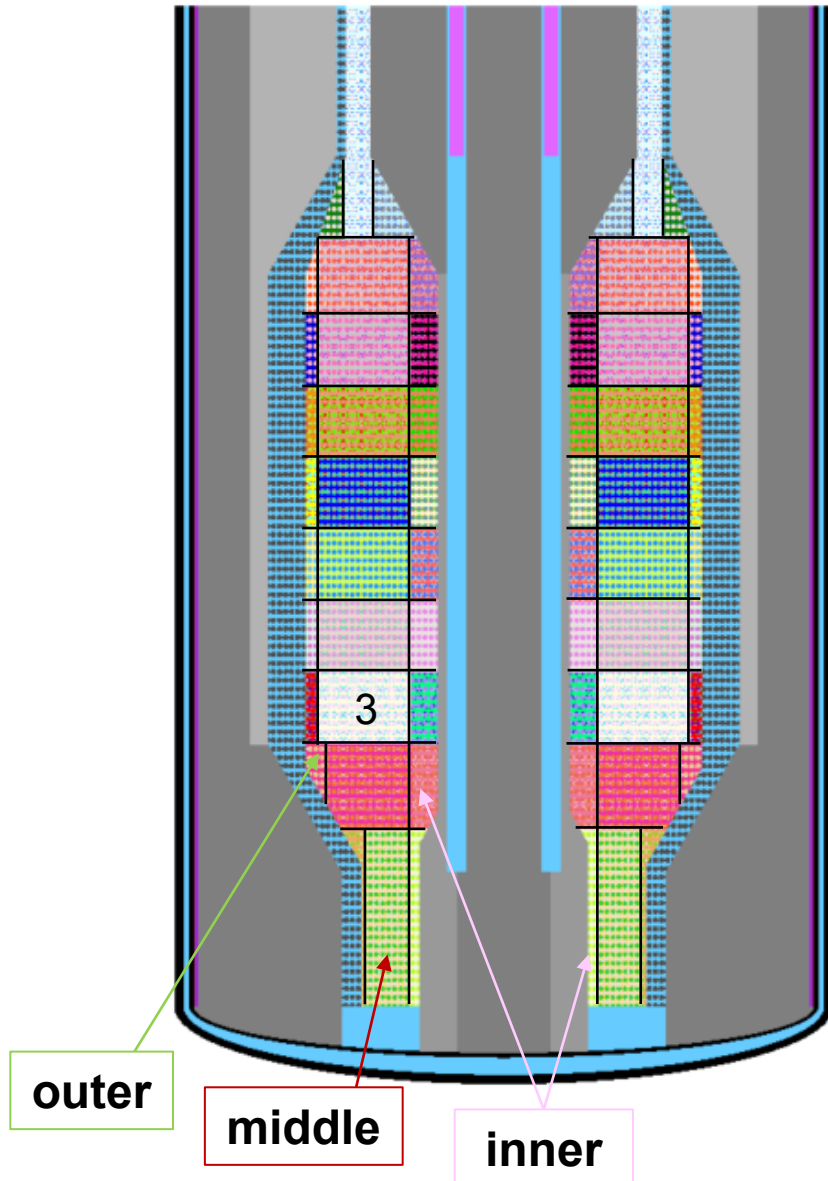
Axial variation, middle radial zone



Axial variation:

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

6. Radial variation of 1-group removal cross section



Radial variation:
Significant radial variation for various nuclides

7. Tritium production

- At equilibrium, an FHR produces hundreds of times more tritium per unit energy than an LWR
- Various reactions in the coolant produce tritium
 - ${}^6\text{Li} + n \rightarrow {}^4\text{He} + {}^3\text{H}$ (~65%)
 - ${}^7\text{Li} + n \rightarrow {}^4\text{He} + {}^3\text{H} + n'$ (~35%)
 - ${}^{19}\text{F} + n \rightarrow {}^{17}\text{O} + {}^3\text{H}$ (<1%)
- Mass of FLiBe defined in the ORIGEN model is the total FLiBe mass in the entire system
- ORIGEN Flux is equal to $\phi \left(\frac{V_{core}}{V_{Loop}} \right)$

TRITON

- Determine the flux spectrum and 1-group cross sections in FLiBe in this core

ORIGEN

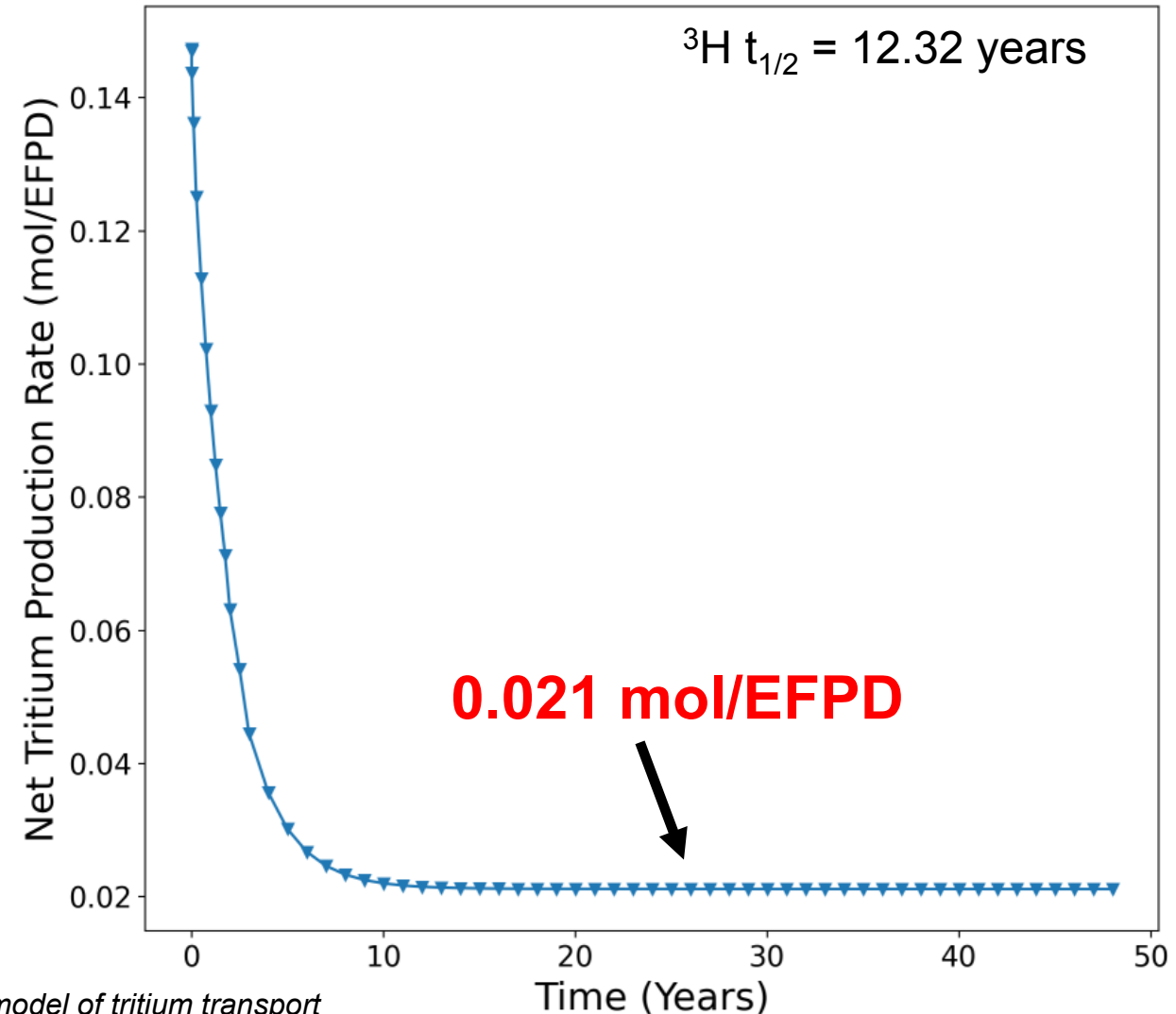
- Irradiate FLiBe using explicit flux magnitude scaled based on the fraction of system FLiBe in the core at any given time

7. Equilibrium tritium production rate

Equilibrium value from SCALE is **0.021 mol/EFPD**, consistent with previous analyses:

- Equilibrium value from Cisneros was 0.023 mol/EFPD
- Equilibrium is mainly a balance between Li-6 production and destruction
 - ${}^9\text{Be} + n \rightarrow {}^4\text{He} + {}^6\text{Li}$
 - ${}^6\text{Li} + n \rightarrow {}^4\text{He} + {}^3\text{H}$
- The calculated behavior is consistent with previously established trends
- At equilibrium, the PB-FHR Mk 1 produces 0.099 mol ${}^3\text{H}$ /GWd as compared to 0.00042 (BWR) or 0.00047 (PWR)*

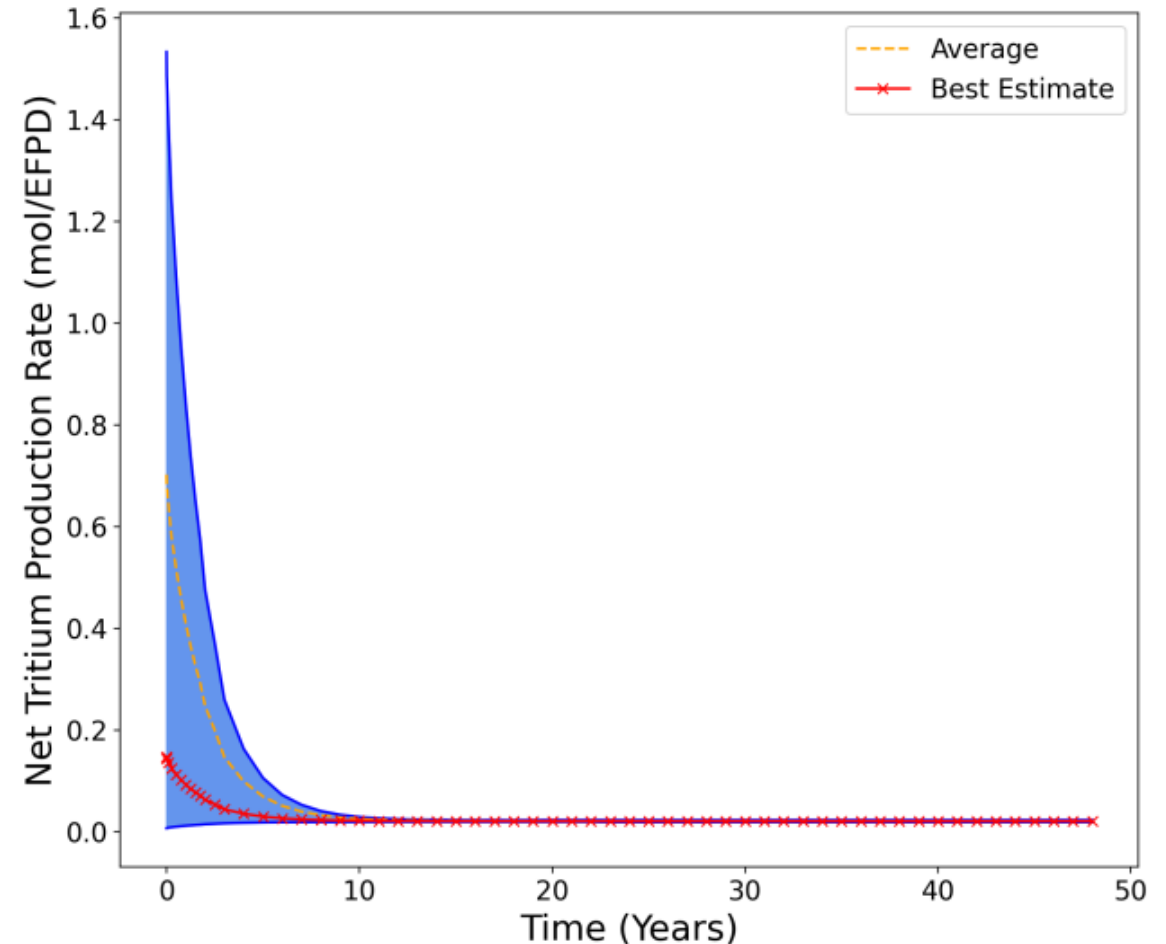
*Stempien, J. D., Ballinger, R. G., Forsberg, C. W., "An integrated model of tritium transport and corrosion in FHRs," *Nuclear Engineering and Design*, Vol 310, pp. 257-272, (2016).



7. Sensitivity analysis on tritium production

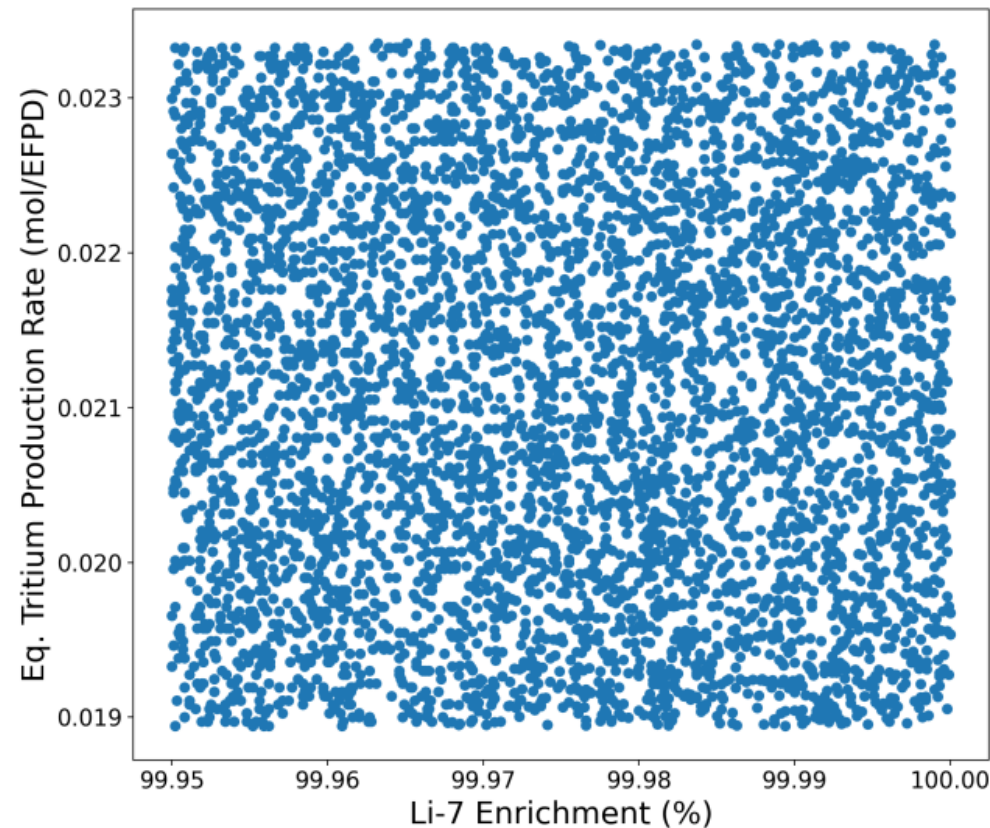
- We ran 5,000 combinations of initial Li-7 enrichment and flux using SAMPLER to determine their impact on equilibrium tritium production
- Variations in initial tritium production rate are quite large and depend on flux and initial Li-7 enrichment
 - Li-6 is a poison, so FHR systems seek to enrich coolant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

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

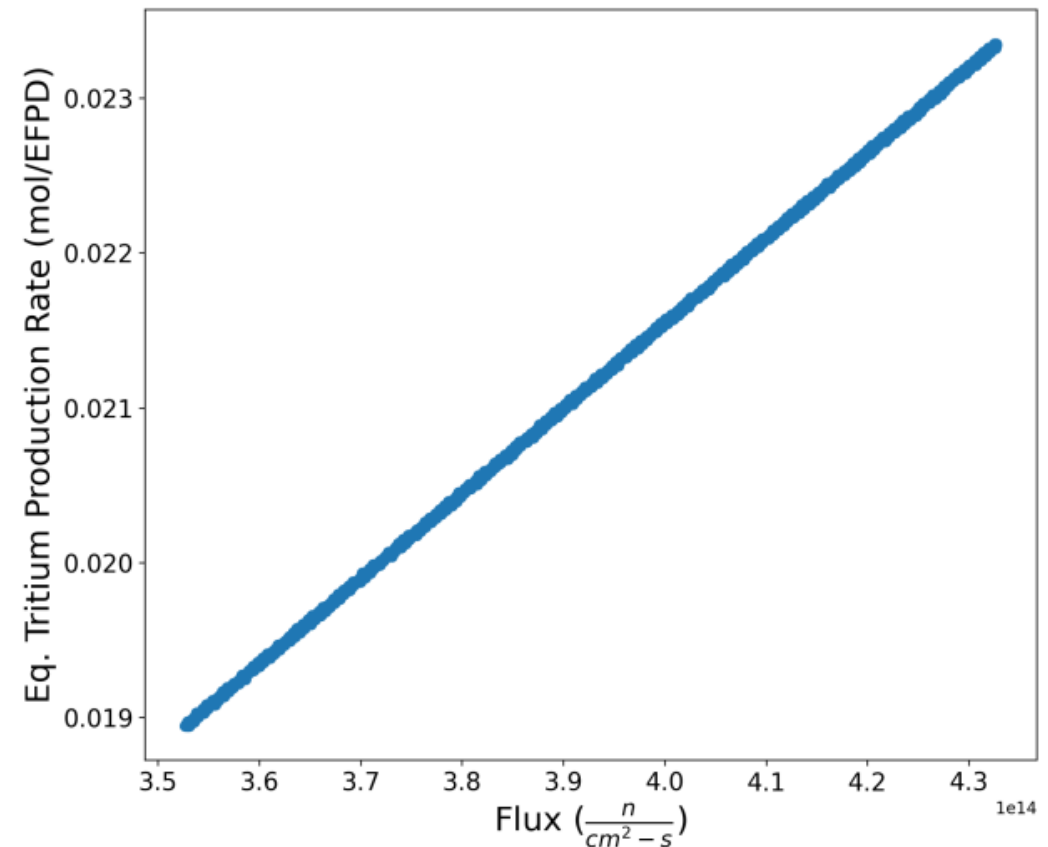


7. Sensitivity analysis on tritium production

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



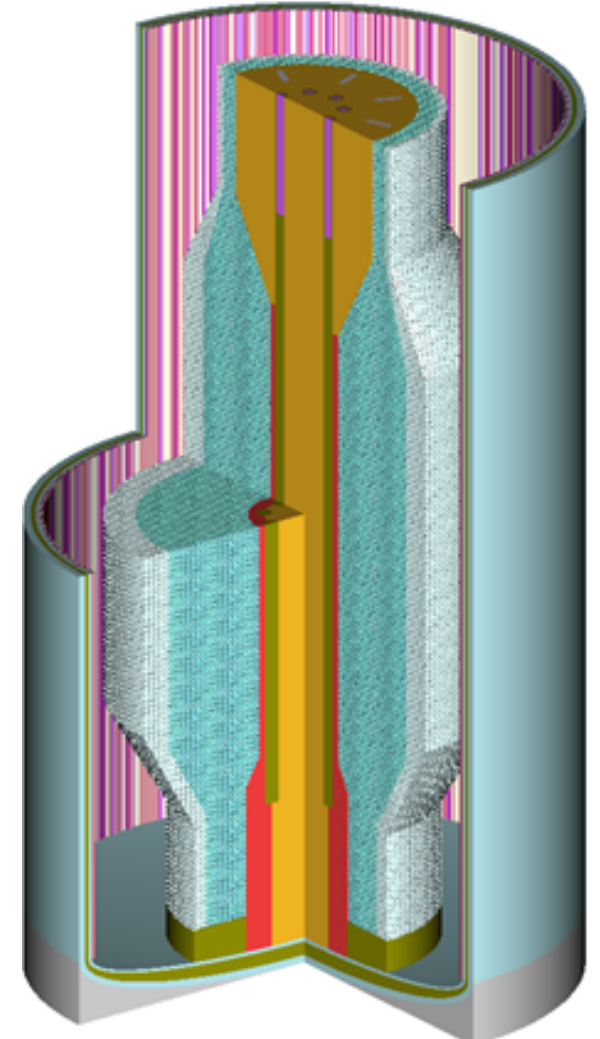
No correlation for initial Li-7 enrichment



Strong correlation for neutron flux

Neutronics Summary

- SCALE's MG physics was confirmed adequate for application in UCB Mark 1: k_{eff} bias smaller than 260 pcm, while achieving 24 times faster runtime
- Fuel compositions for a UCB Mark 1 equilibrium core were developed using an iterating scheme
- Power profiles and decay heat were determined for equilibrium core and provided to MELCOR team
- Temperature feedback: linear behavior found for fuel and salt, nonlinear trend for materials containing graphite
- Strong radial variation for 1-group xs was observed, while axial variation was limited to inlet/outlet regions
- Tritium production rate in coolant salt was determined: larger than LWR, independent of initial Li-7 enrichment, strongly dependent on flux



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

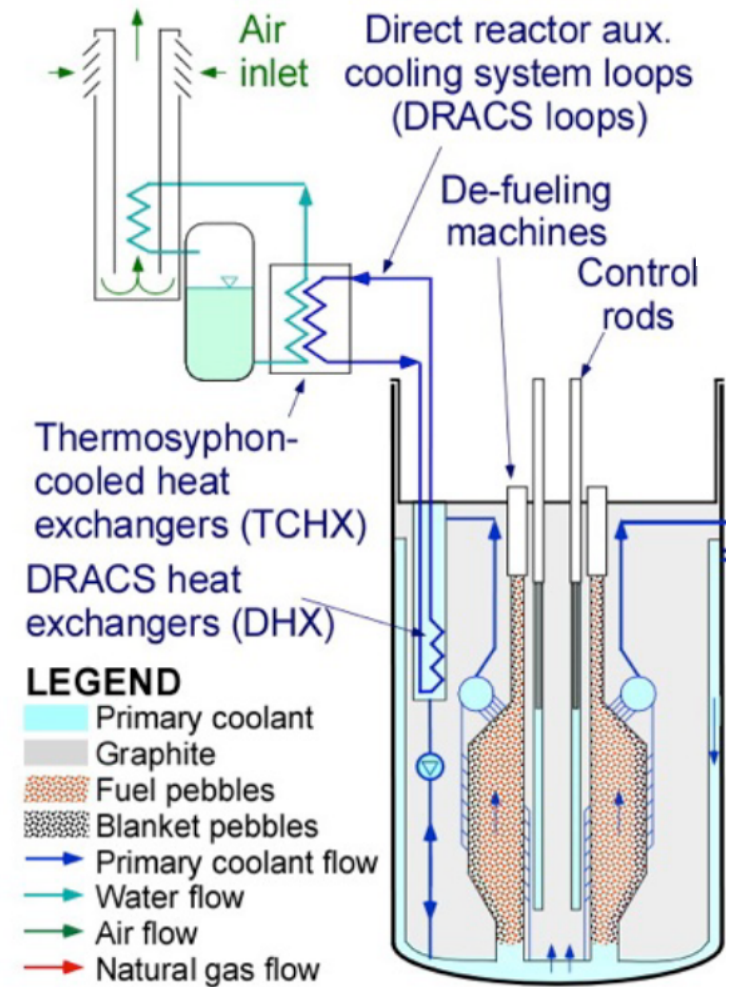
Fission product release

- 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)



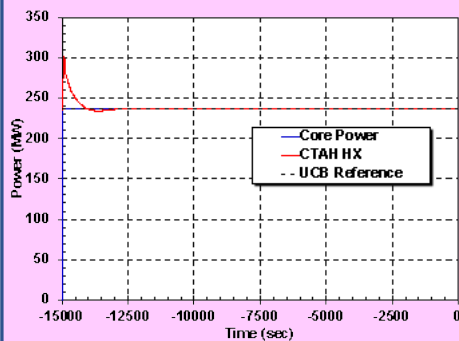
Transient/Accident Solution Methodology

Stage 0:
Normal Operation
Establish thermal state

Time constant in FHR graphite structures is very large

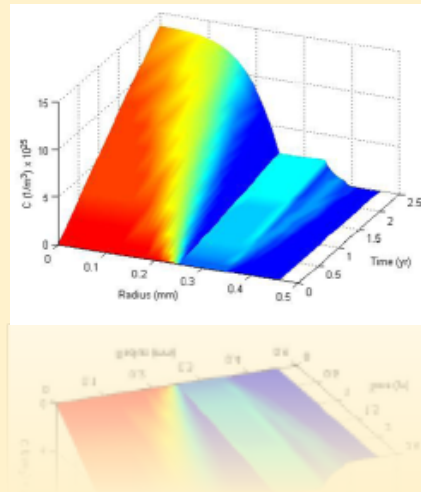
Reduce heat capacities for structures to reach steady state thermal conditions.

Reset heat capacities after steady state is achieved.



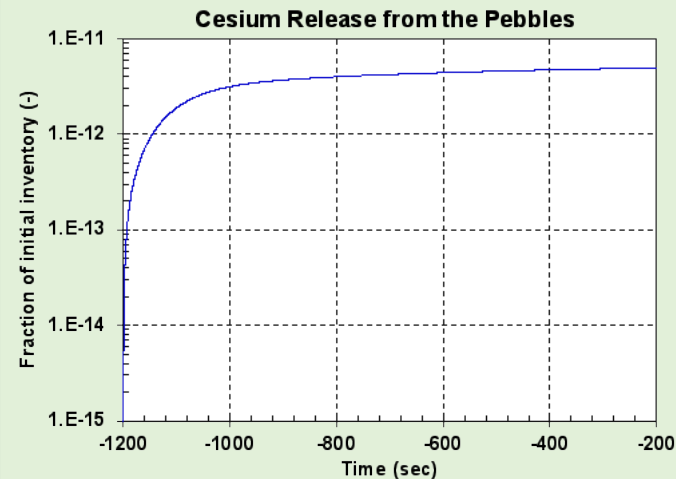
Stage 1:
Normal Operation
Diffusion Calculation

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



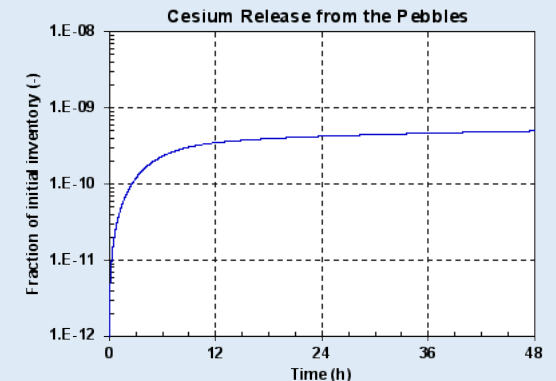
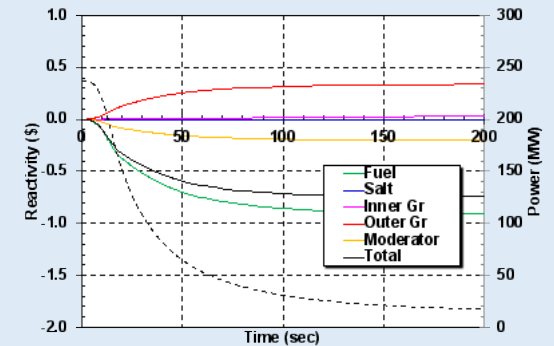
Stage 2:
Normal Operation
Transport Calculation

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

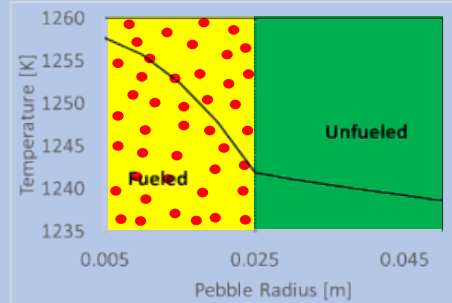
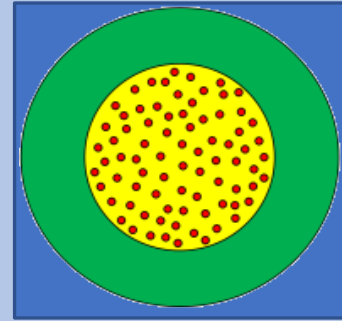


Core components

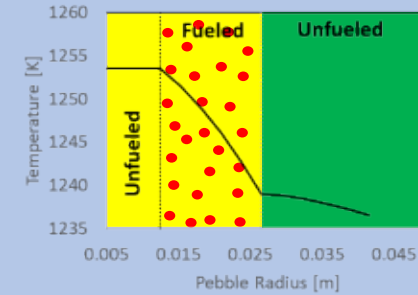
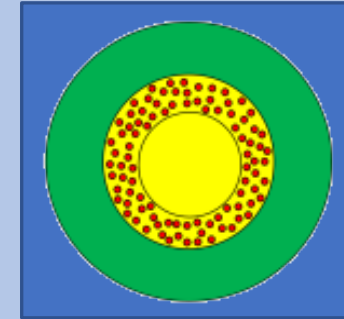
• Pebble Bed Reactor Fuel/Matrix Components

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

Fueled pebble core

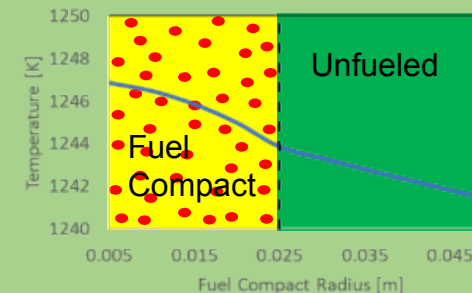
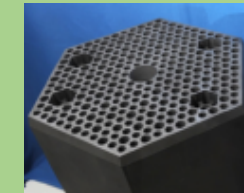
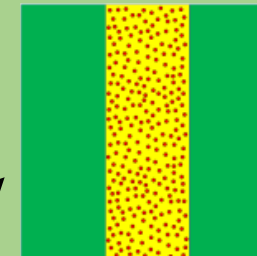
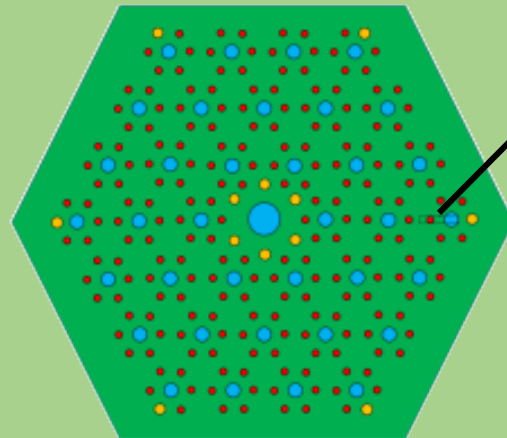


Unfueled pebble core

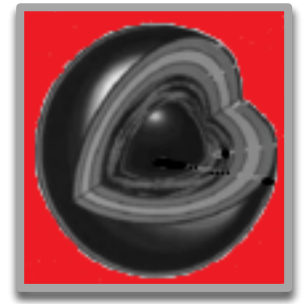
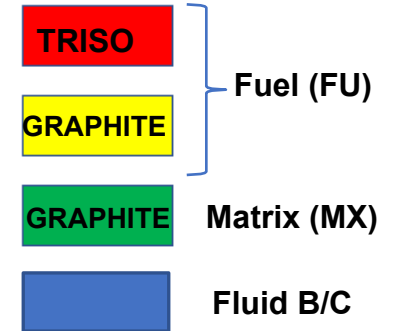


• Prismatic Modular Reactor Fuel/Matrix Components

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



Legend



TRISO (FU)

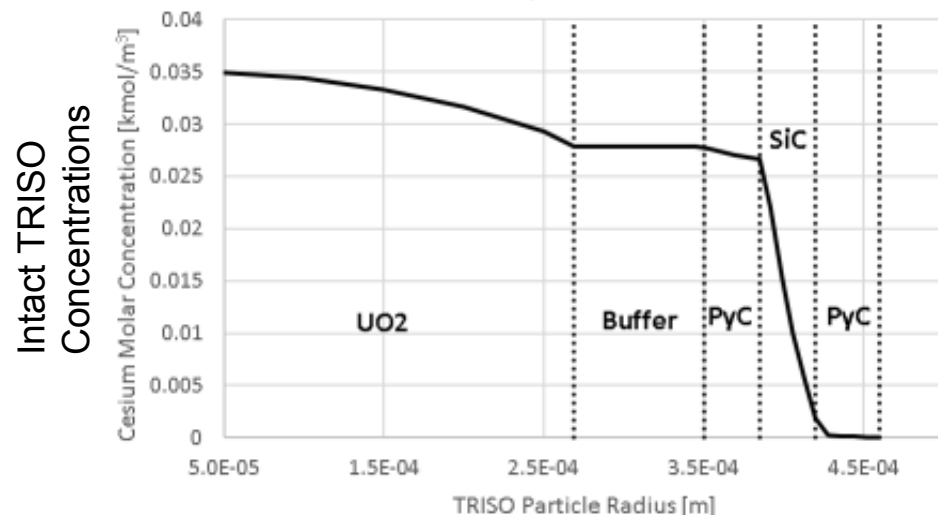
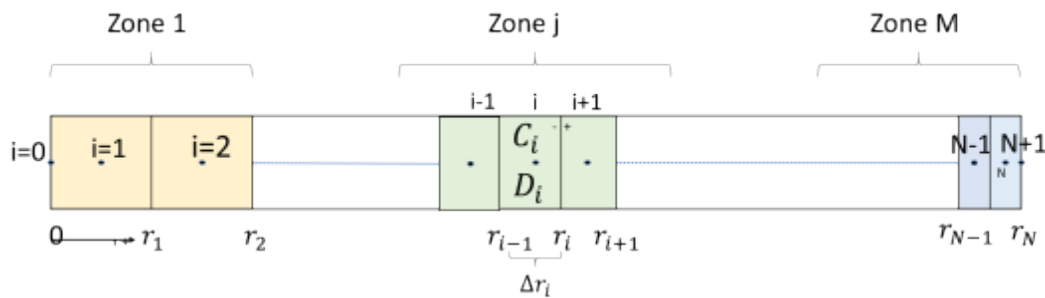
Sub-component model for zonal diffusion of radionuclides through TRISO particle

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 ₂	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
Kr	Some		Some		Not found	Some	Some
Sr	Some		Some		Extensive	Some	Some
Xe	Some		Some		Some	Some	Not found

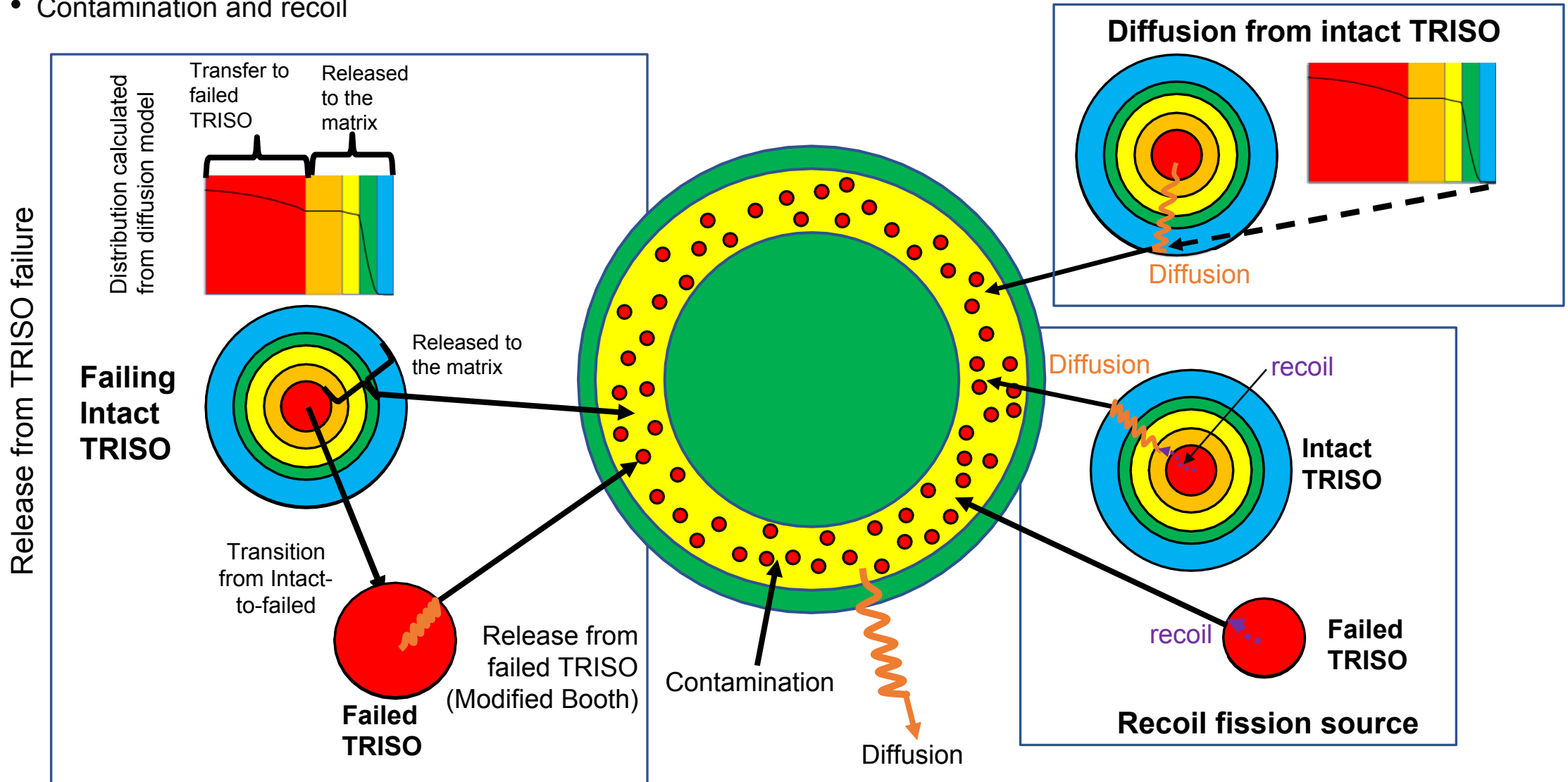
Data used in the demo calculation [IAEA TECDOC-0978]

Layer	FP Species							
	Kr		Cs		Sr		Ag	
	D (m ² /s)	Q (J/mole)	D (m ² /s)	Q (J/mole)	D (m ² /s)	Q (J/mole)	D (m ² /s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6-8	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

Radionuclide Release Models

- Recent failures – particles failing within latest time-step (burst release, diffusion release in time-step)
- Previous failures – particles failing on a previous time-step (time history of diffusion release)
- Contamination and recoil



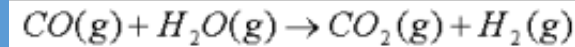
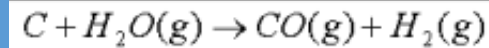
Graphite Oxidation

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

Steam oxidation

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

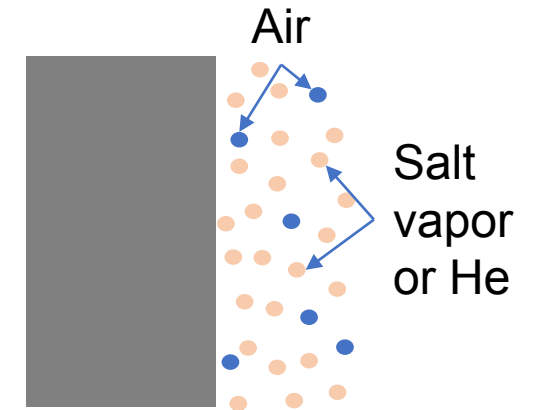
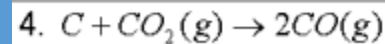
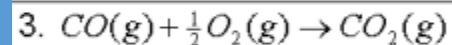
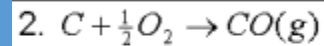
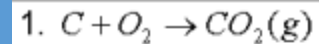
Reactions



Air oxidation

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

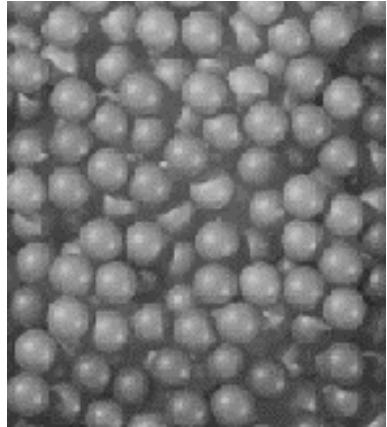
Reactions



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

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

where:

ε = Bed porosity [-]

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

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

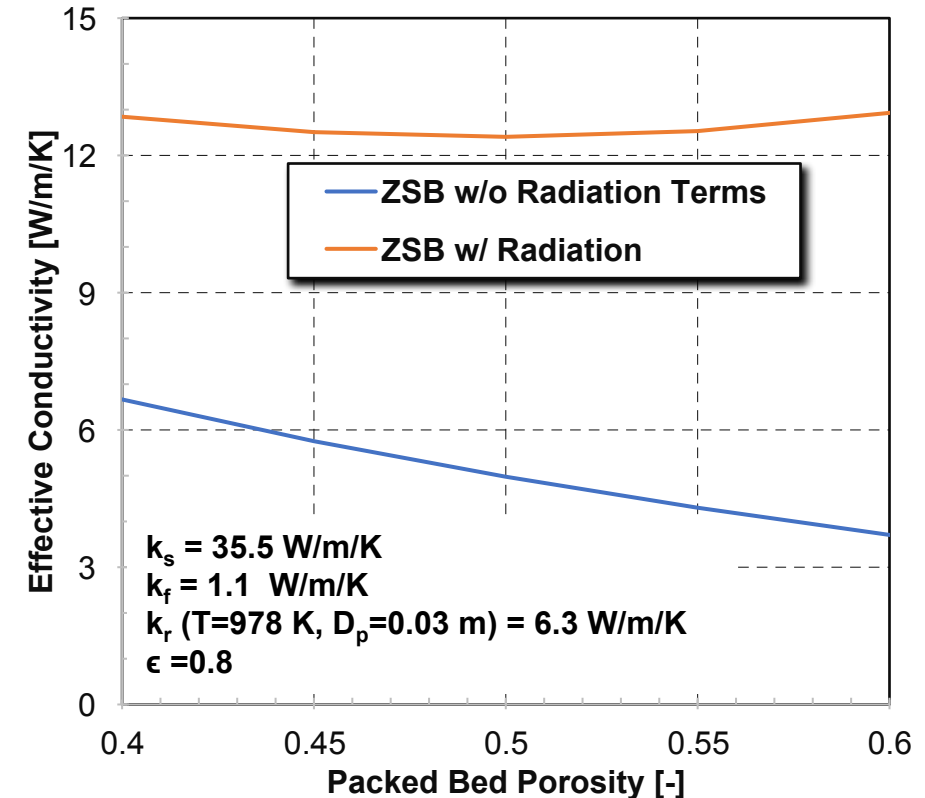
k_s = Solid conductivity [W/m/K]

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

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

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



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

$$Nu_{\text{Free}} = 2.0 + 0.6 Gr_f^{1/4} Pr_f^{1/3}$$

$$Nu_{\text{Forced}} = 2.0 + 0.6 Re_f^{1/2} Pr_f^{1/3}$$

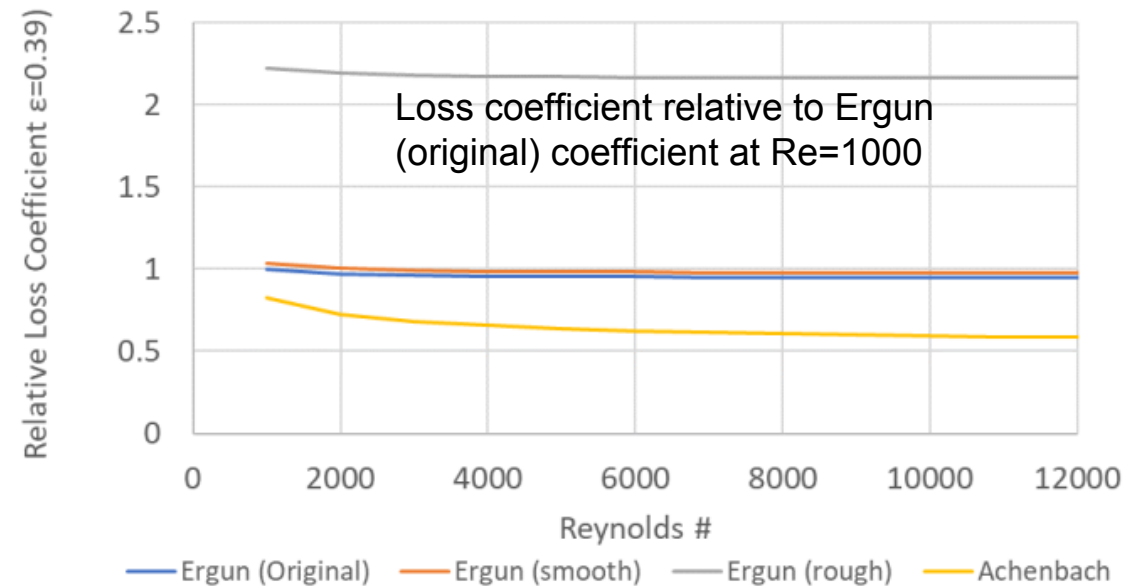
- Constants and exponents accessible by sensitivity coefficient

Flow resistance

- Packed bed pressure drop

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

Correlation	C ₁	C ₂	C ₃	C ₄
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 (HTGR/FHR)

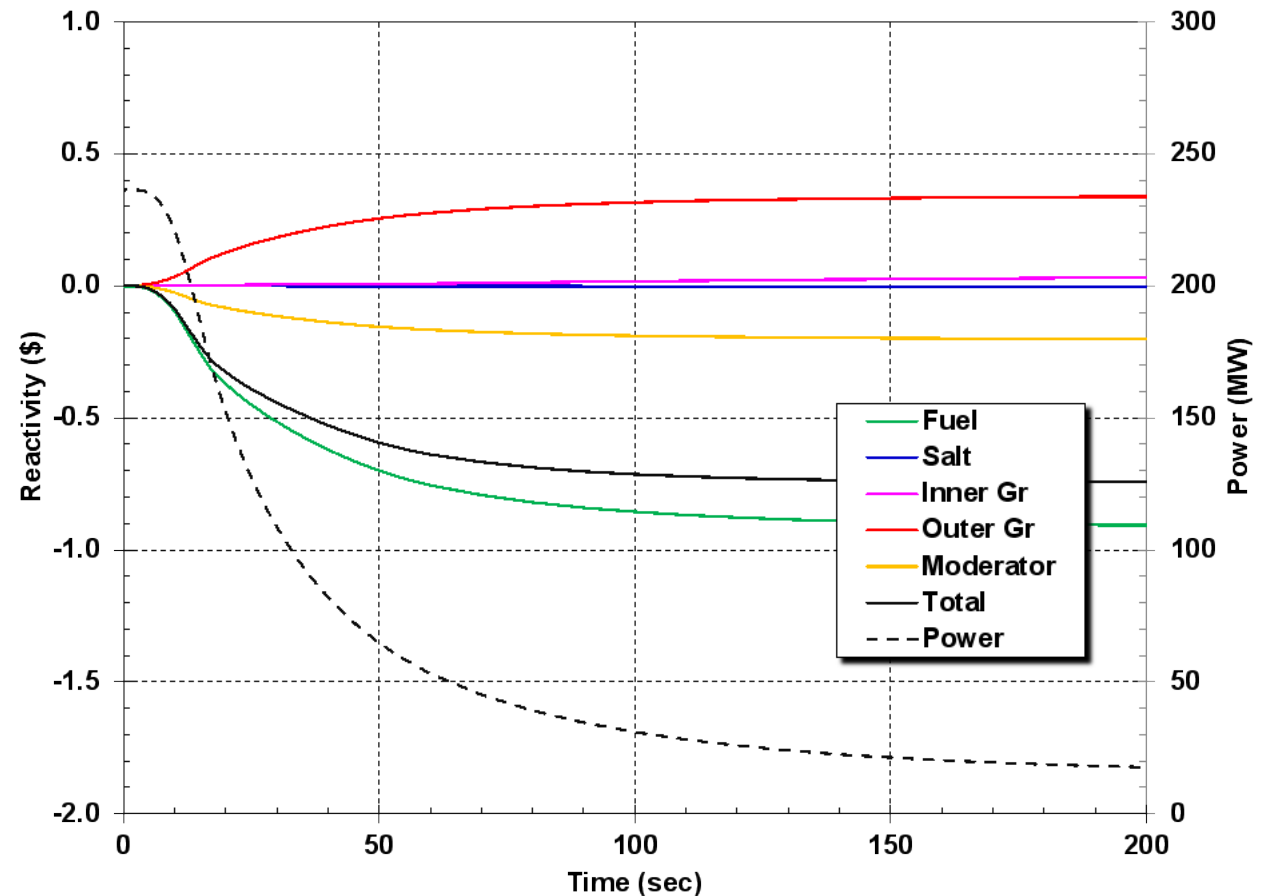
Standard treatment

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

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

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

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

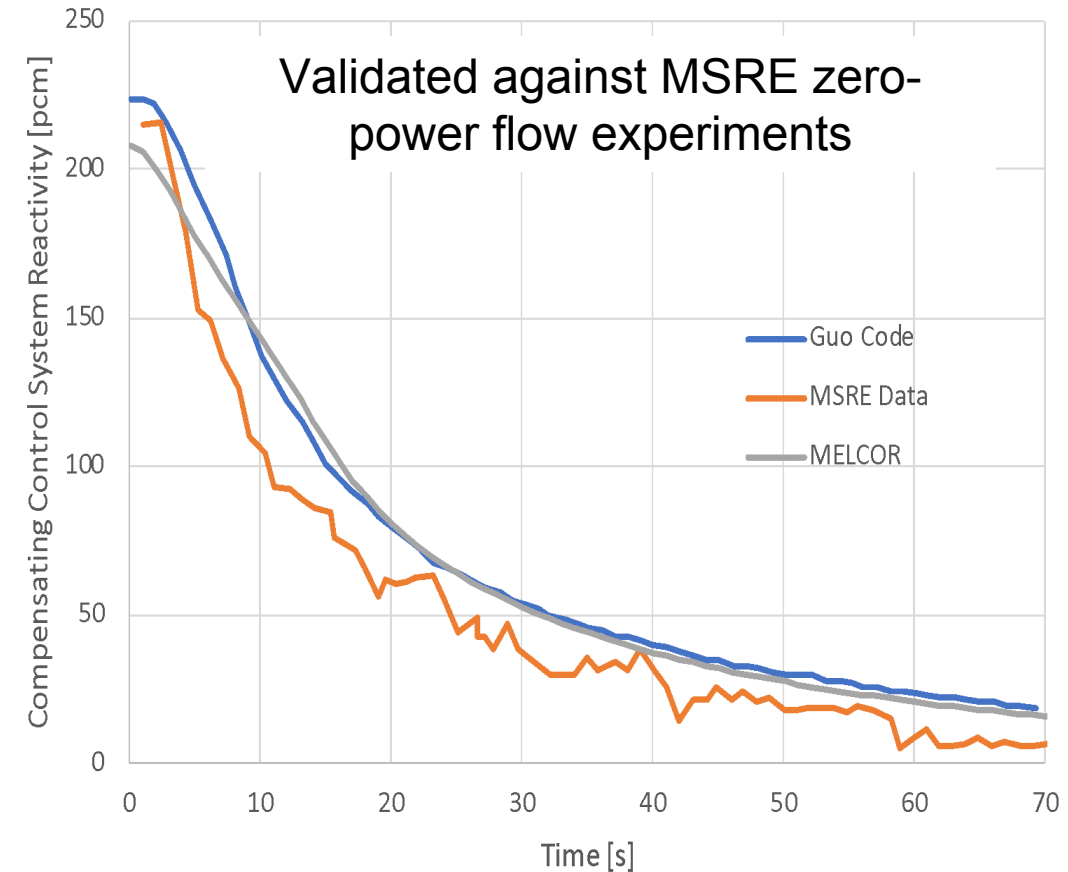
$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda} \right) P(t) - (\lambda_i + 2/\tau_C) C_i^C(t) + \left(\frac{V_L}{V_C} \right) (\lambda_i + 2/\tau_L) C_i^L(t), \quad i = 1 \dots 6$$

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

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

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 6 forms as found in the Molten Salt Reactor Experiment

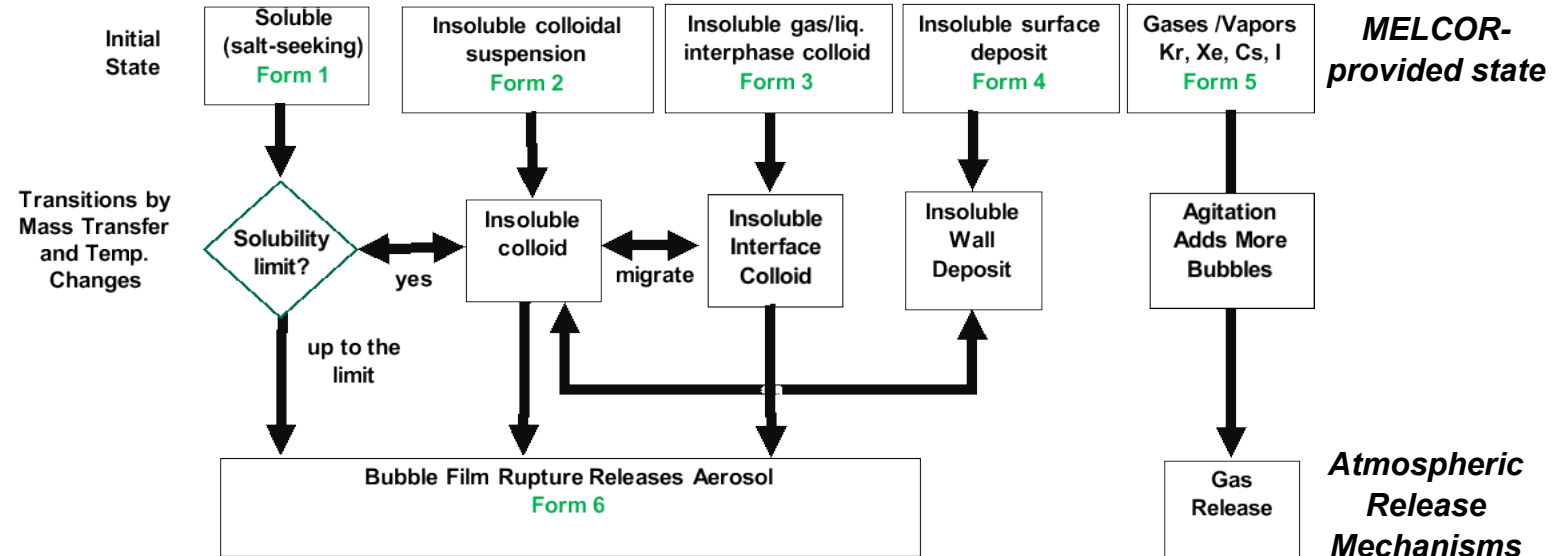
Model Scope

Evaluation of thermochemical state

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

Thermodynamic database

- Generalized approach to utilize any thermodynamic database
- MSTDB has two systems
 - Pu-U-Th-Nd-Ce-La-Cs-Rb-Ca-K-Na-F-Be-Li
 - Pu-U-Cs-K-Cl-Mg-Na-Li



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



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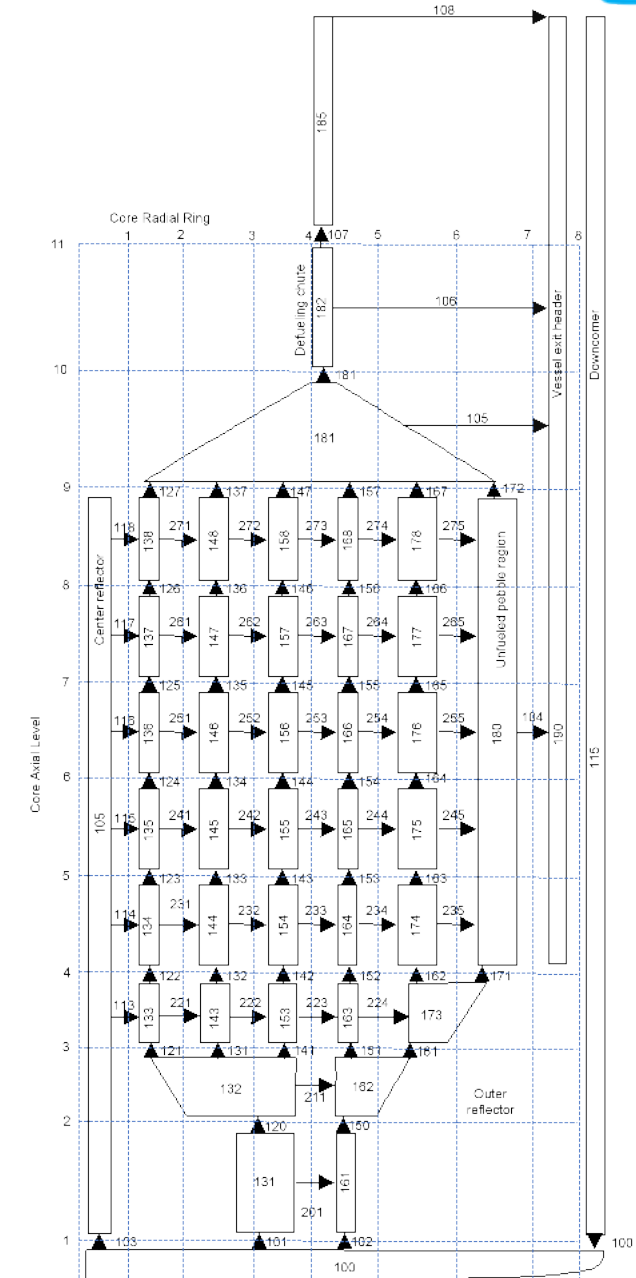
Core and reactor vessel

Core nodalization – light blue lines

- Assumes azimuthal symmetry
- Subdivided into 11 axial levels and 8 radial rings
- Each cell models 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”



Molten salt has free surface in the hotwell and the standpipes

- 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

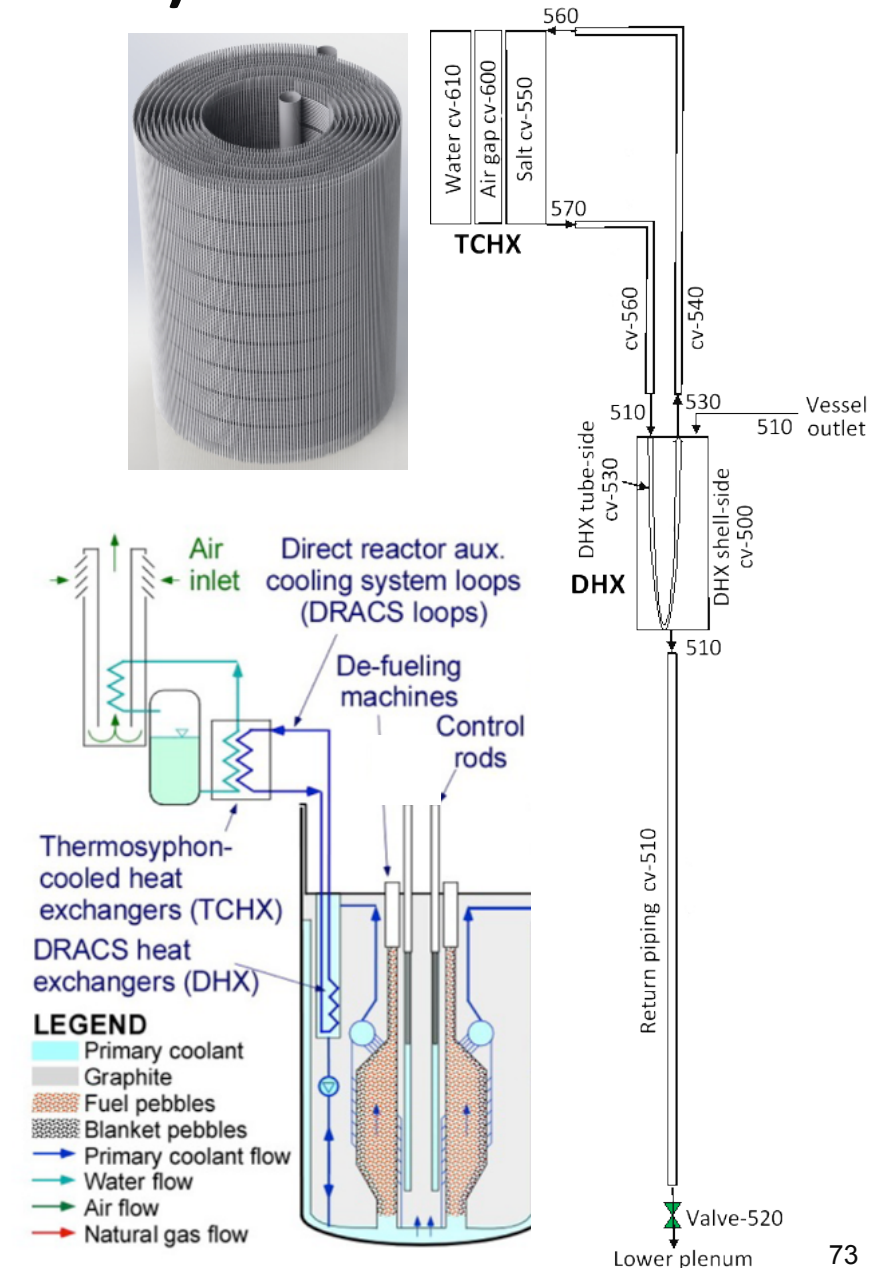
Each train has 4 loops in series

- 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

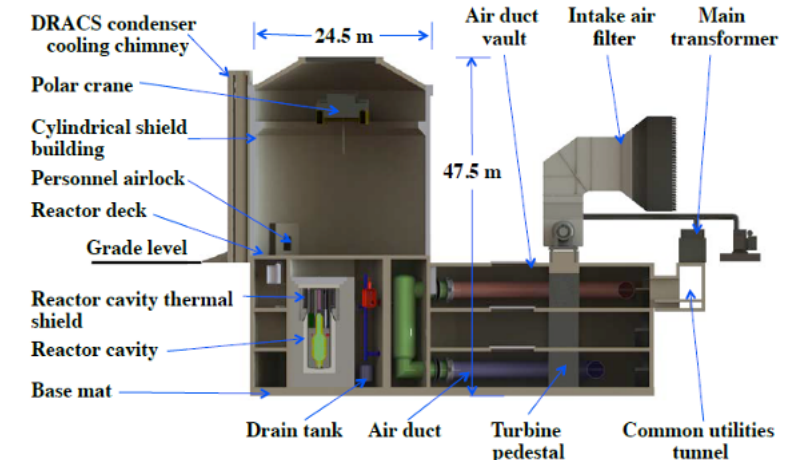
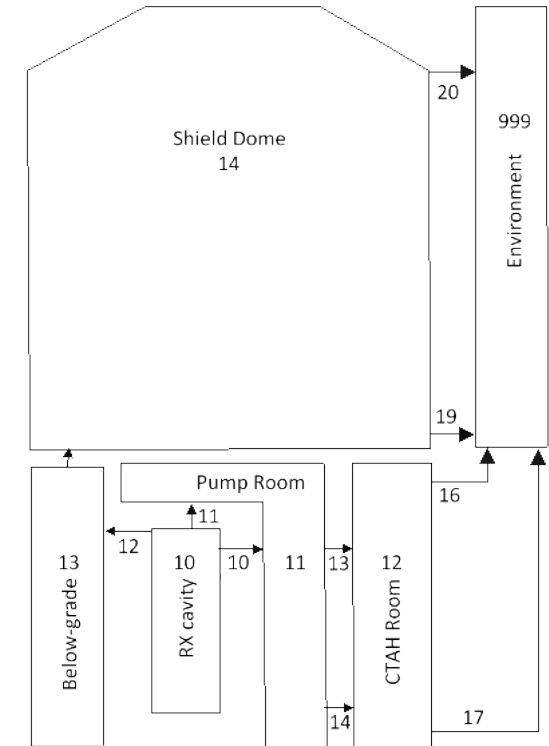
- Below-grade compartment includes the cover-gas enclosure for reactor cavity over-pressurization

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

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

- $$K_{loss} = a \left(\frac{(1 - \epsilon)}{Re} \right) + b \left(\frac{(1 - \epsilon)}{Re} \right)^c$$

Pebble to fluid heat transfer within a cell

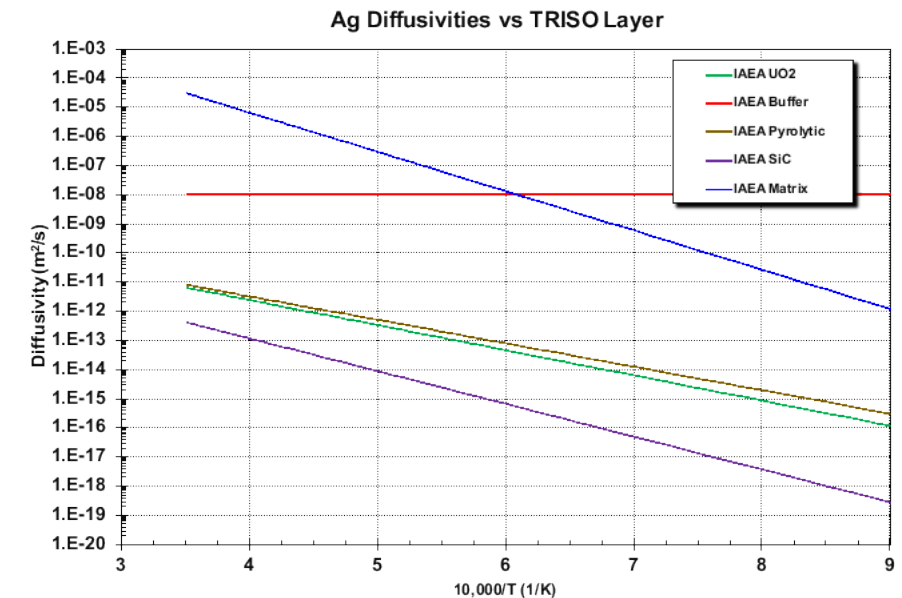
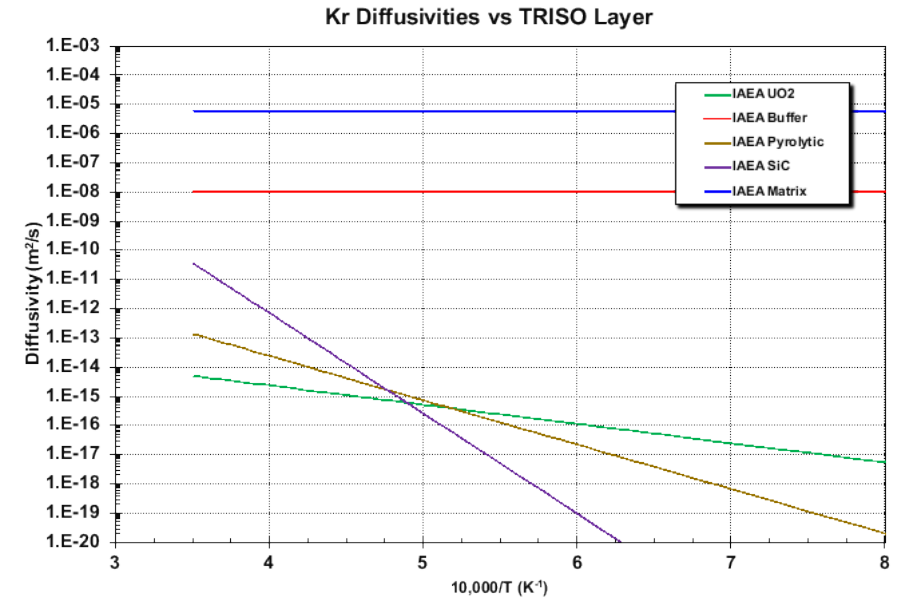
- Forced convection using Wakao correlation, $Nu = 2 + 1.1 Re^{0.66} Pr^{0.33}$

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
 - UCO 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

Applied MELCOR to 3 scenario with loss-of-secondary heat removal

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

Sensitivity calculations included

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

Loss-of-onsite power with failure to SCRAM

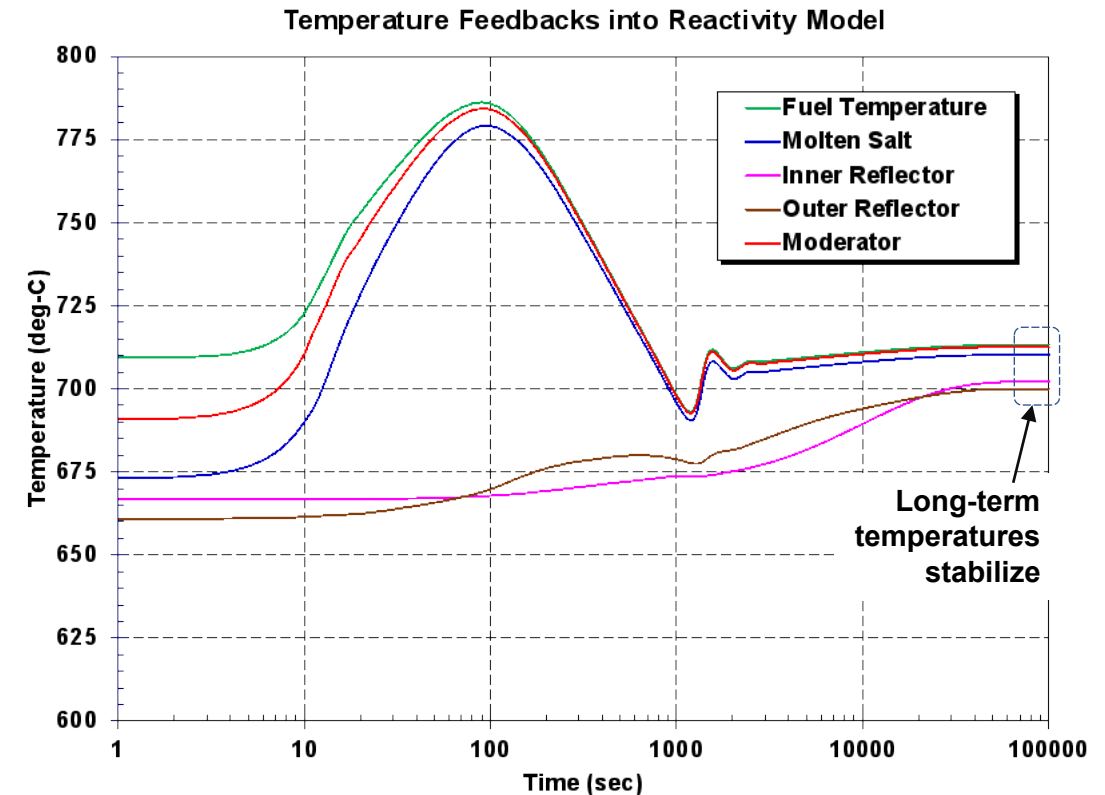
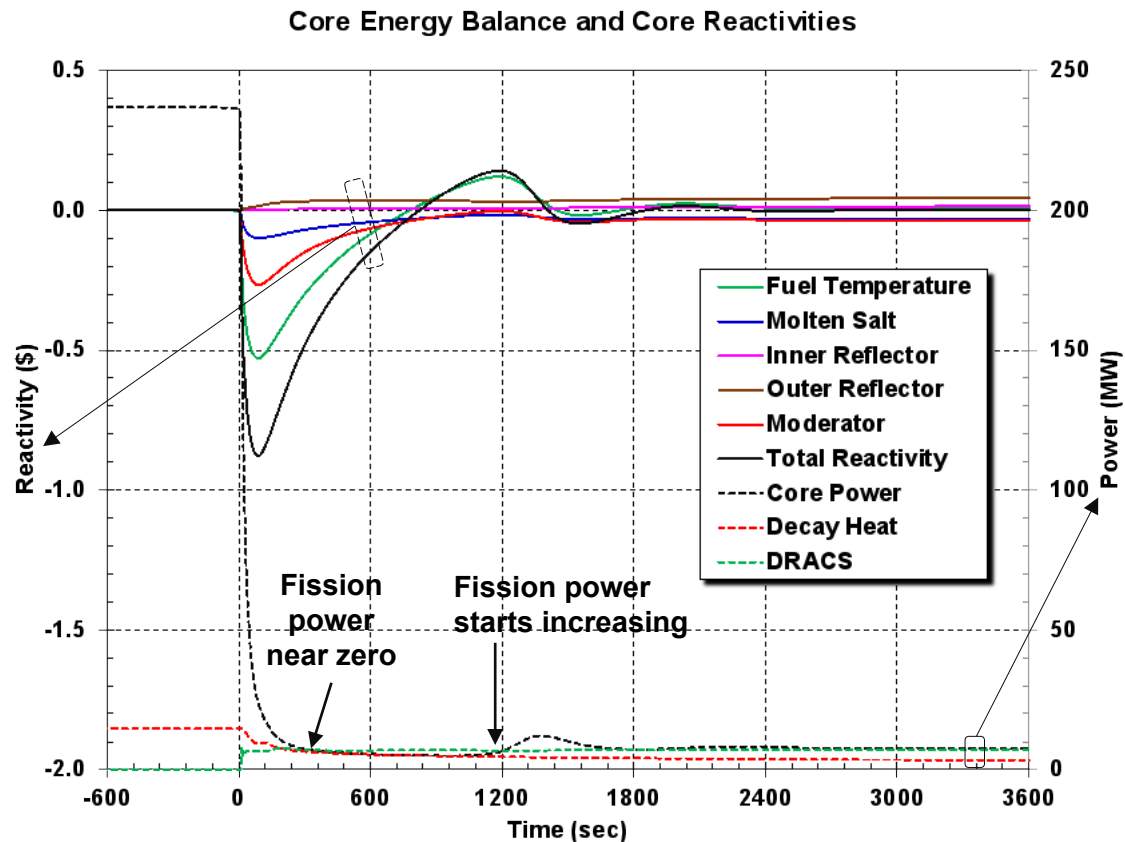
- Salt pumps shut off
- Reactor fails to SCRAM
- Secondary heat removal ends
- 0 to 3 trains of DRACS operating

ATWS with 3xDRACS

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

3xDRACS exceeds core power after 330 s

Long-term core power balanced by DRACS heat removal (~7.2 MW)



* Power response does not include xenon transient

ATWS with variable DRACS

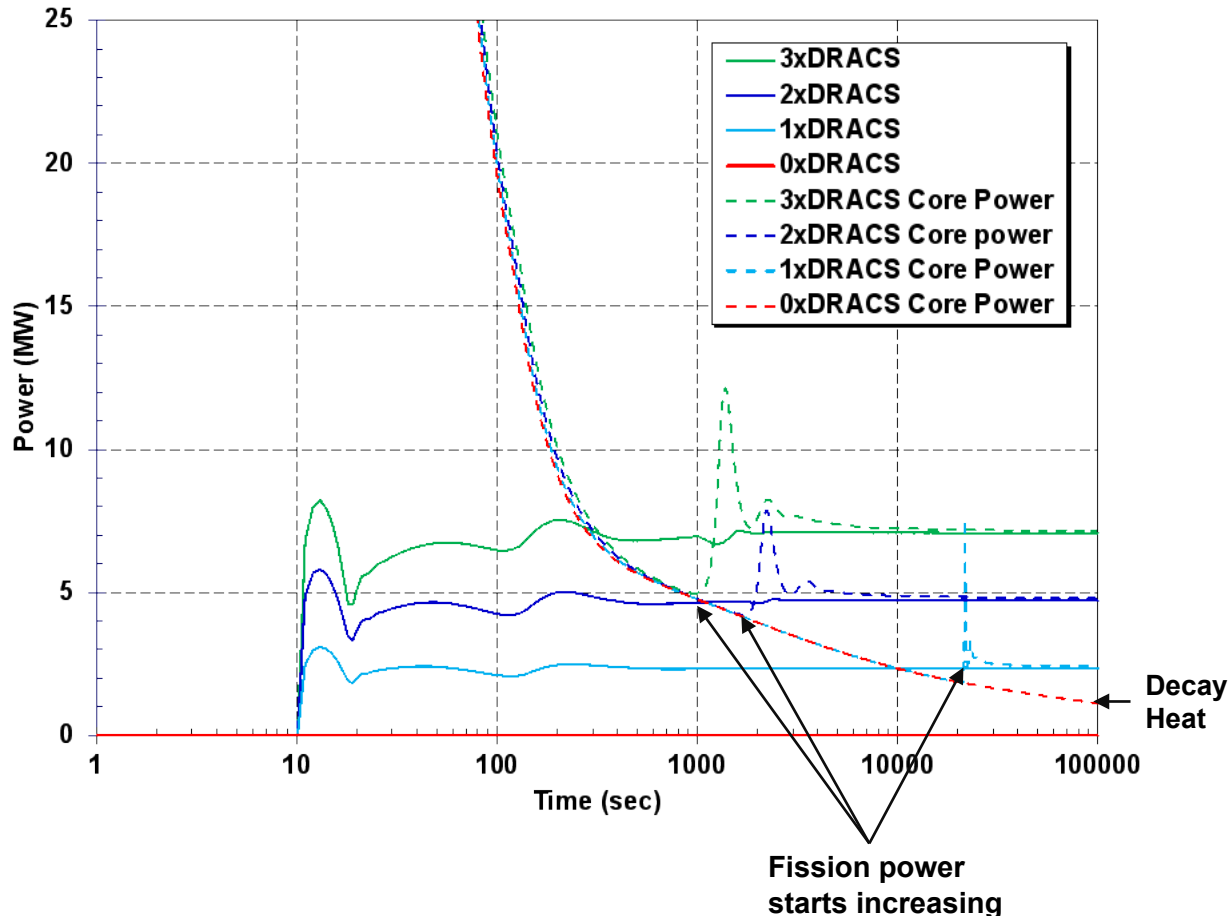
Core power eventually balances to DRACS heat removal *

- Fission power + decay heat = DRACS heat removal

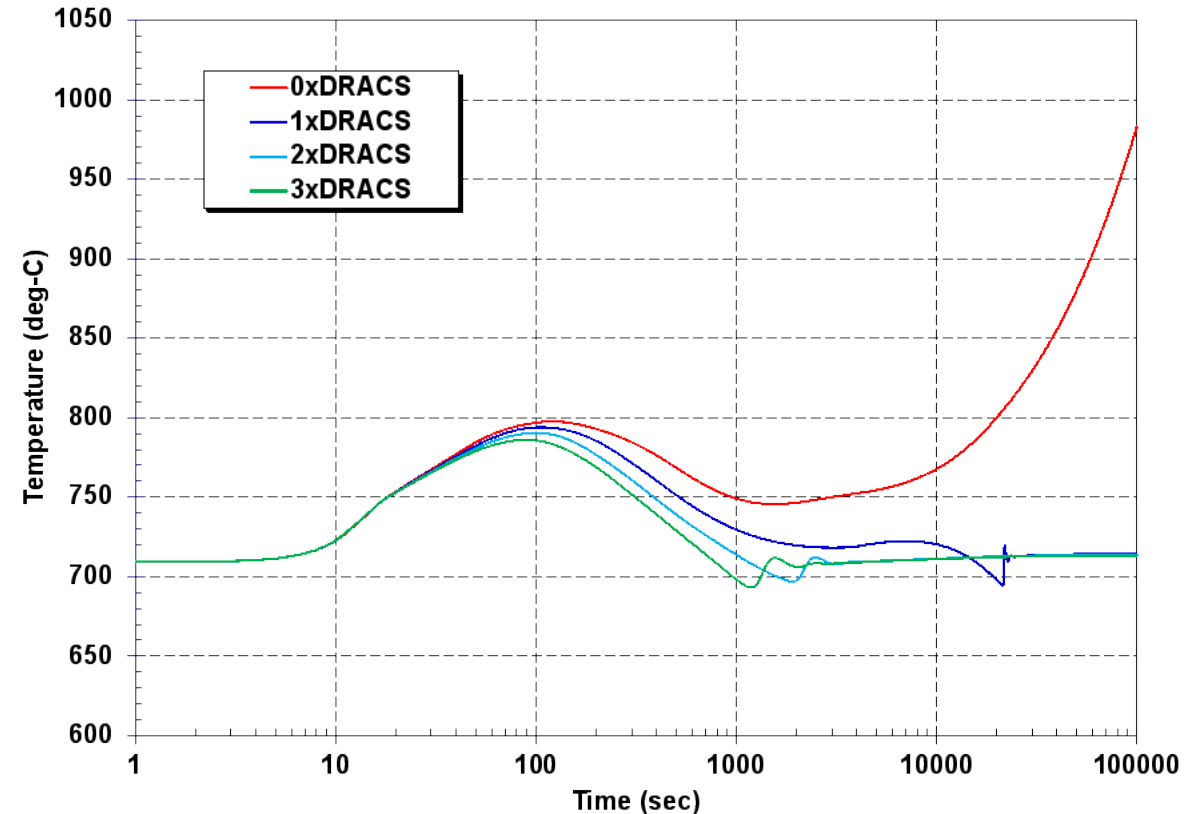
Long-term fuel temperatures are similar except for the 0xDRACS case

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

Fuel Temperature Feedbacks into Reactivity Model



Fuel Temperature Feedbacks into Reactivity Model



* Power response does not include xenon transient

Station Blackout

Loss-of-onsite power with SCRAM

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

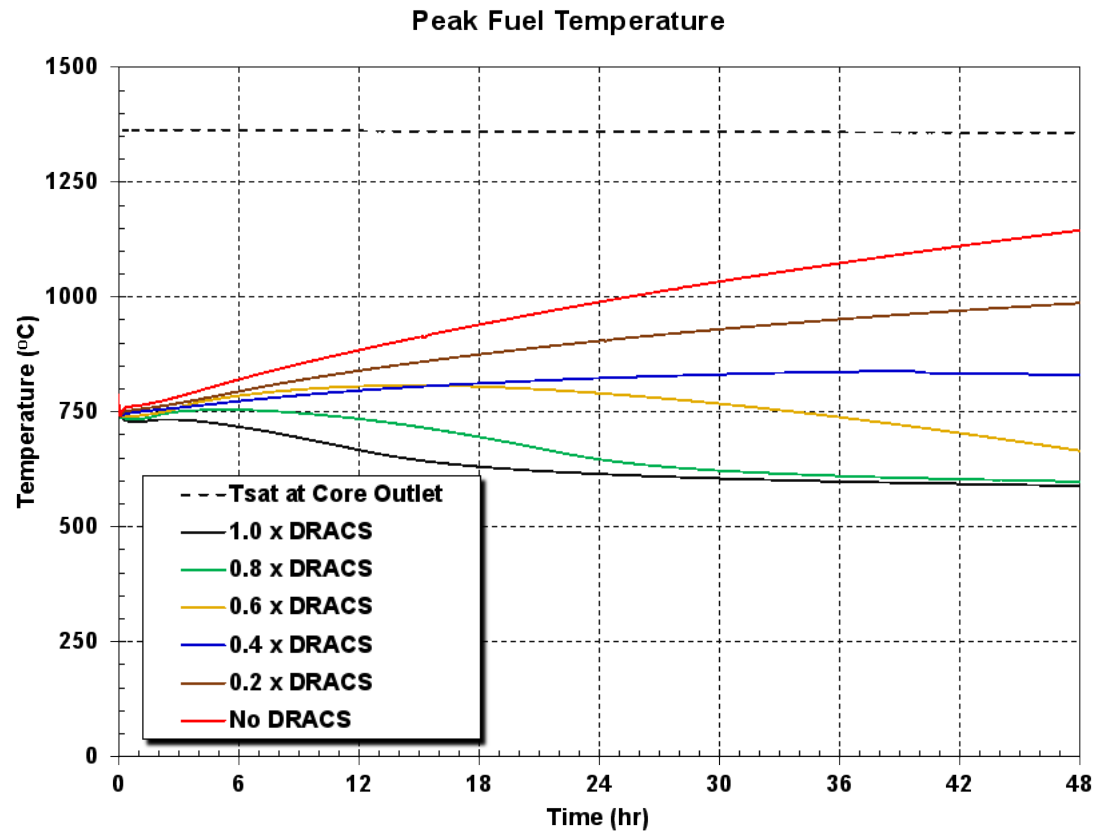
Unmitigated sensitivity case

- No DRACS and extended calculation to 7 days

SBO results (1/3)

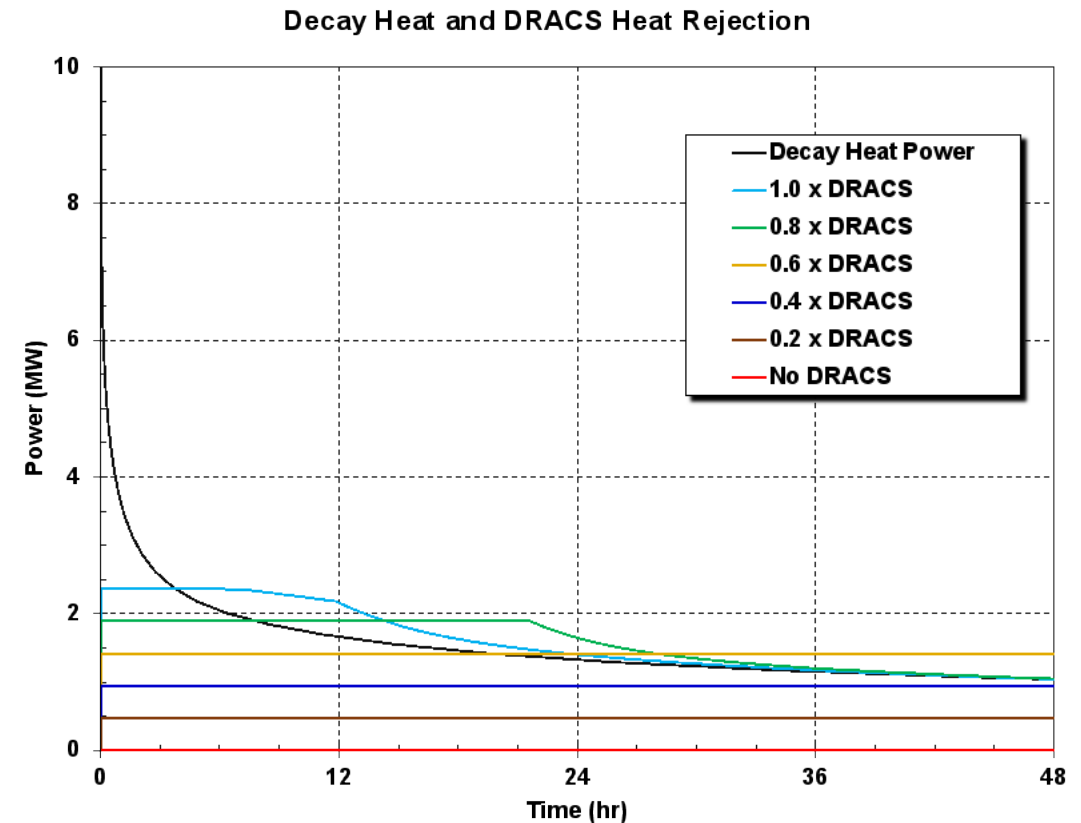
DRACS cases illustrate degraded response

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



DRACS power follows heat removal requirements

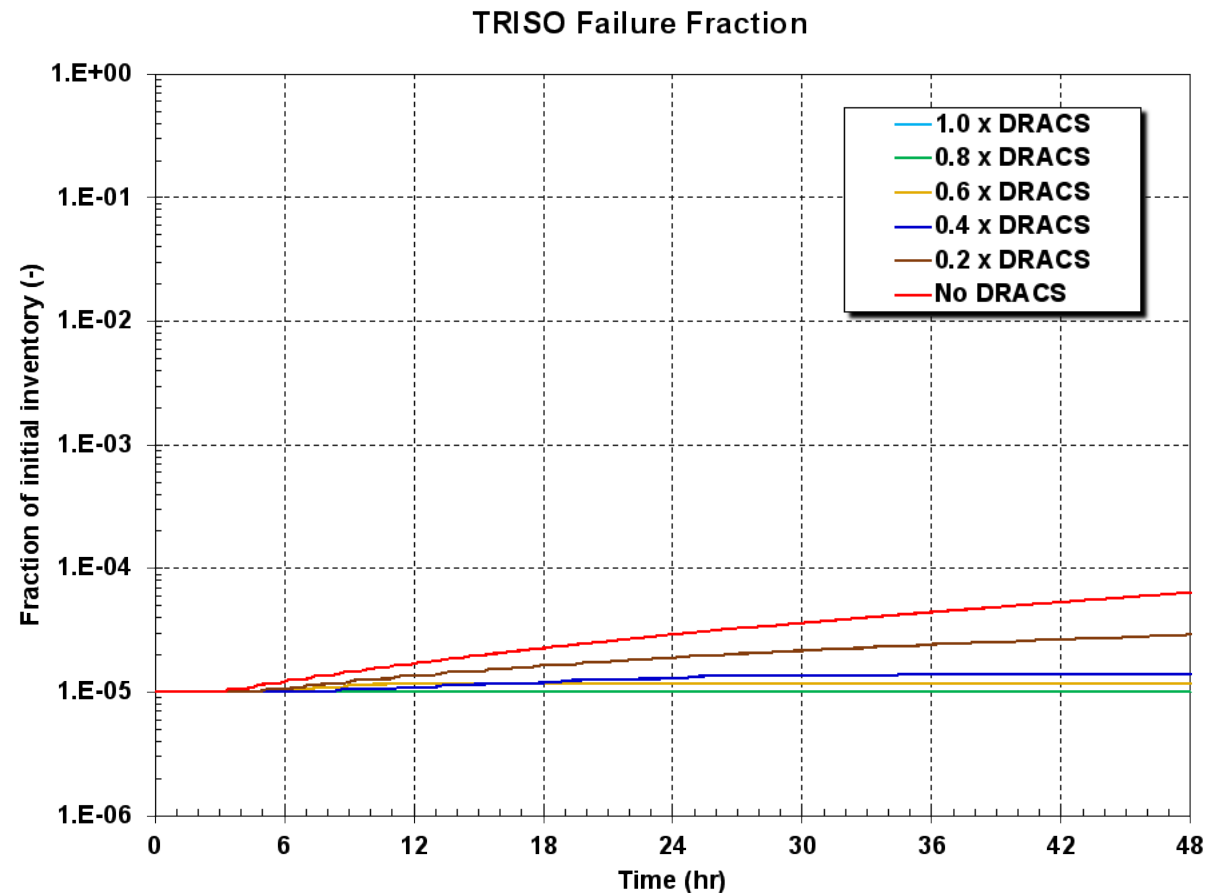
- 1xDRACS exceeds decay heat within 3 hr



SBO results (2/3)

The TRISO failure fraction remains low (1×10^{-5}) in the LOPA with one DRACS operating *

- Higher TRISO failures were calculated as the DRACS degrades

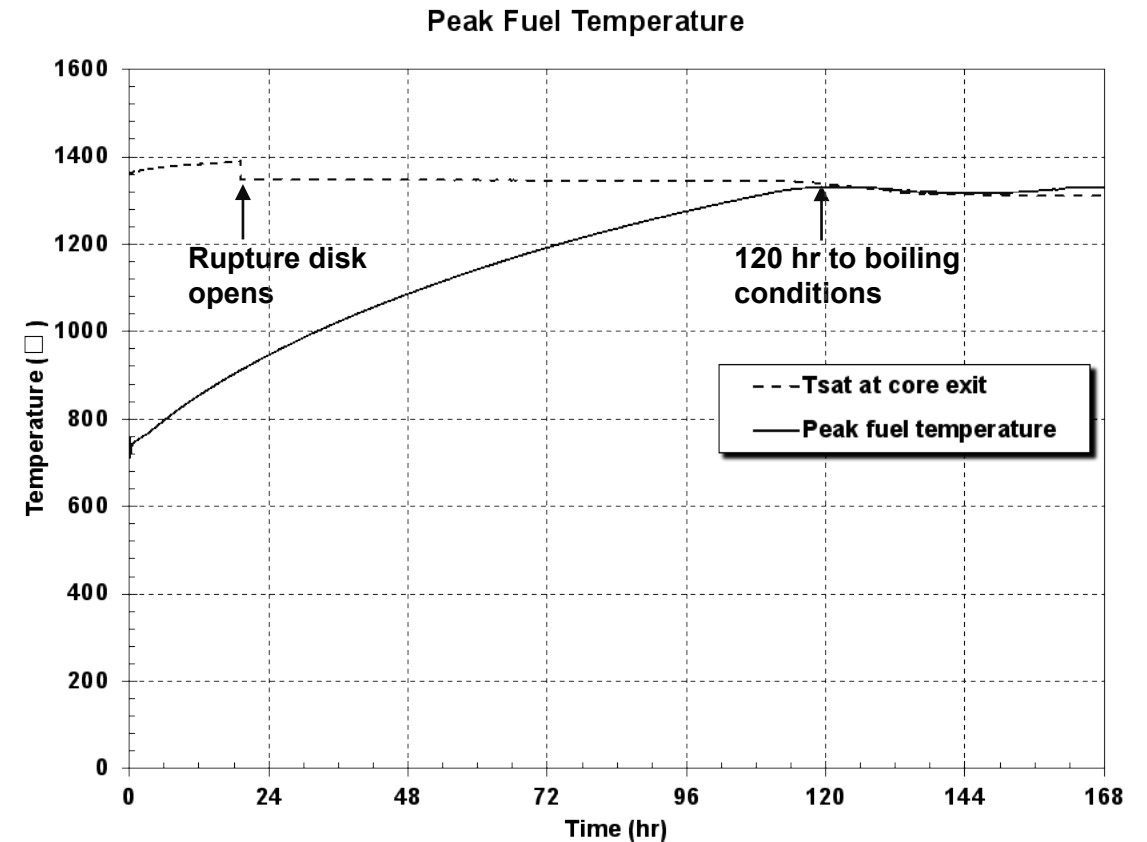
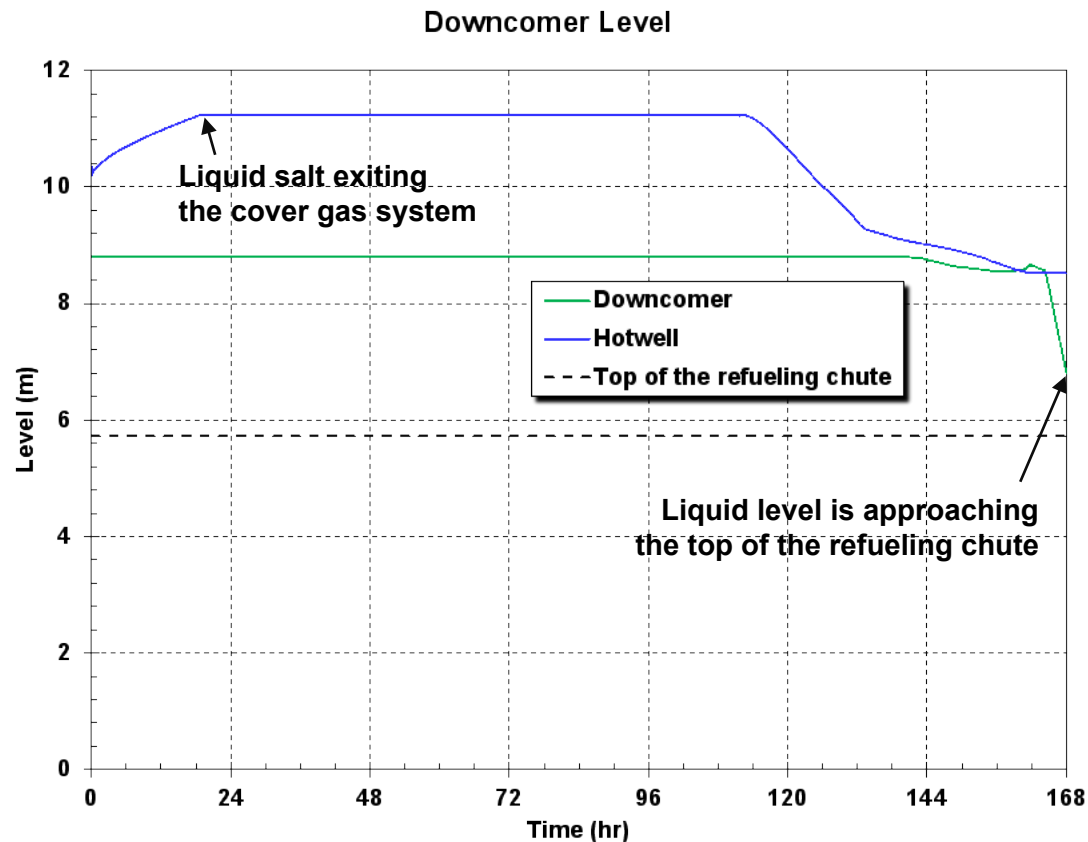


* UCO TRISO thermal failure characteristics were not available, so UO_2 TRISO diffusivity and UO_2 failure data were used. Both are changeable through user input with design-specific data.

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)



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

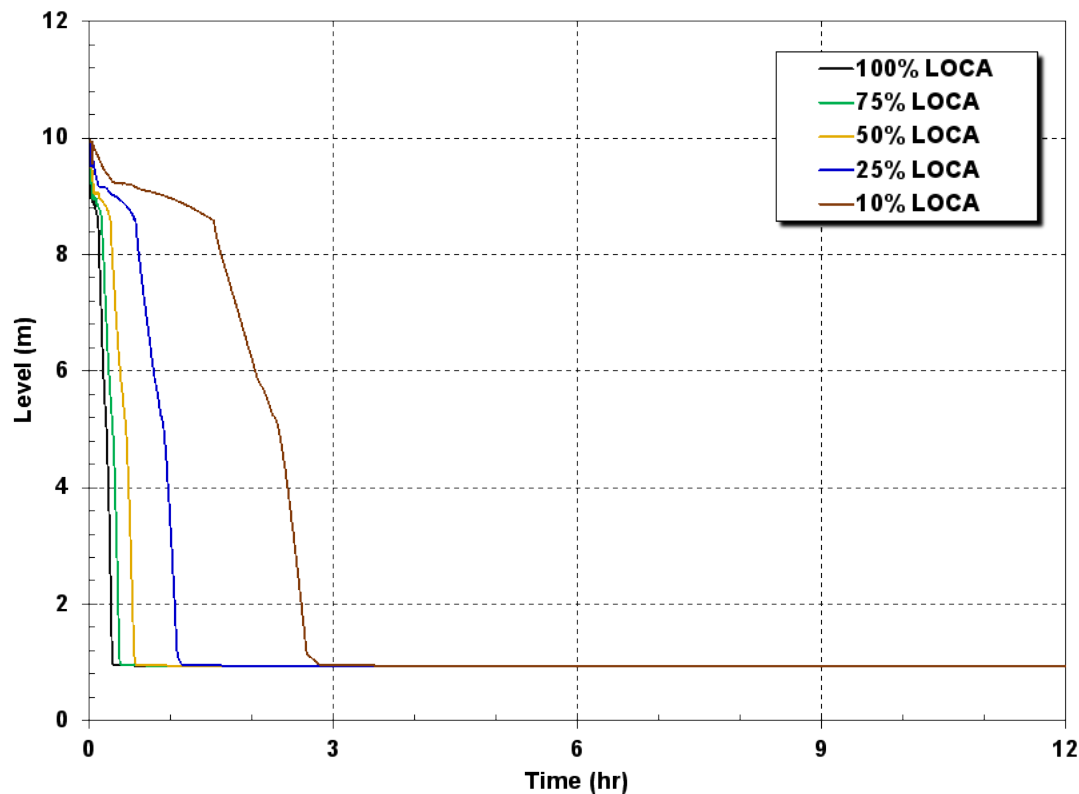
LOCA results (1/6)

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

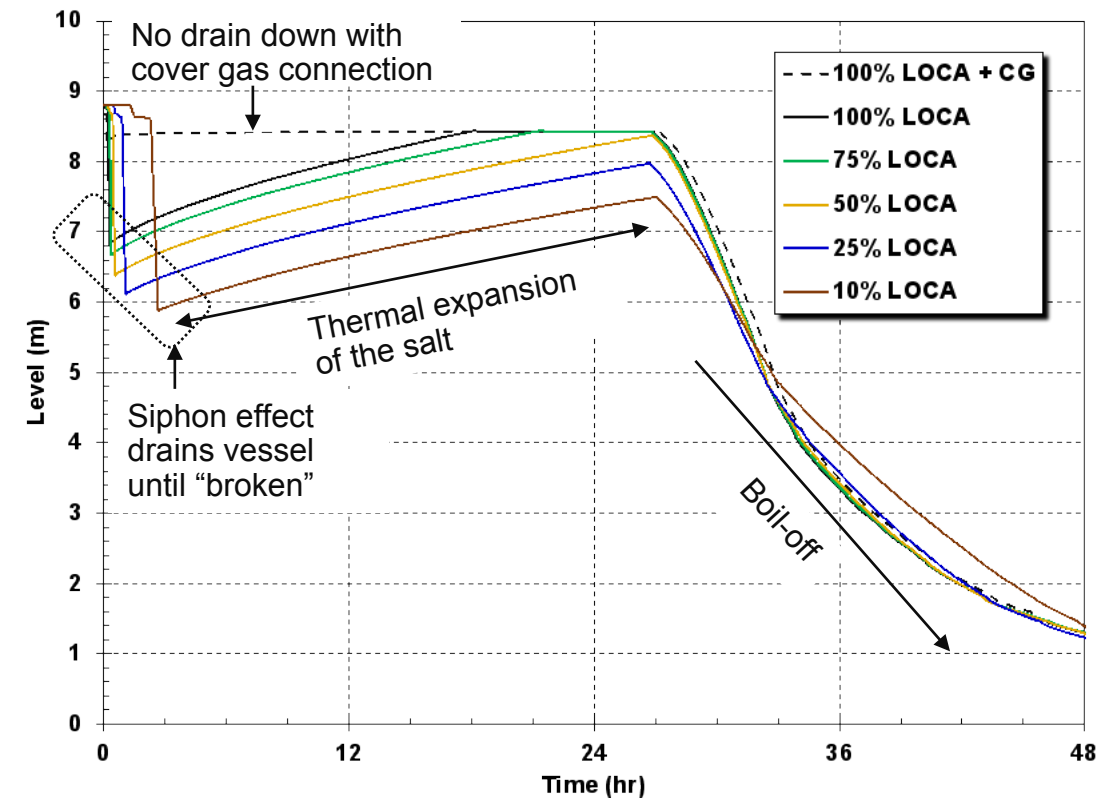
Cover gas connection (+ CG) between hotwell and standpipe prevents siphon

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

Standpipe Level



Downcomer Level



LOCA results (2/6)

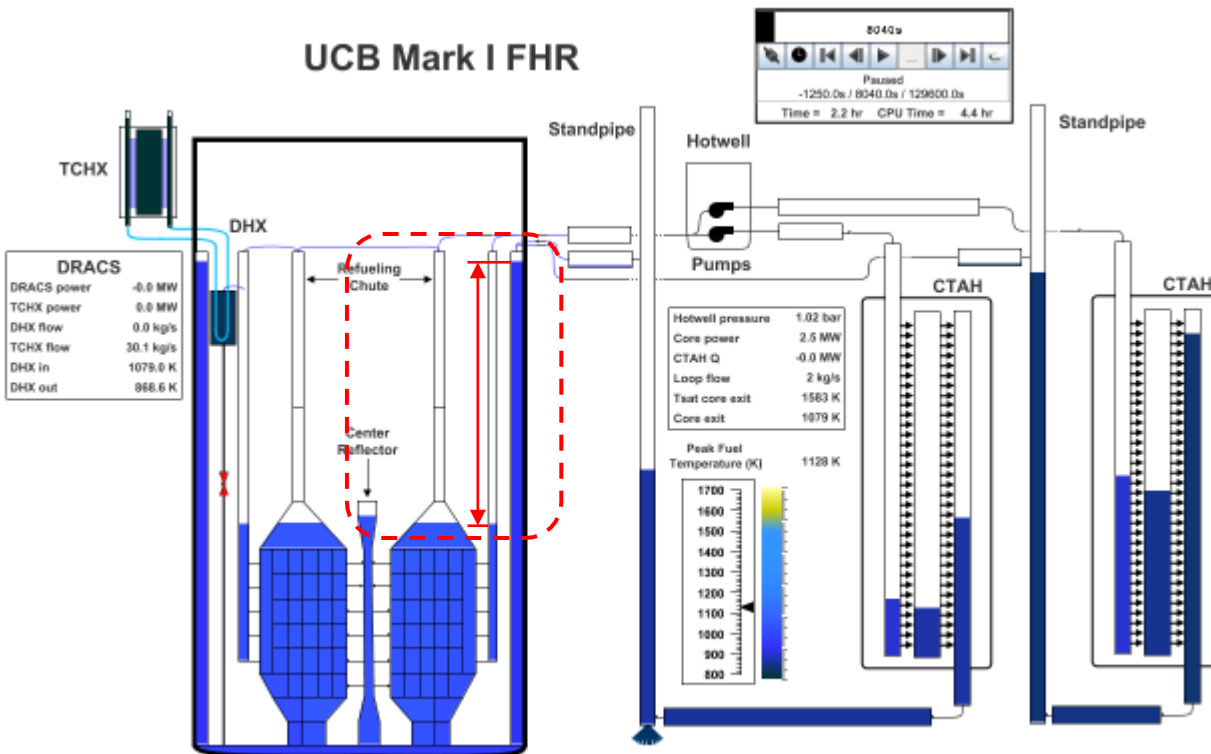
Liquid drain down initially creates siphon and then low pressure region

- Level difference between the core and downcomer

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

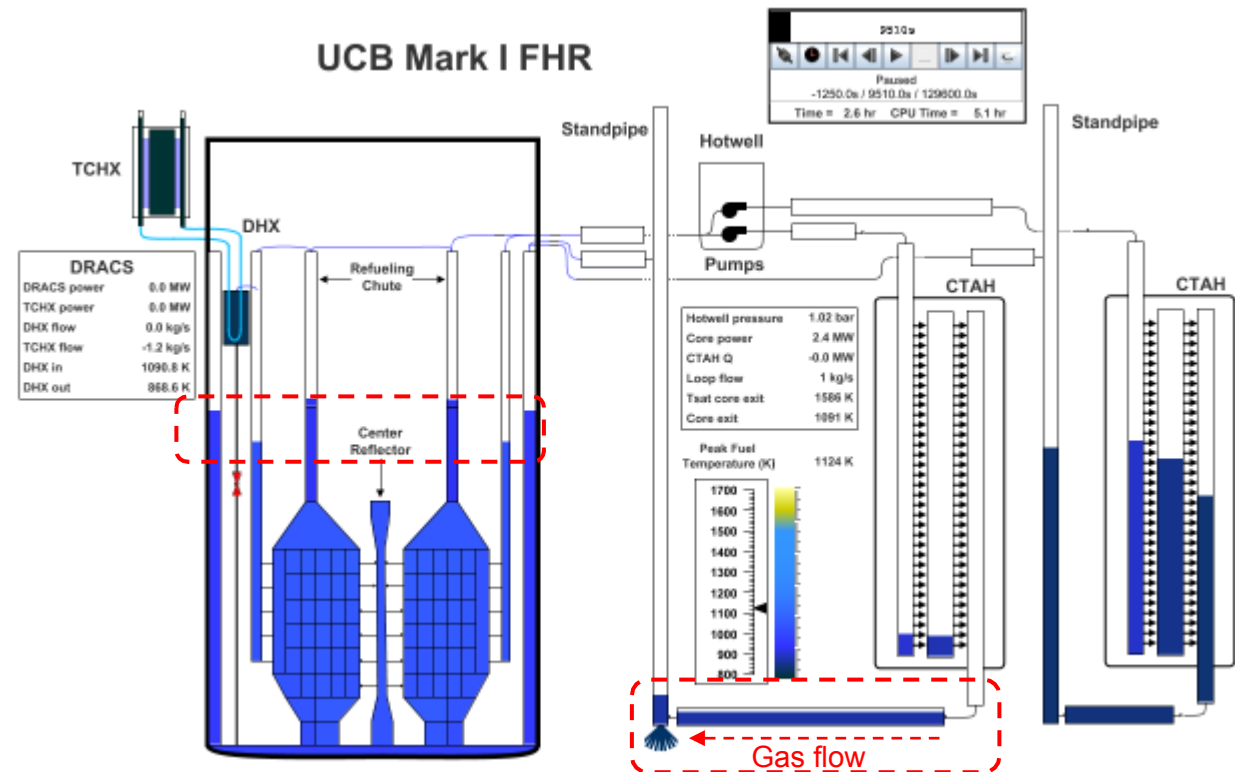
- Standpipe connections to the cover gas system are closed

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10% LOCA at maximum point in the "siphon"

UCB Mark I FHR



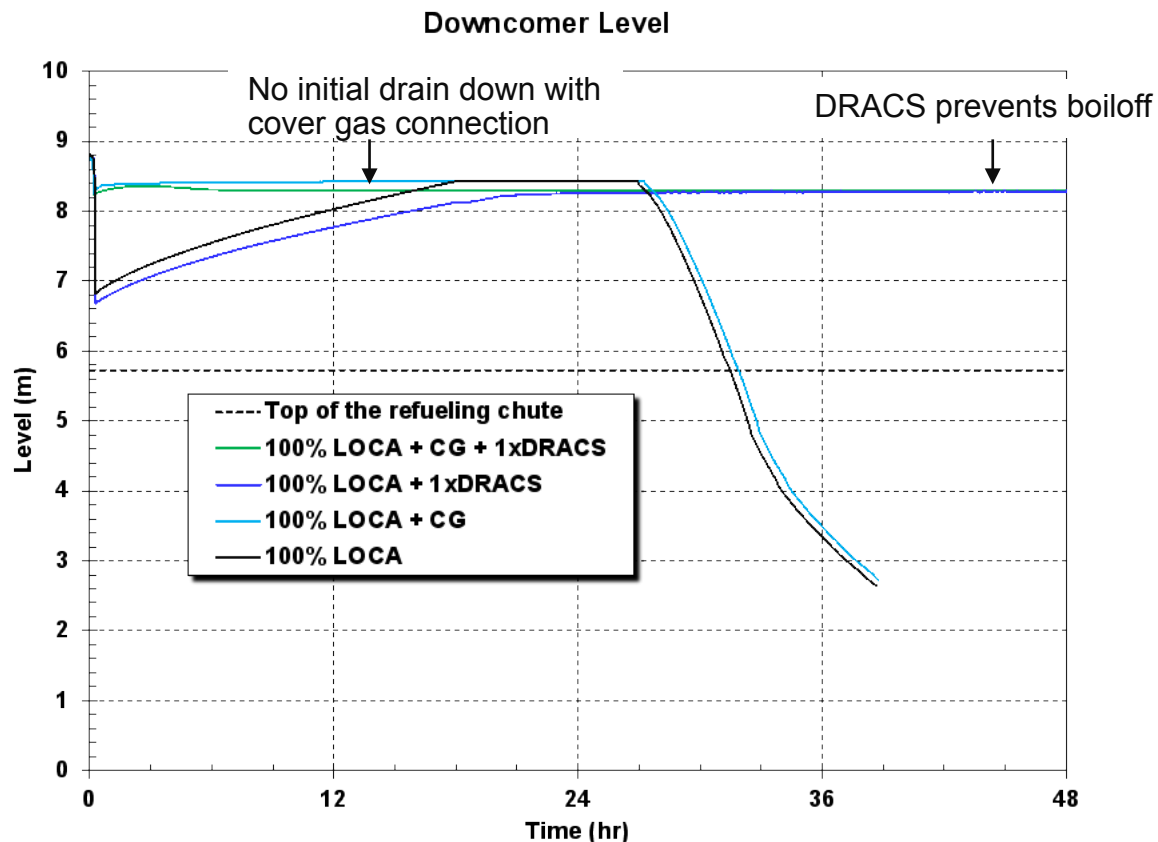
10% LOCA after equilibration

LOCA results (3/6)

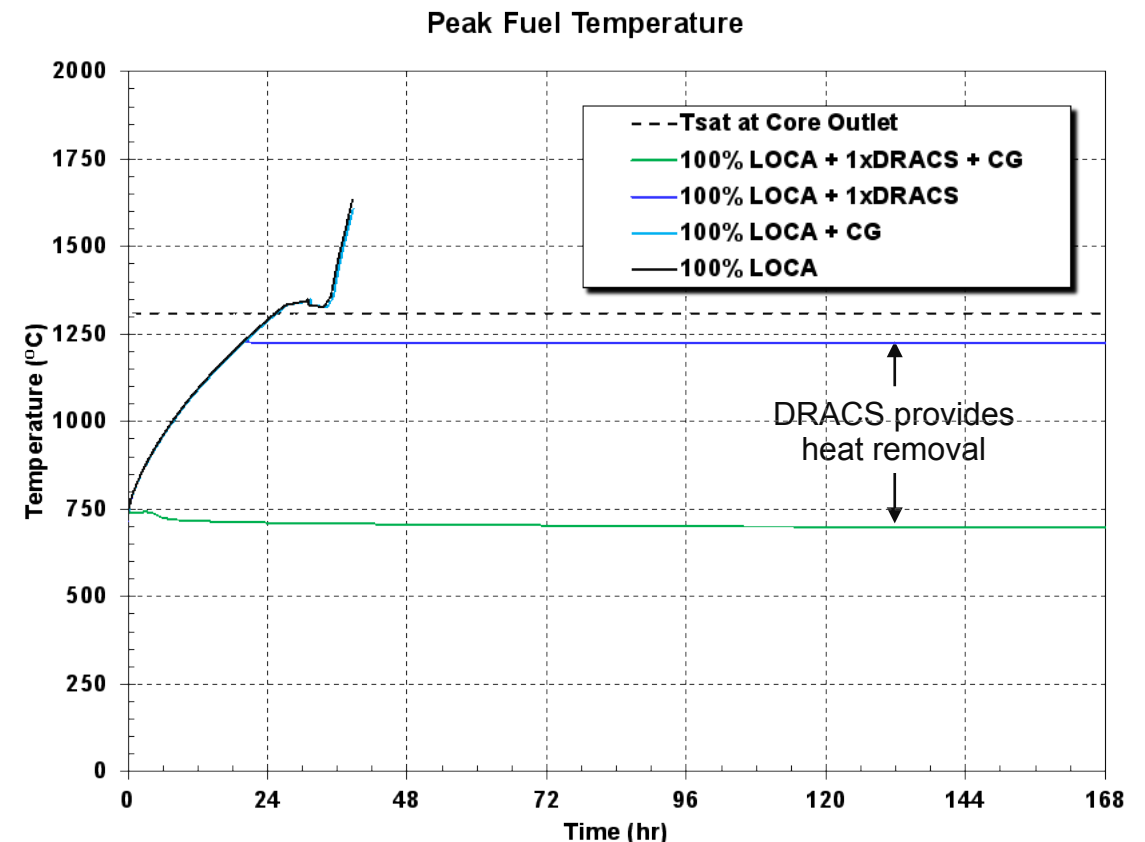
LOCA cases without DRACS proceed to fuel uncover at ~31 hr

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

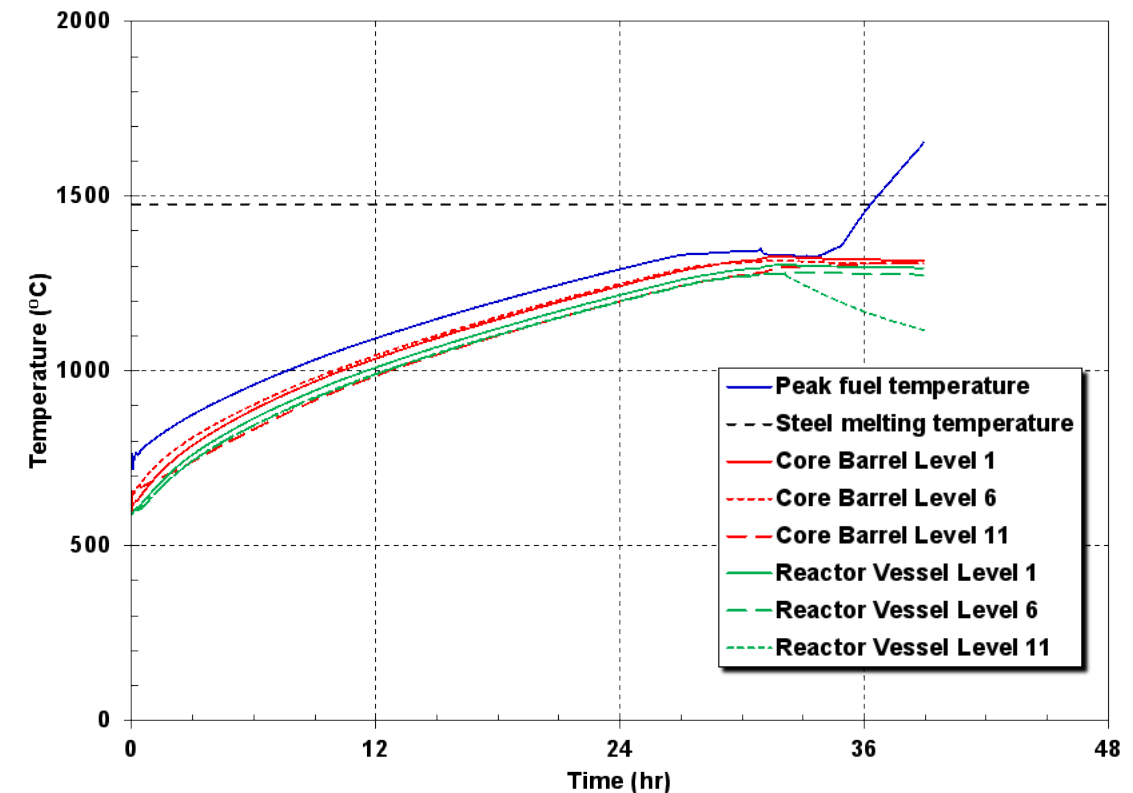
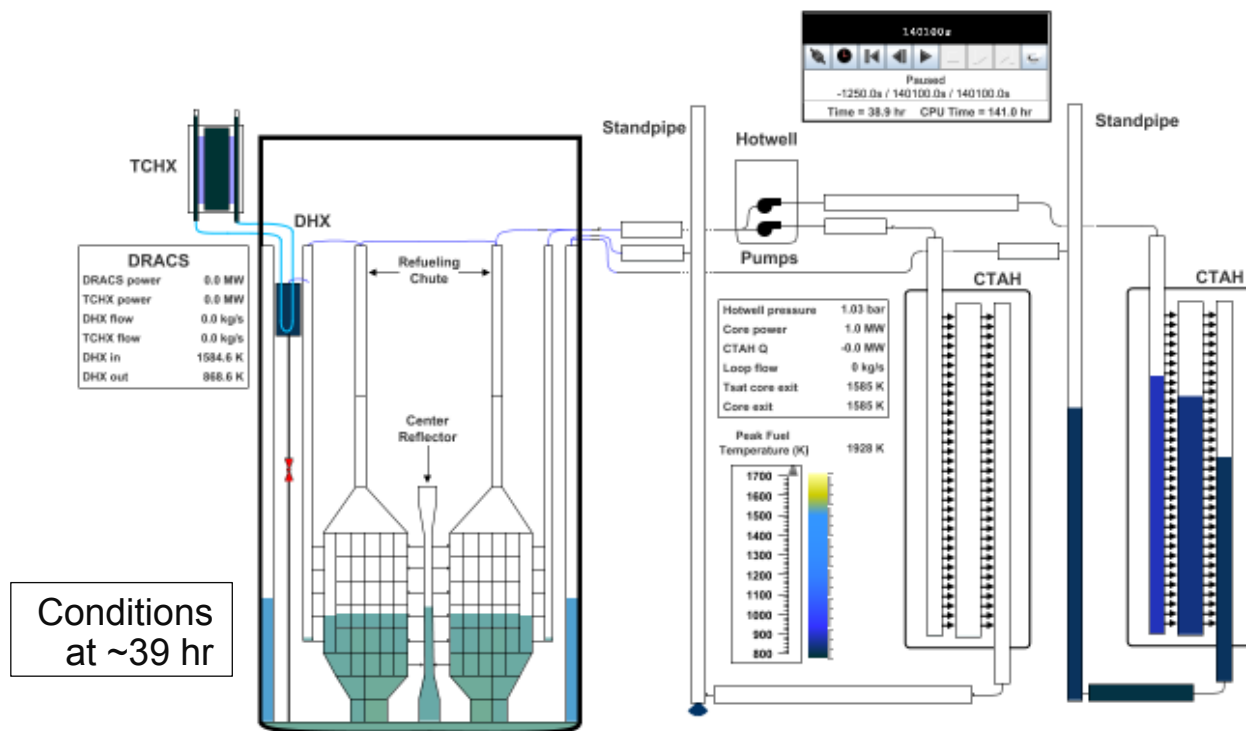


100% LOCA cases

LOCA results (4/6)

We terminated the calculation at ~?? hrs, when the fuel kernel melting starts

- Reactor vessel wall below steel melting temperature
- Upper core barrel (level 6) reaches the steel melting temperature
- Residual molten salt keeps the bottom level (level 1) at T_{sat}
- Pebbles and reflectors below graphite sublimation temperature (3600°C)

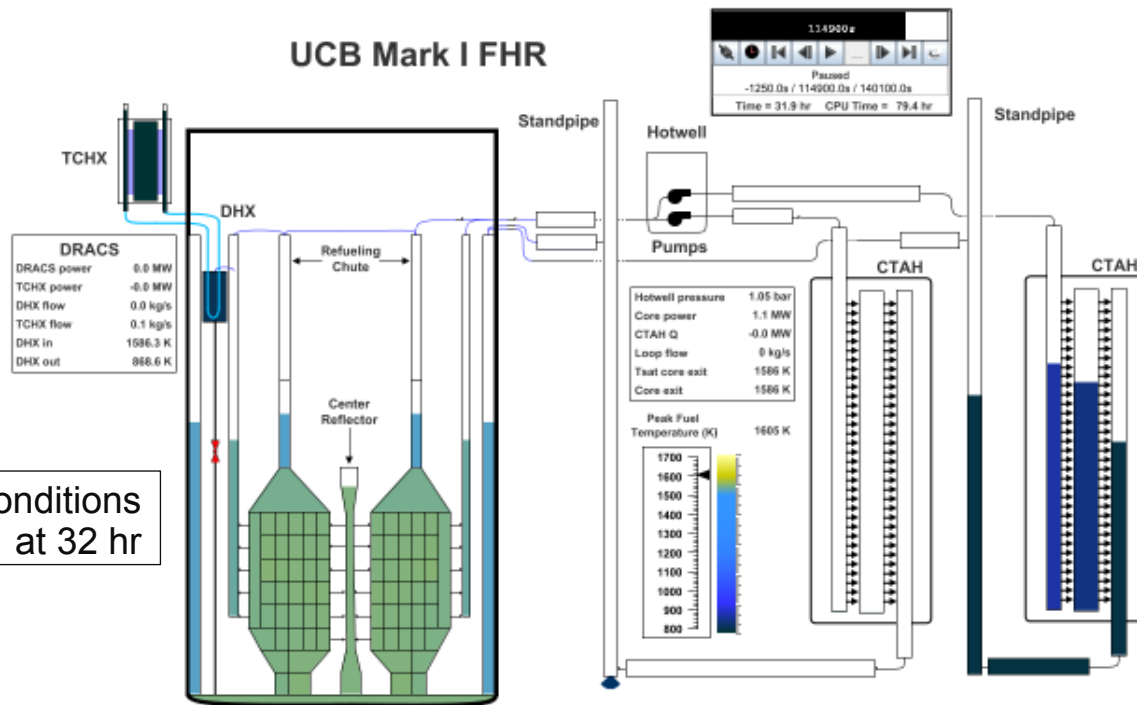


LOCA results (5/6)

TRISO failure rate extrapolated from available UO_2 TRISO data

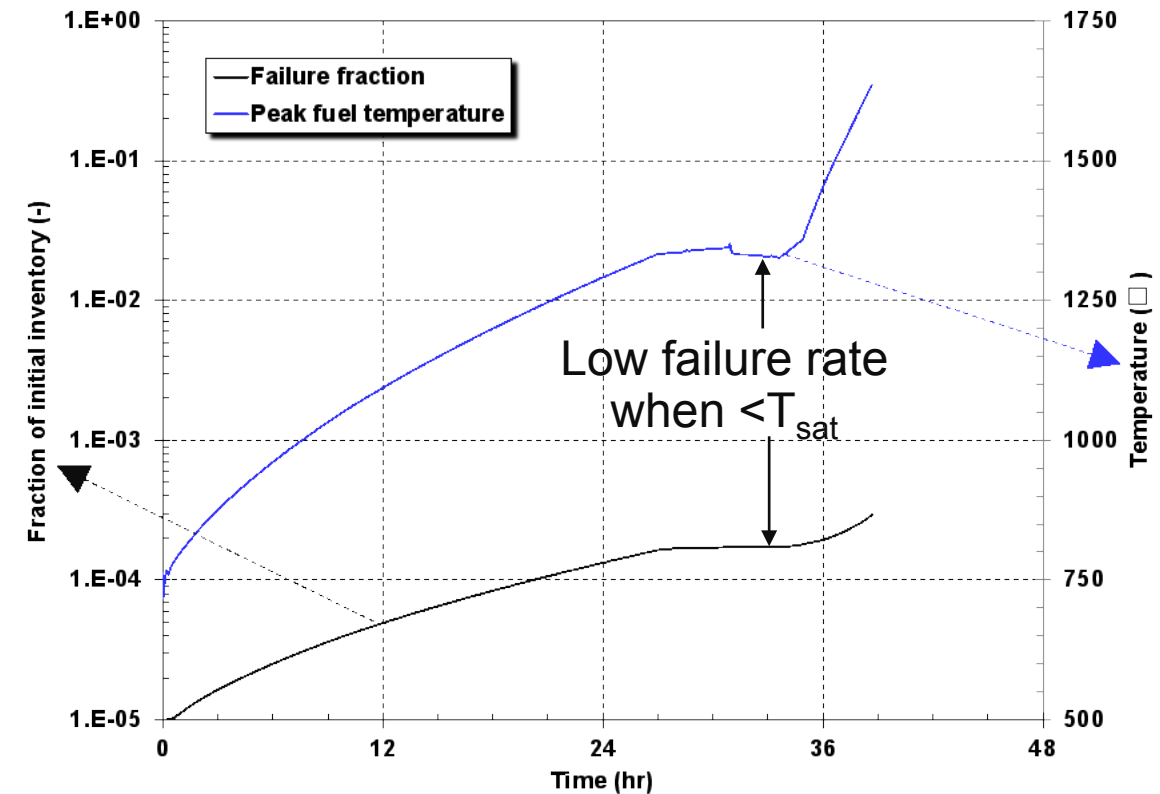
- Correlation is based on data to 1800°C
- Initial failures set to 10^{-5}
- 1.7×10^{-4} of the TRISOs failed at 32 hr
- ?% of the TRISOs failed by 48 hr

UCB Mark I FHR



Conditions
at 32 hr

TRISO Failure Fraction and Peak Fuel Temperature



Note:

** Fuel used thermal-physical properties of UO_2 .

LOCA results (6/6)

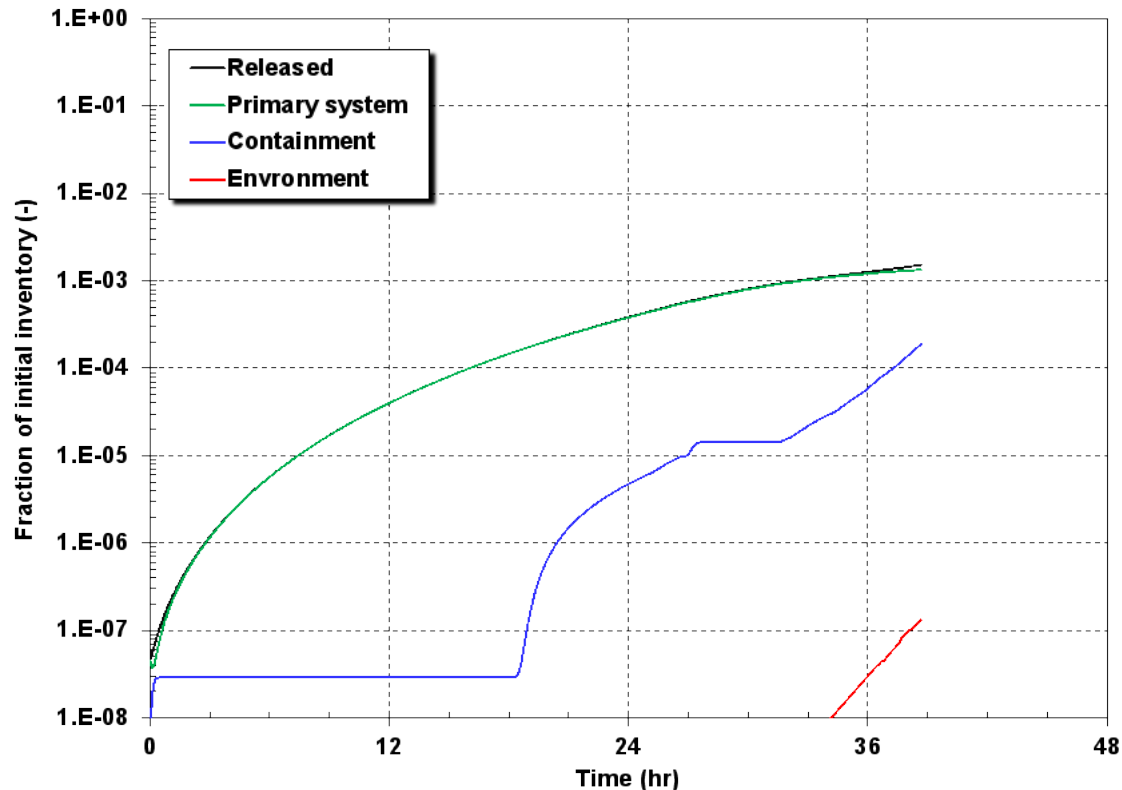
Most of the fission product release from fuel is retained in the containment

- Assumed hole size equivalent to 100% volume per day at 0.25 psig (8.7 in²)

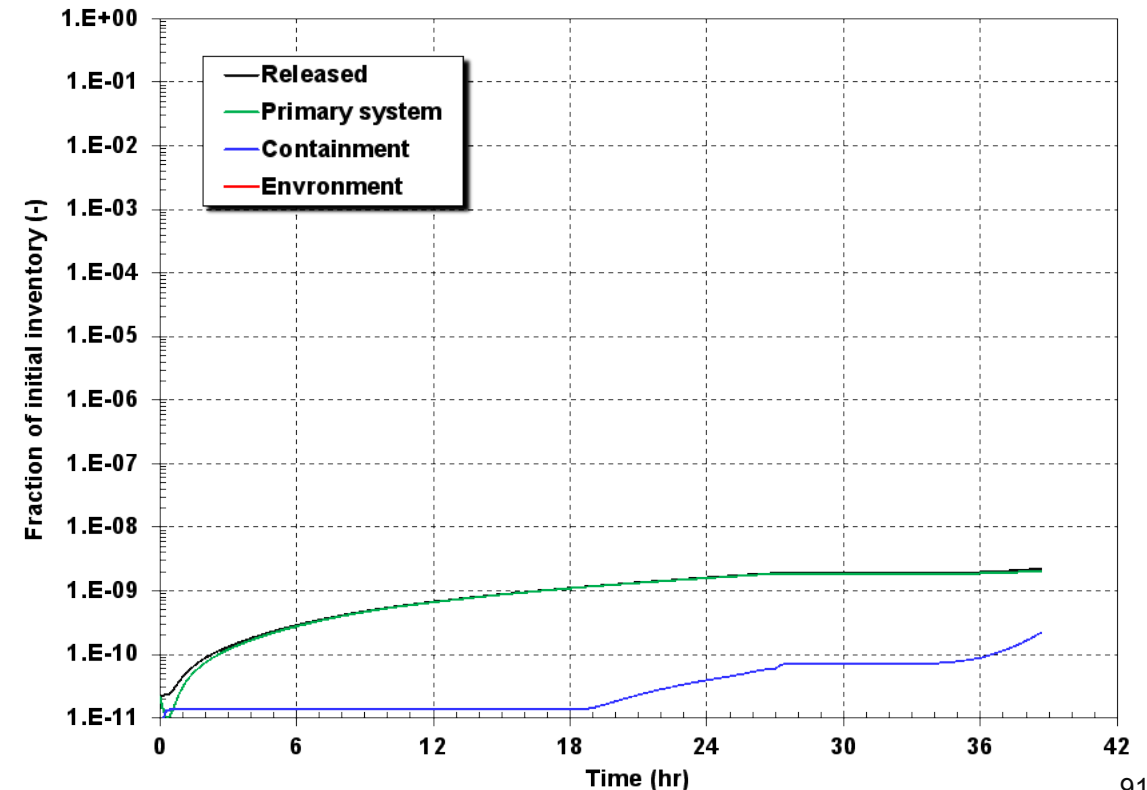
The radionuclide distribution is affected by the timing of the release from the TRISO

- Iodine release from the pebbles occurred later during the robust boiling phase
- Most aerosols leaving the primary system settle in the containment

Cesium Release and Distribution



Iodine Release and Distribution



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



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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 ³)	22.7	12.9	105.2	4.8	321.1
Fuel average surface heat flux (MWt/m ²)	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 ³)	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 ³)	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

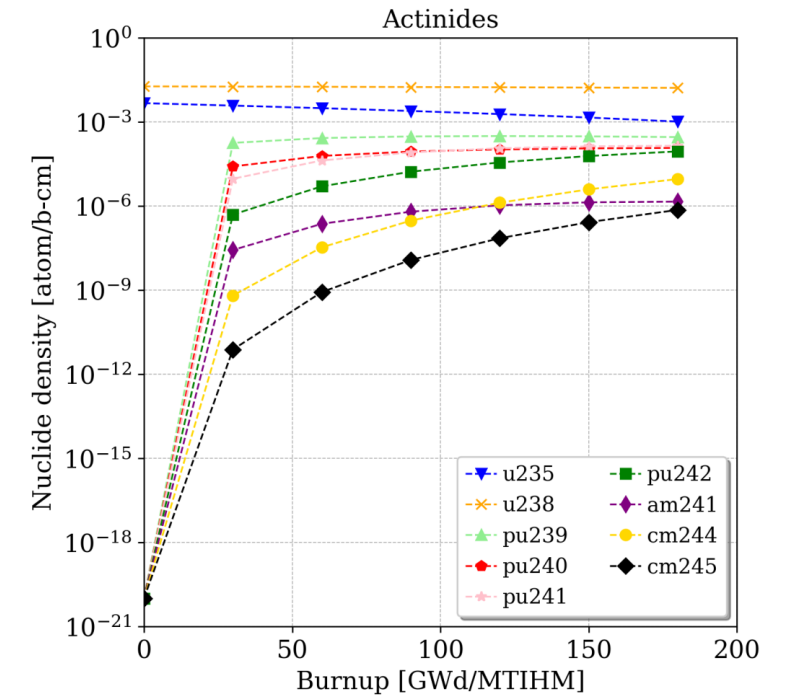
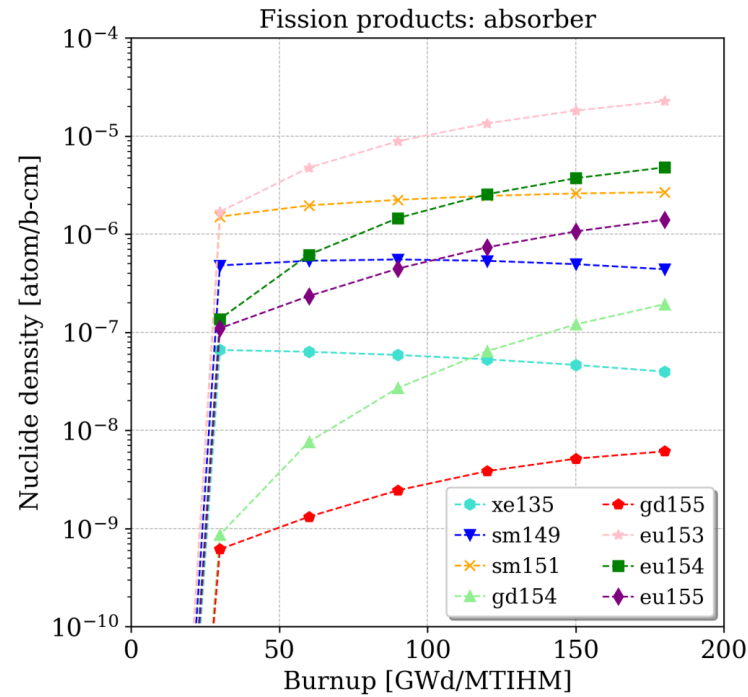
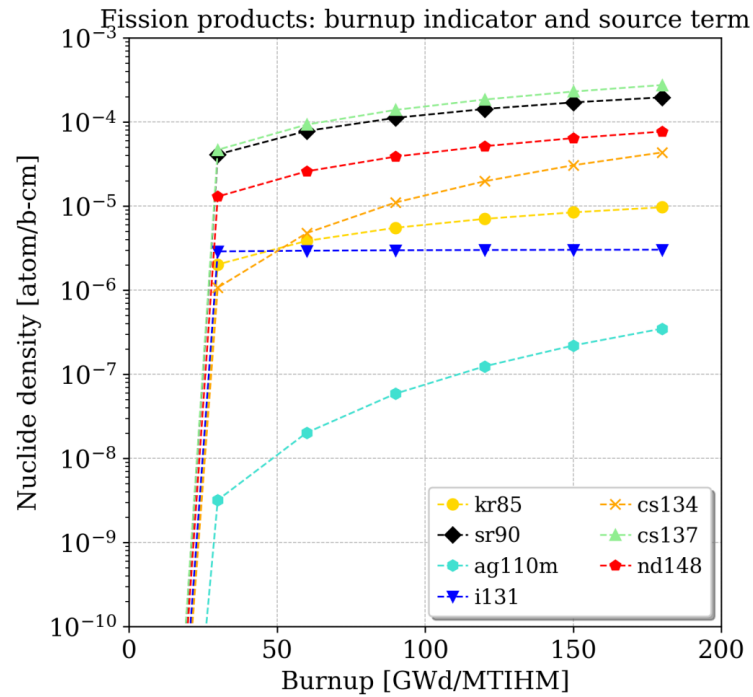
* End of Cycle (EOC) life value (fixed fuel) or equilibrium value (pebble fuel)

** 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.

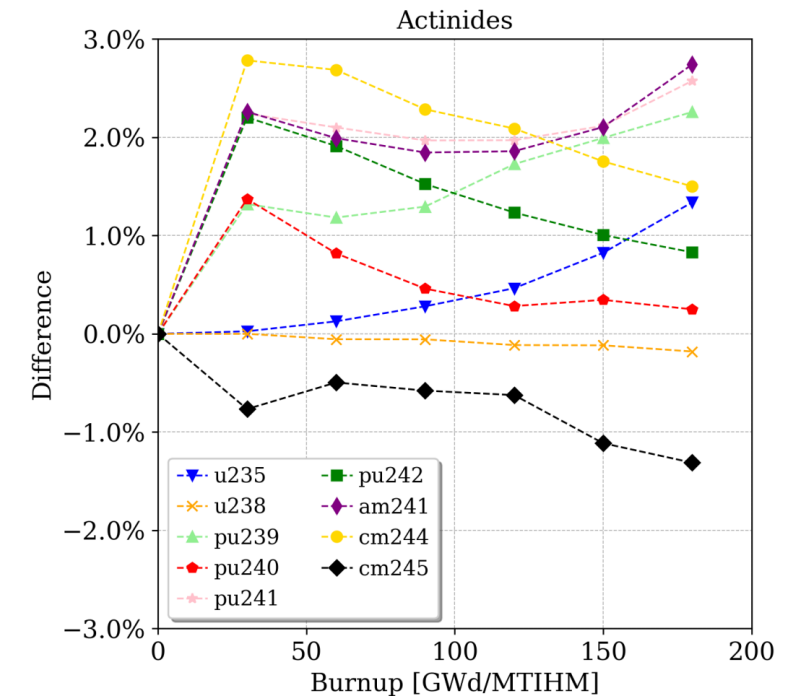
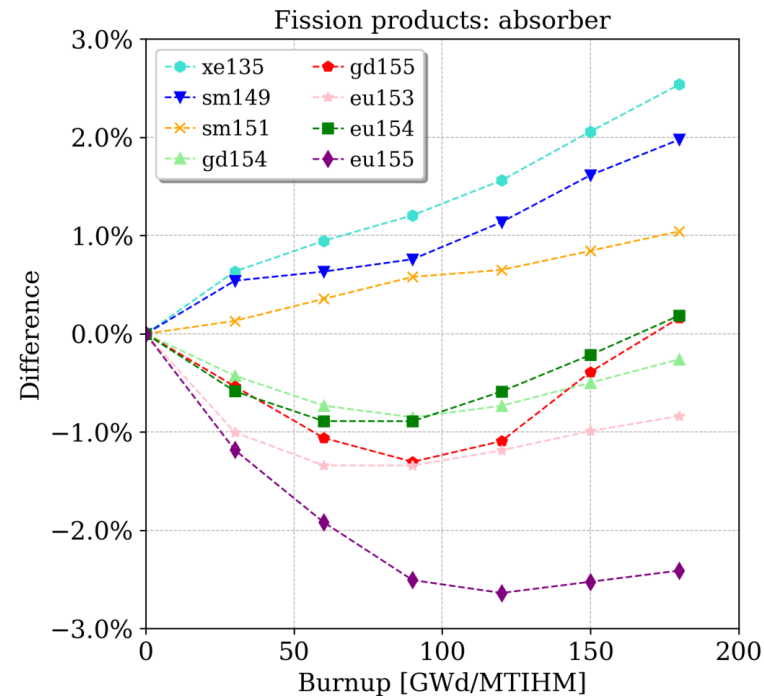
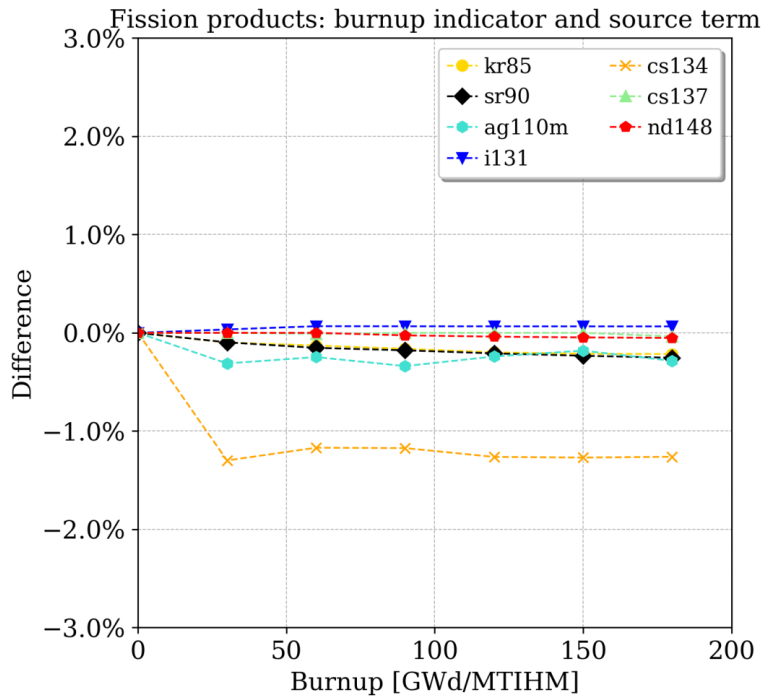
1. Single pebble nuclide density over depletion

CE random results:



1. Single pebble nuclide density comparison over depletion

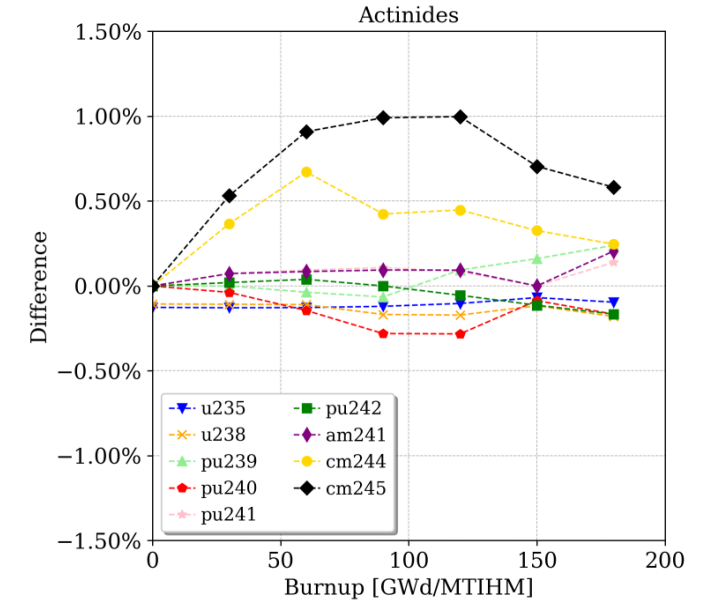
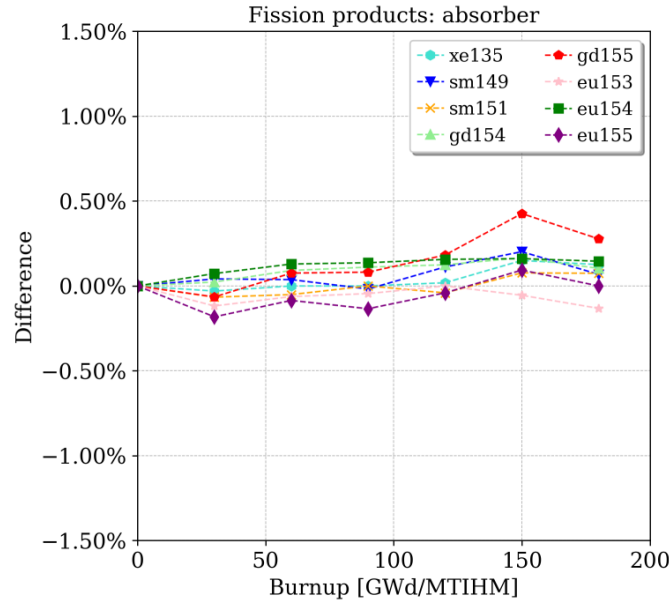
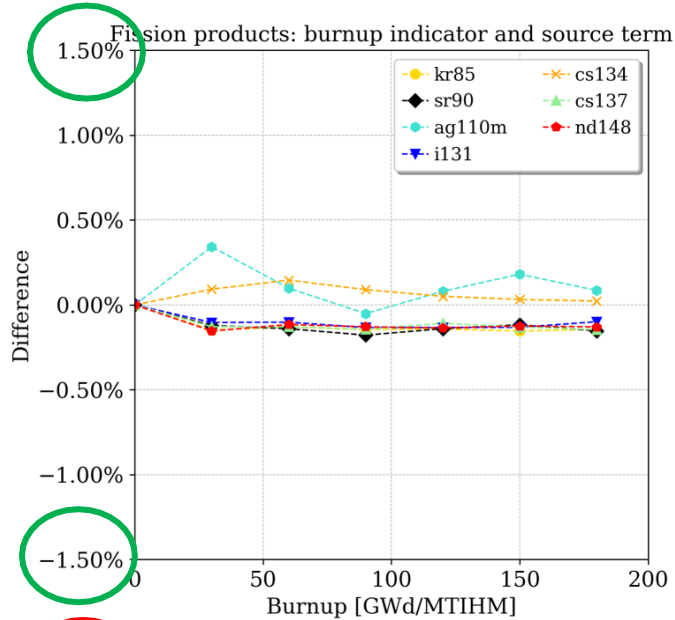
Comparison of MG against CE random:



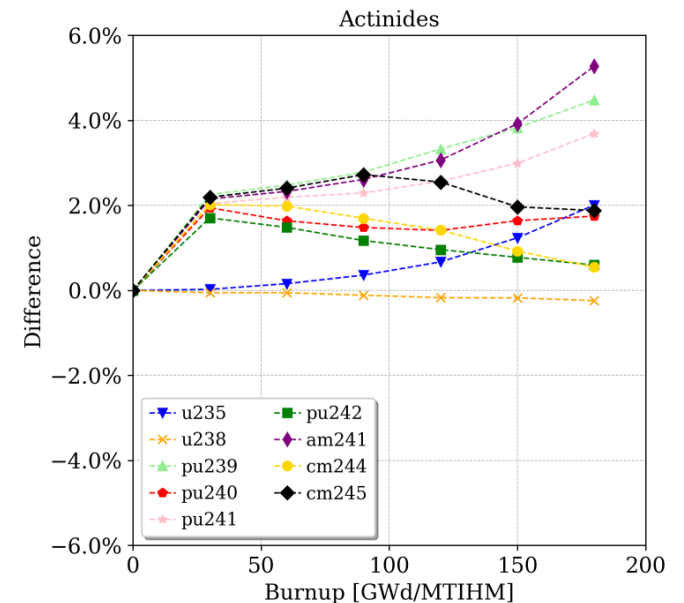
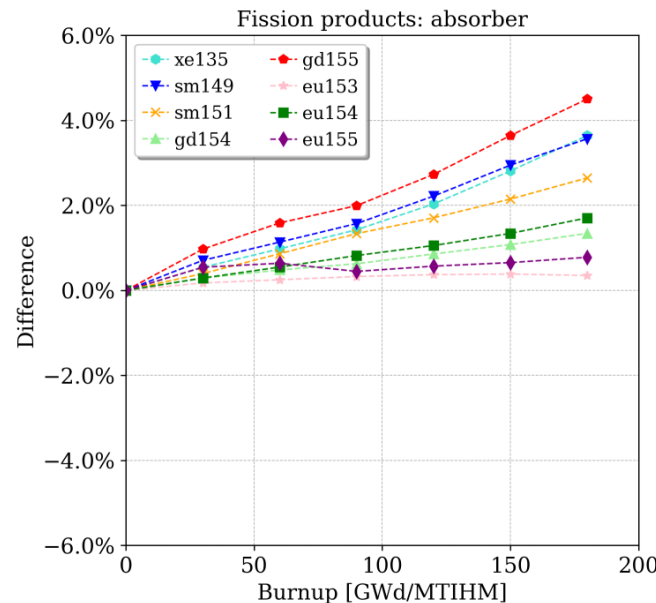
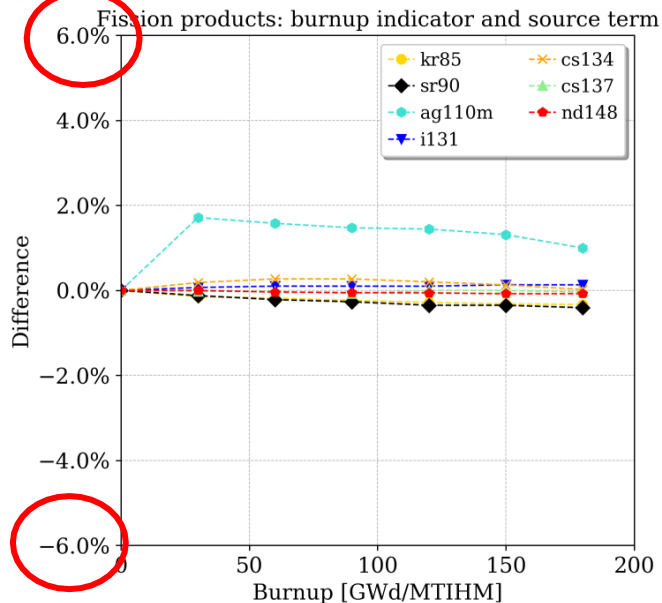
Result: MG bias remains below 3% for relevant nuclide densities over depletion

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

CE, lattice, unclipped



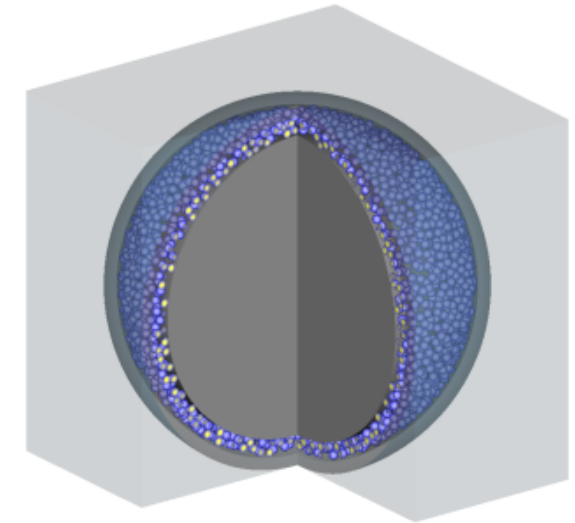
CE, lattice, clipped



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

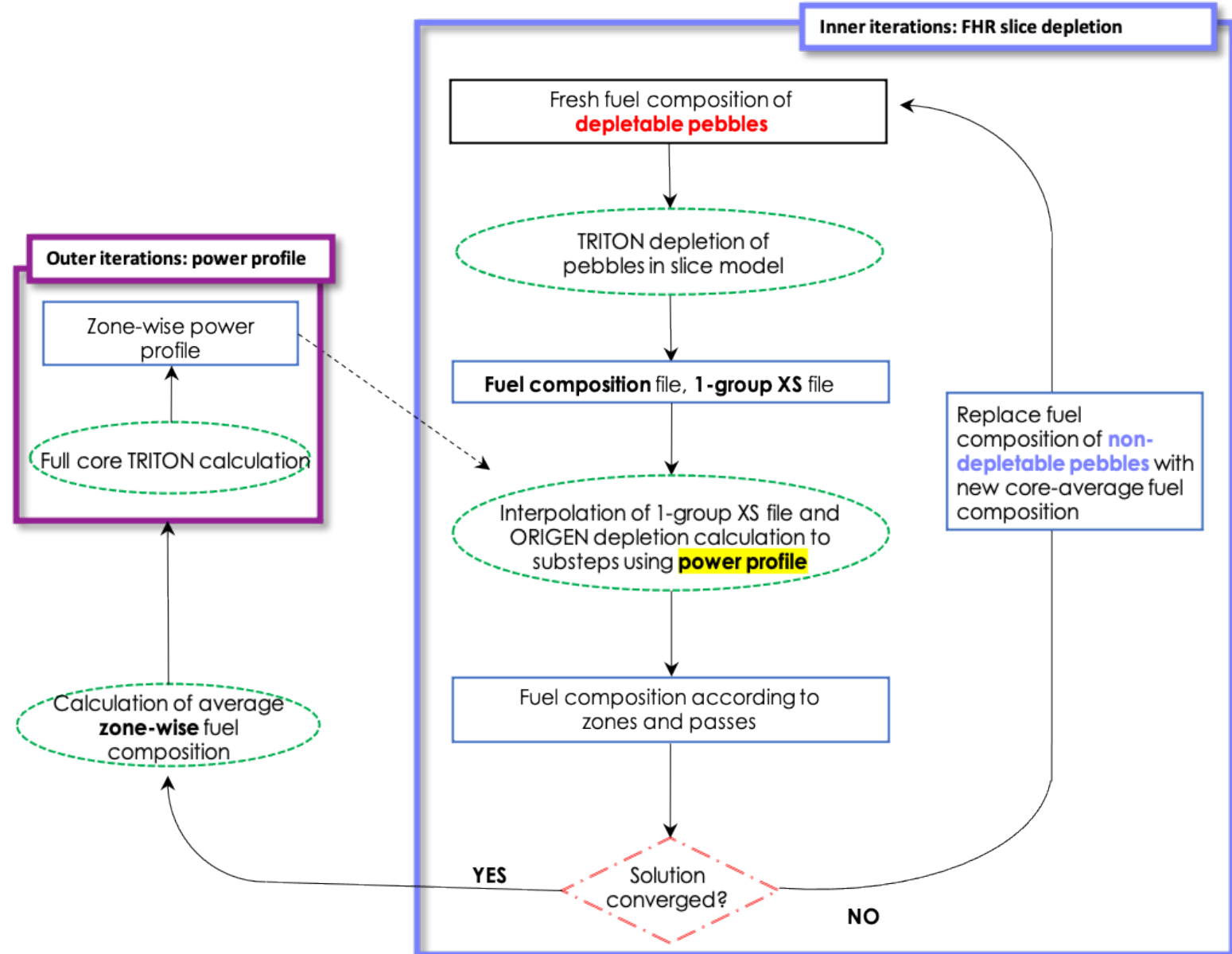


SCALE model a UCB Mark 1 pebble
in a cube surrounded by FLiBe

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)	$\frac{bu_{final}}{180 \text{ } GWd/tHM} - 1$	k_{eff}	$k_i - k_{i-1}$ (pcm)	$N_D^{235}U$ ($atoms/b-cm$)	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$	$N_D^{239}Pu$ ($atoms/b-cm$)	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$
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)	$\frac{bu_{final}}{180 \text{ } GWd/tHM} - 1$	k_{eff}	$k_i - k_{i-1}$ (pcm)	$N_D^{235}U$ ($atoms/b-cm$)	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$	$N_D^{239}Pu$ ($atoms/b-cm$)	$\frac{N_{D_i}}{N_{D_{i-1}}} - 1$
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

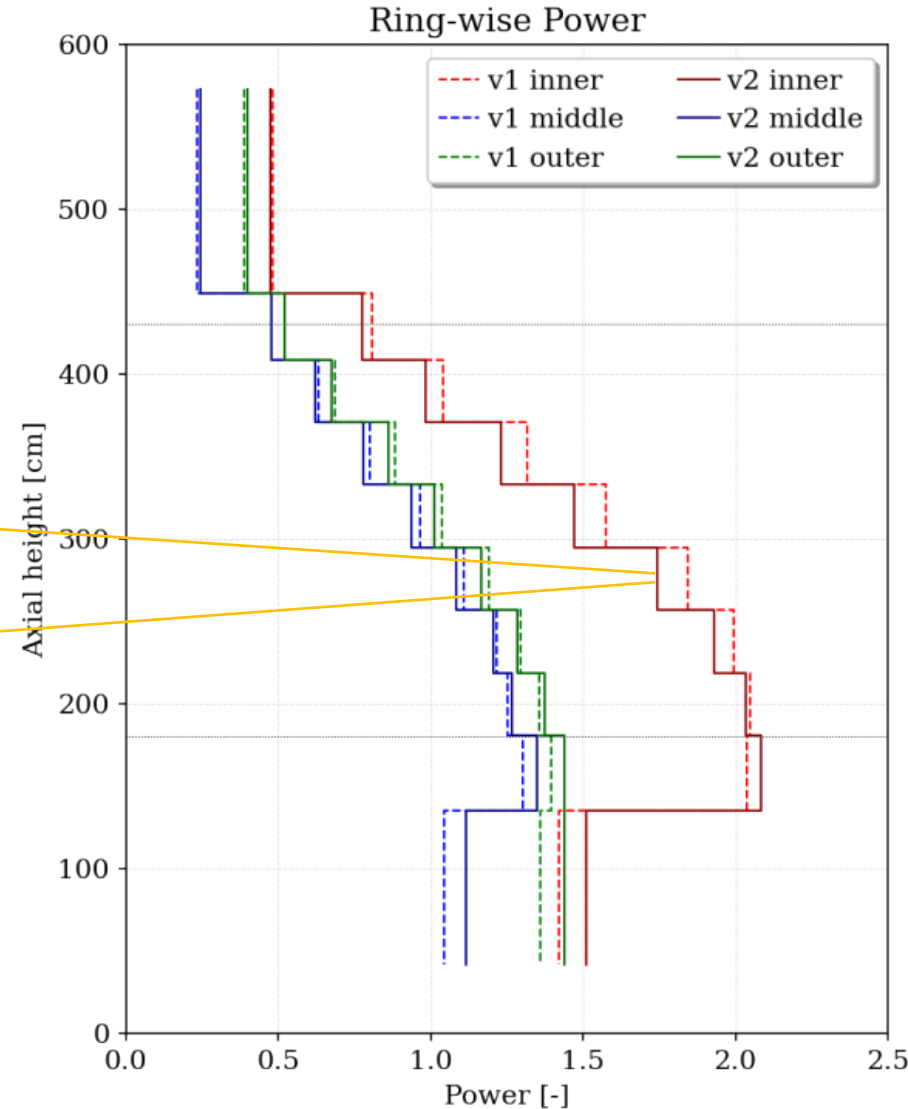
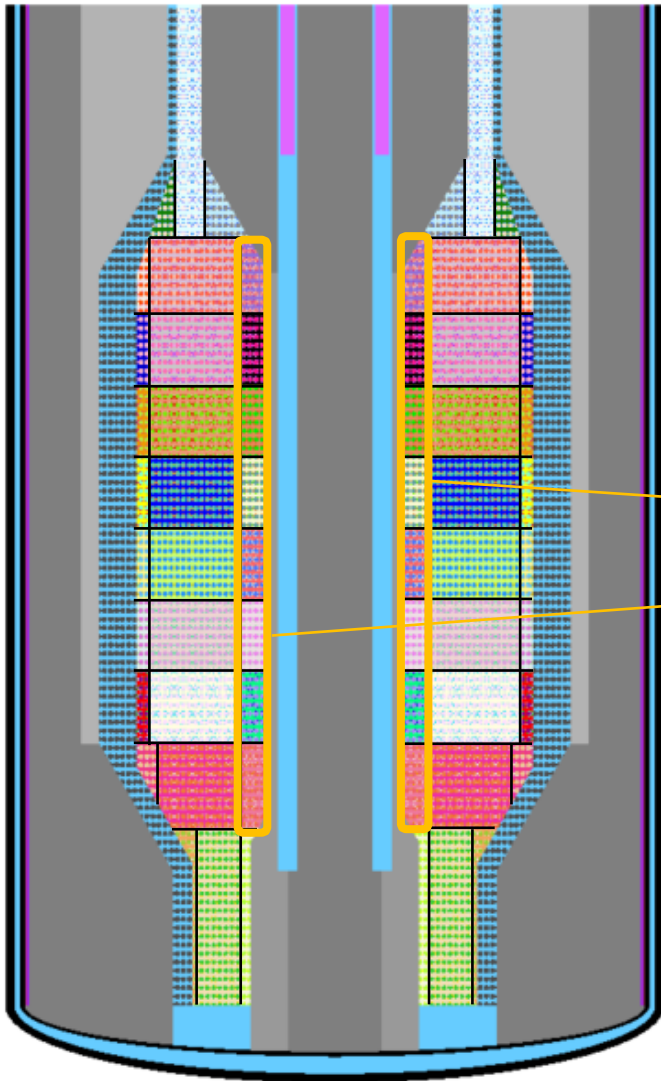
2. Comparison of final core average fuel compositions

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



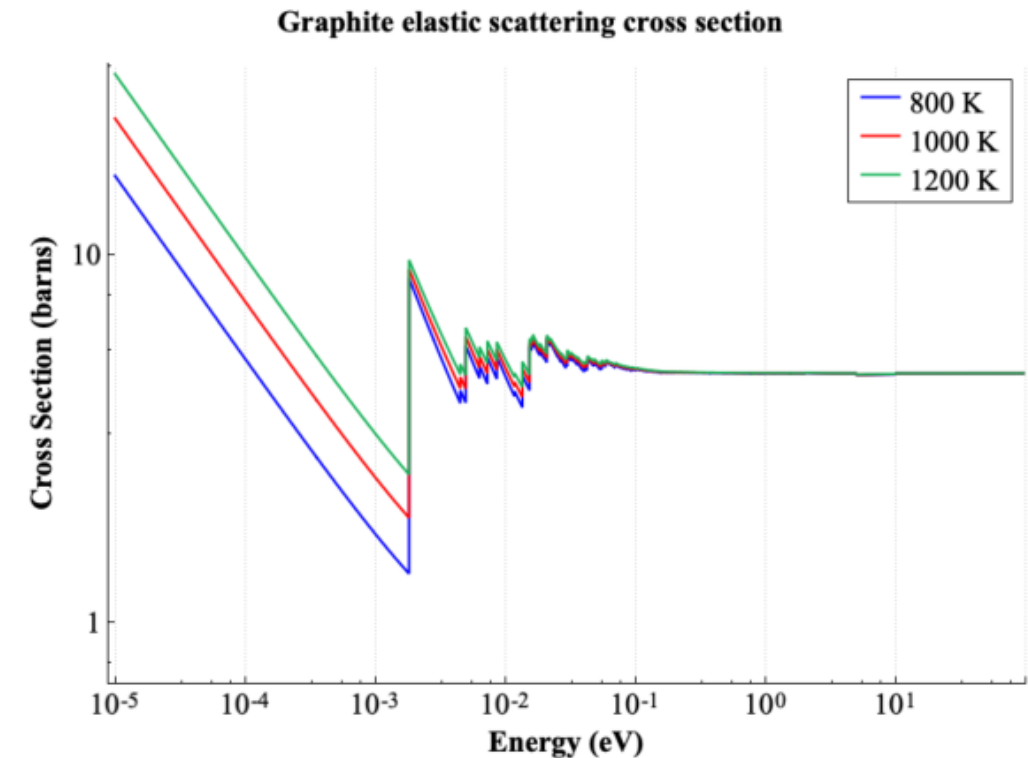
Results:

- 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 ρ to determine coefficient

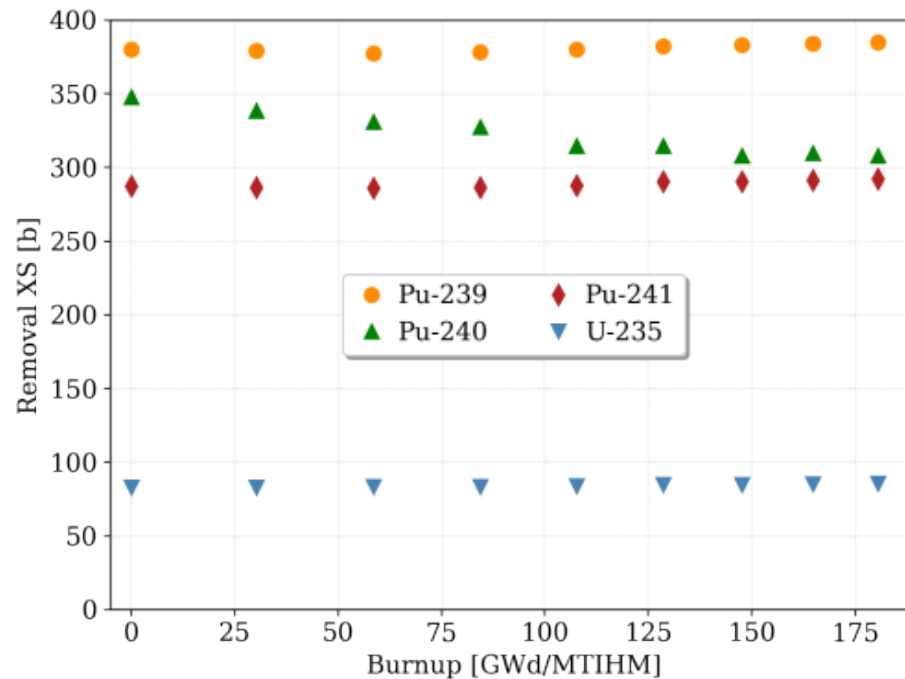
Component	Temperature Reactivity Coefficient [pcm/K]	
	Cisneros [1]	ORNL
Fuel	-3.8	-4.388
Salt coolant	-1.8	-0.479
Graphite moderator	-0.7	N/A
Inner graphite reflector	+0.9	N/A
Outer graphite reflector	+0.9	N/A



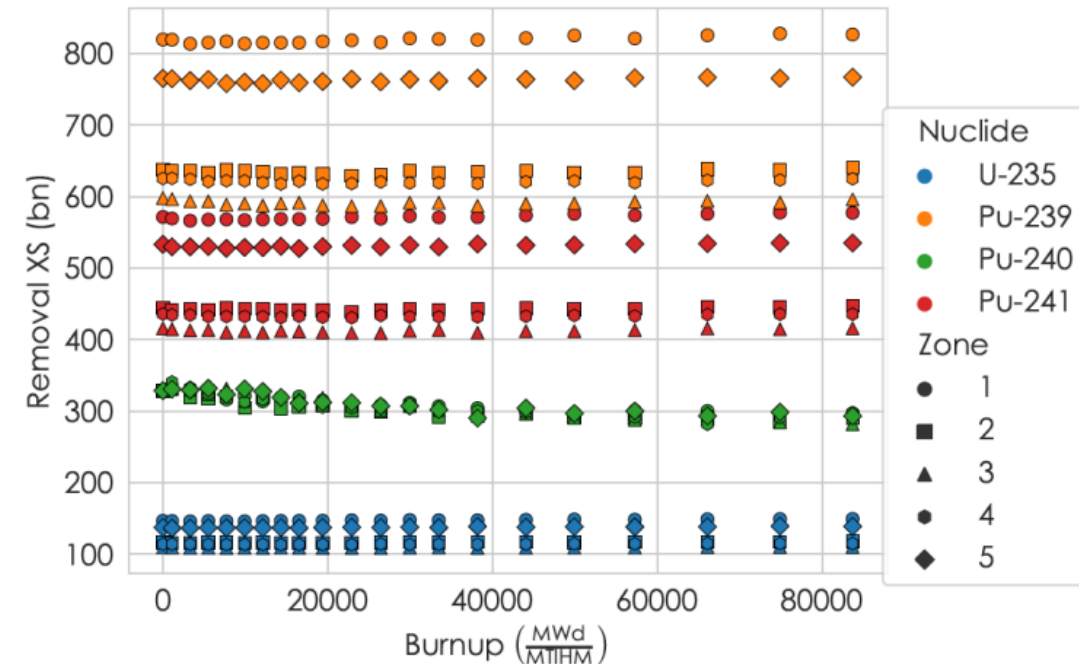
[1] A. T. Cisneros, "Pebble Bed Reactors Design Optimization Methods and their Application to the Pebble Bed Fluoride Salt Cooled High Temperature Reactor (PB-FHR)," University of California, Berkeley, 2013.

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



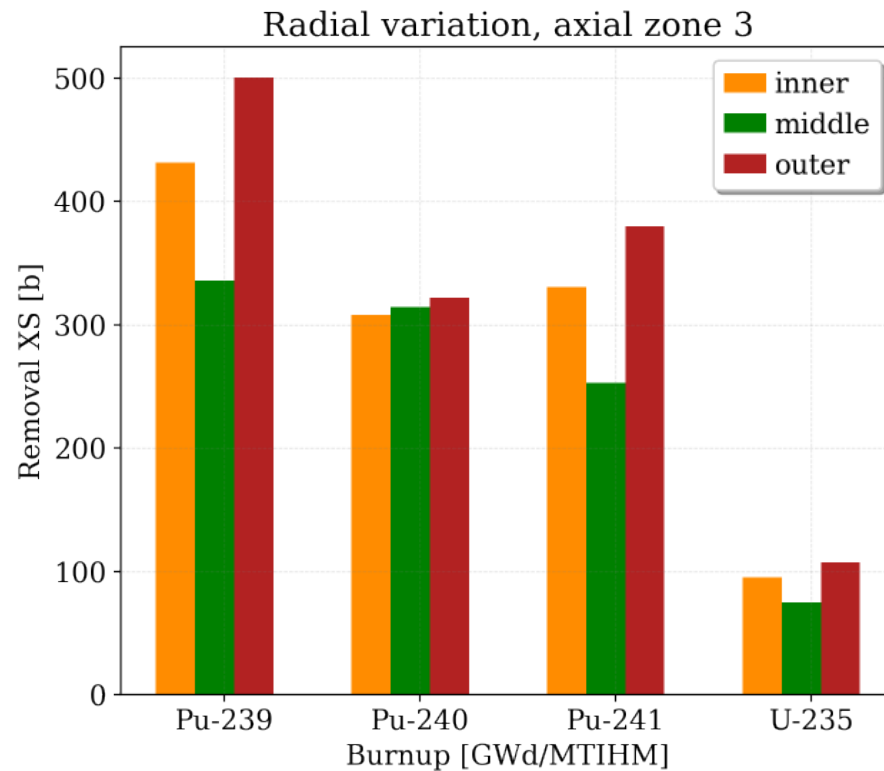
UCB Mark 1 slice depletion (HFP)



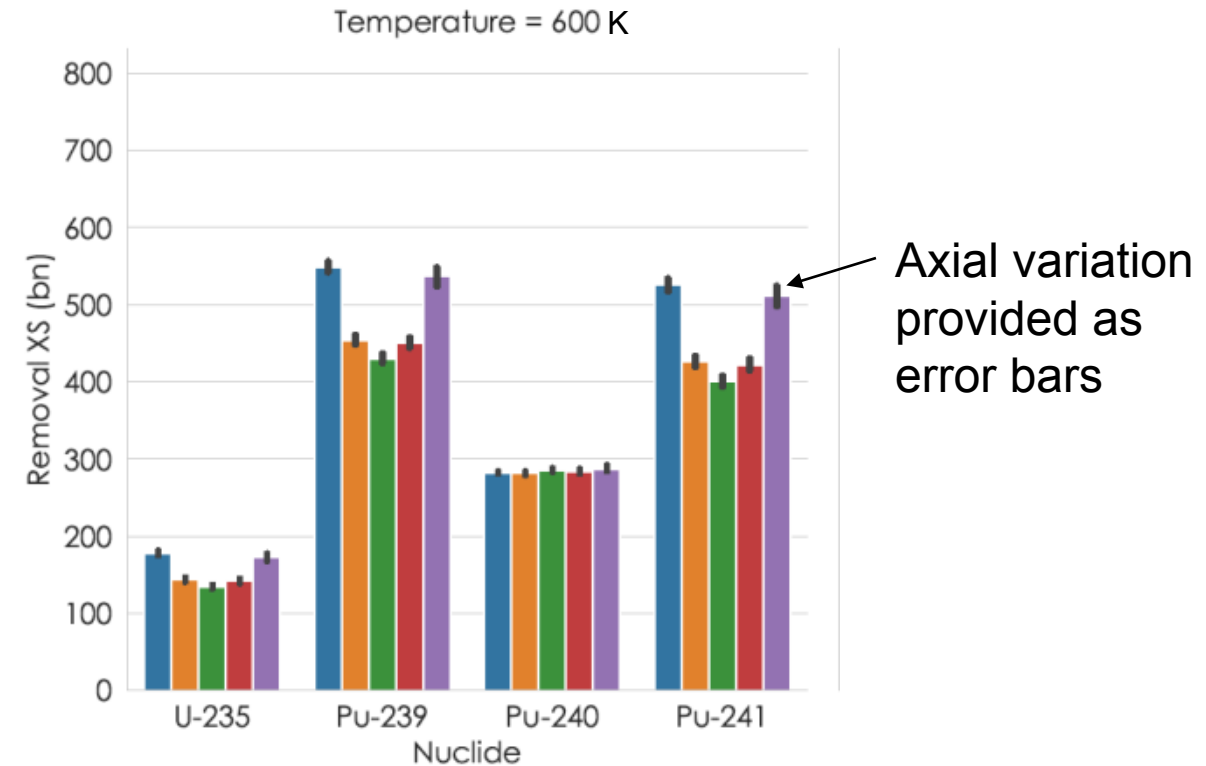
PBMR-400 slice depletion*

- 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

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/EFPD**
- Equilibrium value from Cisneros analytical approach: **0.023 mol/EFPD**

*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



U.S. NRC

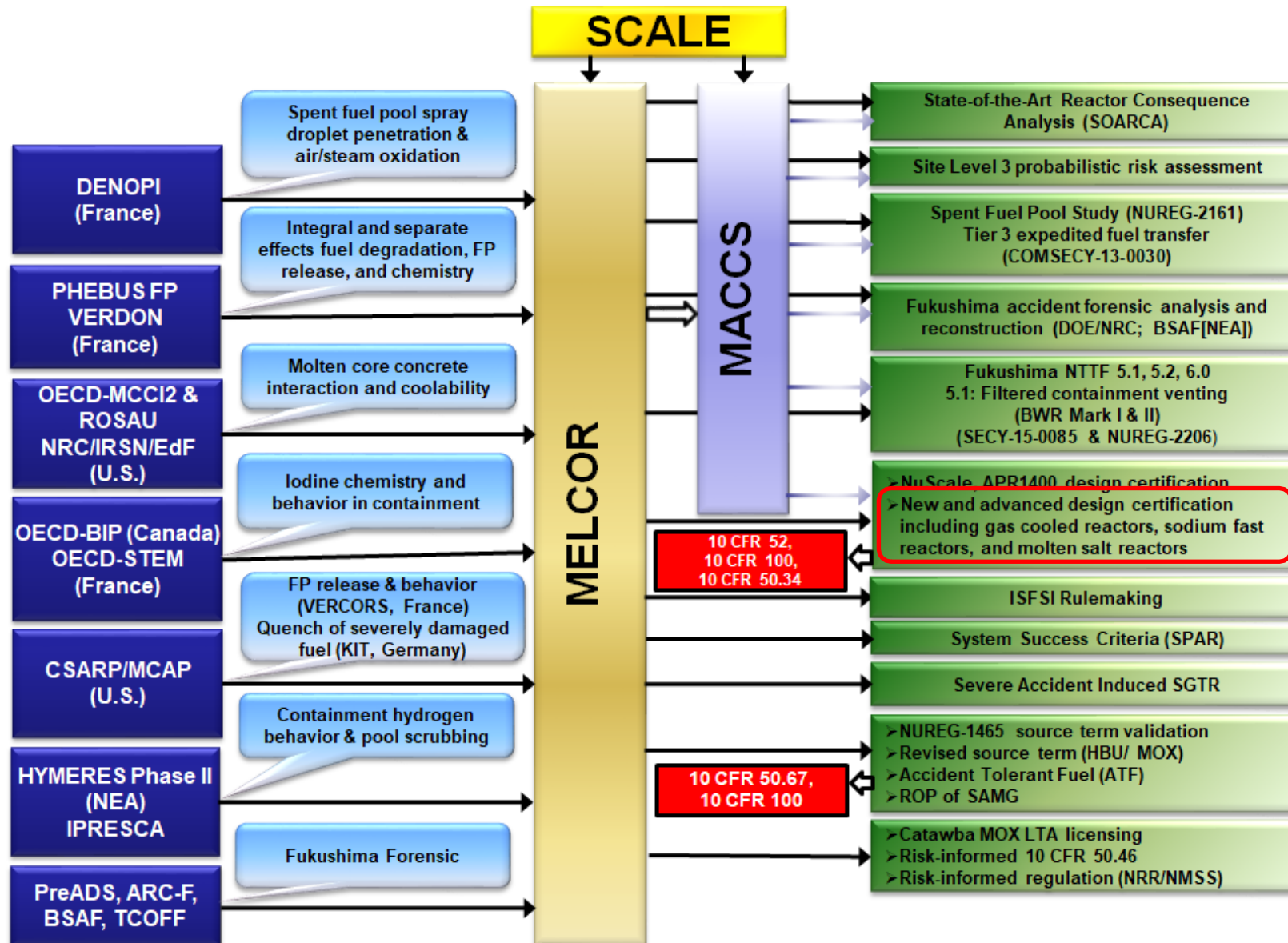


OAK RIDGE
National Laboratory



Sandia
National
Laboratories

MELCOR Development for Regulatory Applications



What Is It?

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

Who Uses It?

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

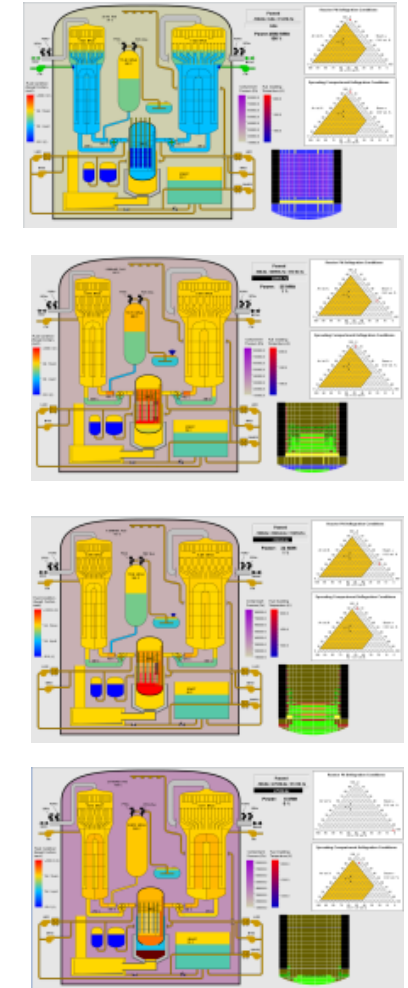
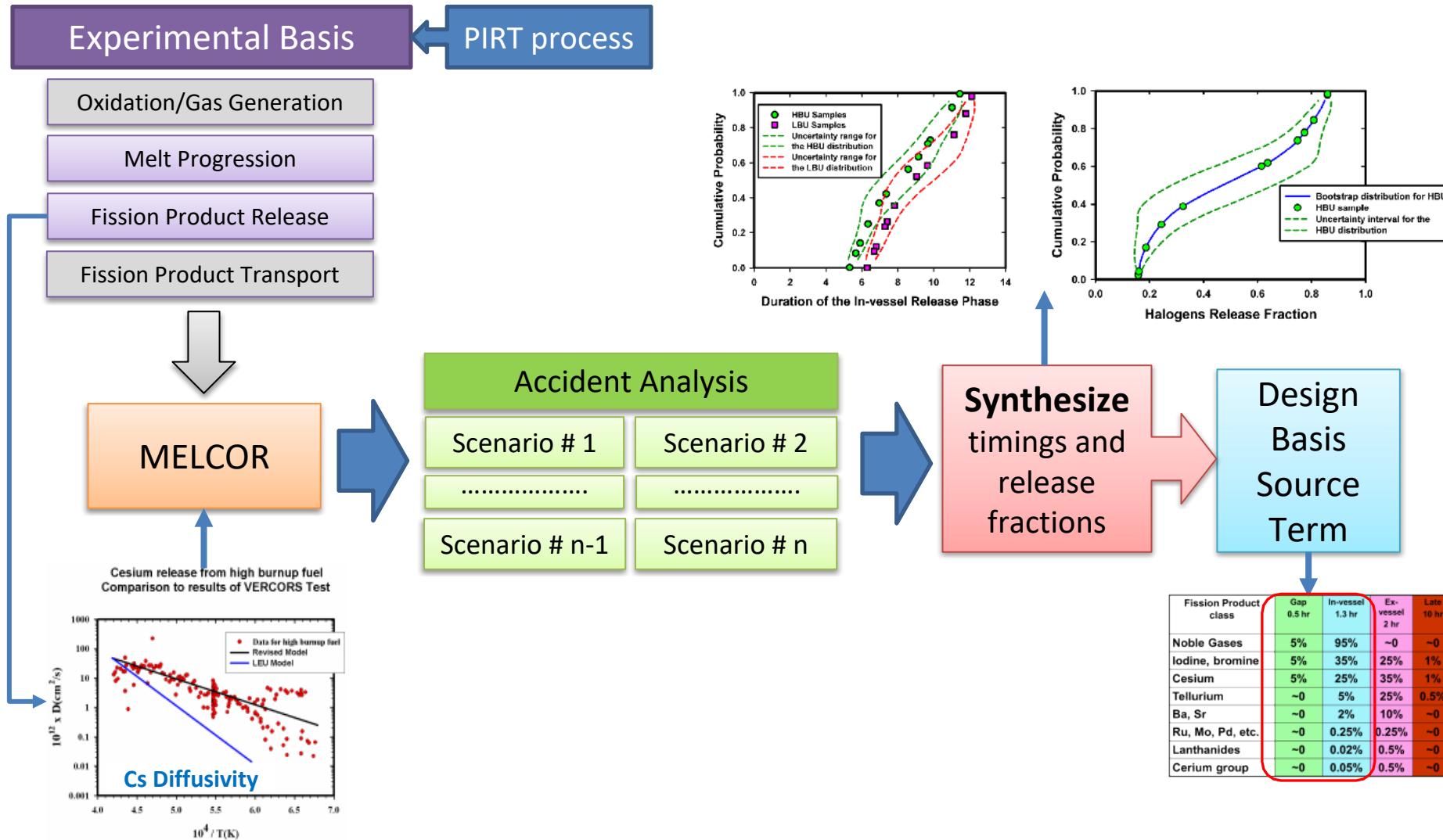
How Is It Used?

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

How Has It Been Assessed?

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

Source Term Development Process



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 (H³)

Spent Fuel

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

Facility Safety

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

MELCOR Attributes

Foundations of MELCOR Development

Fully integrated, engineering-level code

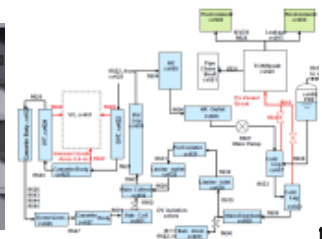
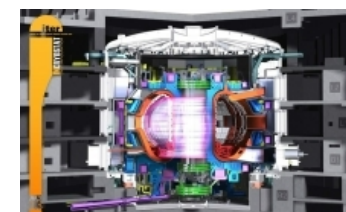
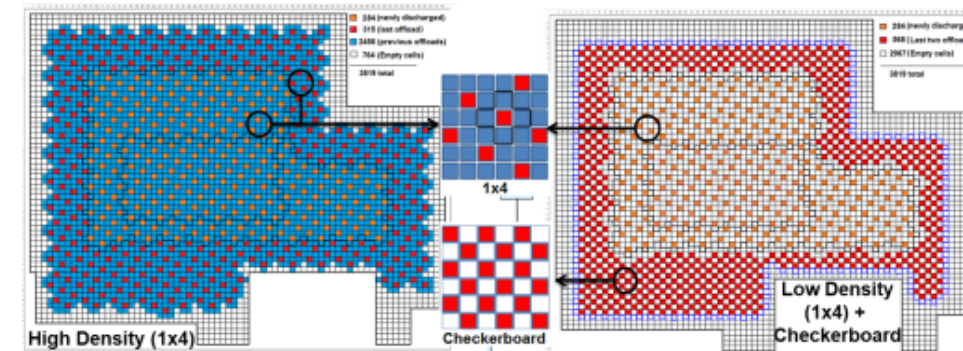
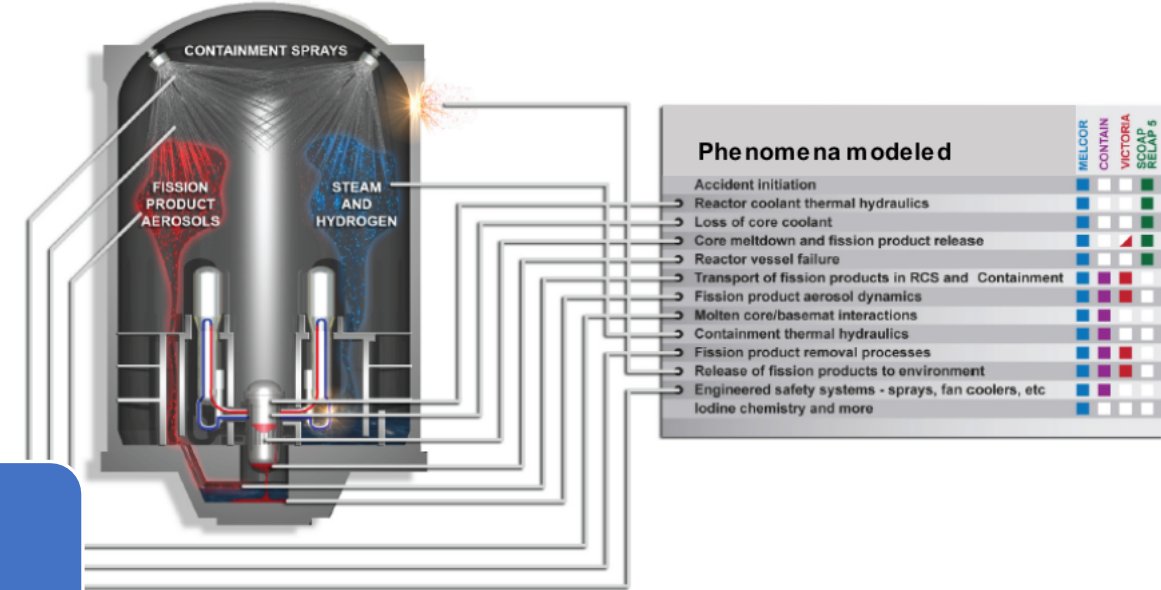
- Thermal-hydraulic response of reactor coolant system, reactor cavity, reactor enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

Level of physics modeling consistent with

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

Traditional application

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



MELCOR Attributes

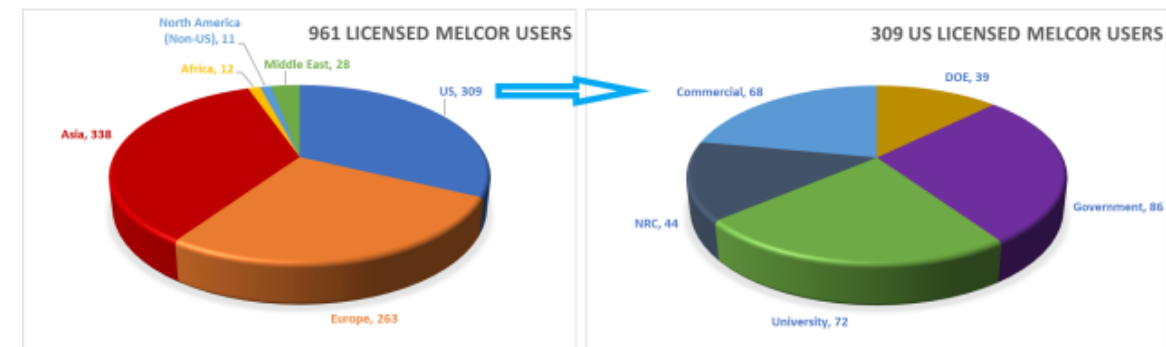
MELCOR Pedigree

Validated physical models

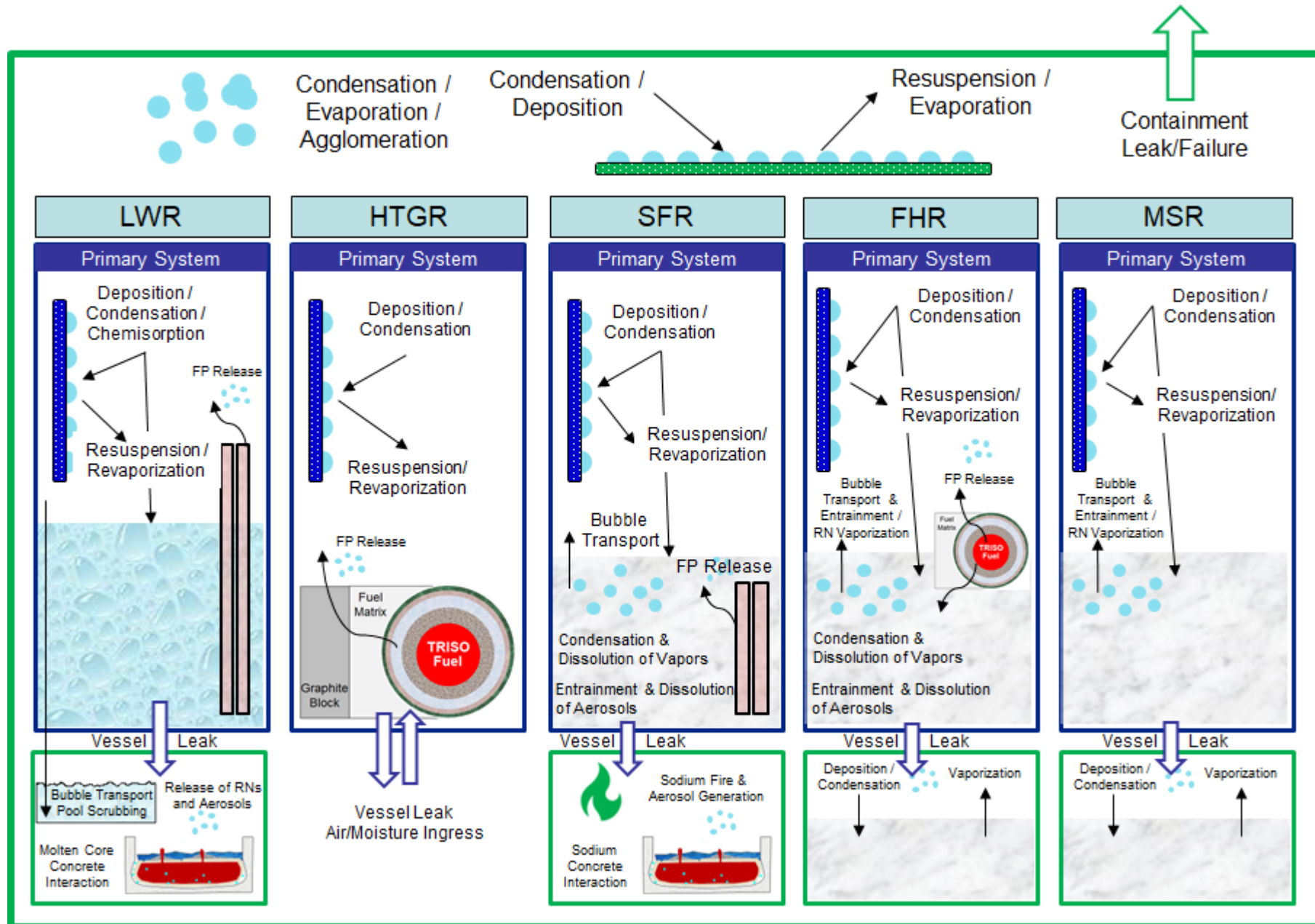
- International Standard Problems, benchmarks, experiments, and reactor accidents
- Beyond design basis validation will always be limited by model uncertainty that arises when extrapolated to reactor-scale

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

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



Common Phenomenology

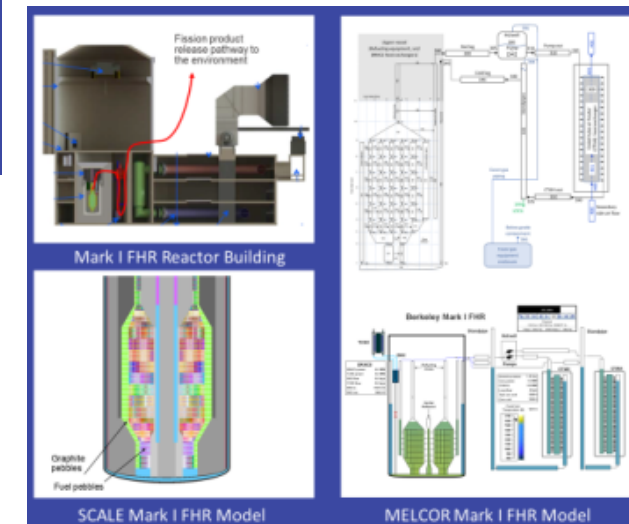
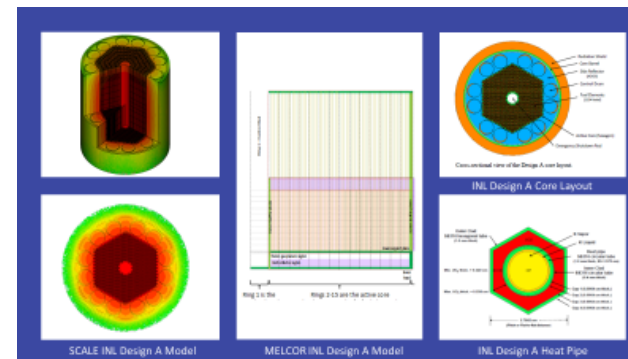
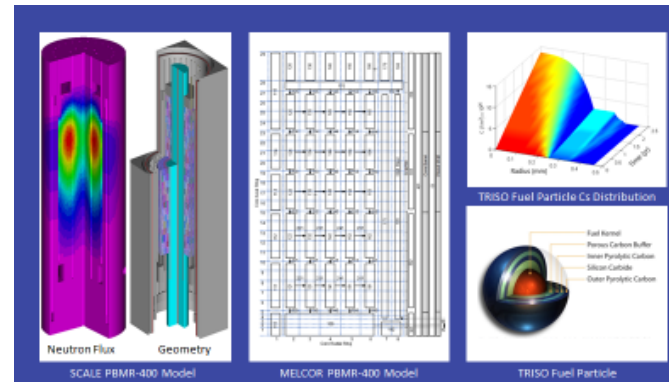
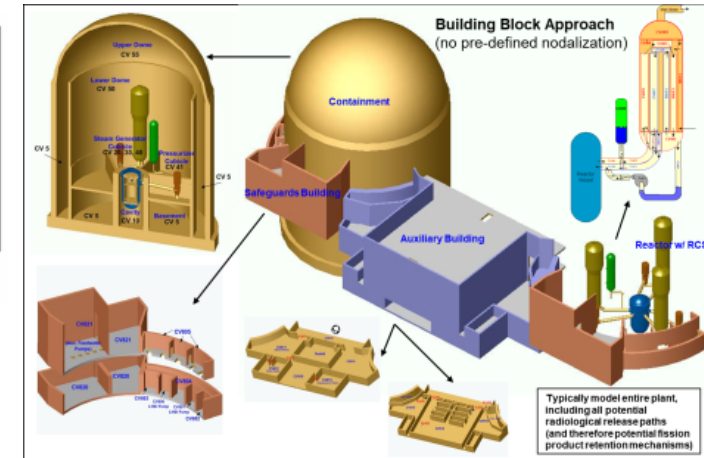


Parametric models enable uncertainties to be characterized

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

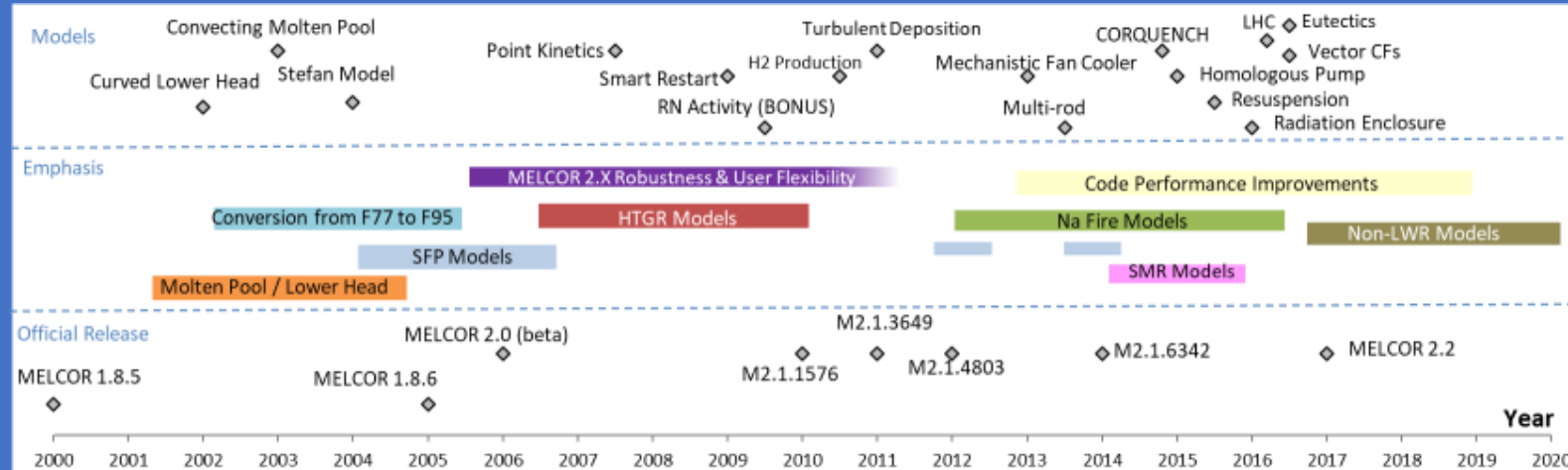
Code models are general and flexible

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



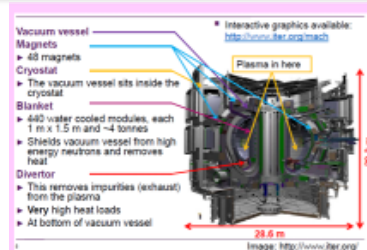
MELCOR State-of-the-Art

MELCOR Code Development



M2x Official Code Releases

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



Fusion

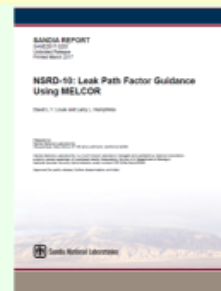
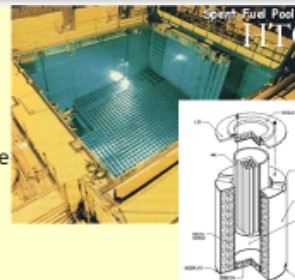
- Neutron Beam Injectors (LOVA)
- Li Loop LOFA transient analysis
- ITER Cryostat modeling
- Helium Lithium
- Helium Cooled Pebble Bed Test Blanket (Tritium Breeding)

Spent Fuel

Spent fuel pool risk studies

Multi-unit accidents (large area destruction)

Dry Storage

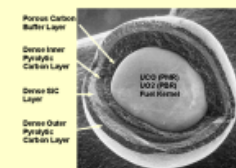


Non-Nuclear Facilities

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

HTGR Reactors

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



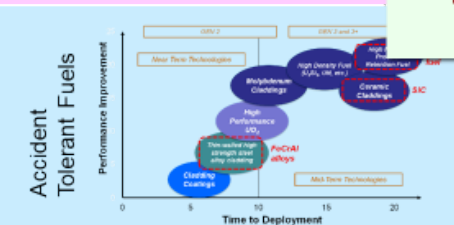
Sodium Reactors

- Sodium Properties
 - Sodium Equation of State
 - Sodium Thermo-mechanical properties
- Containment Modeling
 - Sodium pool fire model
 - Sodium spray fire model
 - Atmospheric chemistry model
 - Sodium-concrete interaction



Molten Salt Reactors

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



MELCOR Software Quality Assurance – Best Practices

MELCOR SQA Standards

SNL Corporate procedure IM100.3.5

CMMI-4+

NRC NUREG/BR-0167

Emphasis is on Automation

Affordable solutions

Consistent solutions



MELCOR Wiki

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

Code Configuration Management (CM)

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

Reviews

- Code Reviews: Code Collaborator
- Internal SQA reviews

Continuous builds & testing

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

Bug tracking and reporting

- Bugzilla online

Code Validation

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

Documentation

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

Project Management

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

Sharing of information with users

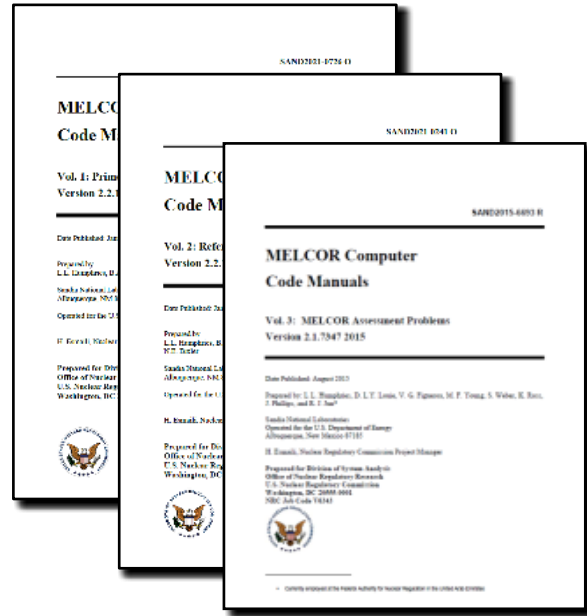
- External web page
- MELCOR workshops
- MELCOR User Groups (EMUG & AMUG)



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

Table 1-1: Physics Package Coverage

MELCOR Verification & Validation Basis



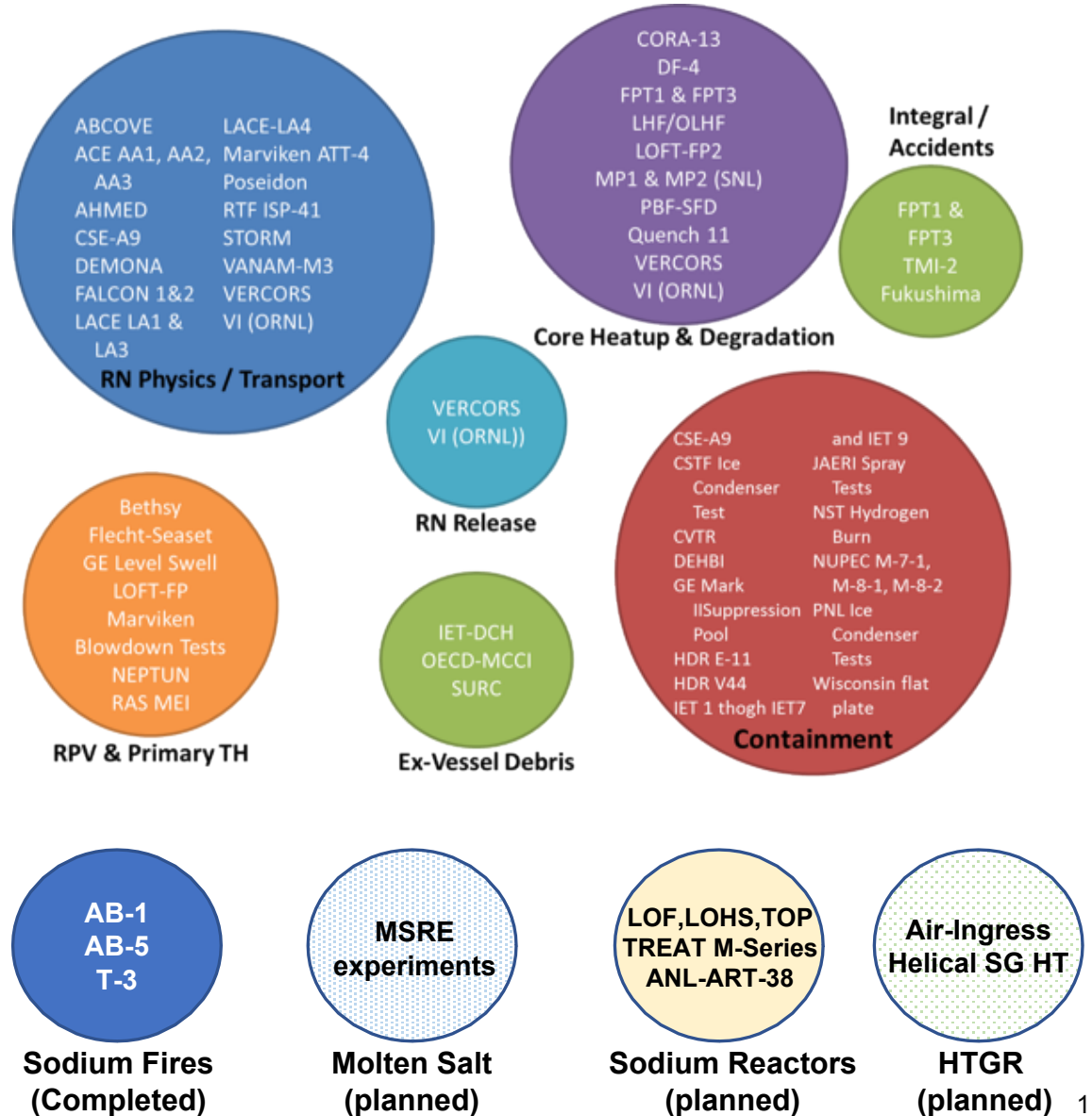
Volume 1: Primer & User Guide
Volume 2: Reference Manual
Volume 3: MELCOR Assessment Problems
[SAND2015-6693 R]

Analytical Problems

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

LWR & non-LWR applications

Specific to non-LWR application



Sample Validation Cases

TRISO Diffusion Release

IAEA CRP-6 Benchmark
Fractional Release

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

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

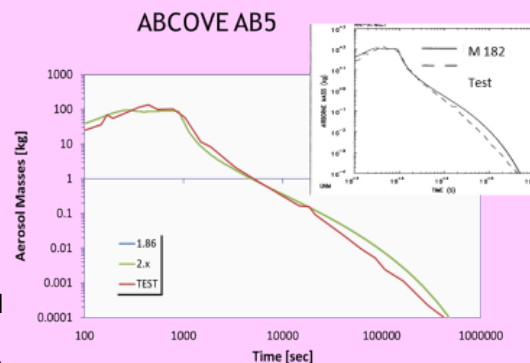
A sensitivity study to examine fission product release from a fuel particle starting with a bare kernel and ending with an irradiated TRISO particle.

Aerosol Physics

- Agglomeration
- Deposition
- Condensation and Evaporation at surfaces

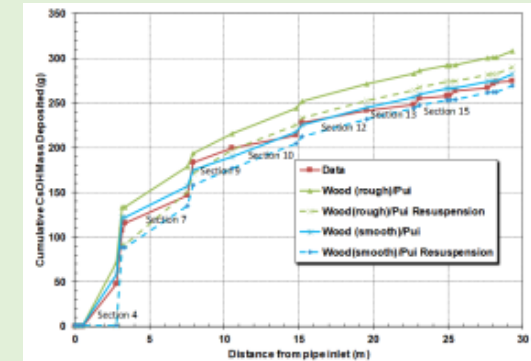
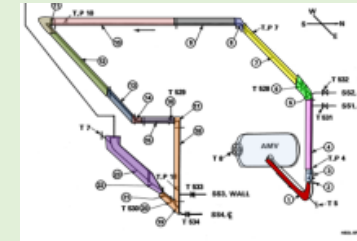
Validation Cases

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



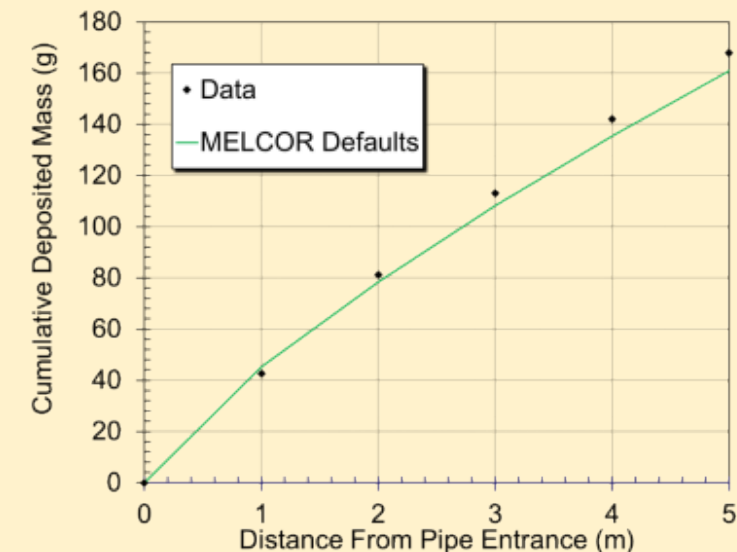
LACE LA1 and LA3 tests experimentally examined the transport and retention of aerosols through pipes with high speed flow

Turbulent Deposition



Resuspension

STORM (Simplified Test of Resuspension Mechanism) test facility



MELCOR Modernization

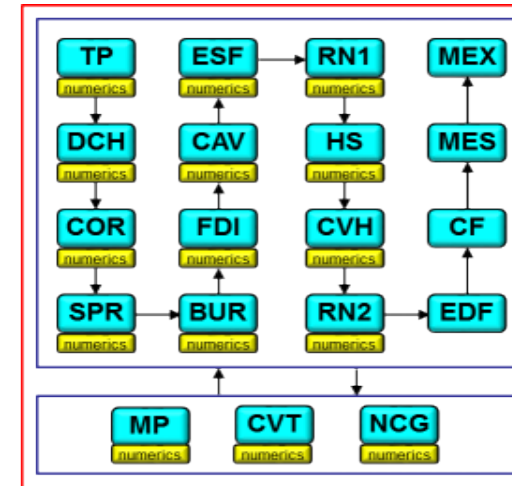
Generalized numerical solution engine

Hydrodynamics

In-vessel damage progression

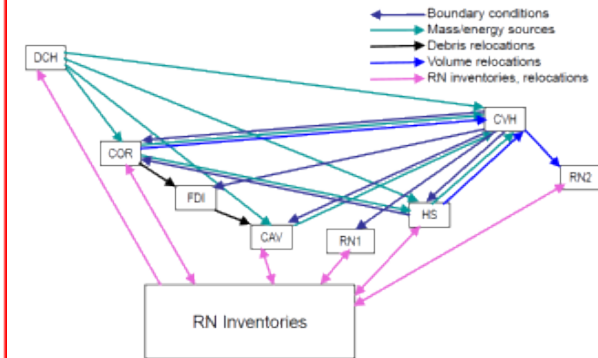
Ex-vessel damage progression

Fission product release and transport

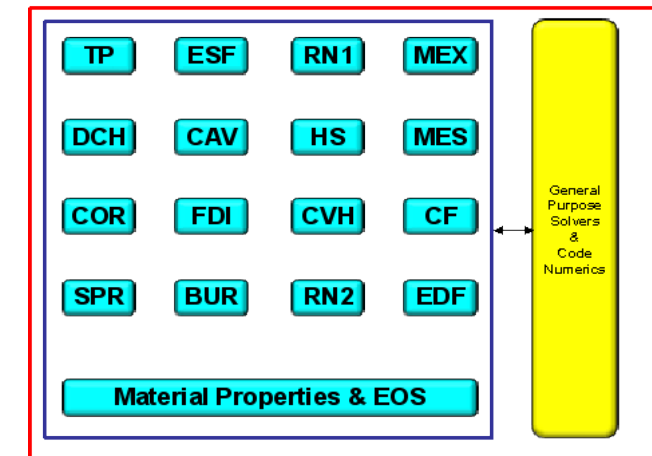


TP = Transfer Process
DCH = Decay Heat
COR = Core
SPR = Containment Spray
BUR = Gas Combustion
FDI = Fuel Dispersal Interaction
CAV = Cavity (MCCI)
ESF = Engineered Safety Features
MP = Material Properties

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

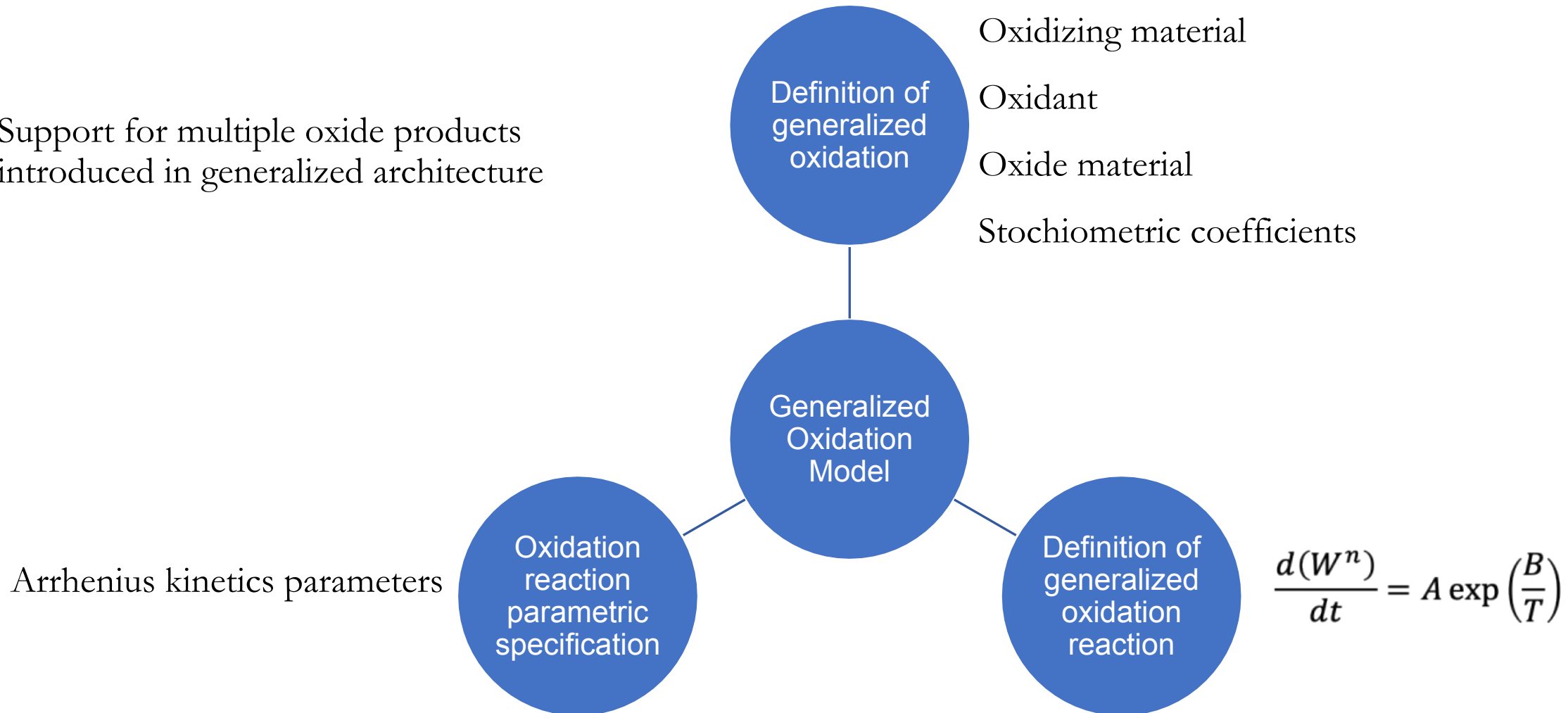


Separate **Physics** & **Numerics**



Generalized Oxidation Model

Support for multiple oxide products
introduced in generalized architecture



Molten Salt Chemistry and Radionuclide Release – Integration into MELCOR

