SCALE/MELCOR Non-LWR Source Term Demonstration Project – High-Temperature Gas-Cooled Reactor

July 2021

Outline

NRC strategy for non-LWR source term analysis

Project scope

High-temperature gas-cooled reactor fission product inventory/decay heat methods and results
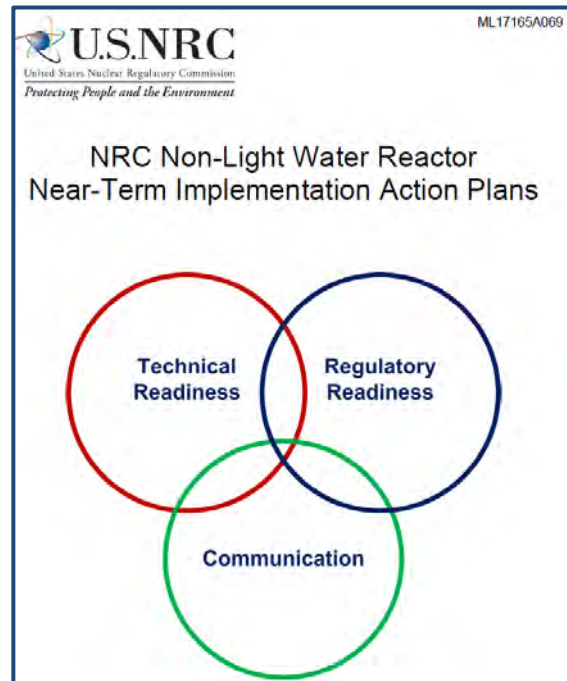
High-temperature gas-cooled reactor plant model and source term analysis
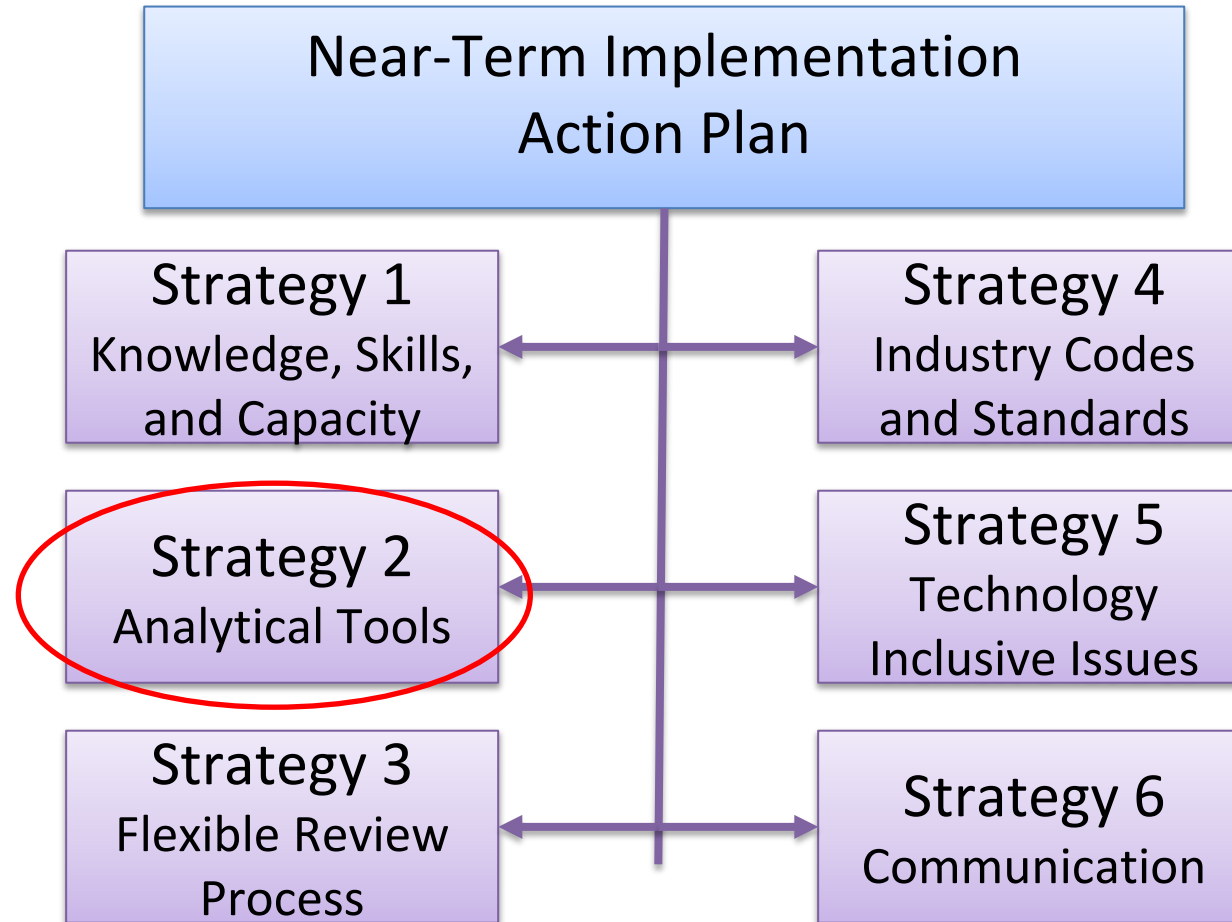
Summary

Appendices

- SCALE overview

- VSOP

- ORIGEN library interpolation

- MELCOR overview

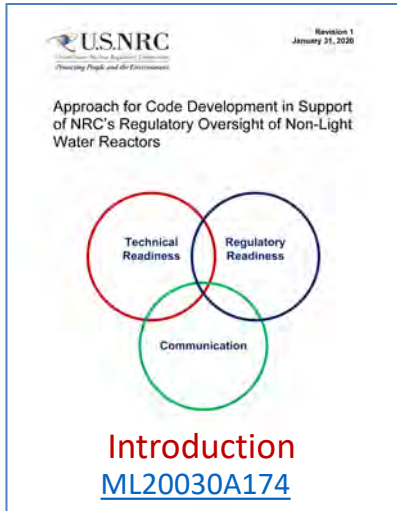- MELCOR default radionuclide classes

Integrated Action Plan (IAP) for Advanced Reactors

ML17165A069

Near-Term Implementation Action Plan
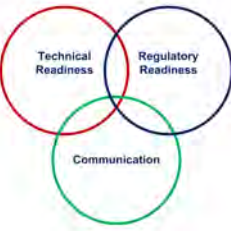
Strategy 1
Knowledge, Skills, and Capacity

Strategy 2
Analytical Tools

Strategy 3
Flexible Review Process

Strategy 4
Industry Codes and Standards

Strategy 5
Technology Inclusive Issues

Strategy 6
Communication

IAP Strategy 2 Volumes
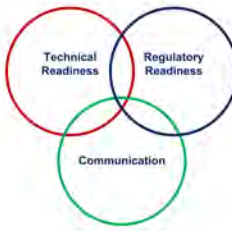
Introduction
ML20030A174
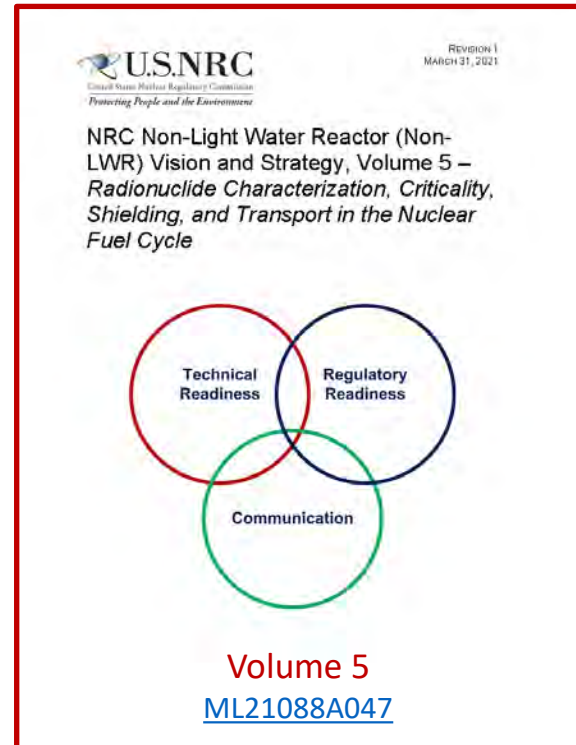
Volume 1
ML20030A176

Volume 2
ML20030A177
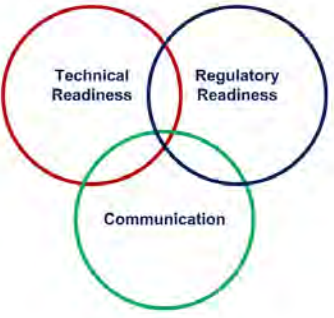
Volume 4
ML21085A484

These Volumes outline the specific analytical tools to enable independent analysis of non-LWRs, "gaps" in code capabilities and data, V&V needs and code development tasks.
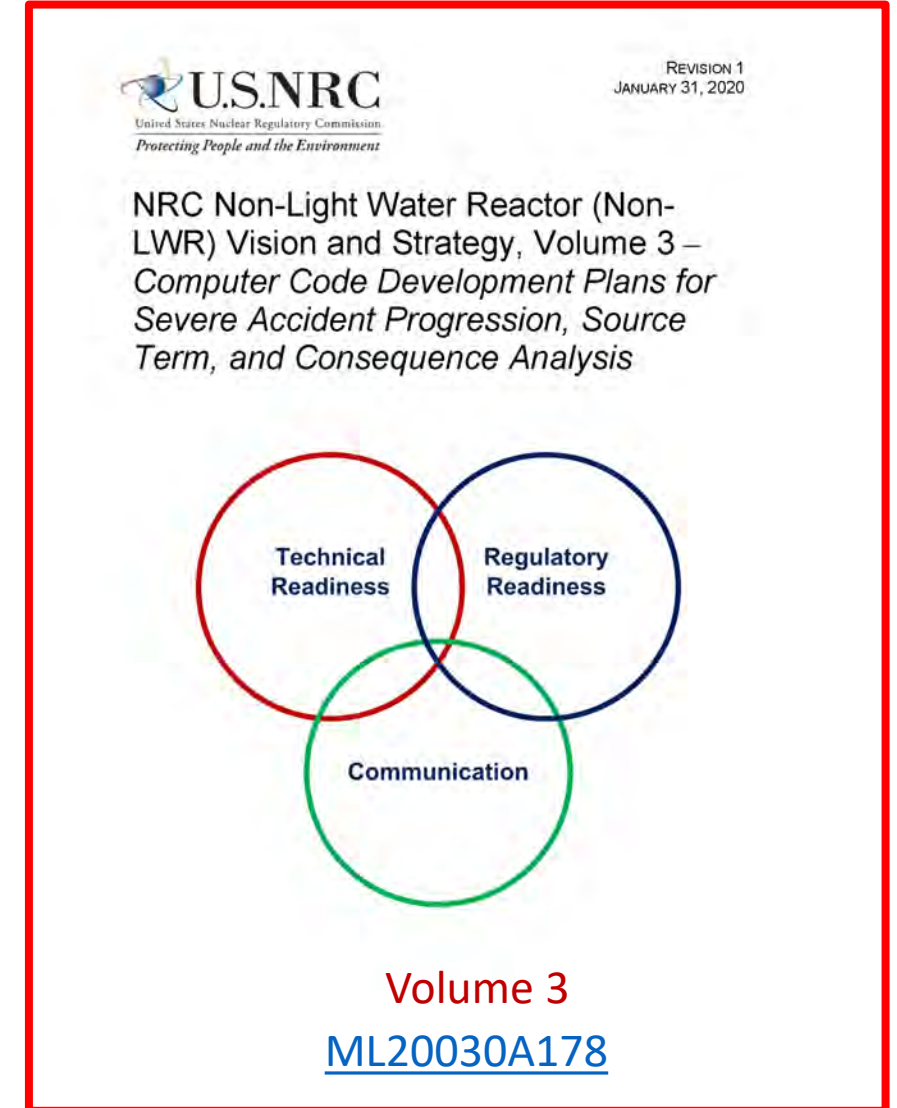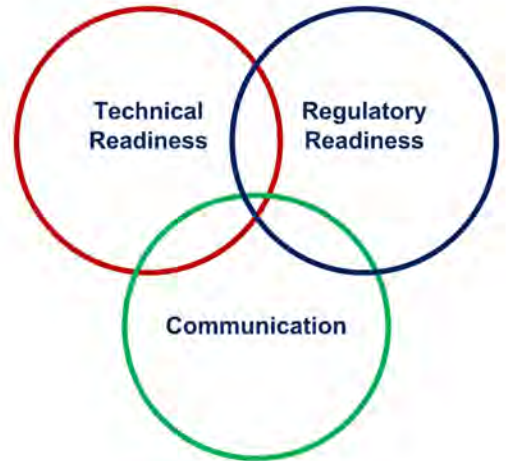
Volume 5
ML21088A047

Volume 3
ML20030A178

NRC strategy for non-LWR analysis (Volume 3)

Evaluation Model and Suite of Codes

Code strategy for source term

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

Role of NRC severe accident codes

RES	NMSS	NRR

SCALE
(w/ Sensitivity/Uncertainty Quantification)

Isotopic Inventories, Decay Heat, Kinetics and Power Distribution Parameters

MELCOR
(w/ Sensitivity/Uncertainty Quantification)

Radionuclide Source Term

MACCS, RADTRAD, RASCAL, etc.
(w/ Sensitivity/Uncertainty Quantification)

Dose, Health Effects, Economic/Societal Consequences

Storage & Transport of Materials

Material Processing for Applicable Designs

Safety Review (Regulations)

- **Siting and Safety Analysis[1,2]** - 10 CFR 100.21, 10 CFR 50.34, Part 52 (various)
- **Control Room Habitability[3]** - 10 CFR 50, Appendix A, GDC-19
- **Technical Support Center Habitability[4]** – 10 CFR 50, Appendix E, 10 CFR 50.47
- **Severe Accidents, FSAR Chapter 19**
- **Emergency Planning** – 10 CFR 50.160 *(expected future use assuming this regulation is promulgated)*
- **Emergency Response** – Nuclear/Radiological Incident Annex (NRIA) to the National Response Framework (NRF)

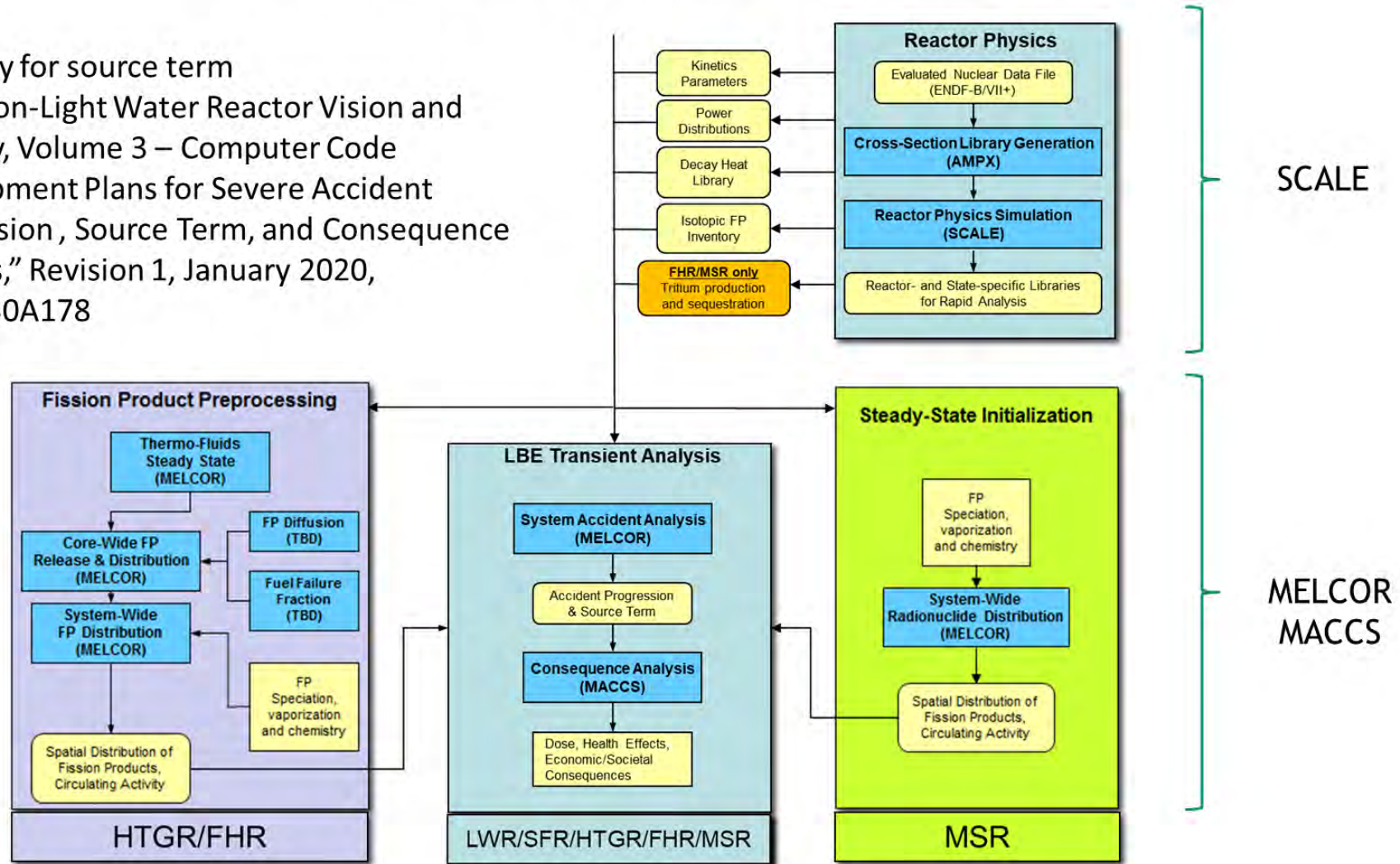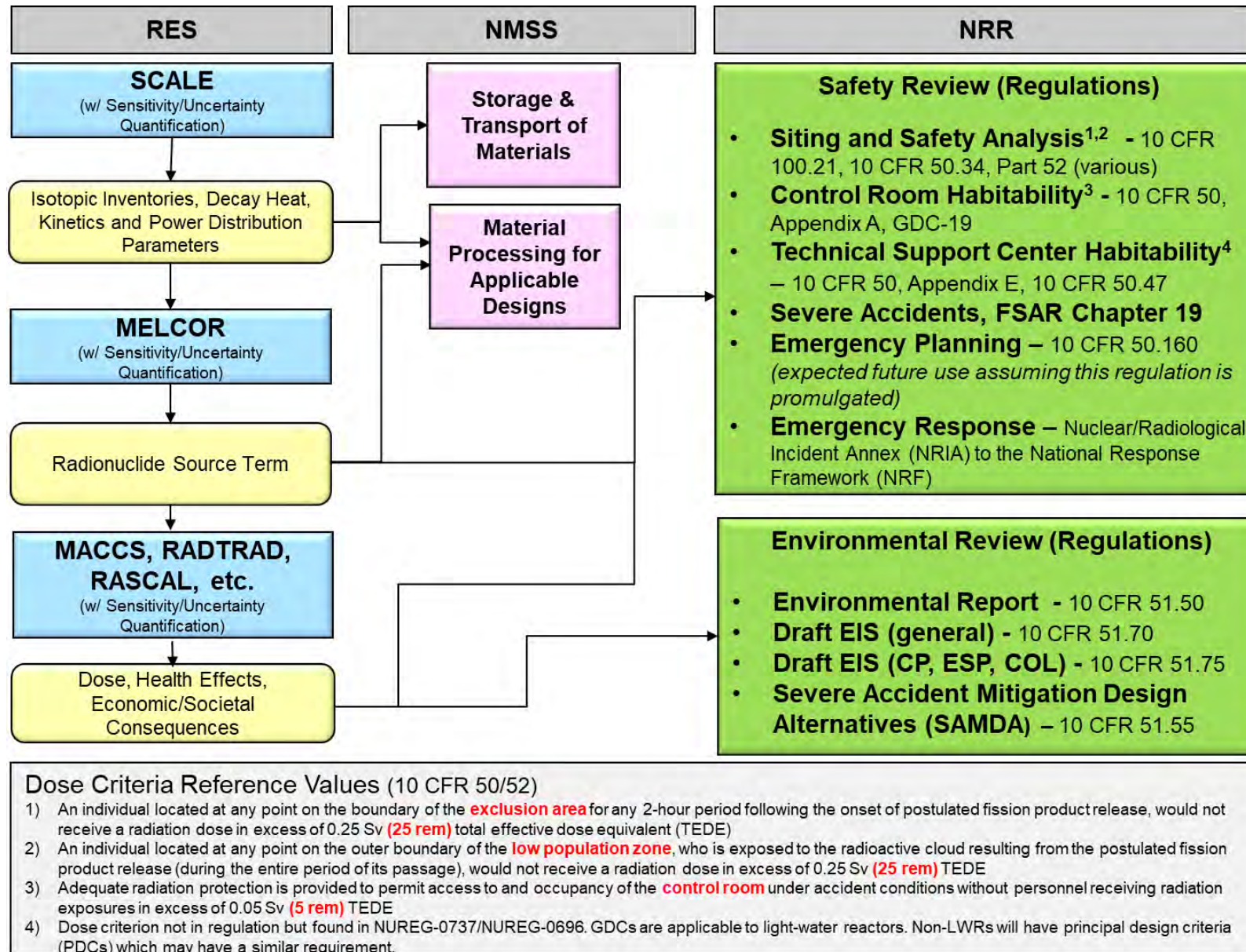**Environmental Review (Regulations)**

- **Environmental Report** - 10 CFR 51.50
- **Draft EIS (general)** - 10 CFR 51.70
- **Draft EIS (CP, ESP, COL)** - 10 CFR 51.75
- **Severe Accident Mitigation Design Alternatives (SAMDA)** – 10 CFR 51.55

Dose Criteria Reference Values (10 CFR 50/52)
1) An individual located at any point on the boundary of the **exclusion area** for any 2-hour period following the onset of postulated fission product release, would not receive a radiation dose in excess of 0.25 Sv **(25 rem)** total effective dose equivalent (TEDE)
2) An individual located at any point on the outer boundary of the **low population zone**, who is exposed to the radioactive cloud resulting from the postulated fission product release (during the entire period of its passage), would not receive a radiation dose in excess of 0.25 Sv **(25 rem)** TEDE
3) Adequate radiation protection is provided to permit access to and occupancy of the **control room** under accident conditions without personnel receiving radiation exposures in excess of 0.05 Sv **(5 rem)** TEDE
4) Dose criterion not in regulation but found in NUREG-0737/NUREG-0696. GDCs are applicable to light-water reactors. Non-LWRs will have principal design criteria (PDCs) which may have a similar requirement.

Project 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 – UC Berkeley Mark I
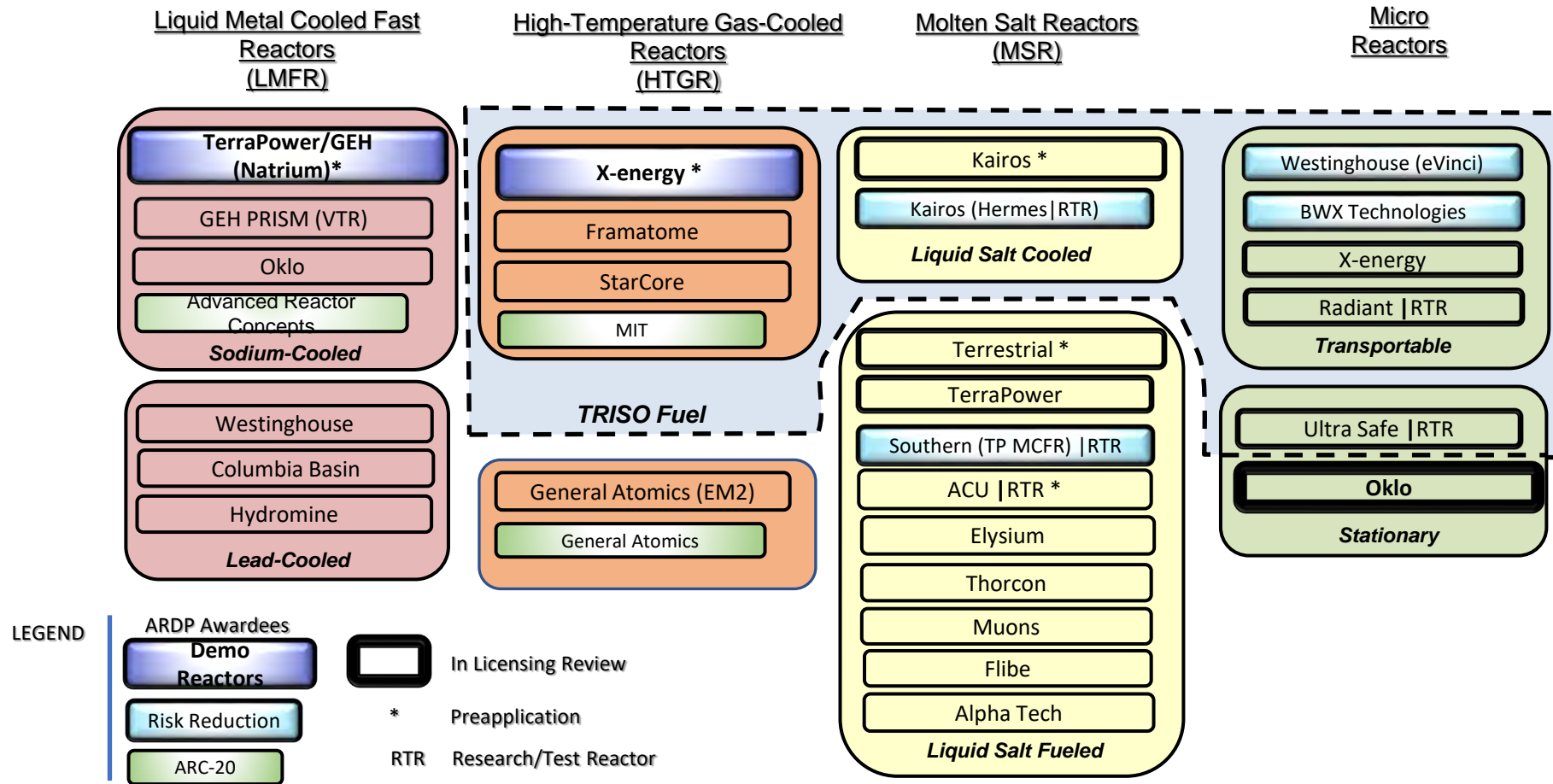
FY22

- 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

Liquid Metal Cooled Fast Reactors (LMFR)

TerraPower/GEH (Natrium)*
GEH PRISM (VTR)
Oklo
Advanced Reactor Concepts
Sodium-Cooled

Westinghouse
Columbia Basin
Hydromine
Lead-Cooled

High-Temperature Gas-Cooled Reactors (HTGR)

X-energy *
Framatome
StarCore
MIT
TRISO Fuel

General Atomics (EM2)
General Atomics

Molten Salt Reactors (MSR)

Kairos *
Kairos (Hermes|RTR)
Liquid Salt Cooled

Terrestrial *
TerraPower
Southern (TP MCFR) |RTR
ACU |RTR *
Elysium
Thorcon
Muons
Flibe
Alpha Tech
Liquid Salt Fueled

Micro Reactors

Westinghouse (eVinci)
BWX Technologies
X-energy
Radiant |RTR
Transportable

Ultra Safe |RTR
Oklo
Stationary

LEGEND

ARDP Awardees
Demo Reactors
Risk Reduction
ARC-20

In Licensing Review
* Preapplication
RTR Research/Test Reactor

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High-temperature gas-cooled reactor (1/2)

High-temperature high-pressure helium transfers heat from core to the secondary system

- Core outlet temperatures to 1000℃
- High temperature increases efficiency
- Fuel in a prismatic or a pebble bed core

Peach Bottom Unit 1

- Operated 1966-1974
- 115 MW thermal power
- 37% efficiency, 88% availability

Fort St. Vrain

- Operated 1979-1989
- 842 MW thermal power

Peach Bottom Unit #1
[https://commons.wikimedia.org/wiki/File:Peach_Bottom_-Aerial_View_1.jpg

High-temperature gas-cooled reactor (2/2)

Department of Energy funded design of the Next Generation Nuclear Plant
- Project as established by Energy Policy Act of 2005
- Project started in 2007
- Initial focus on the PBMR-400 design
  - Pebble Bed Modular Reactor (Pty) Ltd
  - Focus of an Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) neutronics benchmark study [NEA/NSC/DOC(2013)10]
- Areva SC-HTGR design was selected in 2012
- Department of Energy subsequently ended support
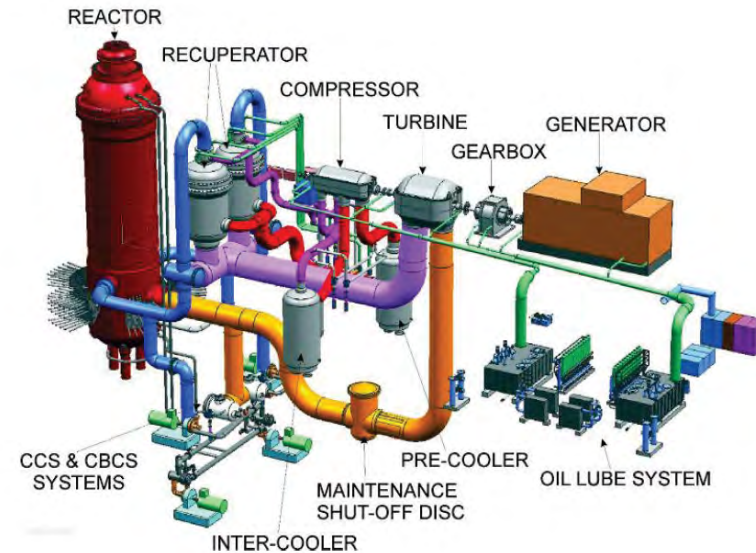
PBMR-400
[NEA/NSC/DOC(2013)10]

Publicly available design

PBMR-400 – Used for SCALE/MELCOR demonstration project

MELCOR model based on data from OECD/NEA neutronics benchmark project

- "Development of MELCOR Input Techniques for High Temperature Gas-cooled Reactor Analysis," James Corson, Master's thesis, Texas A&M University, 2010

No description of confinement or secondary system

- MELCOR confinement model based on NGNP schematics
- Simplified secondary system used to estimate steady-state conditions

PBMR Coupled Neutronics/
Thermal-hydraulics Transient
Benchmark
The PBMR-400 Core Design

Volume 1
The Benchmark Definition

OECD   NEA

PBMR-400 (1/2)

400 MWt

Helium coolant
- Pressure – 9 MPa (1300 psi)
- Core inlet – 500℃
- Core outlet – 900℃
- Core flowrate (downward) – 192 kg/s

452,000 TRISO pebbles in an annular core
- Core inner diameter – 2.0 m
- Core outer diameter – 3.7 m
- Core height – 11 m

92 GWD/MTU target burn-up

Steel vessel with graphite reflectors

Fuel Line
Top Reflector
Fuel Core
Centre Reflector
Side Reflector
Control Rod
SAS Channel
Bottom Reflector
SAS Extraction Point

Pieter J Venter, Mark N Mitchell, Fred Fortier, "PBMR Reactor Design and Development," 18th International Conference on Structural Mechanics in Reactor Technology (SMiRT 18), Beijing, China, August 7-12, 2005, SMiRT18- S02-2
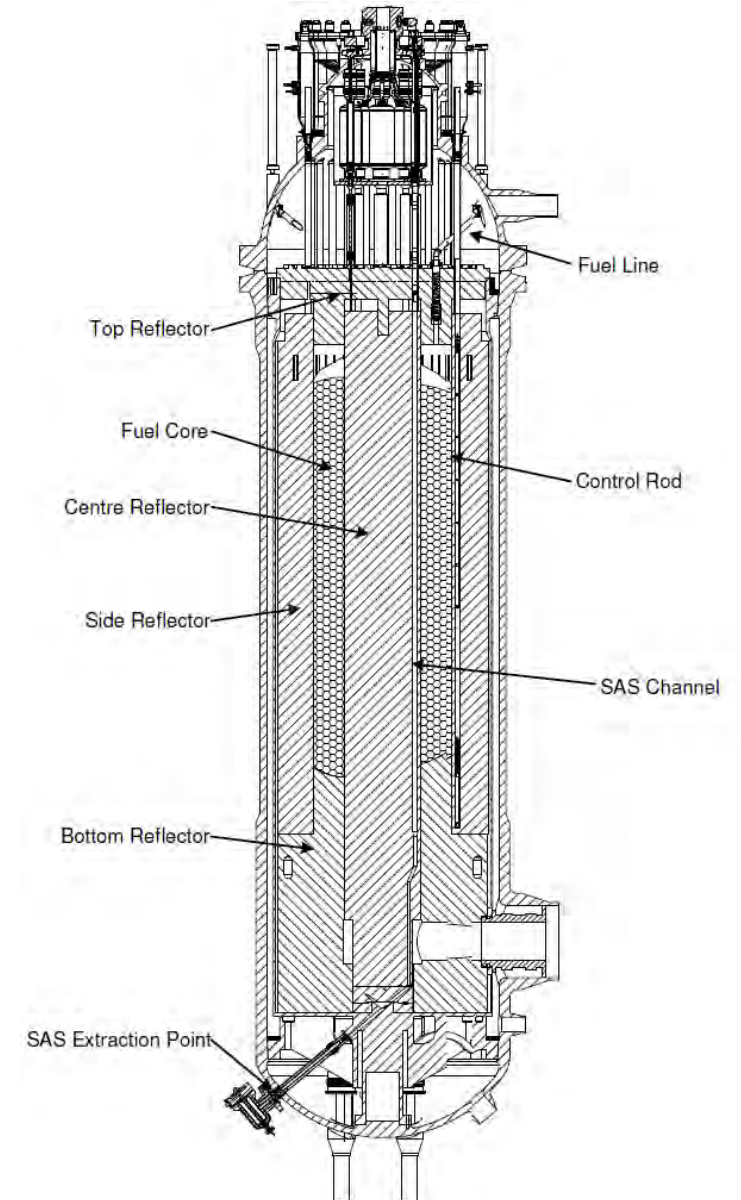
PBMR-400 (2/2)

TRISO particle
- TRISO is a portmanteau for **tr**istructural **iso**tropic
- Kernel – 1.5 g U; 250 μm radius
- Porous carbon buffer layer
- 3 coatings to contain fission products

Fuel Kernel
Porous Carbon Buffer
Inner Pyrolytic Carbon
Silicon Carbide
Outer Pyrolytic Carbon
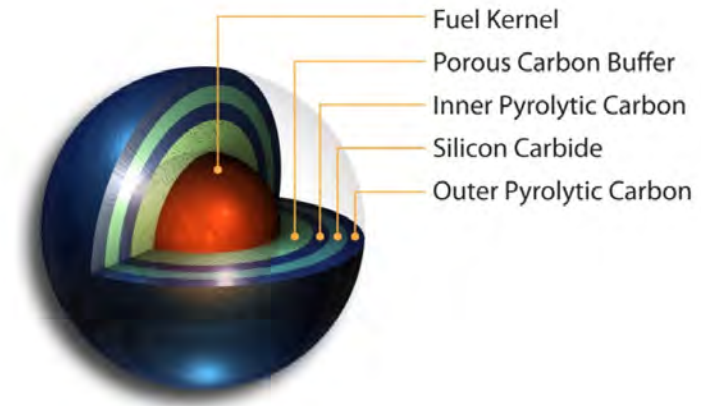
TRISO particle
[INL/EXT-08-14497]

TRISO pebble
- Contains 14,500 TRISO particles
- 25 mm radius
- 5 mm graphite outer shell

TRISO pebble
[https://www.energy.gov/ne/articles/x-energy-developing-pebble-bed-reactor-they-say-cant-melt-down]

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PBMR-400 benchmark used to represent PBR concepts

INL/MIS-17-43095, "AGR-5/6/7 Irradiation Experiment Test Plan", 1/25/2018

- Fuel Kernel
- Porous Carbon Buffer
- Inner Pyrolytic Carbon
- Silicon Carbide
- Outer Pyrolytic Carbon

Typical TRISO particle layer structure

Design features

- Fueled by graphite "pebbles" composed of UO_2-bearing TRISO fuel particles (5-10% ^{235}U)
- Pebbles circulate multiple passes through the core to high discharge burnup (~90 GWd/MTIHM)
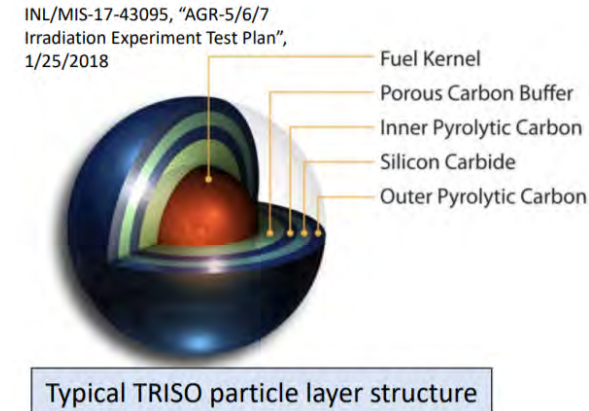
Two cases evaluated

- **Startup core:** 1/3 fuel pebbles, 2/3 graphite "dummy" pebbles
- **Equilibrium core:** 110 material zones with pre-specified material compositions (100% fuel)

PBMR-400 SCALE geometry
(S. Skutnik, ORNL)

References:
1. "Status and Prospects for Gas Cooled Reactor Fuels", IAEA-TECDOC-CD-1614, April 2009
2. OECD/NEA, "PBMR Coupled Neutronics / Thermal-hydraulics Transient Benchmark I: The PBMR-400 Core Design," NEA/NSC/DOC(2013)10, July 2010

Prior SCALE validation for HTGR systems (1/2)

- **HTR-10 initial core critical benchmark**
  - Based on International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE) benchmark for HTR-10 initial core
  - Graphite-coated, spherical fuel elements with TRISO fuel particles
    - 3 cm fuel spheres at 17% ^{235}U enrichment
  - SCALE 6.0 with ENDF/B-VIII.0 nuclear data
  - **Figure of merit:** System k-eigenvalue (k_{eff})
    - SCALE consistent with MCNP to within -73±34 pcm
    - MCNP and SCALE calculations both showed a moderate positive reactivity bias (1.4 ± 0.4)%

Active core region

Dummy pebbles' region
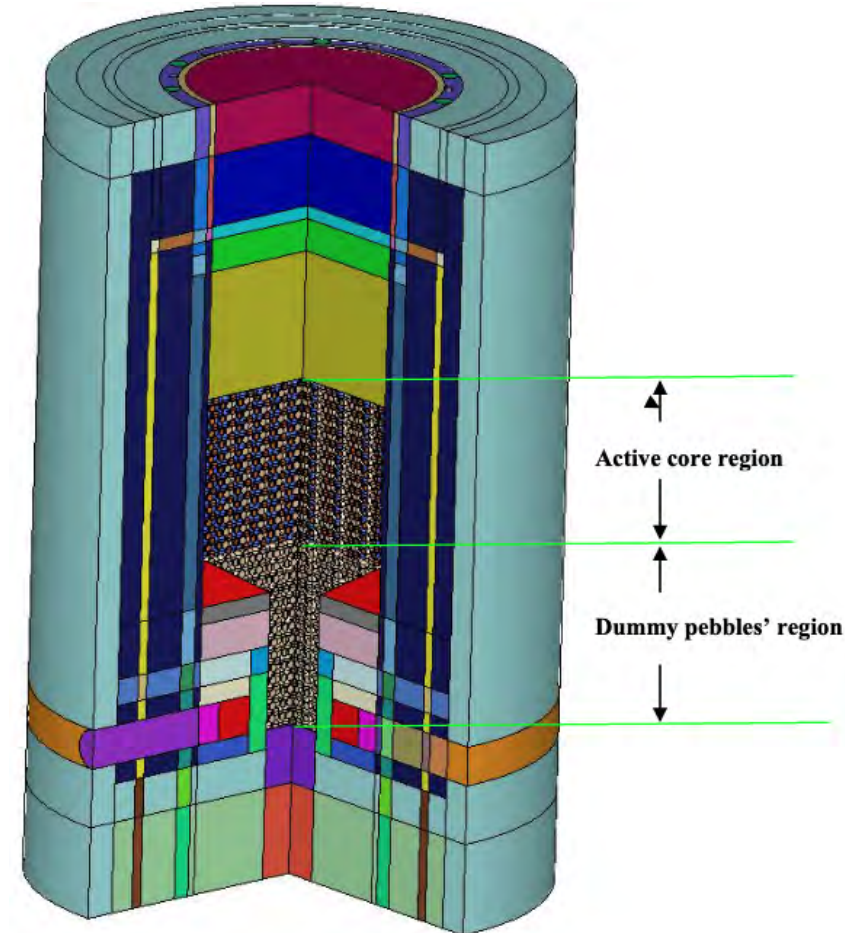
Image: NUREG/CR-7107

G. Ilas, D. Ilas, R. P. Kelly, and E. E. Sunny, "Validation of SCALE for High Temperature Gas-Cooled Reactor Analysis," NUREG/CR-7107(ORNL/TM-2011/161), Jul. 2012
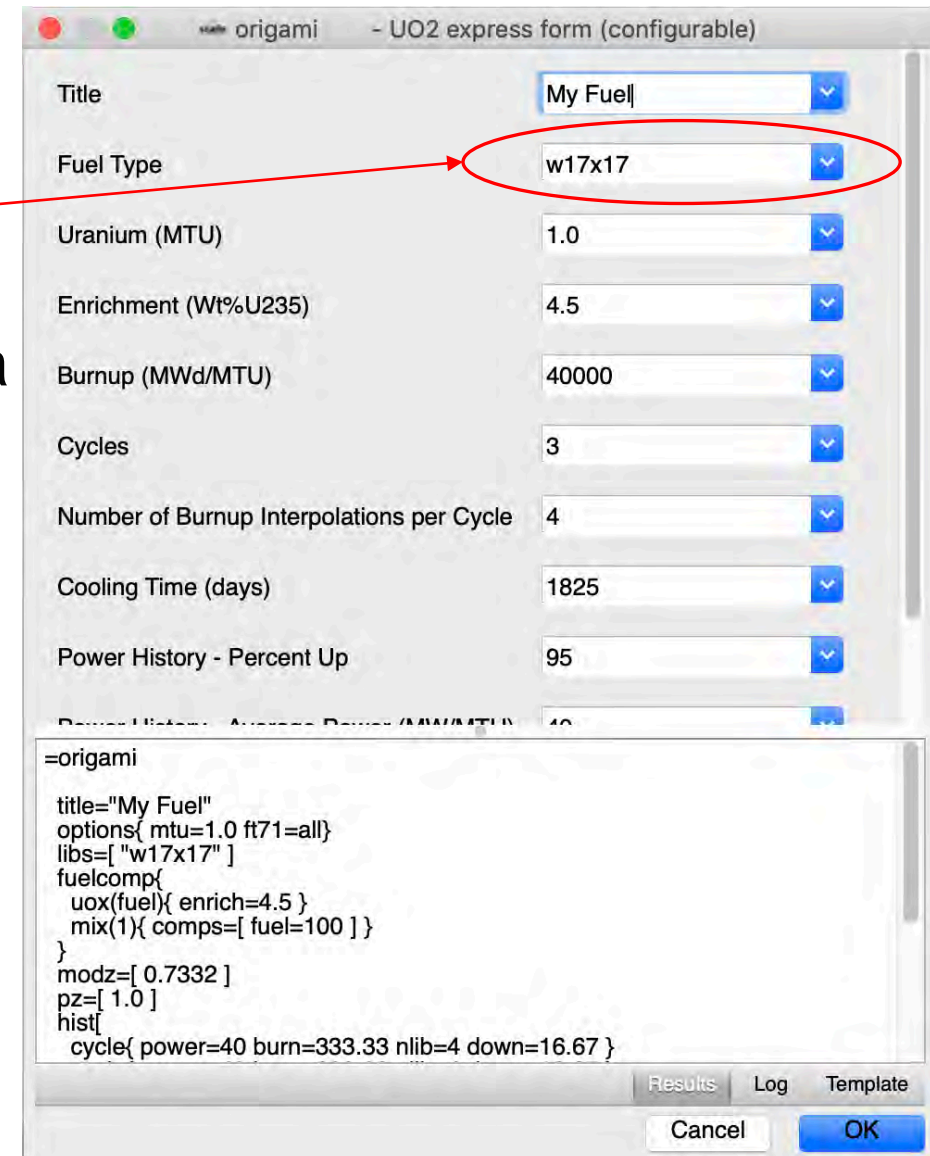
Prior SCALE validation for HTGR systems (2/2)

- **HTR-PROTEUS critical benchmark**
  - IRPhE benchmark based upon critical experiments performed at PROTEUS facility (Paul Scherrer Institut, Switzerland)
    - 10 deterministic pebble packing arrangements with 3 random close-packed arrangements
    - Graphite-coated spherical fuel elements with TRISO fuel particles
    - 3 cm radius graphite spheres (2.35 cm fuel region radius), 16.7% ^{235}U enrichment
  - **Figure of merit:** System k-eigenvalue (k_{eff})

| | Difference with MCNP5 (pcm) | | | |
| | ENDF/B-VI | | ENDF/B-VII.0 | |
	Average	**Maximum**	**Average**	**Maximum**
Columnar hexagonal point-on-point (CHPOP)	422 ± 93	667 ± 82	804 ± 87	1302 ± 811
Hexagonal close-packed (HCP)	252 ± 93	353 ± 84	782 ± 95	801 ± 85

G. Ilas, D. Ilas, R. P. Kelly, and E. E. Sunny, "Validation of SCALE for High Temperature Gas-Cooled Reactor Analysis," NUREG/CR-7107(ORNL/TM-2011/161), Jul. 2012

Workflow

SCALE specific | Generic | End-user specific

SCALE → **SCALE Binary Output** → **Inventory Interface File** → **Other**, **MACCS Input**, **MELCOR Input**

SCALE → **SCALE Text Output** → **Power distributions**, **Kinetics data** → **MELCOR Input**
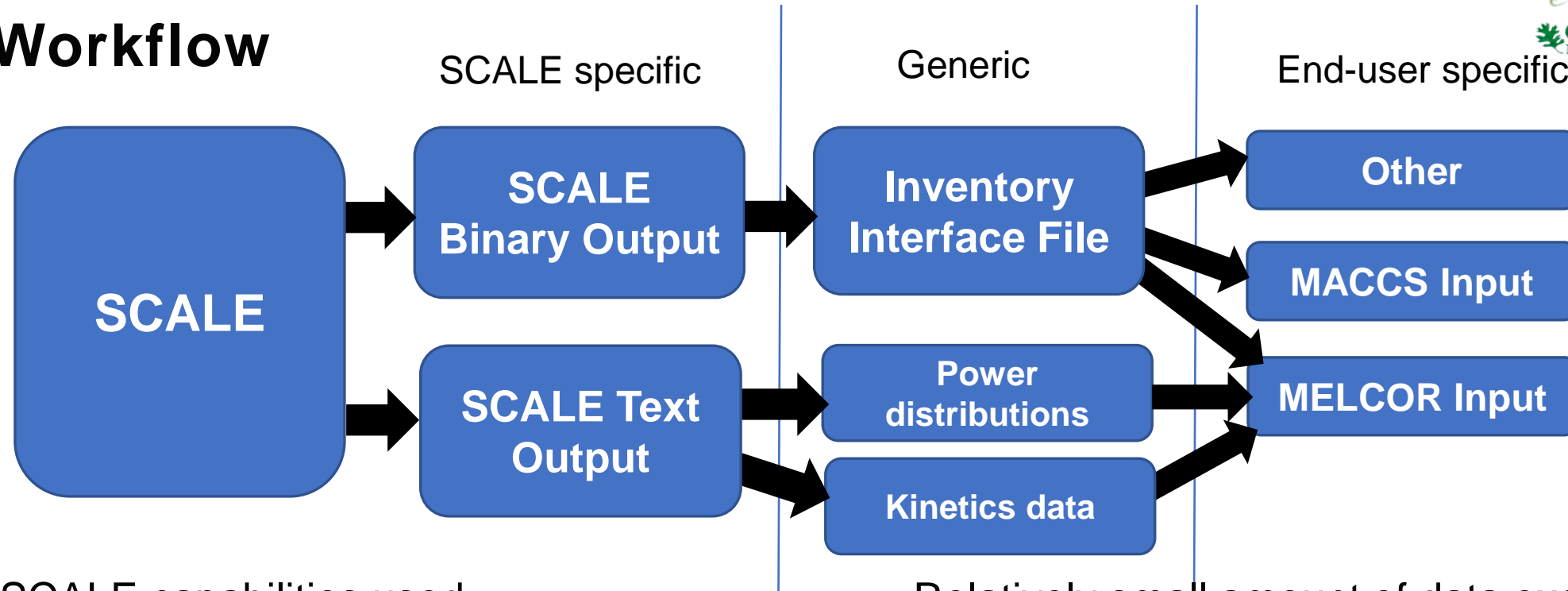
- SCALE capabilities used
  - KENO or Shift[*] 3D Monte Carlo transport
  - ENDF/B-VII.1 continuous energy physics
  - ORIGEN for depletion
  - Sequences
    - CSAS for reactivity (e.g. rod worth)
    - TRITON for reactor physics & depletion

[*]To be released with SCALE 6.3

- Relatively small amount of data except for nuclide inventory
  - new interface file developed for inventory using standard JSON format
  - easily read in python and post-processed into MELCOR or MACCS input
  - contains nuclear data such as decay Q-value for traceability when performing UQ studies

General ORNL Methodology for Fuel Inventory

- ORNL has used a methodology with the Oak Ridge Isotope GENeration (ORIGEN) code to rapidly generate inventories using ORIGEN reactor libraries

- SCALE/ORIGEN use of fundamental nuclear data allows the following to be calculated from nuclide inventory (moles of each nuclide in a system)
  - mass
  - decay heat
  - activity
  - gamma emission
  - neutron emissions

- With SCALE 6.2 (2016), the sequence ORIGAMI was released which is the modern approach of using ORIGEN reactor libraries


```
=origami

title="My Fuel"
options{ mtu=1.0 ft71=all}
libs=[ "w17x17" ]
fuelcomp{
  uox(fuel){ enrich=4.5 }
  mix(1){ comps=[ fuel=100 ] }
}
modz=[ 0.7332 ]
pz=[ 1.0 ]
hist[
  cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
```

Plans for SCALE/ORIGAMI and HTGR

- Soon ORIGAMI will have a new **PBMR-400 fuel type** and the ability to generate (in seconds)
  - fuel inventory for a PBMR-400 pebble
  - initial enrichment
  - specific power history
  - cooling time

- Generalizing what we learn for the PBMR-400 will enable future **HTGR fuel types**

Current Fuel Types

>50 different fuel types supported!

HTGR analysis with SCALE: Overview

- **Key assumptions**
  - License applications will specify pebble circulation strategy and equilibrium core
  - Analyzing the equilibrium core is the limiting case from an inventory/decay heat standpoint

- **Main goals**
  - Evaluate neutronic characteristics
  - Generate inventory and decay heat for the MELCOR nodalization **which may differ** from how the application specifies their equilibrium core isotopics
  - Generate individual pebble inventory within a core zone/batch (e.g., difference between fresh vs. once-through pebble in a single core zone)
  - Generate discharge pebble inventory/decay heat with sensitivity/uncertainty analysis

PBMR-400 equilibrium core
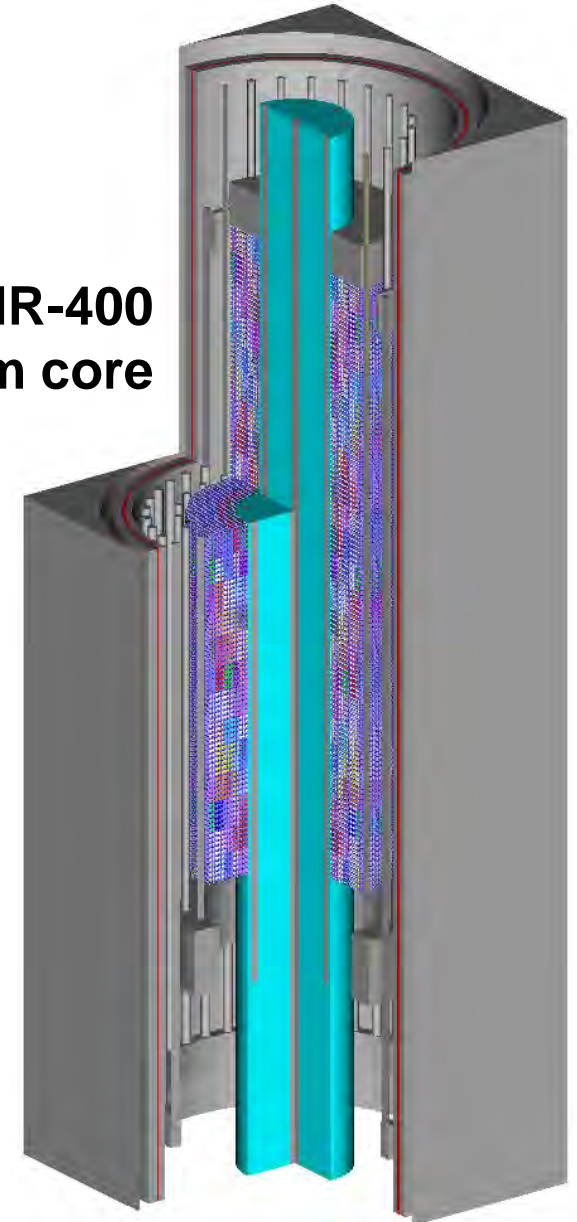
Analysis areas

1. Pebble packing

2. Temperature feedback

3. Radial/axial spectral variation

4. Pebble flow

5. TRITON model scope for ORIGEN library generation

   • (i.e. what matters for producing one-group sections)

**PBMR-400
equilibrium core**
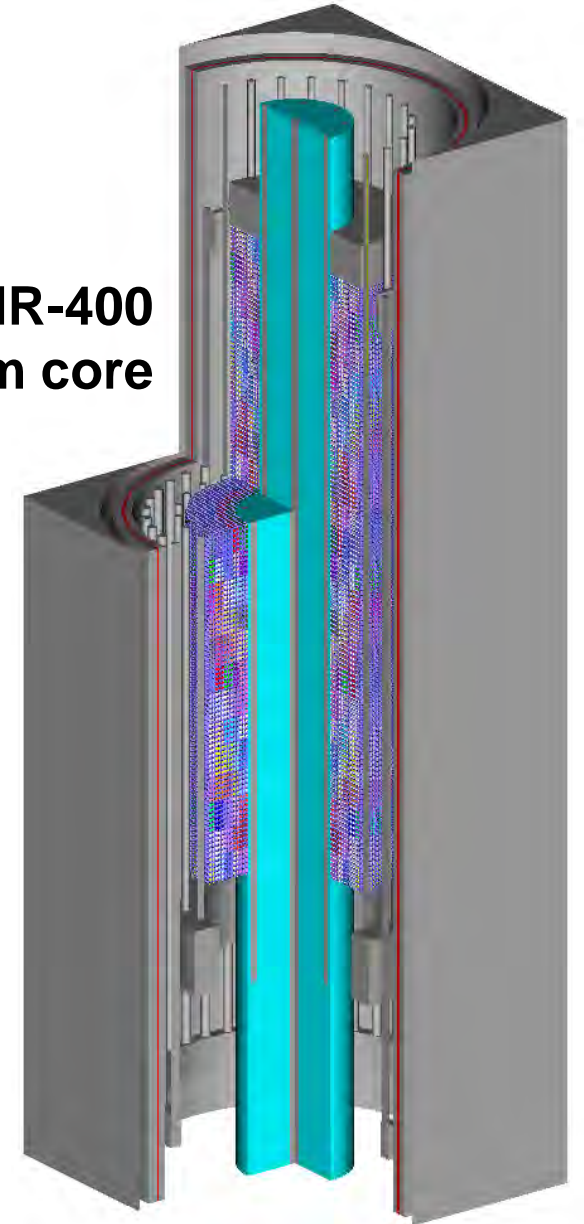
1. Pebble packing

PBMR-400 benchmark specifies ~452,000 fuel pebbles with a packing fraction of 61%

Can be achieved using a BCC lattice (dodecahedral) of unbroken spheres, however substantial negative bias in k_{eff} observed due to local voids near reflector regions

Present best estimate models use "clipped pebbles" at boundary to maintain uniform local packing fraction
- Similar to modeling approaches used for HTR-10[†]
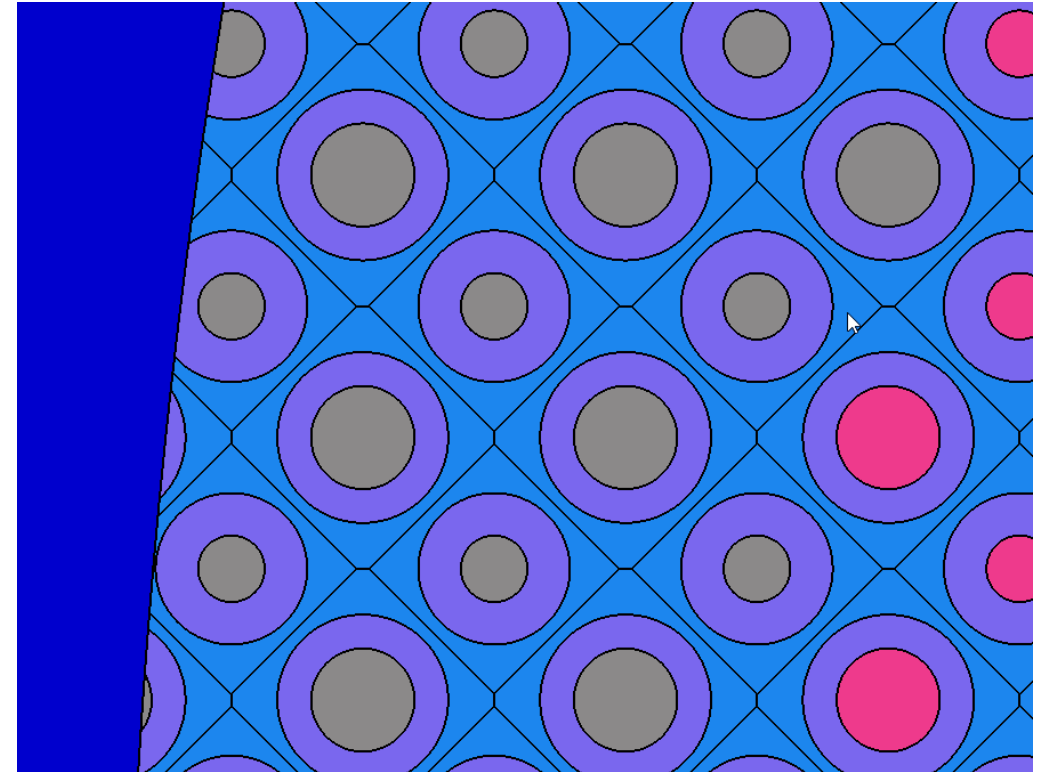
Image: S. Skutnik, ORNL

[†] J.-Y. Hong, S.-R. Wu, S.-C. Wu, D.-S. Chao, J.-H. Liang, "Burnup computations of multi-pass fuel loading scenarios in HTR-10 using a pre generated fuel composition library," *Nuclear Engineering and Design*, 374 (2021)

2. Temperature feedback (1/2)

Estimation of specific reactivity feedback components (e.g., temperature reactivity coefficients of fuel, moderator) requires detailed thermal hydraulic analysis of core

Strong coupling between neutronics & thermal hydraulics

Approach: Using system isotherms
- All system materials adjusted to a fixed temperature
  - e.g., 300, 600, 900, 1200 K
- Does not afford specific isolation of moderator / fuel temperature coefficients
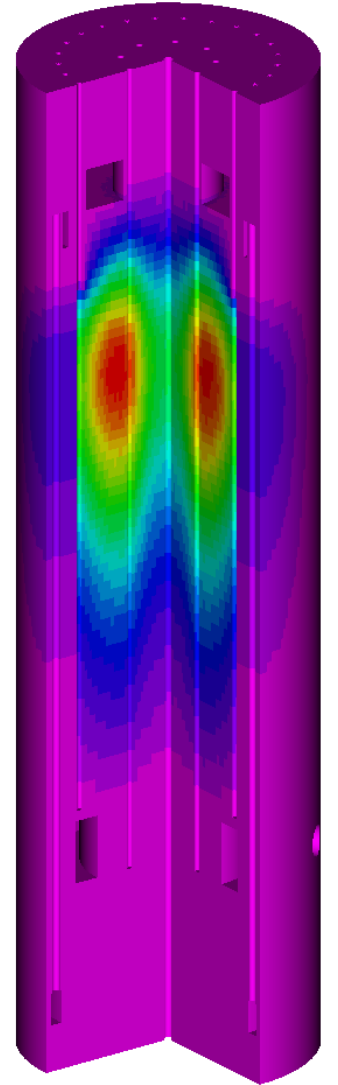
PBMR-400 total neutron flux, from SCALE/Shift
3D Monte Carlo Calculation (S. Skutnik, ORNL)

Strong temperature-driven spectral shifts, especially toward ^{239}Pu low-lying resonance

Fresh core
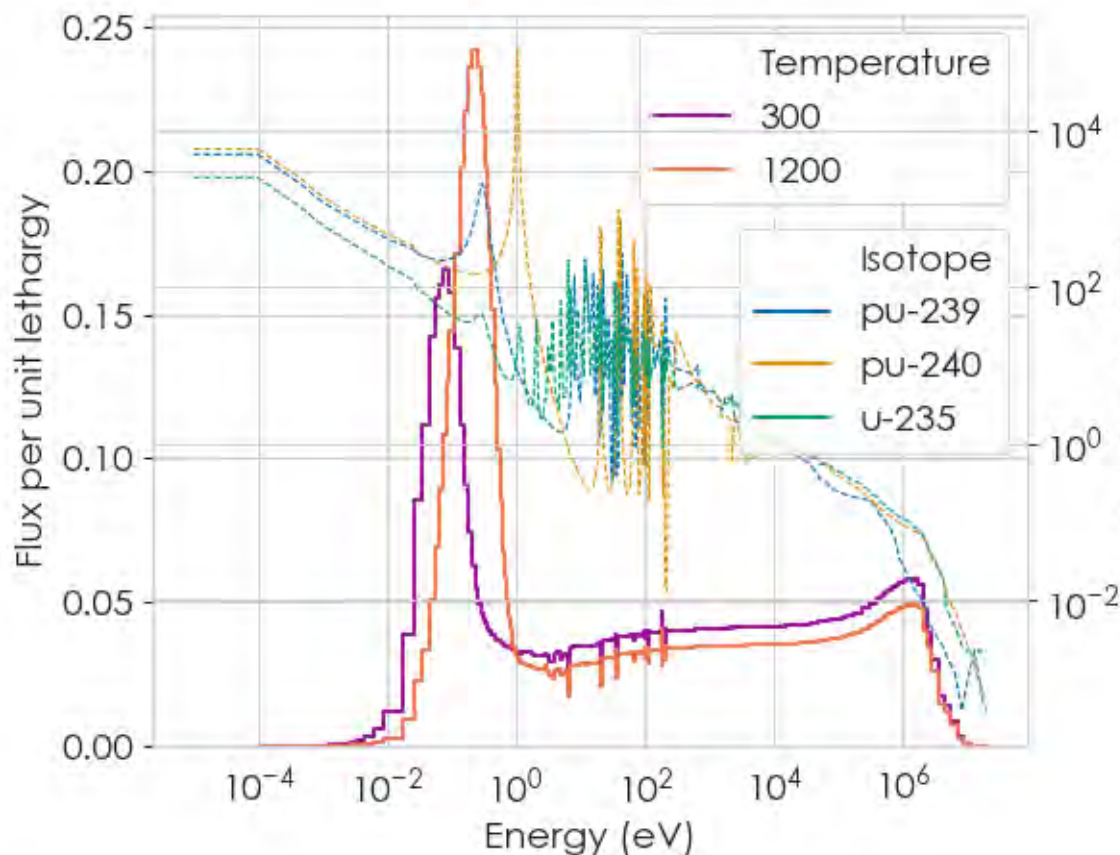
Equilibrium core
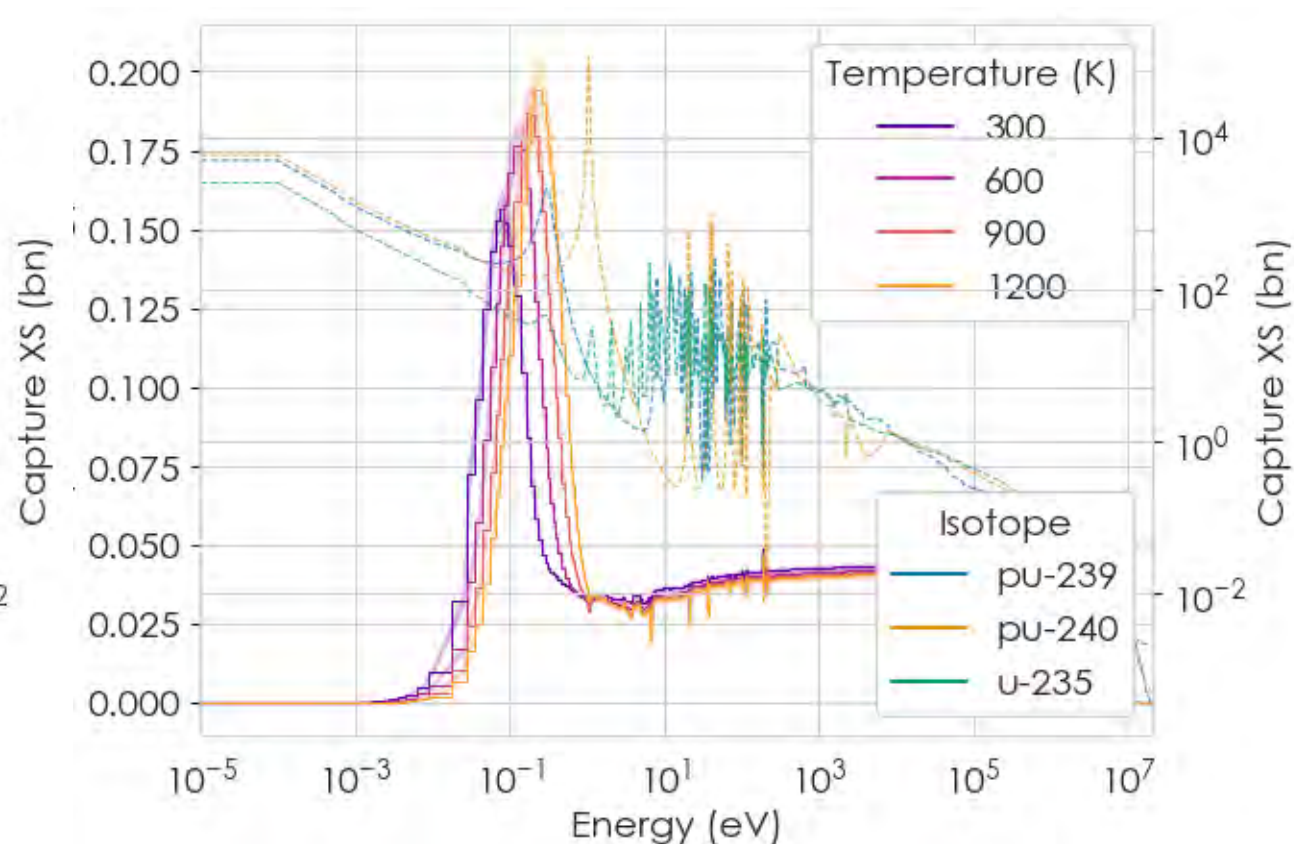
3. Flux shape shows a top-weighted distribution due to pebble loading & depletion

U.S.NRC

OAK RIDGE
National Laboratory
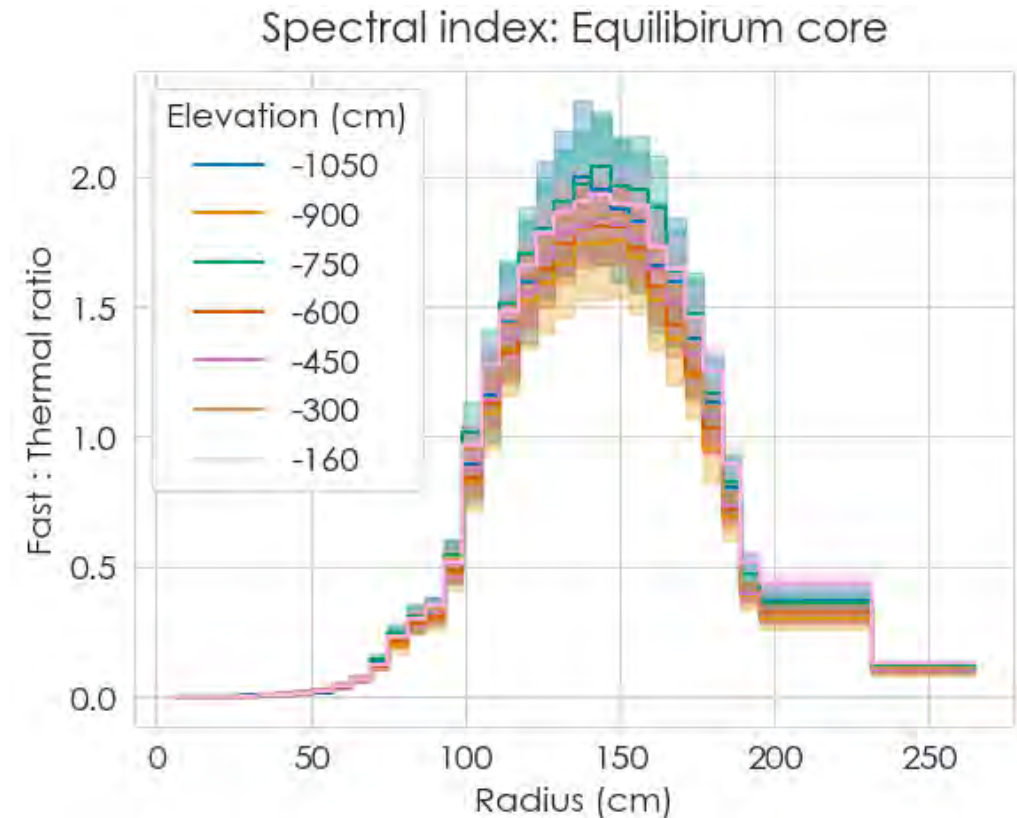
Sandia
National
Laboratories
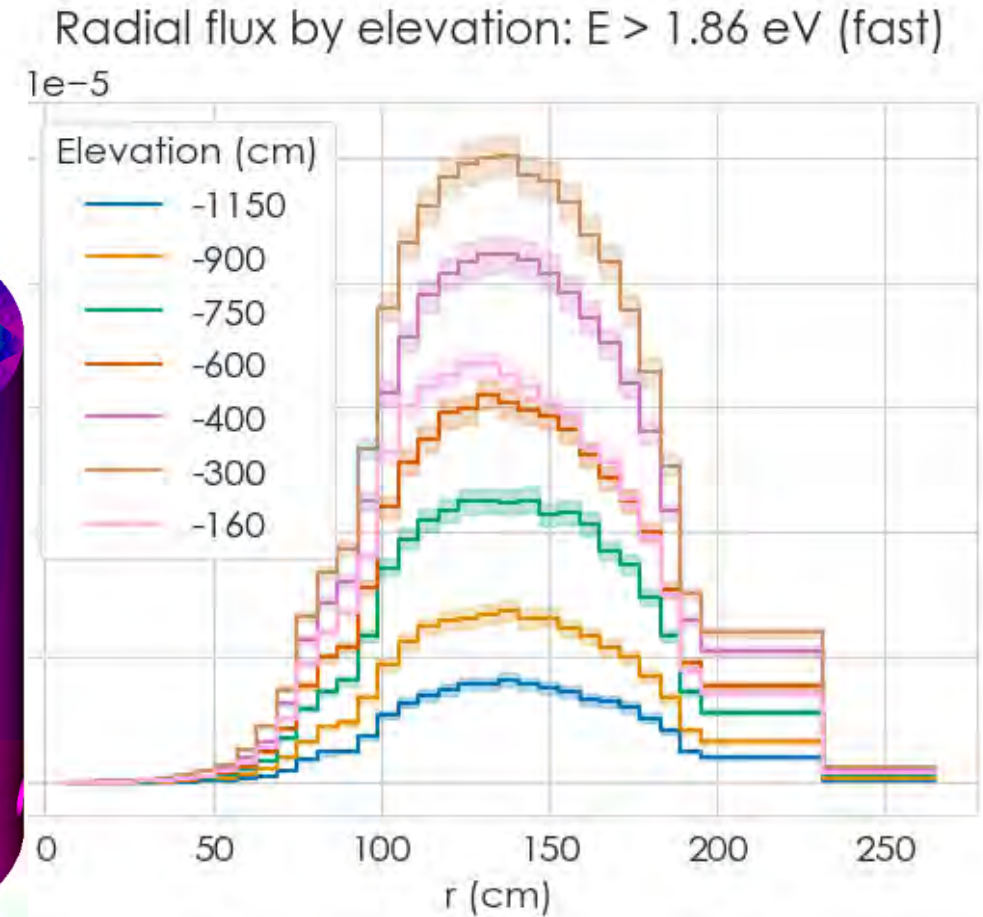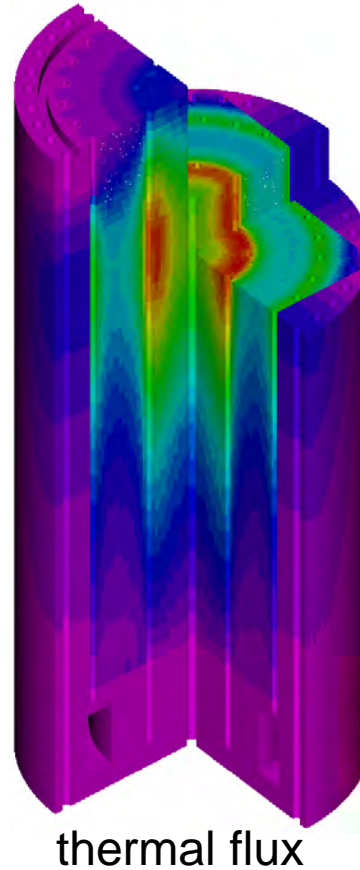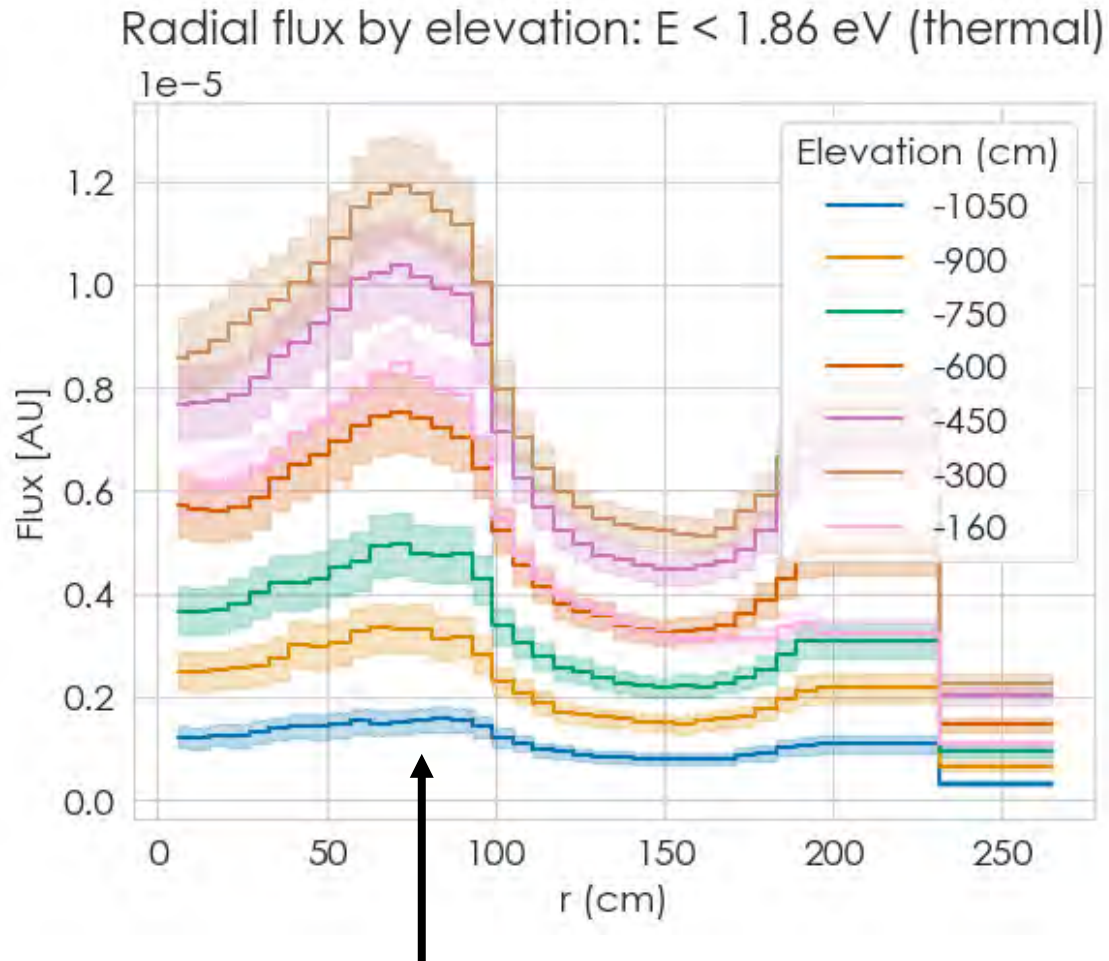
thermal flux

Strong power peaking effects observed
near graphite reflector regions (esp. interior)

3. Fast : thermal flux ratio (spectral index) <u>sensitive</u> to radial zone; relatively invariant axially

Axial
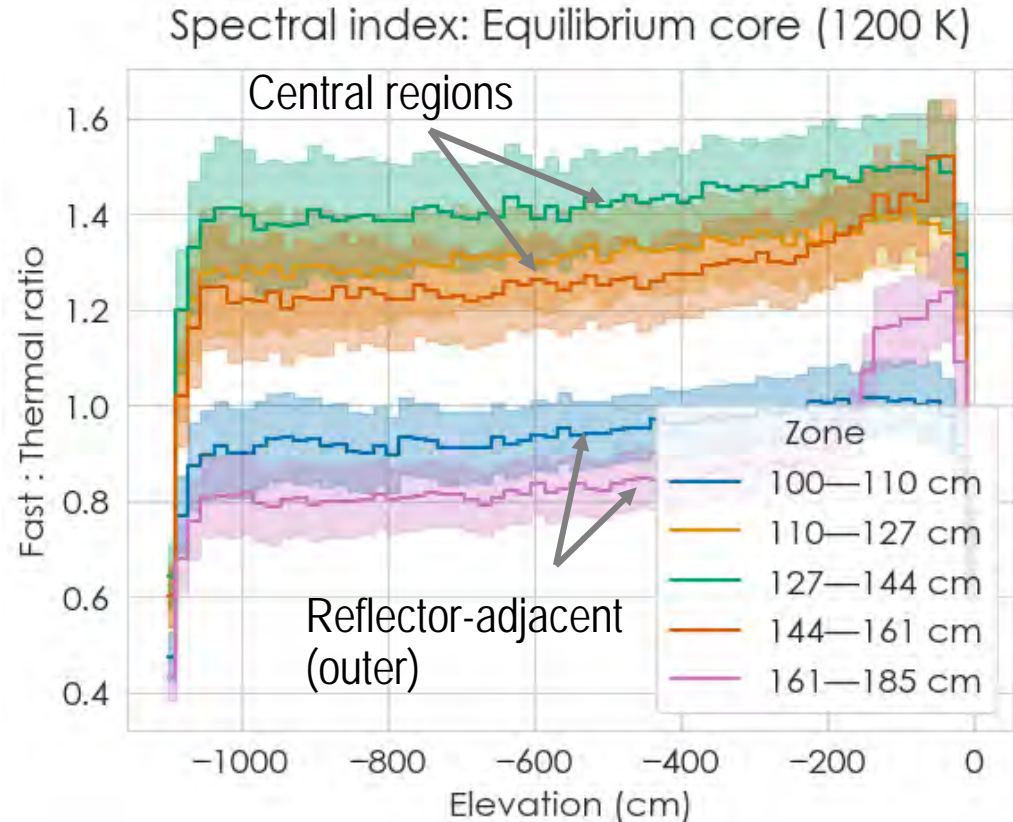
Radial

Major spectral shifts primarily occur across **radial** zones; i.e., primarily need **radial** zone Origen libraries

Approach: "Equilibrium" compositions derived from previous equilibrium core calculation with flowing pebbles (VSOP)

- Pebble locations currently treated as "static" in a full-core, 3-D Monte Carlo neutron transport calculation

- Discrete axial and radial material zones, representing spatially-dependent "average" at equilibrium after several months of operation

Similarity to prior approaches:

- VSOP:[1] Depletion of fixed core compositions to a pre-defined k_{eff}, then shuffle zones downward, reload pebbles at top of core and repeat. Depletion assumes admixture of fresh & burned pebbles exposed to same depleting flux

- HTR-10 multi-pass pebble burnup analysis[2] follows similar procedure to VSOP

References:

1. HJ. Rütten, K.A. Haas, H. Brockmann, W. Scherer, "V.S.O.P. (99/05) Computer Code System" (2005)
2. J.-Y. Hong, S.-R. Wu, S.-C. Wu, D.-S. Chao, J.-H. Liang, "Burnup computations of multi-pass fuel loading scenarios in HTR-10 using a pre generated fuel composition library," *Nuclear Engineering and Design*, 374 (2021)
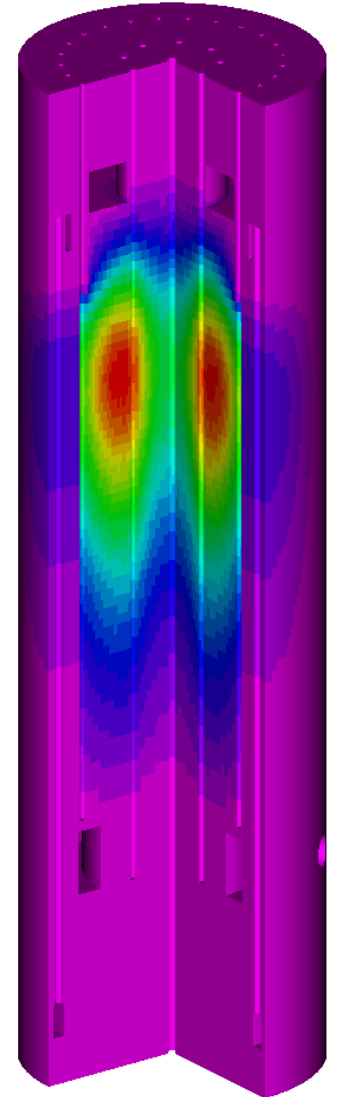
PBMR-400 total neutron flux from SCALE/Shift 3D Monte Carlo calculation (S. Skutnik, ORNL)

4. Capturing possible pebble transit paths through the core (velocity differentials & cross-flow)

Current assumptions:

- Pebble transit dominated by vertical motion; can capture differential velocity across radial regions

- Active core modeled as a right-cylindrical annulus (cylindrical shell)

Similarity to prior approaches:

- VSOP: Pebble transit assumed to be in parallel vertical dimensions unless user specifies otherwise

- HTR-10 burnup analysis normalizes pebble residence time based on assumed transit path (conical funneling)[†]; recycled pebbles uniformly redistributed across top of core

[†]J.-Y. Hong, S.-R. Wu, S.-C. Wu, D.-S. Chao, J.-H. Liang, "Burnup computations of multi-pass fuel loading scenarios in HTR-10 using a pre generated fuel composition library," *Nuclear Engineering and Design*, 374 (2021)

5. ORIGEN library analysis strategy

Evaluate PBMR-400 cross-sections & isotopic responses at different levels of model fidelity

Lower fidelity
Lower computational cost

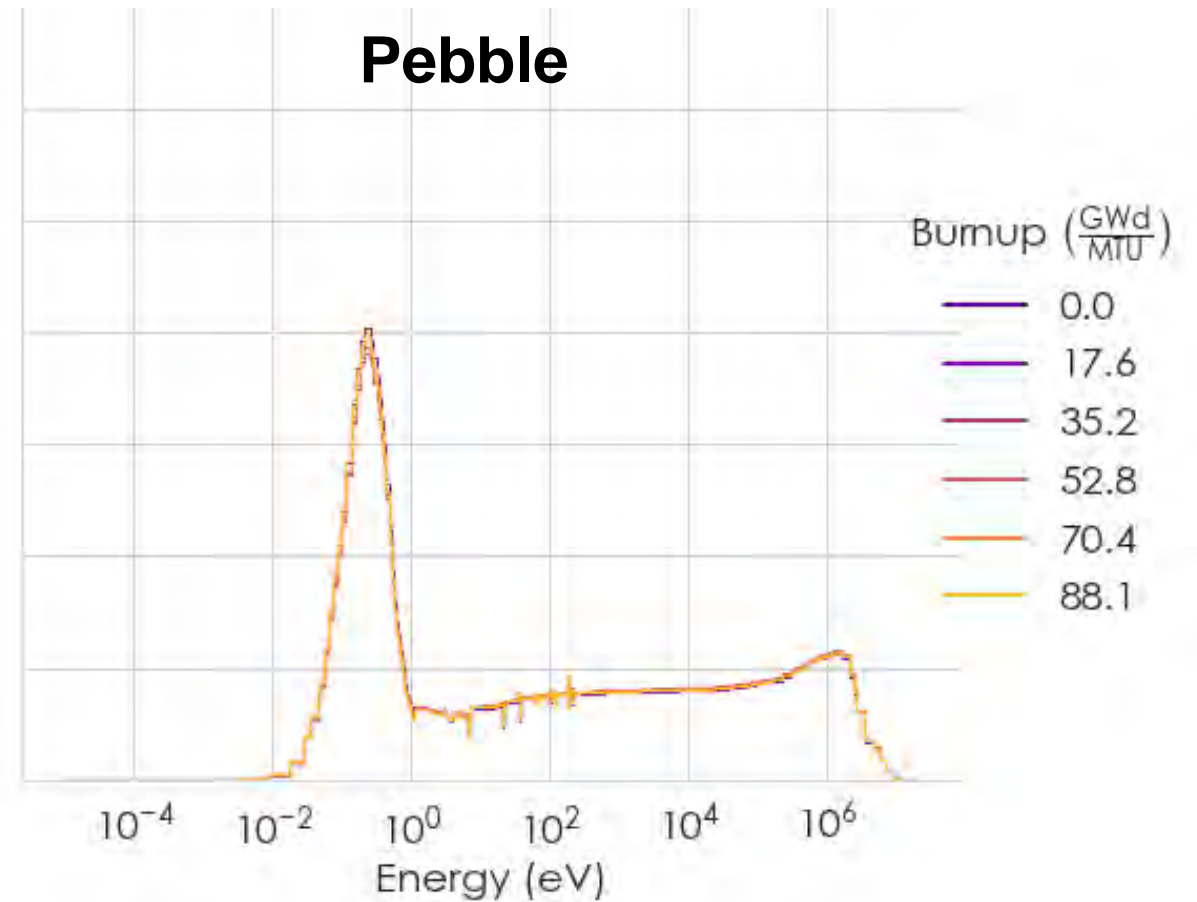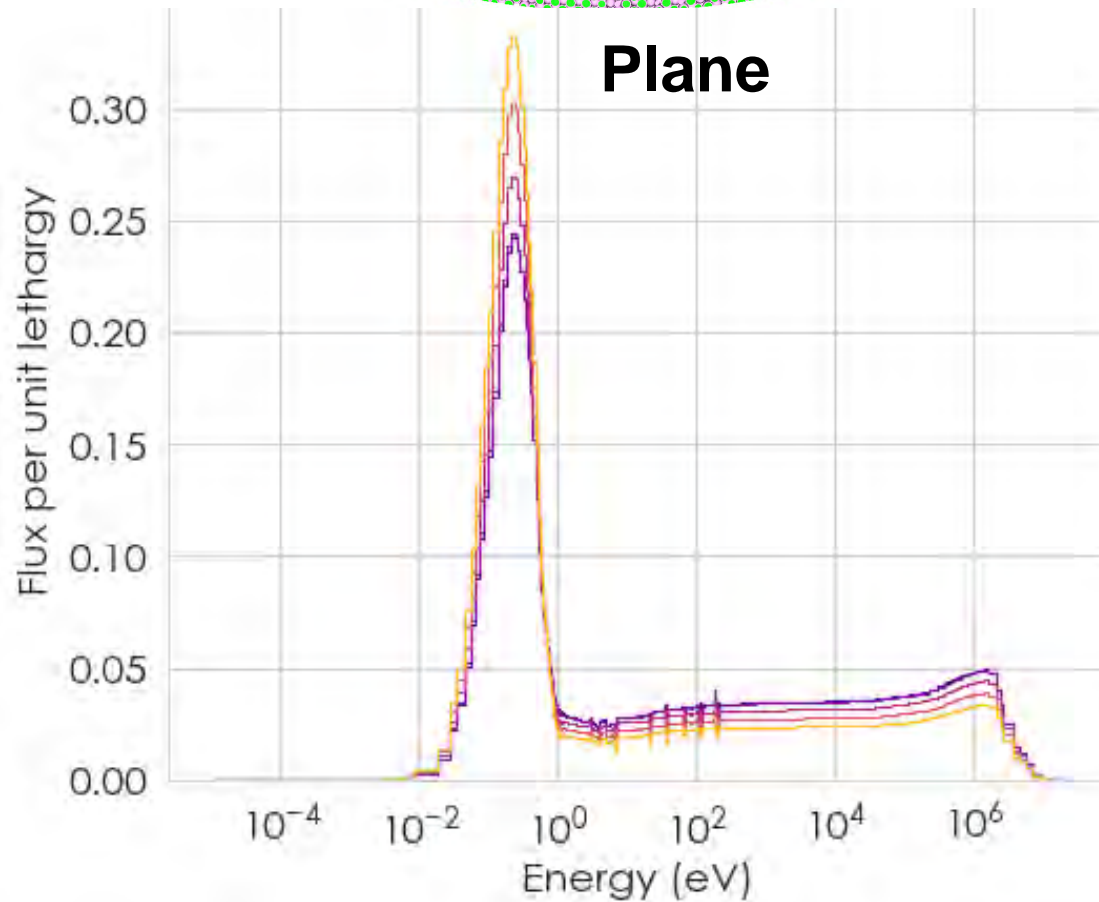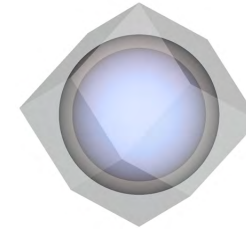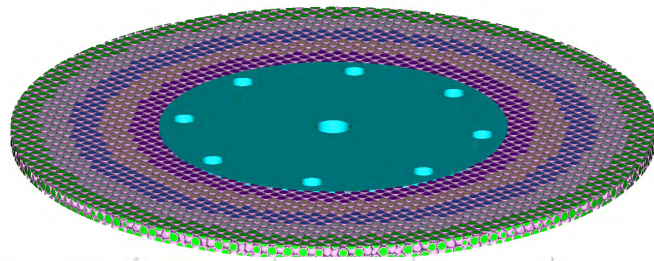High fidelity
High computational cost
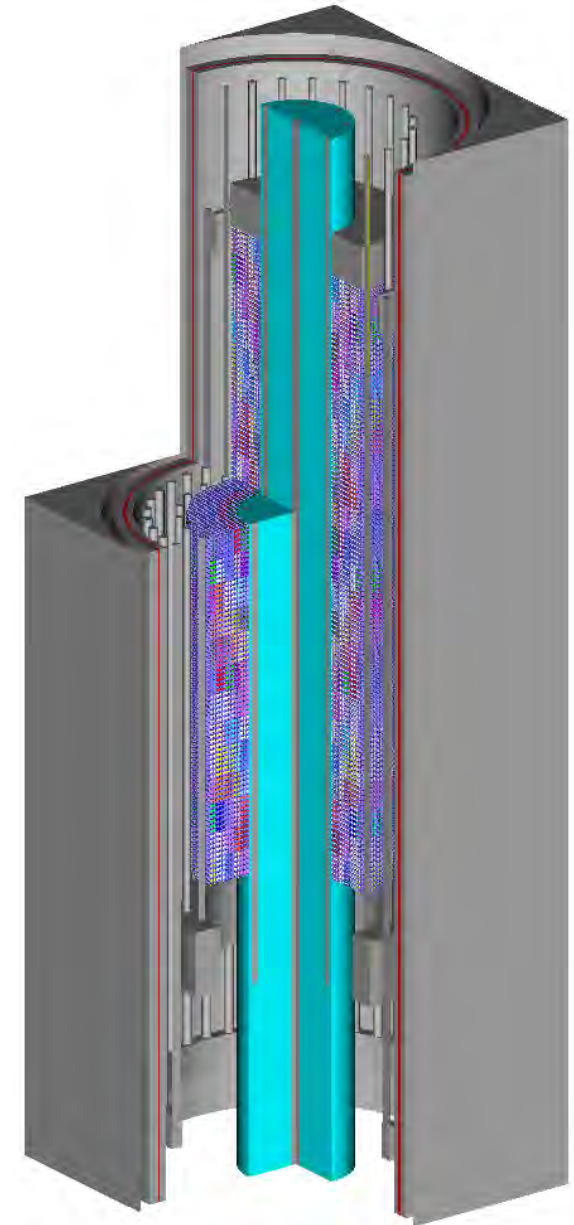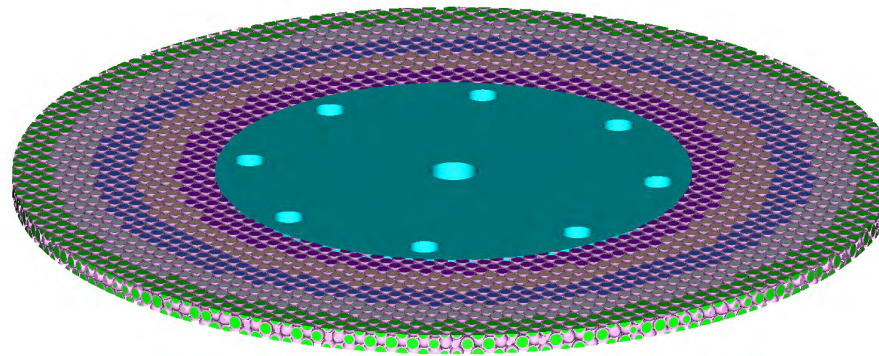
5. ORIGEN library development: "reflected plane" model

- Accounts for important radial effects

  - Proximity to reflector
  - Effects of nearest neighbor pebbles

- Can easily be tuned for different axial zones
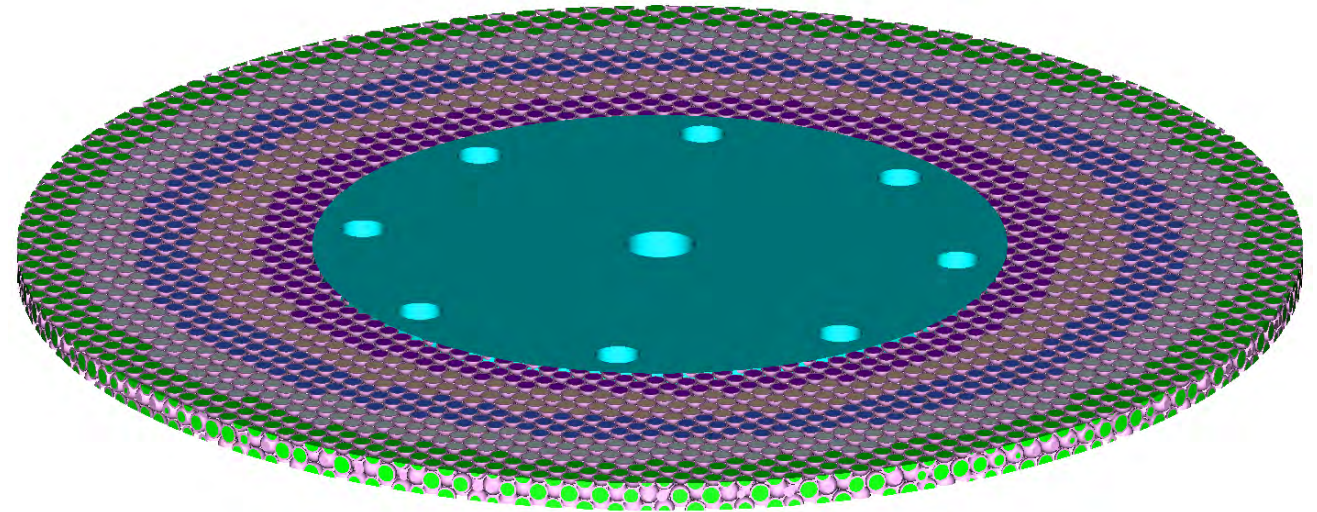
5. Plane model captures important neighbor effects

5. ORIGEN library generation based on 5 spectral zones

- Five separate cases constructed starting with a fresh pebble surrounded by non-depleting neighbors with compositions derived from PBMR-400 benchmark inventory ND-Set3

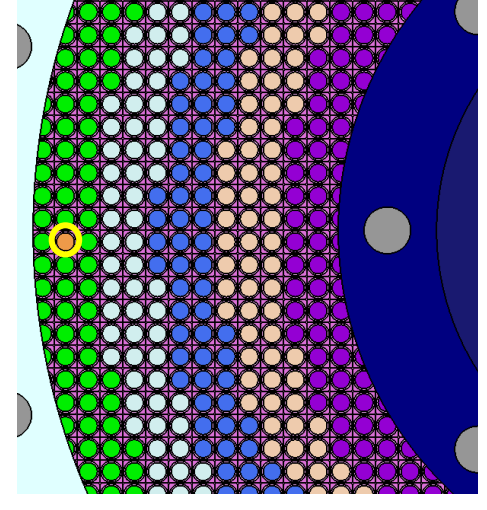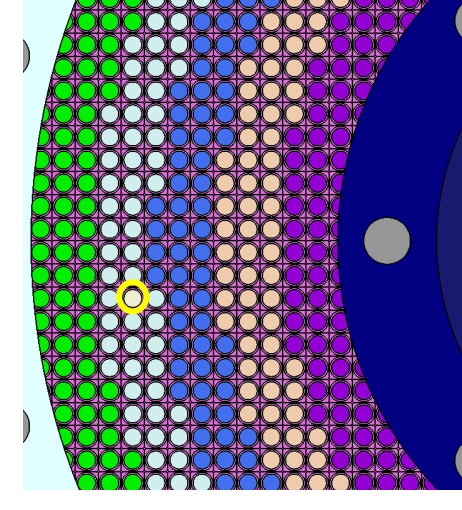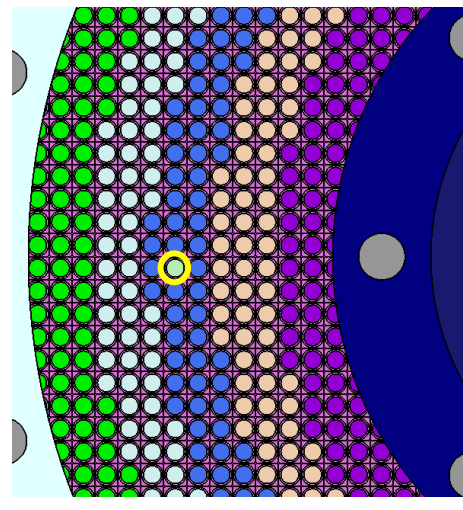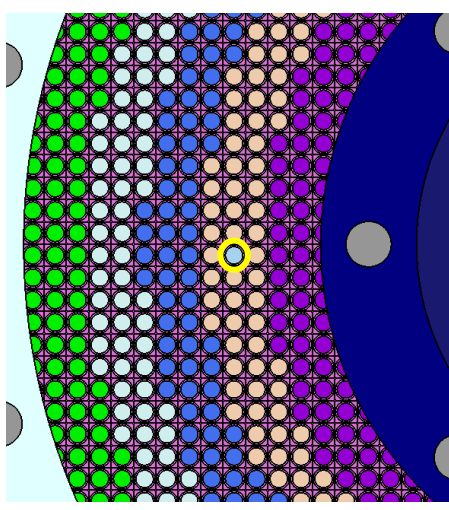- Pebble depleted to discharge burnup surrounded by invariant neighbors
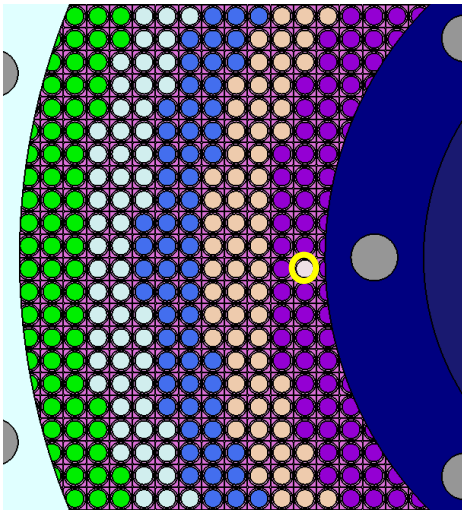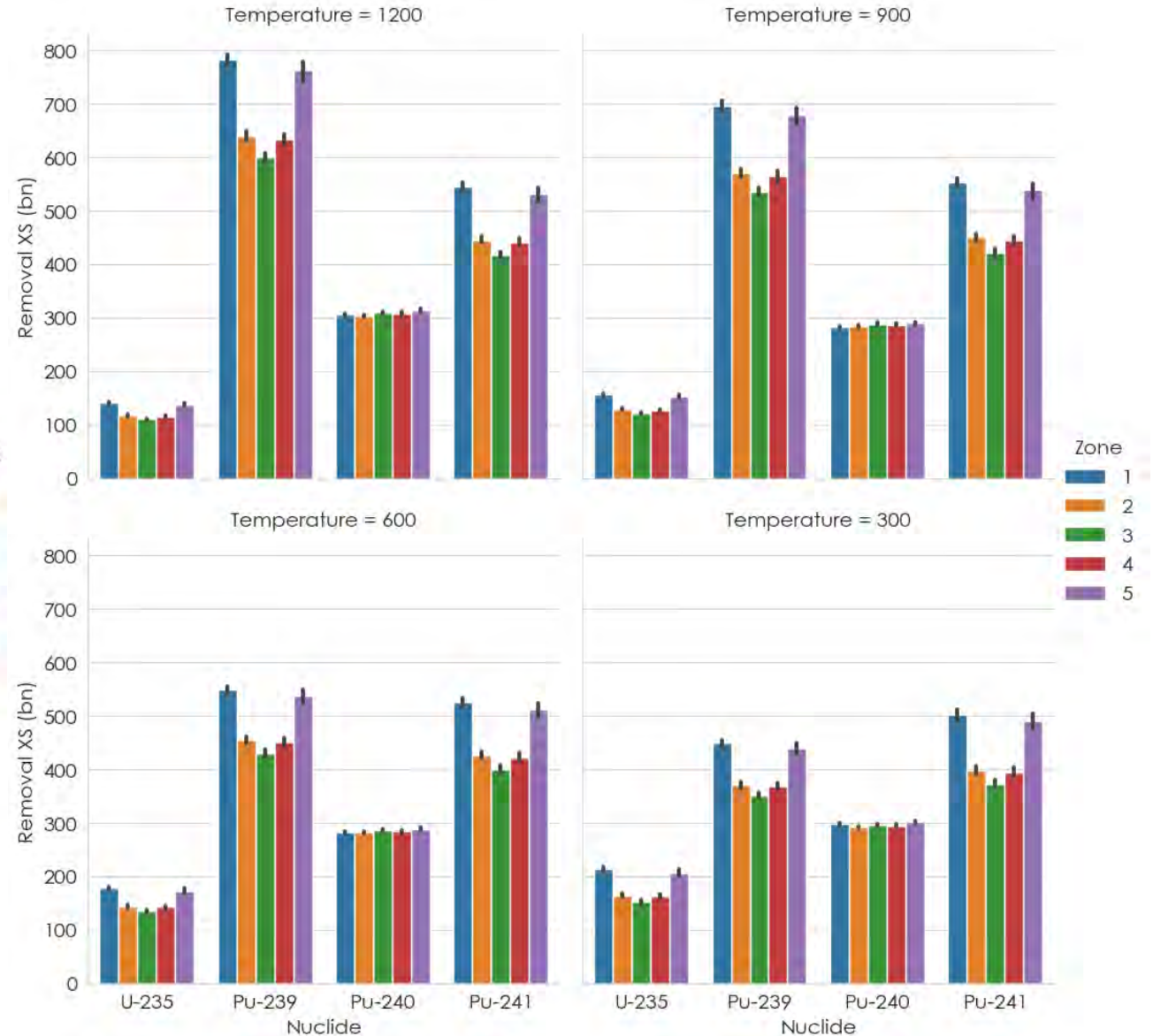
rzone=1   rzone=2   rzone=3   rzone=4   rzone=5

5. Radial, temperature effects drive differences in 1-group XS's ORIGEN libraries
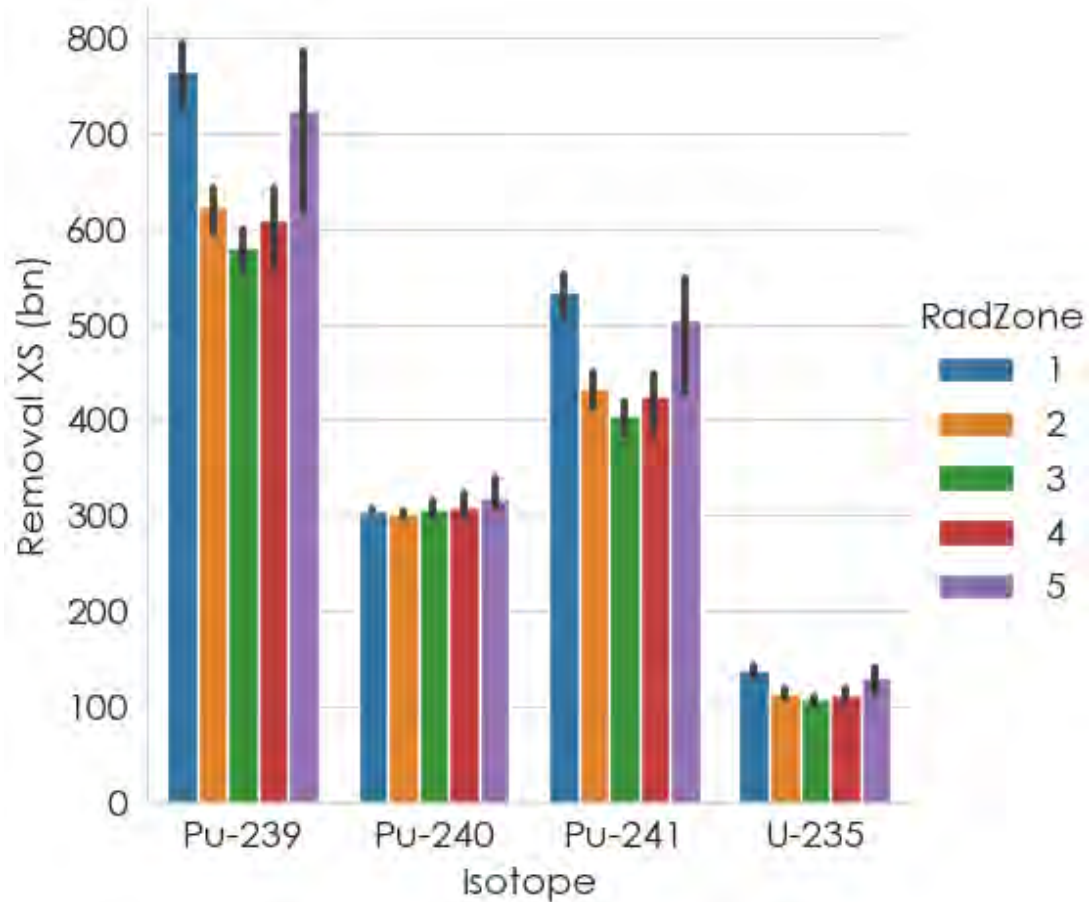
5. Radial zone effects far more prevalent than burnup effects for pebble bed depletion

Outer regions

Central region

Spatial-driven differences in loss cross-sections relatively stable over burnup
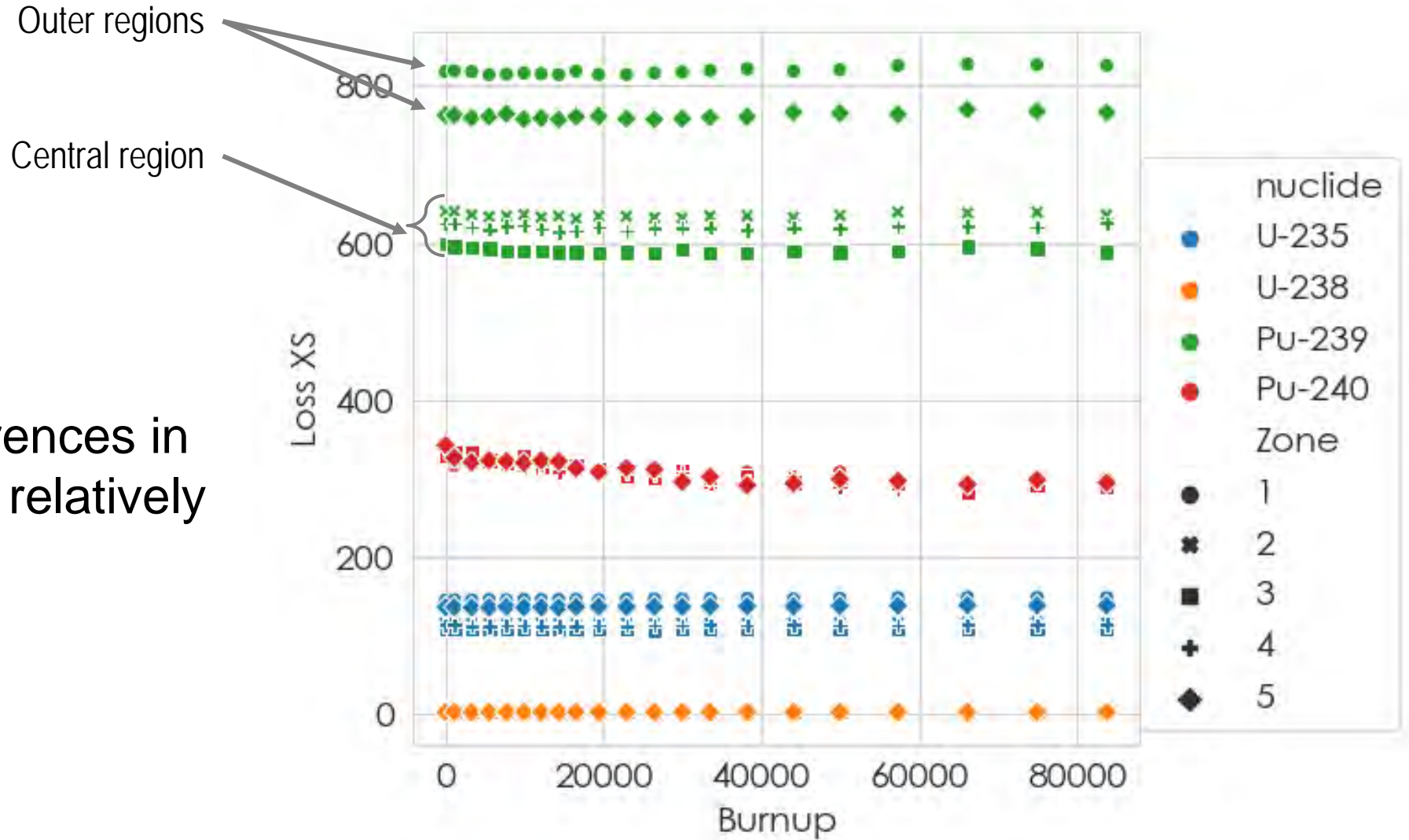
5. Temperature (system isotherm) shows a large, region-dependent effect on 1G removal XS

Magnitude of XS differences due to radial location **increases with system temperature**

- Gap between "inner" and "outer" regions grows with increasing temperature
- Implies a covariant relationship between location & temperature

Conclusions for pebble bed reactor ORIGEN library development

- Analysis areas
  1. Pebble packing
  2. Temperature feedback
  3. Radial/axial spectral variation
  4. Pebble flow
  5. TRITON model scope for ORIGEN library generation
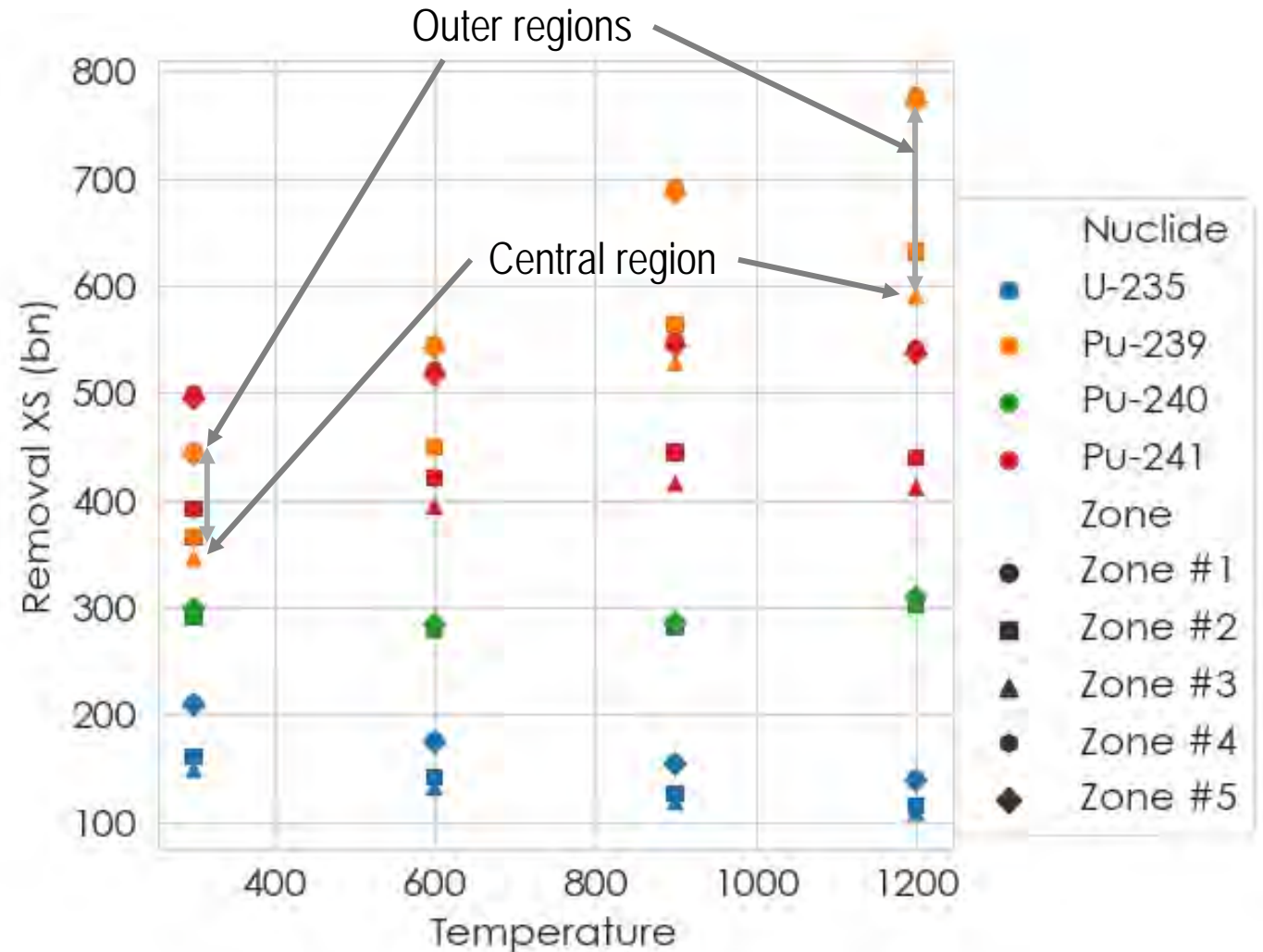
Further details:
S. Skutnik, W. Wieselquist, "Assessment of ORIGEN Reactor Library Development for Pebble-Bed Reactors Based on the PBMR-400 Benchmark," ORNL/TM-2020/1886, July 2021
Available on osti.gov

- For ORIGEN library generation
  - Burnup effects appear to be second-order, roughly linear in nature
  - Radial distance from the reflector is a first-order spectrum characteristic
    - Must be accounted for in library generation
  - Temperature (system isotherm) also a first-order effect
    - Shows covariance with radial position
   - Driven primarily by graphite (reflector) temperature

MELCOR HTGR modeling

Fission product release
- Release from TRISO kernel
- Radionuclide distributions within the layers in the TRISO particle and compact
- Release to coolant

Other core models
- Graphite oxidation
- Intercell and intracell conduction
- Convection & flow
- Point kinetics
- Dust generation and resuspension
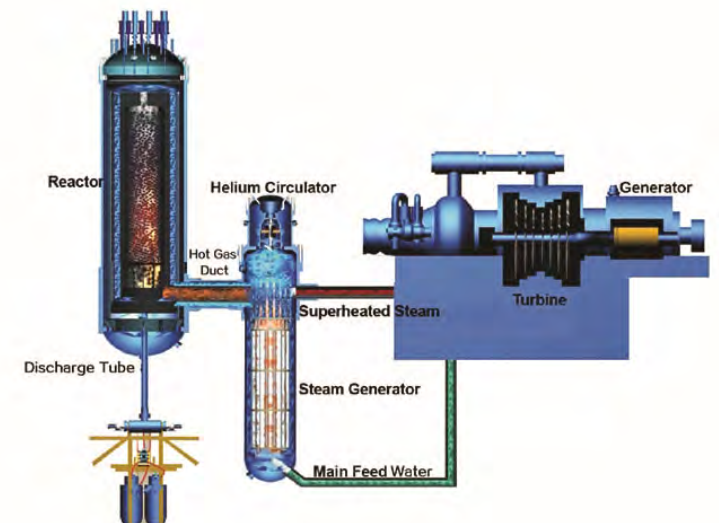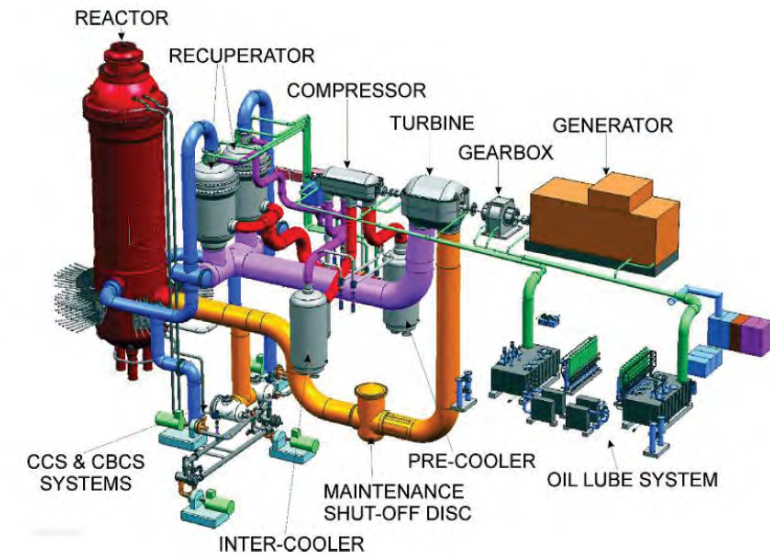
HTGR Components

- 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
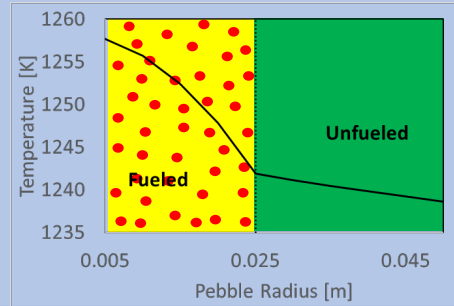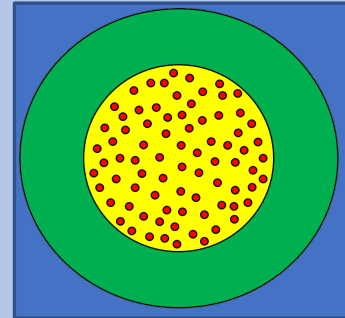
Unfueled pebble core

- 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
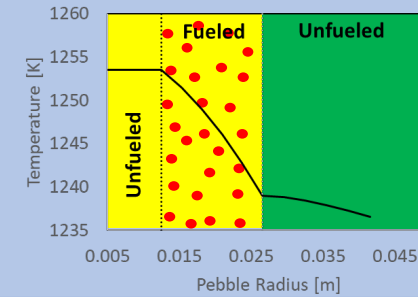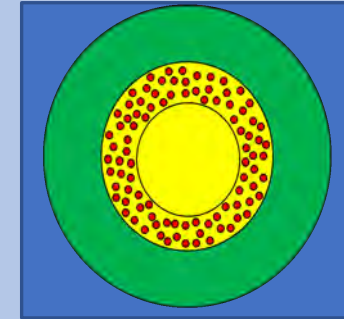
Legend

TRISO — Fuel (FU)
GRAPHITE — Fuel (FU)

GRAPHITE — Matrix (MX)

Fluid B/C

TRISO (FU)

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

44
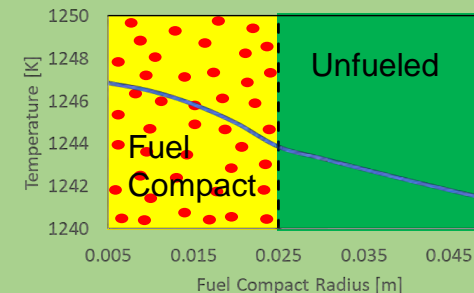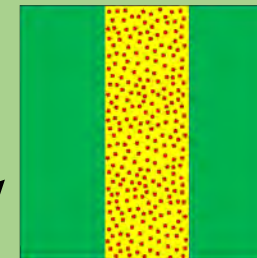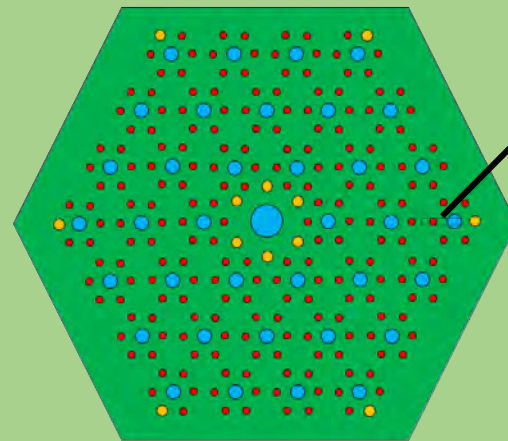
Transient/Accident Solution Methodology

Stage 0:
Normal Operation
Establish thermal state

Time constant in HTGR graphite structures is very large

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

Reset heat capacities after steady state is achieved.

Representative reflector temperature response
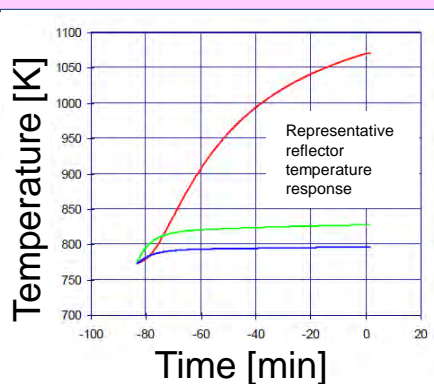
Stage 1:
Normal Operation
Diffusion Calculation

Establish steady state distribution of radionuclides in TRISO particles and matrix
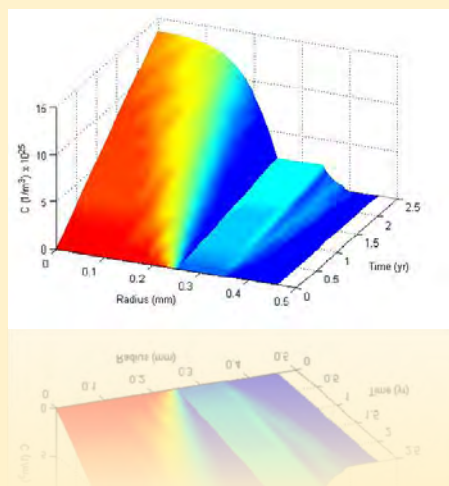
Stage 2:
Normal Operation
Transport Calculation

Calculate steady state distribution of radionuclides and graphite dust throughout system (deposition on surfaces, convection through flow paths)

Circulating Cs Mass

Cs Mass Deposited
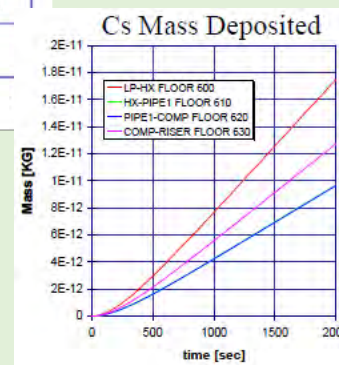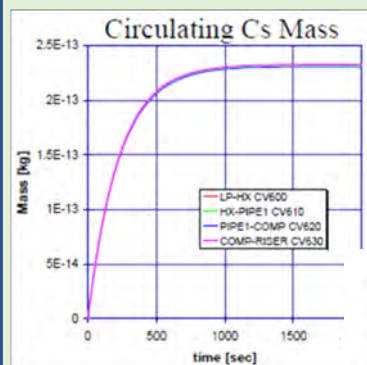
Example:
PBMR-400 Cs Distribution in Primary System

Stage 3:
Accident
Diffusion & Transport calculation

Calculate accident progression and radionuclide release
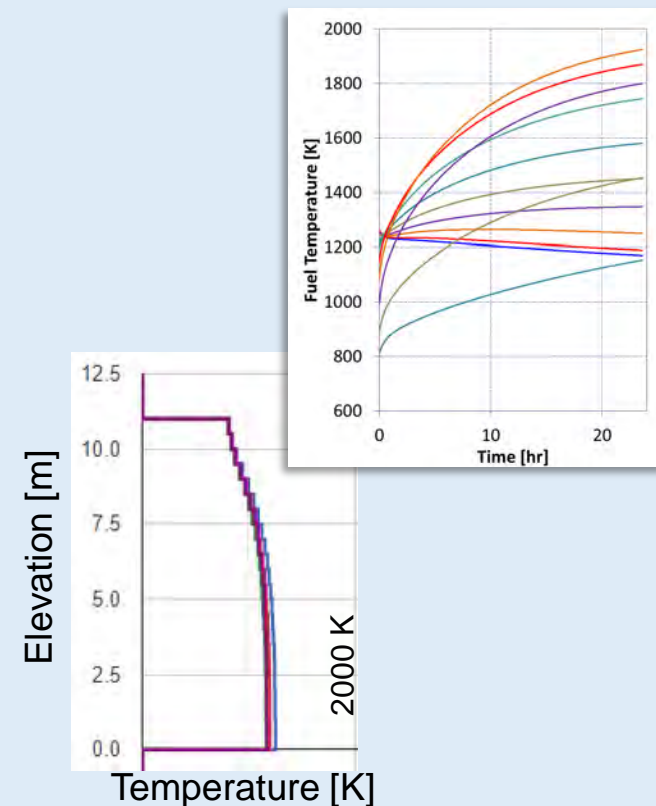
HTGR Radionuclide Diffusion Release Model

Intact TRISO Particles

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

$$\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n D \frac{\partial C}{\partial r}\right) - \lambda C + \beta$$

$$D(T) = D_0 e^{-\frac{Q}{RT}}$$
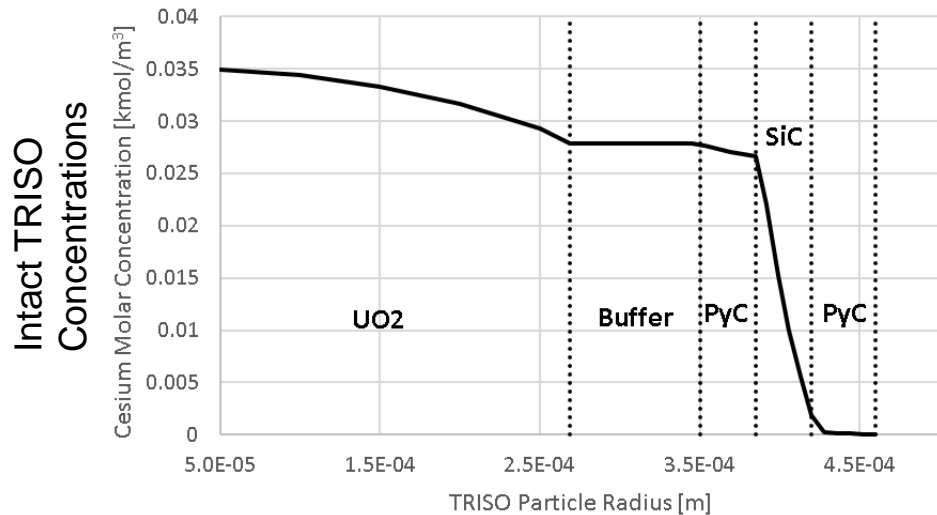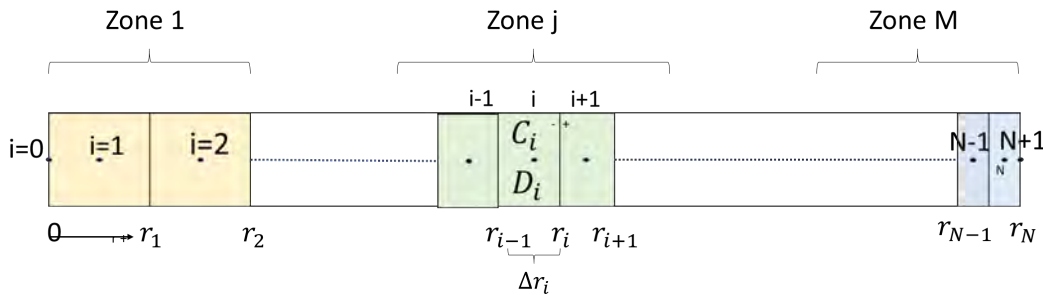
Diffusivity Data Availability

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 (m2/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
CORSOR-Booth LWR scaling used to estimate other radionuclides

HTGR Radionuclide Release Models

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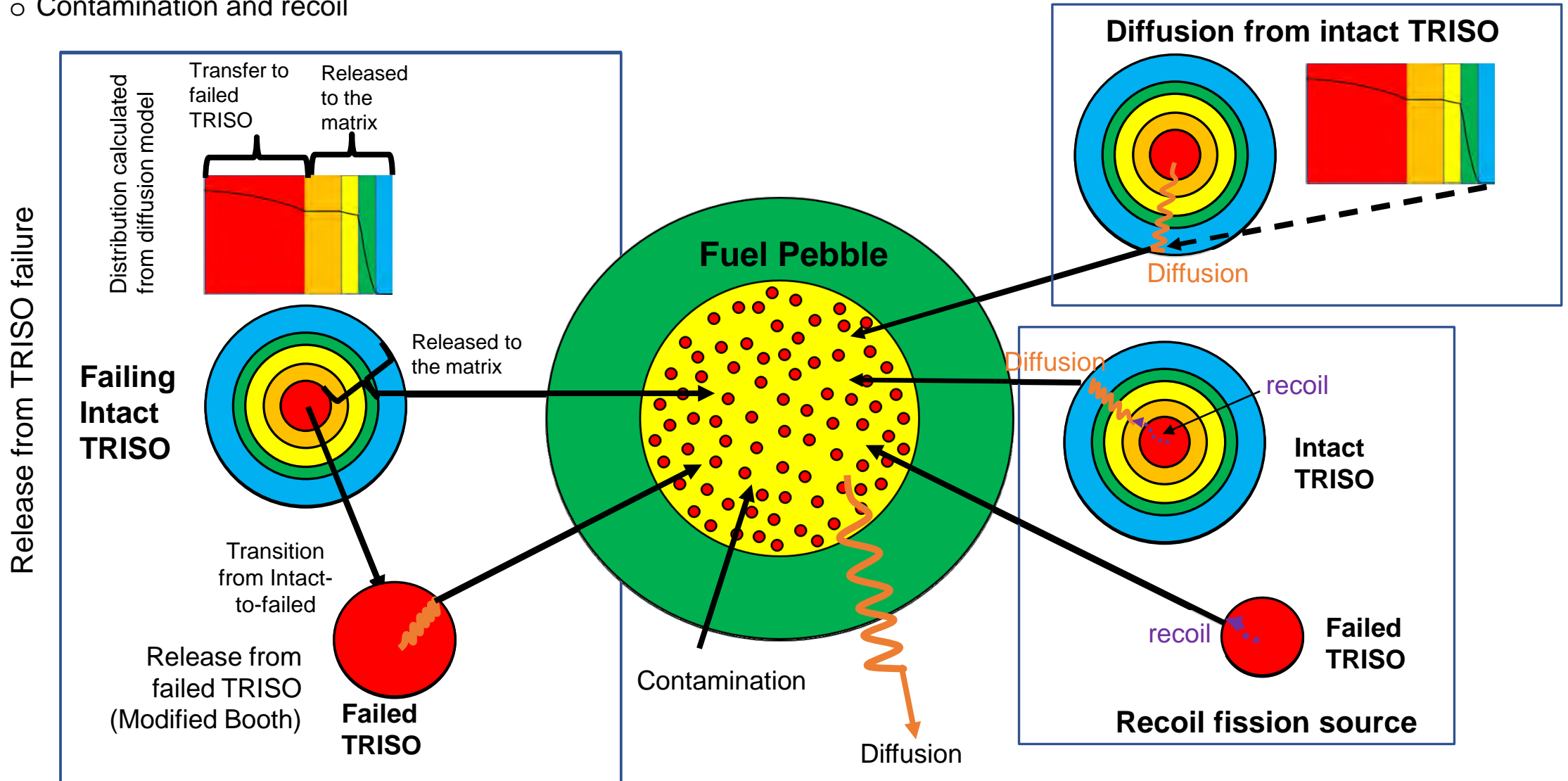
Graphite Oxidation

Steam oxidation

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

Air oxidation

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

Reactions

$$C + H_2O(g) \rightarrow CO(g) + H_2(g)$$

$$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$$

Reactions

1. $C + O_2 \rightarrow CO_2(g)$

2. $C + \frac{1}{2}O_2 \rightarrow CO(g)$

3. $CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g)$

4. $C + CO_2(g) \rightarrow 2CO(g)$

H$_2$O or Air

He
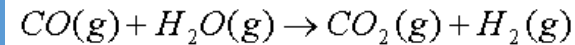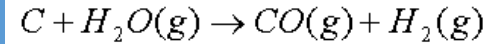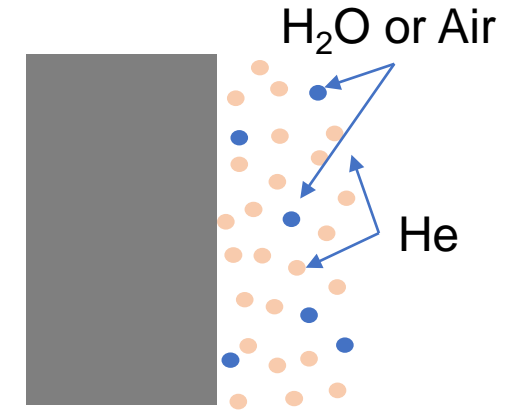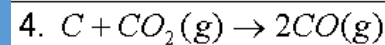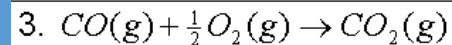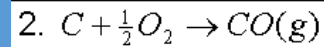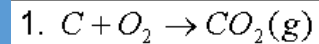
Both steam and air include rate limit due to steam/air diffusion towards active oxidation surface

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

COR Intercell Conduction
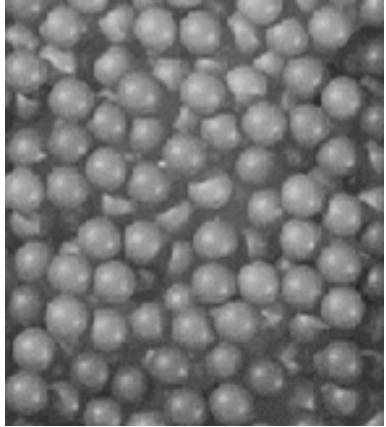
Effective conductivity prescription for pebble bed (bed conductance)

- Zehner-Schlunder-Bauer with Breitbach-Barthels modification to the radiation term

$$k_{eff} = \left(1 - \sqrt{1-\varepsilon}\right)\varepsilon\, 4\sigma T^3 D_p + \left(1 - \sqrt{1-\varepsilon}\right)k_f + \sqrt{1-\varepsilon}\, k_c(T, D_p, \varepsilon, k_f, k_s, k_r)$$

D_p=.06 m
K_f=.154 W/m-K
K_s = 26 W/m-K

ε=0.6
ε=0.39
ε=0.00001
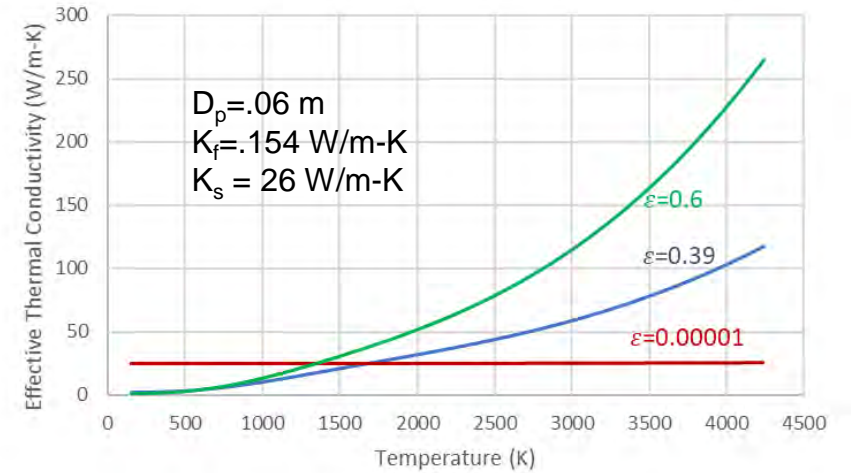
Effective conductivity prescription for prismatic (continuous solid with pores)

- Tanaka and Chisaka expression for effective radial conductivity (of a single PMR hex block)

$$k_{eff} = k_s\left[A + (1-A)\frac{\ln\left(1 + 2B(k_{por}/k_s - 1)\right)}{2B(1 - k_s/k_{por})}\right]$$

- A radiation term is incorporated in parallel with the pore conductivity

- Thermal resistance of helium gaps between hex block fuel elements is added in parallel via a gap conductance term

K_s = 26 W/m-K
K_f=.154 W/m-K

ε=0.6
ε=0.39
ε=0.00001
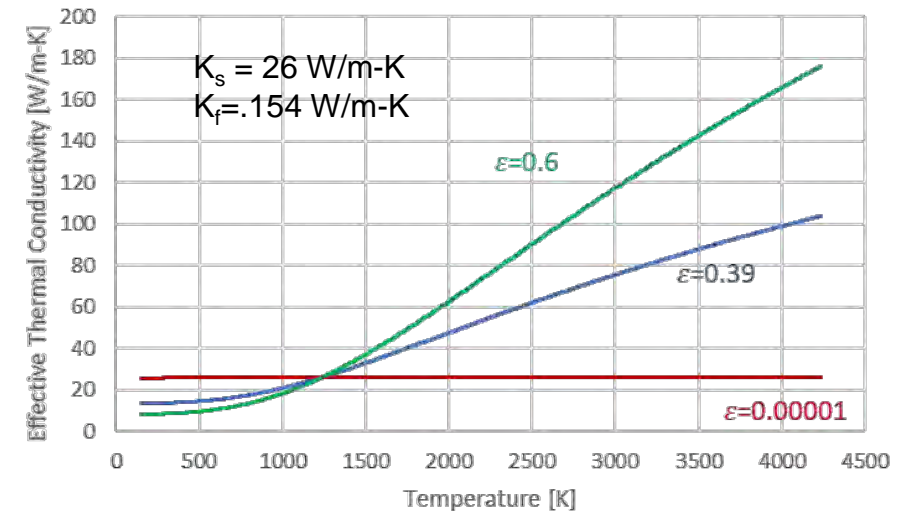
Interface Between Thermal-hydraulics and Pebble Bed Reactor Core Structures

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

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

- Constants and exponents accessible by sensitivity coefficient

Flow resistance

- Packed bed pressure drop

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

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

Loss coefficient relative to Ergun (original) coefficient at Re=1000

Relative Loss Coefficient ε=0.39 — Reynolds #

Ergun (Original) — Ergun (smooth) — Ergun (rough) — Achenbach
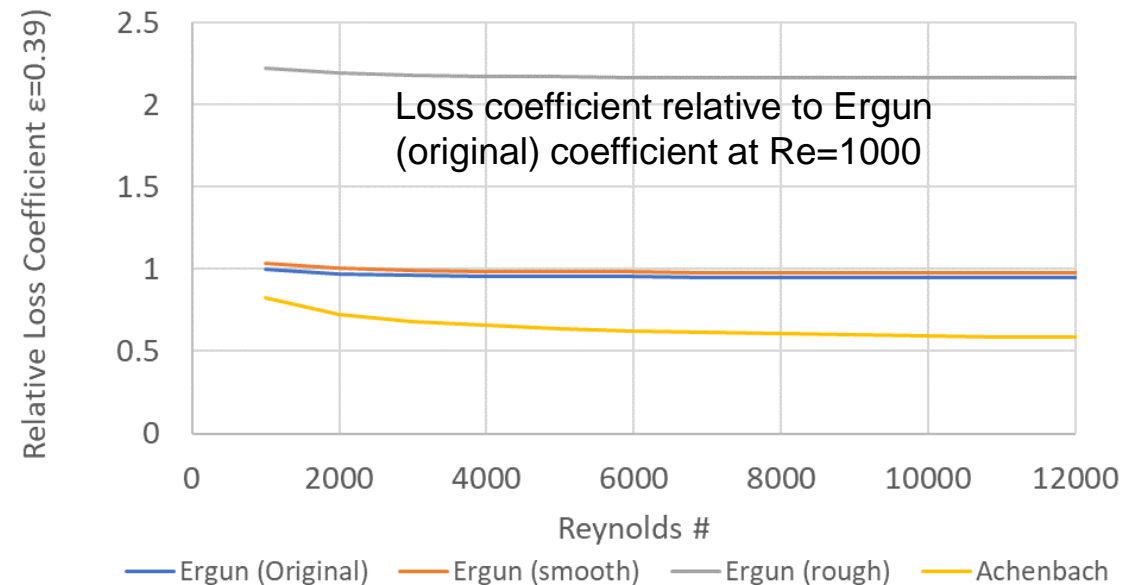
Point kinetics modeling

Standard treatment

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

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

Feedback models
- User-specified external input
- Doppler
- Fuel and moderator density
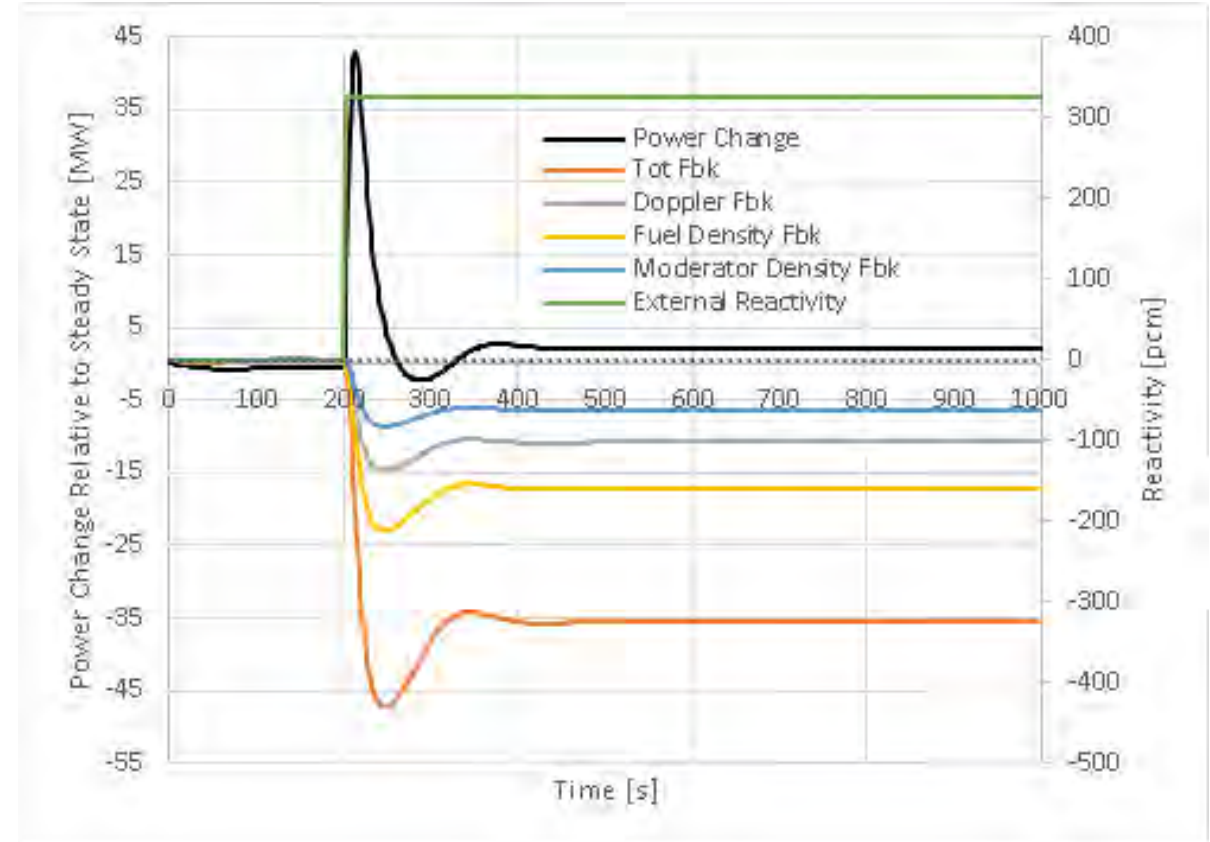
High-Temperature Gas-Cooled Reactor Plant Model and Source Term Analysis

Reactor vessel and core

Pebble bed
Rings 2-6,
Axial levels 6-27
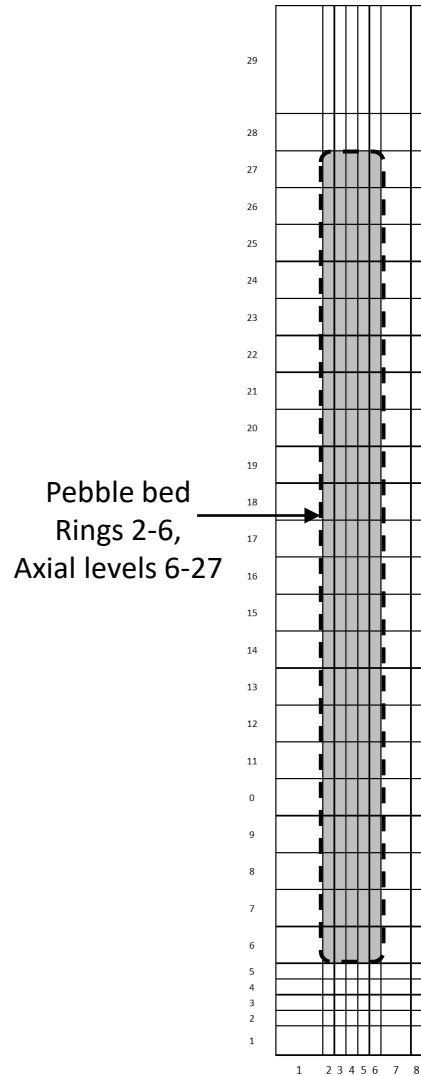
Vessel core package nodalization
(8 rings x 29 axial levels)
Correct aspect ratio
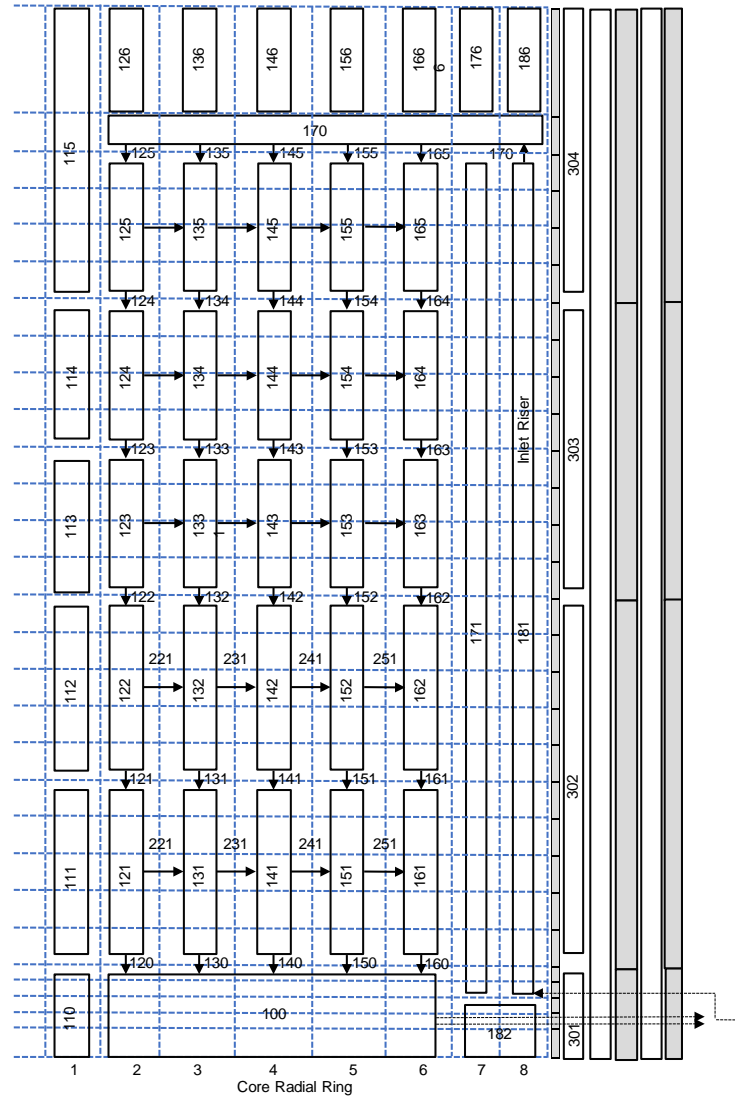
Vessel control volume, flow path, and heat structure
nodalization with core package boundaries in blue
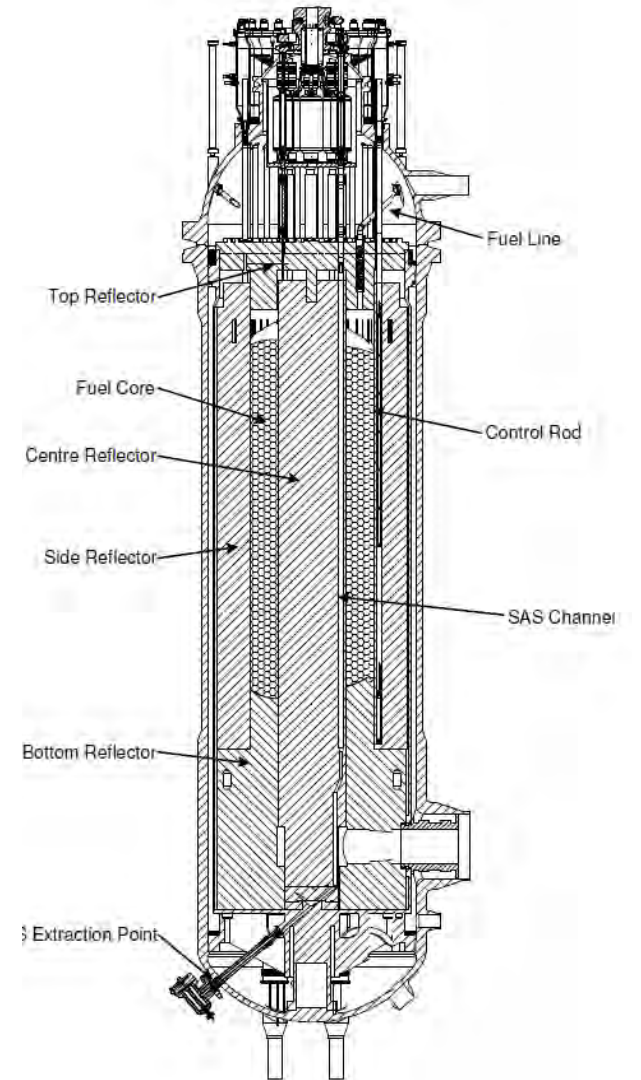
[P.J. Venter, M.N. Mitchell, F. Fortier, PBMR reactor design
and development, in: Proceedings from the 18th
International Conference on Structural Mechanics in
Reactor Technology (SMiRT 18), Beijing, China, Aug. 2005]

Reactor building

Nodalization guided by NGNP layout
- Passive air-flow Reactor Cavity Cooling System (RCCS)

Leakage assumed to be the same as BWR Mark I reactor building surrounding the containment
- 100% vol/day at 0.25 psig

rb_upper
cv-83

RCCS Outlet Plenum cv-76

RCCS Inlet Plenum cv-70

RPV

RPV HS4

RPV HS3

RPV HS2

RPV HS1

CAV-CV51 cv-51

RCCS HS4

RCCS HS3

RCCS HS2

RCCS HS1

RCCS Riser 4 cv-75

RCCS Riser 3 cv-74

RCCS Riser 2 cv-73

RCCS Riser 1 cv-72

RCCS Down Comer cv-71

sg_compt cv-81

CAV-CV50 (Around the RPV Lower head)

rb_cavity CV-80

rb_lower cv-82

Reactor equipment maintenance and repair building

Positioner

Refueling machine

Reactor auxiliary building

Crane central room

Electrical-technical building

Power conversion system

Reactor cavity cooling system

Reactor

Reactor Building

"HTGR Mechanistic Source Terms White Paper," July 2010, [INL-EXT-10-17999]

Picture above shows a water-cooled RCCS but demo model uses air-cooled RCCS.

Recirculation loop and secondary heat removal

Recirculation system and secondary heat removal

- Recirculation loop and secondary heat removal provide boundary conditions to the vessel
  - Flow rate
  - Heat removal & inlet temperature

Pipe break nodalization allows counter-current natural circulation flow

- MELCOR counter-current flow model used to represent adjacent stream drag forces
- Geometry similar to PWR hot leg natural circulation [NUREG-1922]
- Allows for air ingression

Scenario: depressurized loss of forced circulation (DLOFC)

- Assumes double-ended break of the hot leg
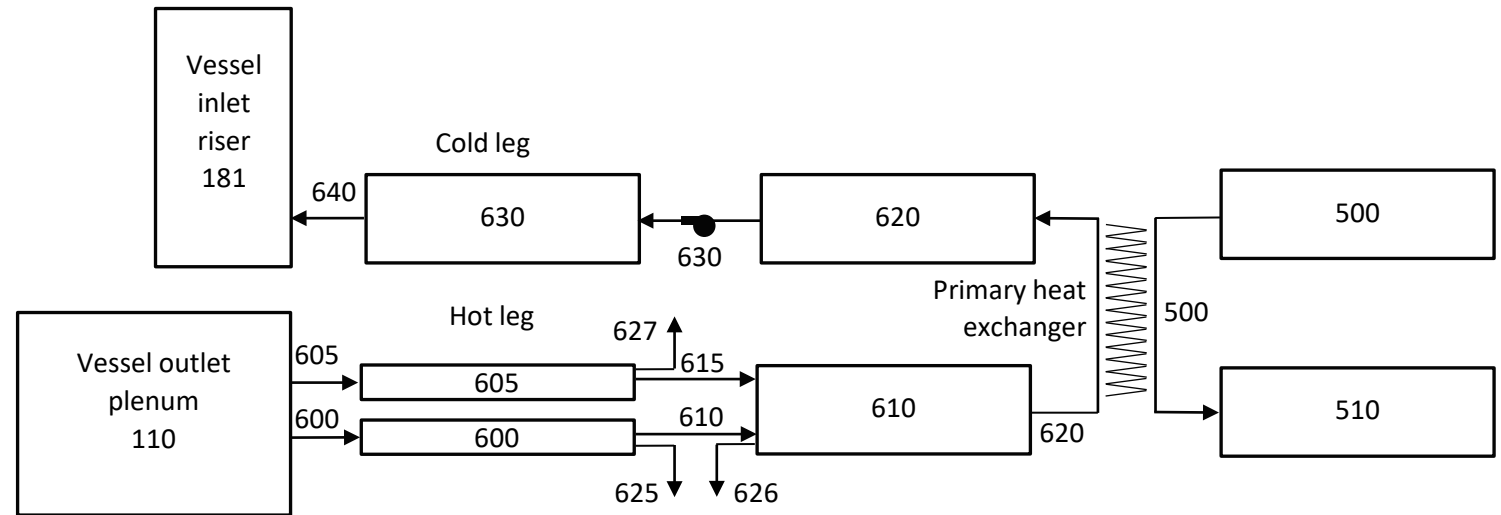
DLOFC scenario

DLOFC is initiated after 900 days of operation
- Long-term fission product concentrations developed in TRISO and pebble
- 24 kg/yr graphite dust generation based on German AVR experience
- TRISO initialized with 10^{-5} failure fraction during the steady state

Provisions for air ingression

Reactor cavity cooling system (RCCS) is operational

Individual sensitivity calculations to explore variations in the model response to uncertainty in input parameters

DLOFC reference case results (1/7)

Following pipe break
- Control rods insert to terminate fission
- The vessel depressurizes in seconds as the high-pressure helium escapes out both sides of the broken pipe
- Peak velocity in the pebble bed is 45 m/s (normal flow rate is 11-18 m/s)

Counter-current flow established on the vessel side of the pipe break
- Hot gases from the exit plenum escape on the top side of the broken hot leg pipe and cooler gases enter along the bottom of the pipe

Vessel Pressure

9.3 MPa initial pressure

Pipe Break Flowrates

Vessel side lower
Vessel side upper
SG side

Positive flow is out of the reactor

Negative flow is into the reactor
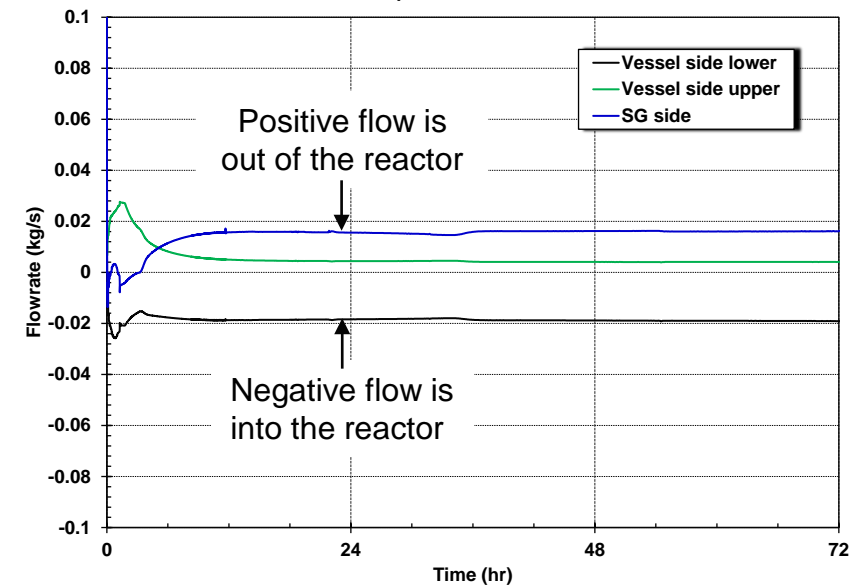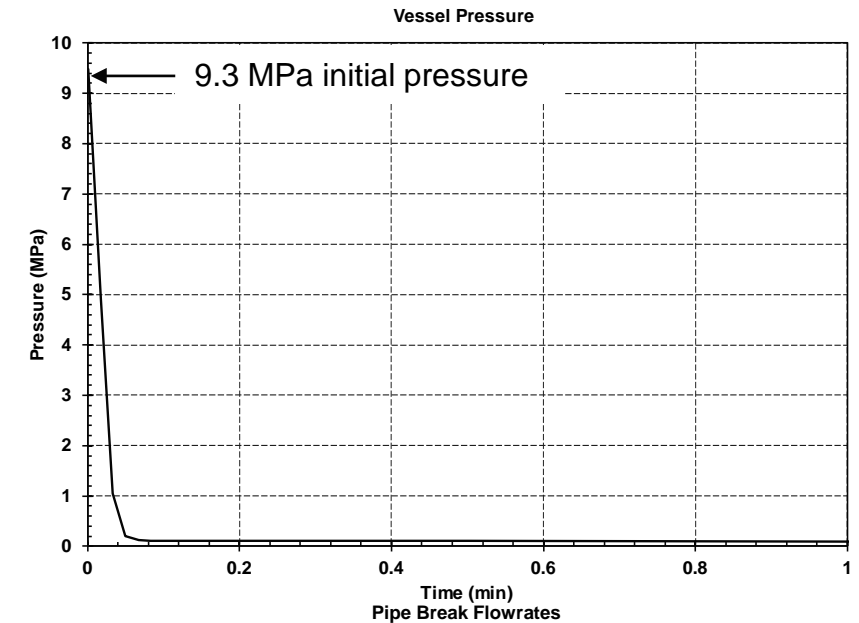
DLOFC reference case results (2/7)

In-vessel natural circulation flow after blowdown
- Upward flow in the inner region of the core where the fuel temperatures and decay power heating are higher
- Downward flow in the outer region of the core where the fuel temperatures and decay power heating are lower
- Flow increases when the fuel starts to cool

The fuel temperatures in the inner region of the pebble bed shift from cooler at inlet and hot at the outlet due to the flow reversal
- The axial fuel temperatures are affected by the local decay heat power (highest in the center) and the flow direction
  - During normal operation, the fuel at the exit (bottom) is the hottest
  - The exit becomes the coolest location (low power and cooler gases entering from the exit plenum)

Positive flow is downward

Axial flow velocities in outer region of the core

Negative flow is upward

Axial flow velocities in inner region of the core

Exit hottest at the bottom of the pebble bed

Exit is cooler due to the flow reversal and cooler air entering from the exit plenum

Top (inlet) is coolest when helium circulator is operating
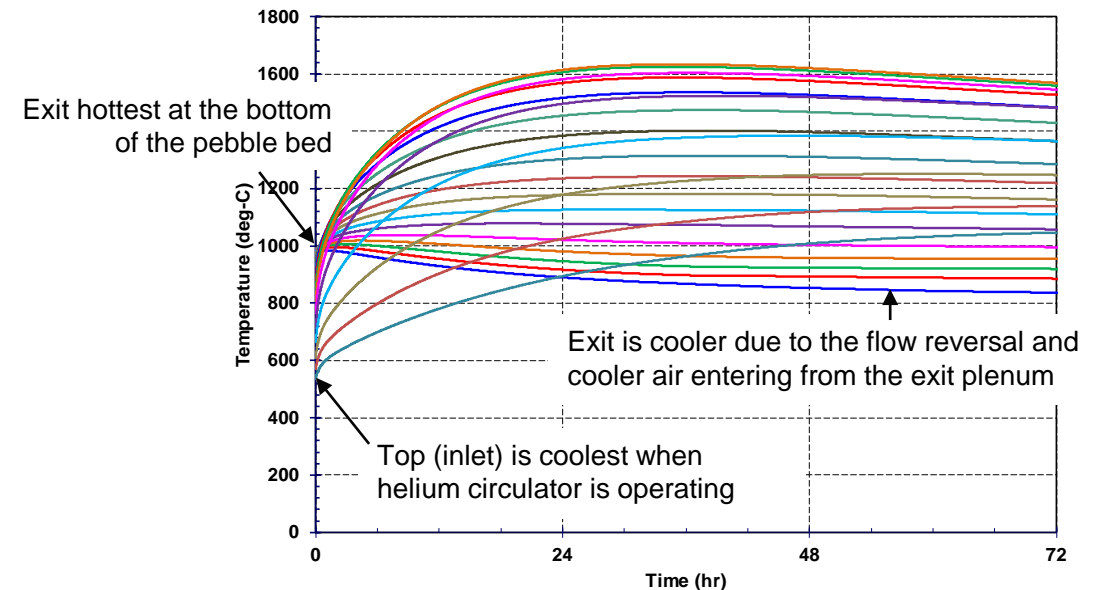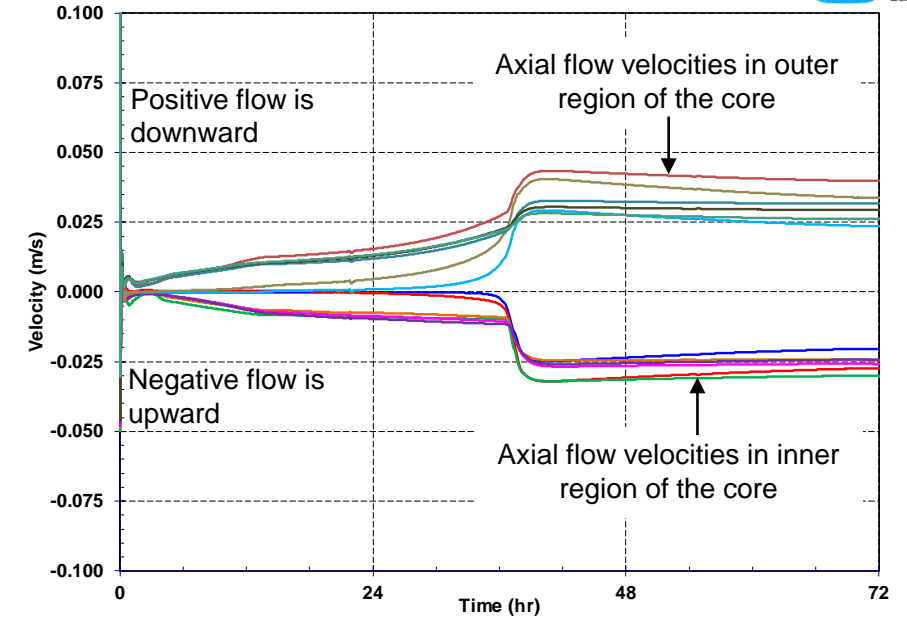
DLOFC reference case results (3/7)

The core heatup is dominated by the decay heat
- The air oxidation power is relatively small at <25 kW
- Although the vessel is thermally-stratified with a low exit path, a small natural circulation flow persists to bring air into the vessel
  - Pebble bed inlet and circulation velocities are <0.04 m/s

The graphite oxidation produces significant quantities of CO and CO_2
- Approximately 50% of the oxidation occurs in the graphite reflector structures around the inlet plenum and 50% in the lower portion of the pebble bed.
- ~1% of the pebble matrix oxidized after 168 hr
  - 17% peak pebble oxidation at the bottom center

Decay Heat Power

Maximum oxidation power is <25 kW

Graphite Oxdidation By-products
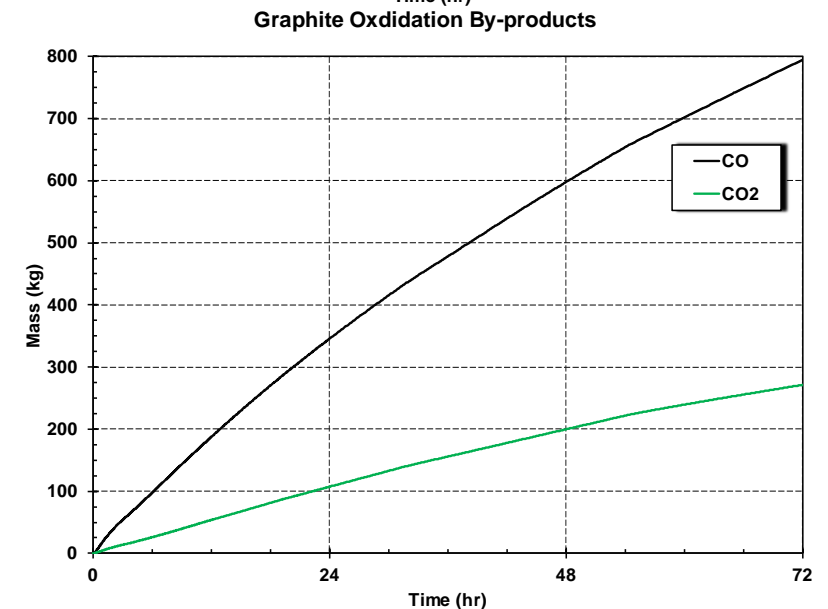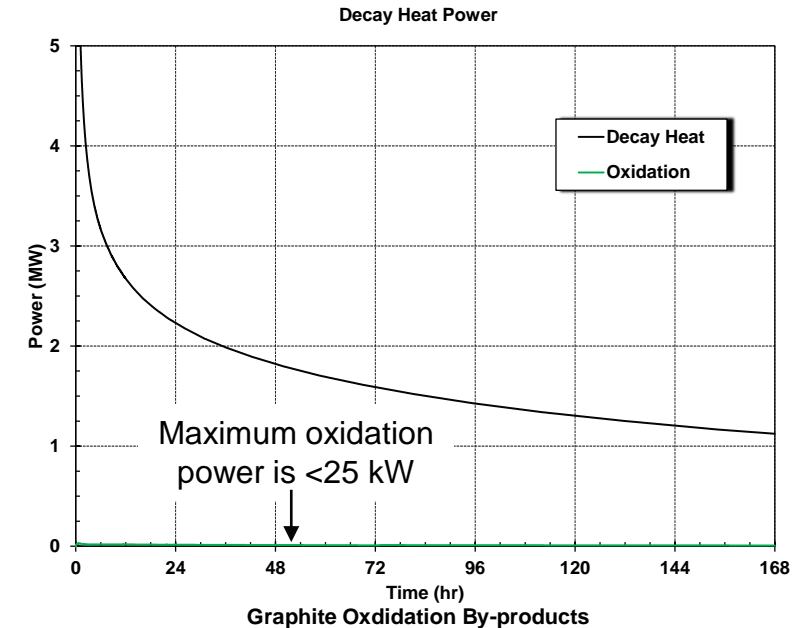
Potential for combustion in the reactor building

- MELCOR lower limit for CO combustion with an ignition source is 12.9% (~2X higher than for hydrogen)
- Highly dependent on local concentrations and building design and interconnectivity
- Demo reactor building assumes high inter-connectivity
  - Allows air and CO circulation
- No carbon-dioxide burns were predicted through 168 hr

CO Reactor Building Mole Fraction
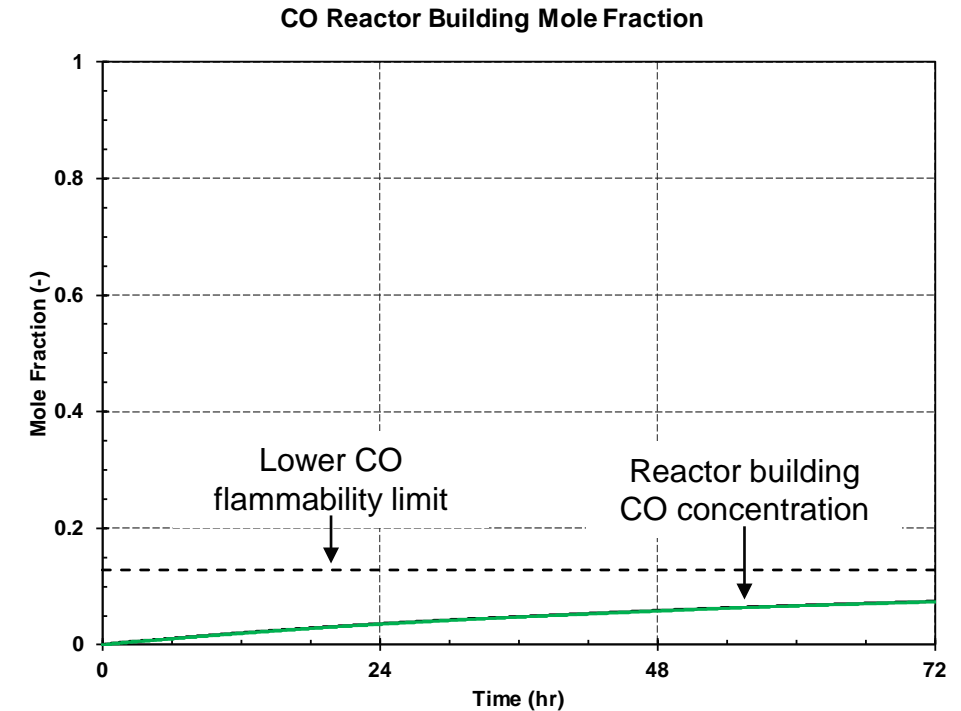
DLOFC reference case results (5/7)

MELCOR predicts release and transport from fuel to the environment

- Fuel heat-up
- TRISO layers – Initial failure fraction + failures during heat-up
- Pebble matrix and pebble outer shell – Higher diffusivity at elevated temperatures, recoil, and air oxidation
- Primary system – Failed with the initiating event
- Reactor building – Design leakage

TRISO Failure Fraction vs Temperature

Specified failure versus temperature

Failure Fraction (-) vs Temperature (°C)

TRISO Failure Fraction

~2×10^{-4} failure fraction calculated in the reference case

Failure Fraction (-) vs Time (hr)
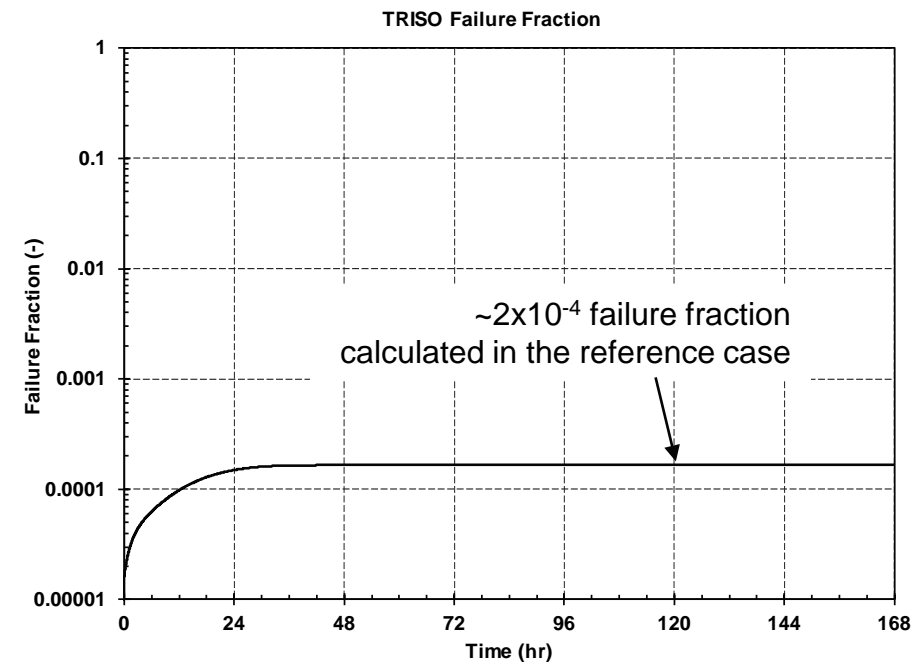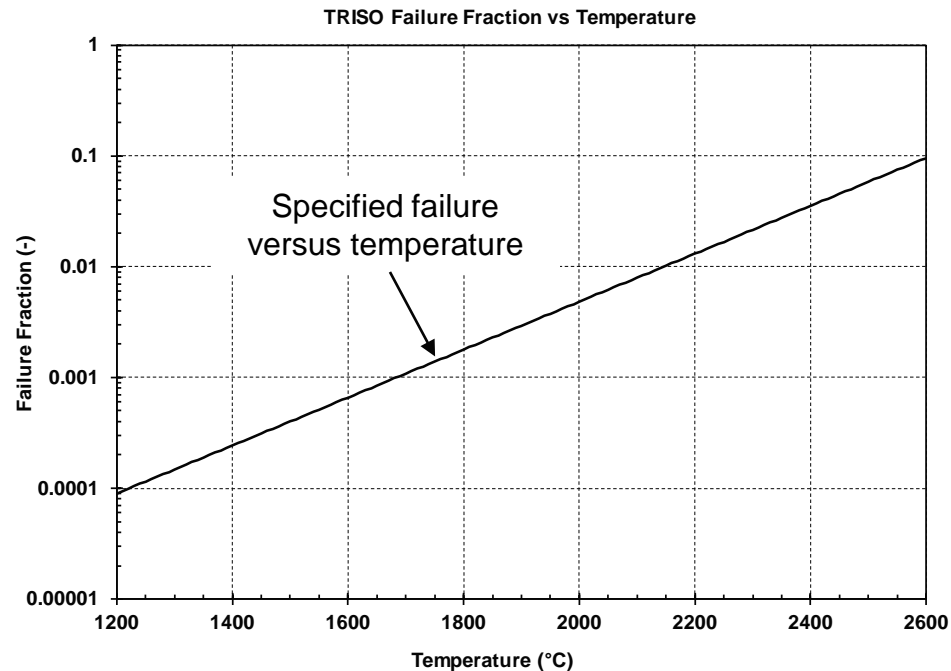
DLOFC reference case results (6/7)

The impact of the low TRISO failure fraction leads to small releases

- Iodine diffusivity assumed to be same as krypton
- Assumes most iodine reacts with cesium
- Larger cesium release due its the higher diffusivity
- Ag release to the environment is 1.2×10^{-3} (highest diffusivity)

Iodine Distribution

Legend:
- Release
- In-vessel
- Reactor building
- Environment

Y-axis: Fraction of initial inventory (-) — 1.E-06, 1.E-07, 1.E-08, 1.E-09, 1.E-10, 1.E-11, 1.E-12

X-axis: Time (hr) — 0, 24, 48, 72

Initial release dominated by airborne dust from steady operation

Cesium Distribution

Legend:
- Release
- In-vessel
- Reactor building
- Environment

Y-axis: Fraction of initial inventory (-) — 1.E-03, 1.E-04, 1.E-05, 1.E-06, 1.E-07, 1.E-08, 1.E-09, 1.E-10, 1.E-11

X-axis: Time (hr) — 0, 24, 48, 72

Initial release dominated by airborne dust from steady operation

DLOFC reference case results (7/7)

Of the small release from the fuel…

34% and 62% of iodine and cesium, respectively, retained in the vessel

- Thermally-stratified orientation limits vessel releases
- Low flowrate combined with aerosol deposition
- Inclusion of graphite oxidation reaction products (CO and CO_2) promotes more flow and therefore more releases from the vessel

58% and 34% of iodine and cesium, respectively, retained in the reactor building

- No strong driving force for reactor building leakage
  - Reference model uses a hole size equivalent to 100% leakage per day at a design pressure of 0.25 psig (3.2 in^2)

Iodine Distribution at 7 days

8.9%
33.6%
57.5%

■ In-vessel ■ Reactor building ■ Environment

Cesium Distribution at 7 days

3.9%
34.4%
61.7%

■ In-vessel ■ Reactor building ■ Environment
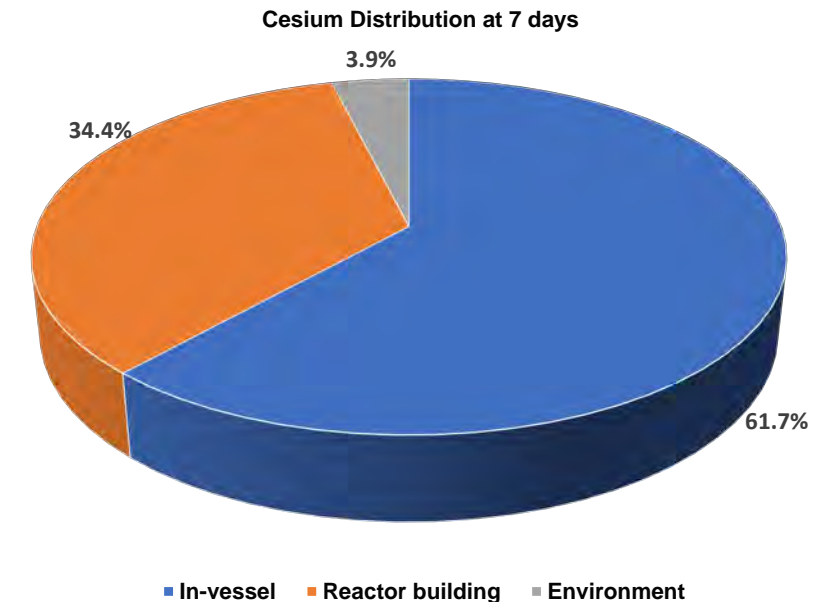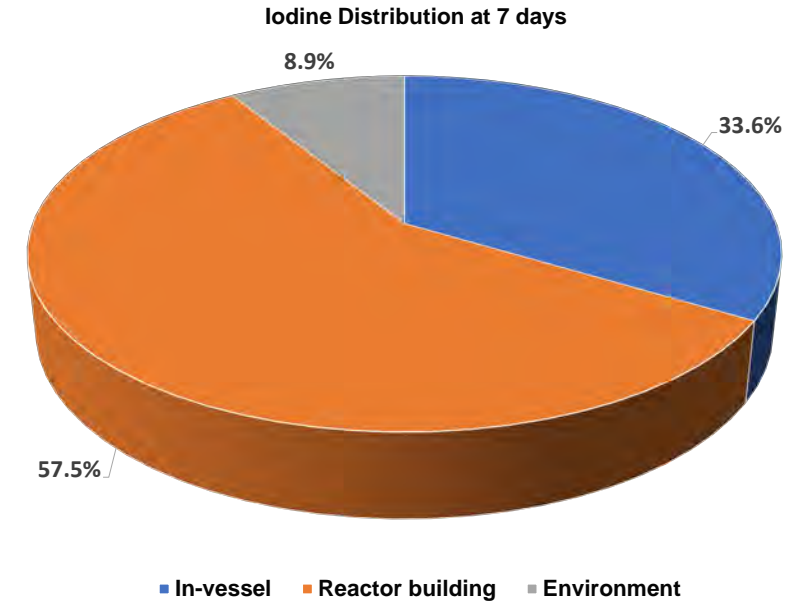
MELCOR can be used to explore the variability of the results to uncertainties

Model	Parameter	Distribution	Range
TRISO Model Parameters	Initial TRISO Failure Fraction (fraction of inventory)	Log uniform	$10^{-5} - 10^{-3}$
	TRISO Failure Rate Multiplier (-)	Log uniform	$0.1 - 10.0$
	Intact TRISO Diffusivity Multiplier (-)	Log uniform	$0.001 - 1000.0$
	Failed TRISO Diffusivity Multiplier (-)	Log uniform	$0.001 - 1000.0$
	Matrix Diffusivity Multiplier (-)	Log uniform	$0.001 - 1000.0$
	TRISO Pebble Emissivity (-)	Uniform	$0.5 - 0.999$
	TRISO Pebble Bed Porosity (-)	Uniform	$0.3 - 0.5$
	TRISO recoil fraction (-)	Uniform	$0 - 0.03$
Radionuclide Model Parameters	Shape Factor (-)	Uniform	$1.0 - 5.0$
	Gaseous Iodine Multiplier (Base = 5% I_2)	Uniform	$0.02 - 1.0$
Design Parameters	Graphite Conductivity Multiplier (-)	Uniform	$0.5 - 1.5$
	Decay Heat Multiplier (-)	Uniform	$0.9 - 1.1$
	RCCS Blockage Multiplier (-)	Log uniform	$0.001 - 1.0$
	RCCS Emissivity (-)	Uniform	$0.1 - 1.0$
	Reactor Building Leakage Multiplier (-)	Log uniform	$0.1 - 100.0$
	Wind speed (m/s)	Uniform	$0 - 10$

Single parameter sensitivity results (1/4)

The sensitivity parameters were sampled at the minimum and maximum values to illustrate their impacts

- A low graphite conductivity has the largest impact on the peak fuel temperature

  - Graphite conductivity varies considerably with irradiation (>10X) and also varies with temperature

- ±10% decay heat has next largest impact on the peak fuel temperature

- High/low emissivity, the next most important single factor, is used as a surrogate for the relative importance of radiative exchange in the pebble bed

- Debris bed porosity had a small effect on the peak fuel temperature

- Heat dissipation limits the magnitude of the initial peak for a blocked RCCS

  - Slow heat-up to 1800℃ by 7 days

Peak Fuel Temperature

Legend:
- Base case
- Low Gr k
- High Gr k
- 1.1X decay heat
- 0.9X decay heat
- Low pebble emissivity
- High pebble emissivity
- Low pebble porosity
- High pebble porosity
- Blocked RCCS

Y-axis: Temperature (°C); X-axis: Time (hr)
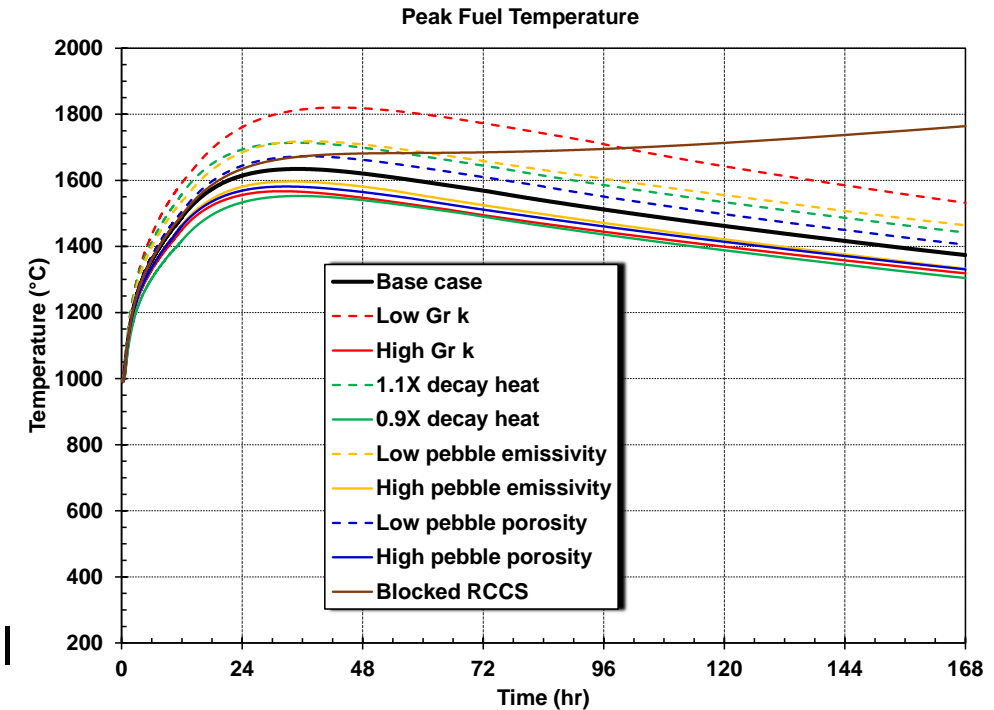
Examples of single parameter sensitivity results (2/4)

As the peak fuel temperature rises, the TRISO failure fraction increases
- Blocked RCCS does not have impact for several days

The cesium environmental release shows an order of magnitude variation
- Reflects variations in release from the pebbles
- Graphite conductivity had the largest impact
- Variations in emissivity = uncertainty in radiative heat transport (similar to ±10% in decay heat power)
- Pebble porosity had a small impact

TRISO Failure Fraction

Legend:
- Base case
- Low Gr k
- High Gr k
- 1.1X decay heat
- 0.9X decay heat
- Low pebble emissivity
- High pebble emissivity
- Low pebble porosity
- High pebble porosity
- Blocked RCCS

Y-axis: Failure Fraction (-)
X-axis: Time (hr)

Cesium Release Fraction from the Pebbles

Legend:
- Base case
- Low Gr k
- High Gr k
- 1.1X decay heat
- 0.9X decay heat
- Low pebble emissivity
- High pebble emissivity
- Low pebble porosity
- High pebble porosity
- 2x recoil
- No recoil
- Blocked RCCS

Y-axis: Release Fraction (-)
X-axis: Time (hr)

Larger hole size in the building and higher wind speed causes higher releases to environment

- 100X building leakage has less than a 10X impact
- External wind has small effect

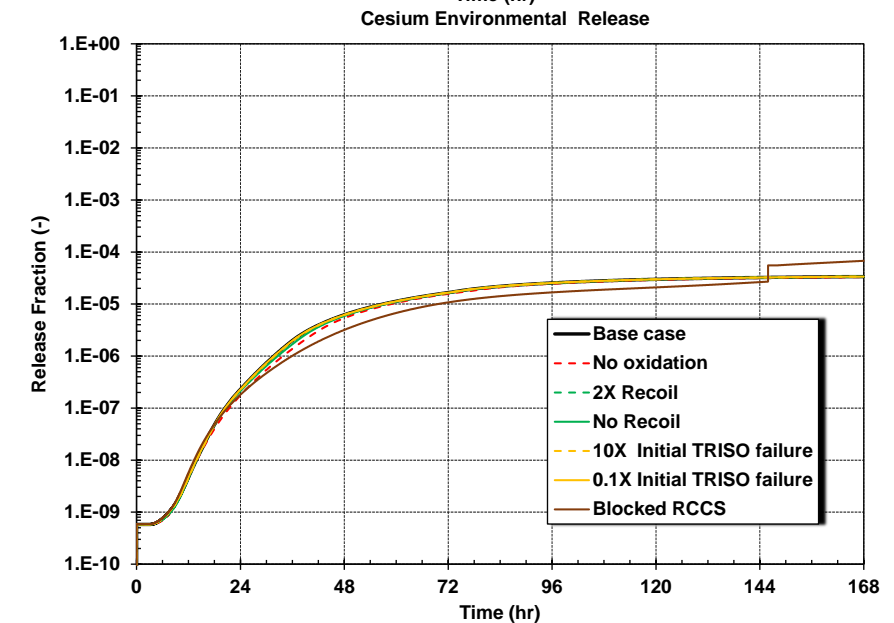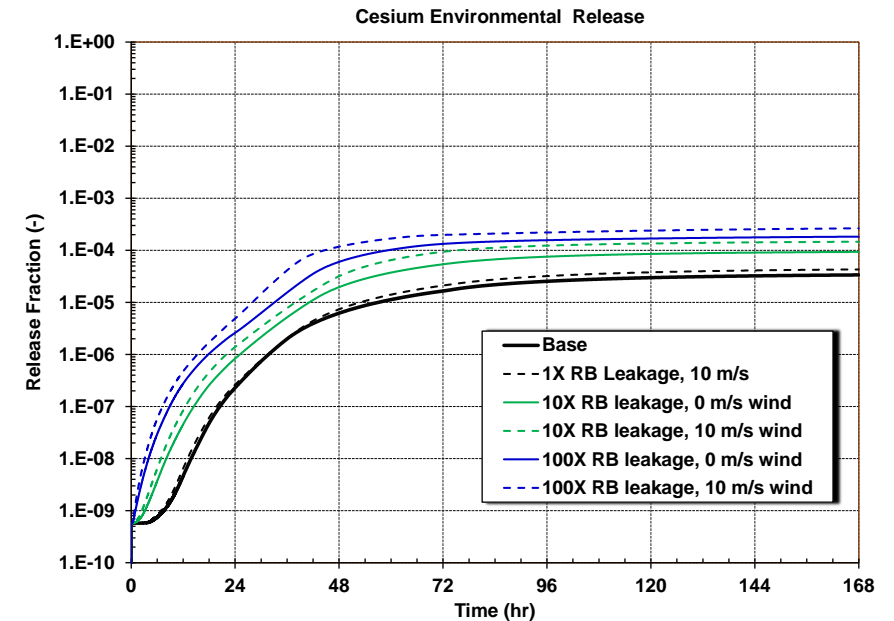Graphite oxidation and the associated CO/CO_2 production did not increase the source term

- CO/CO_2 gas production did not increase environment release

Early impacts of the recoil and initial TRISO failure fraction did not impact long-term environmental release

- Magnitude of the release dominated by the fuel temperature response and the TRISO failure model

Late step change in the blocked RCCS release is due to a carbon monoxide burn

- Building pressurization forces out airborne radionuclides

Cesium Environmental Release

Legend:
- Base
- 1X RB Leakage, 10 m/s
- 10X RB leakage, 0 m/s wind
- 10X RB leakage, 10 m/s wind
- 100X RB leakage, 0 m/s wind
- 100X RB leakage, 10 m/s wind

Cesium Environmental Release

Legend:
- Base case
- No oxidation
- 2X Recoil
- No Recoil
- 10X Initial TRISO failure
- 0.1X Initial TRISO failure
- Blocked RCCS

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Blocked RCCS leads to higher CO generation
- Ratio of reaction products is dependent on the temperature of the graphite
- Blocked RCCS generates ~9% more moles of CO and CO_2

Higher CO generation led to a burn in the steam generator compartment (pipe break location)
- Incomplete burn with slow flame speed
  - Low oxygen concentration (6.8%)
- 0.25 bar (3.5 psi) pressure rise
- Burn creates non-condensable CO_2
  - No subsequent condensation

Graphite Oxidation By-products
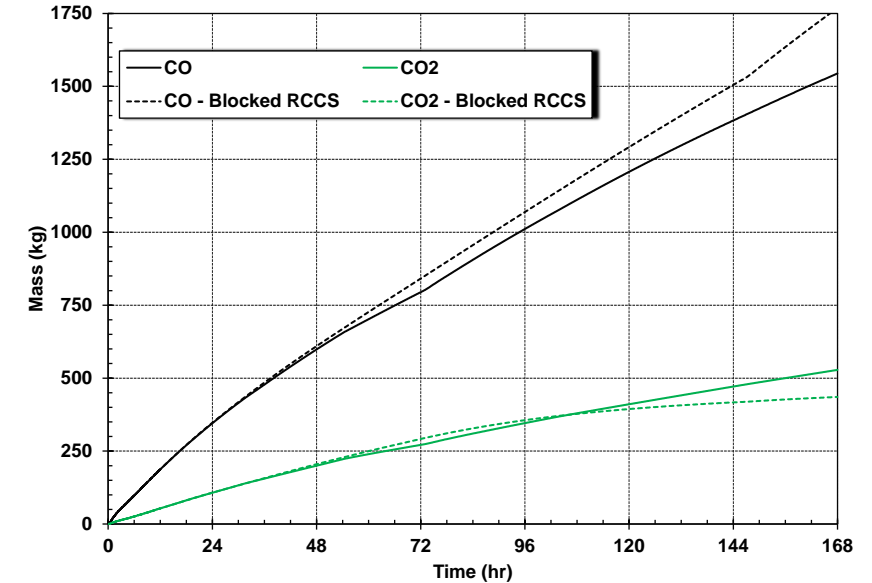
Reactor Building CO Mole Fraction

CO burn in the SG compartment

68
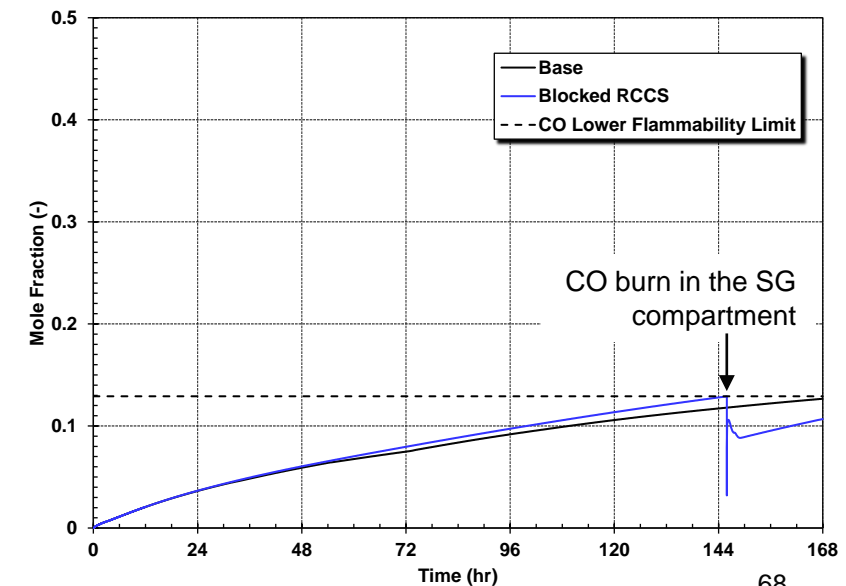
High-Temperature Gas-Cooled Reactor Uncertainty Analysis

Role of MELCOR in Resolving Uncertainty
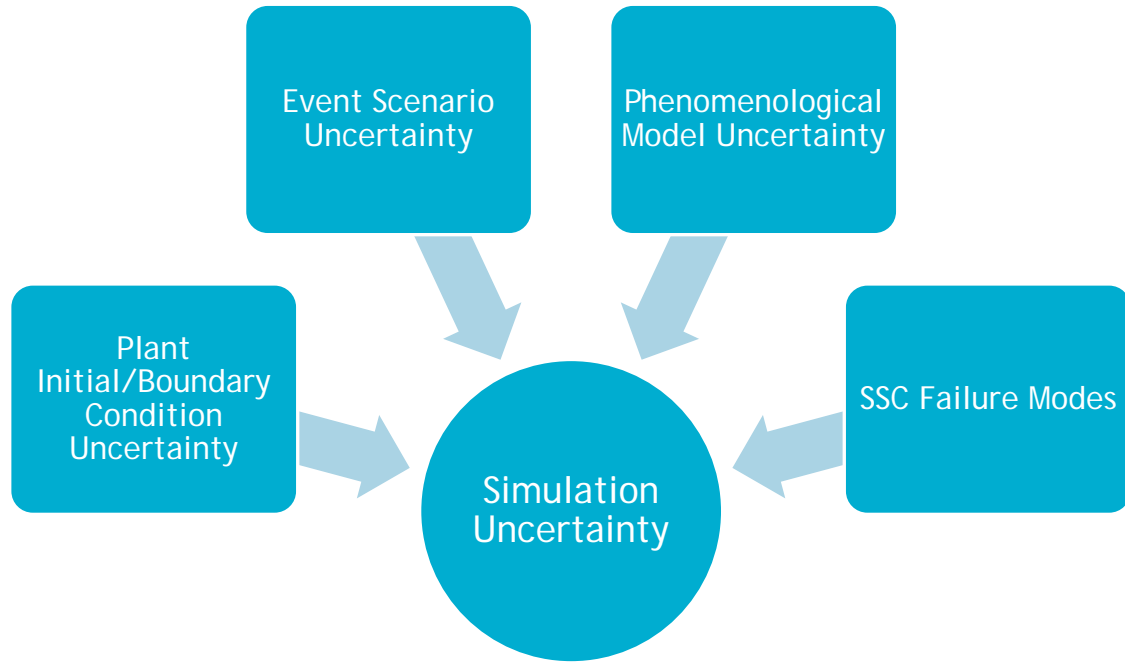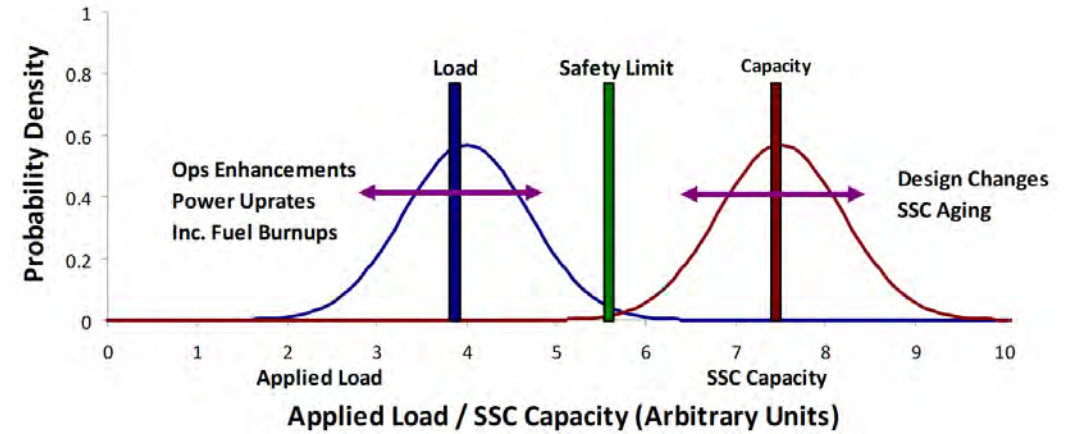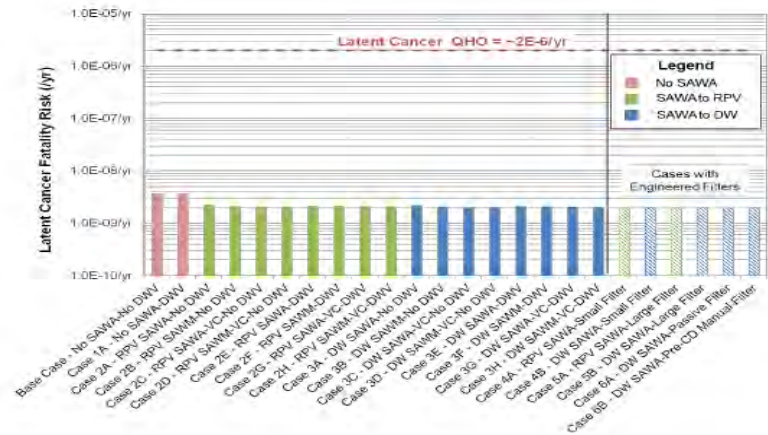
Evolution from MELCOR LWR Uncertainty Analysis

Overall motivation

- A clustering of system responses provides insights on important assumptions and modeling parameters
- Provides a most likely release and range of releases for the scenario

MELCOR application to LWRs

- Range of SOARCA uncertainty studies
- PWR and BWR plant uncertainty studies
- Resolved role of uncertainty in critical severe accident issues

Commonalities between LWR and HTGR

- Chemical form of key elements
- Aerosol physics parameters (e.g., shape factor)
- Operating time before accident happens
- Containment leakage hole size

Parameter selection emphasized potential HTGR-specific uncertainties

- Ran 2000 realizations on High Performance Computer
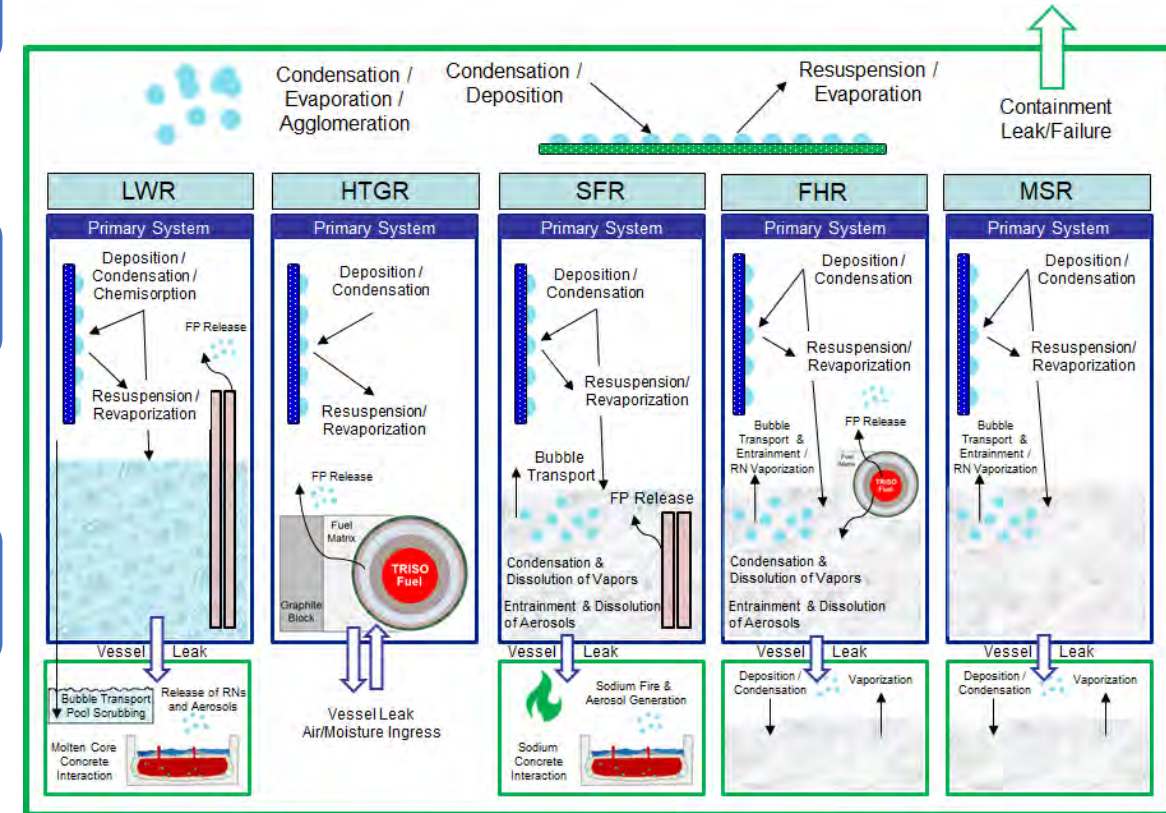
Parametric Uncertainty – Capability Demonstration

Model	Parameter	Distribution	Range
TRISO Model Parameters	Initial TRISO Failure Fraction (fraction of inventory)	Log uniform	$10^{-5} - 10^{-3}$
	TRISO Failure Rate Multiplier (-)	Log uniform	$0.1 - 100.0$
	Intact TRISO Diffusivity Multiplier (-)	Log uniform	$0.001 - 1000.0$
	Failed TRISO Diffusivity Multiplier (-)	Log uniform	$0.001 - 1000.0$
	Matrix Diffusivity Multiplier (-)	Log uniform	$0.001 - 1000.0$
	TRISO Pebble Emissivity (-)	Uniform	$0.5 - 0.999$
	TRISO Pebble Bed Porosity (-)	Uniform	$0.3 - 0.5$
	TRISO recoil fraction (-)	Uniform	$0 - 0.03$
Radionuclide Model Parameters	Shape Factor (-)	Uniform	$1.0 - 5.0$
	Gaseous Iodine Multiplier (Base = 5% I_2)	Uniform	$0.02 - 1.0$
Design Parameters	Graphite Conductivity Multiplier (-)	Uniform	$0.5 - 1.5$
	Decay Heat Multiplier (-)	Uniform	$0.9 - 1.1$
	RCCS Blockage Multiplier (-)	Log uniform	$0.001 - 1.0$
	RCCS Emissivity (-)	Uniform	$0.1 - 1.0$
	Reactor Building Leakage Multiplier (-)	Log uniform	$0.1 - 100.0$
	Wind speed (m/s)	Uniform	$0 - 10$

UO$_2$ Thermal Response
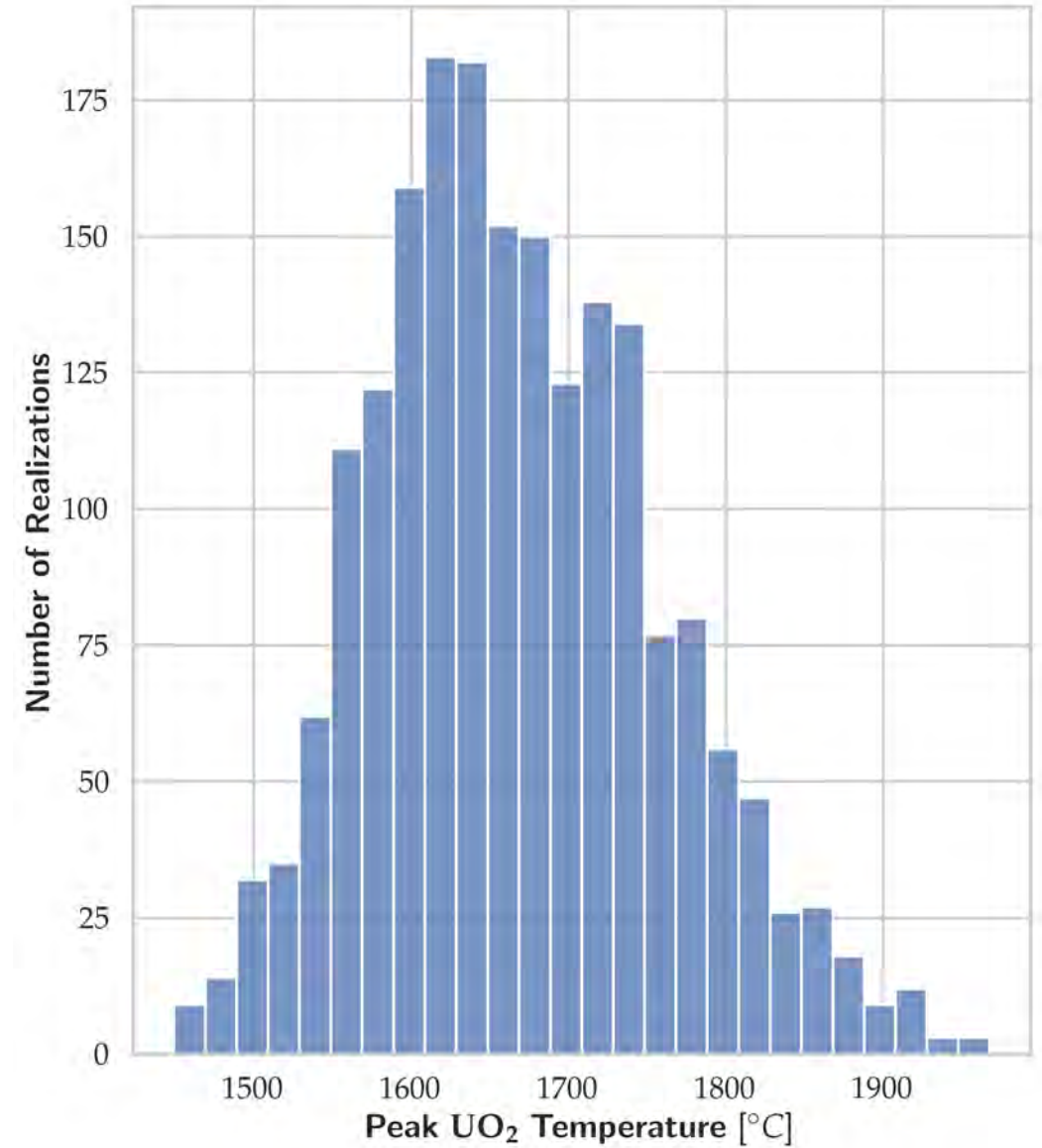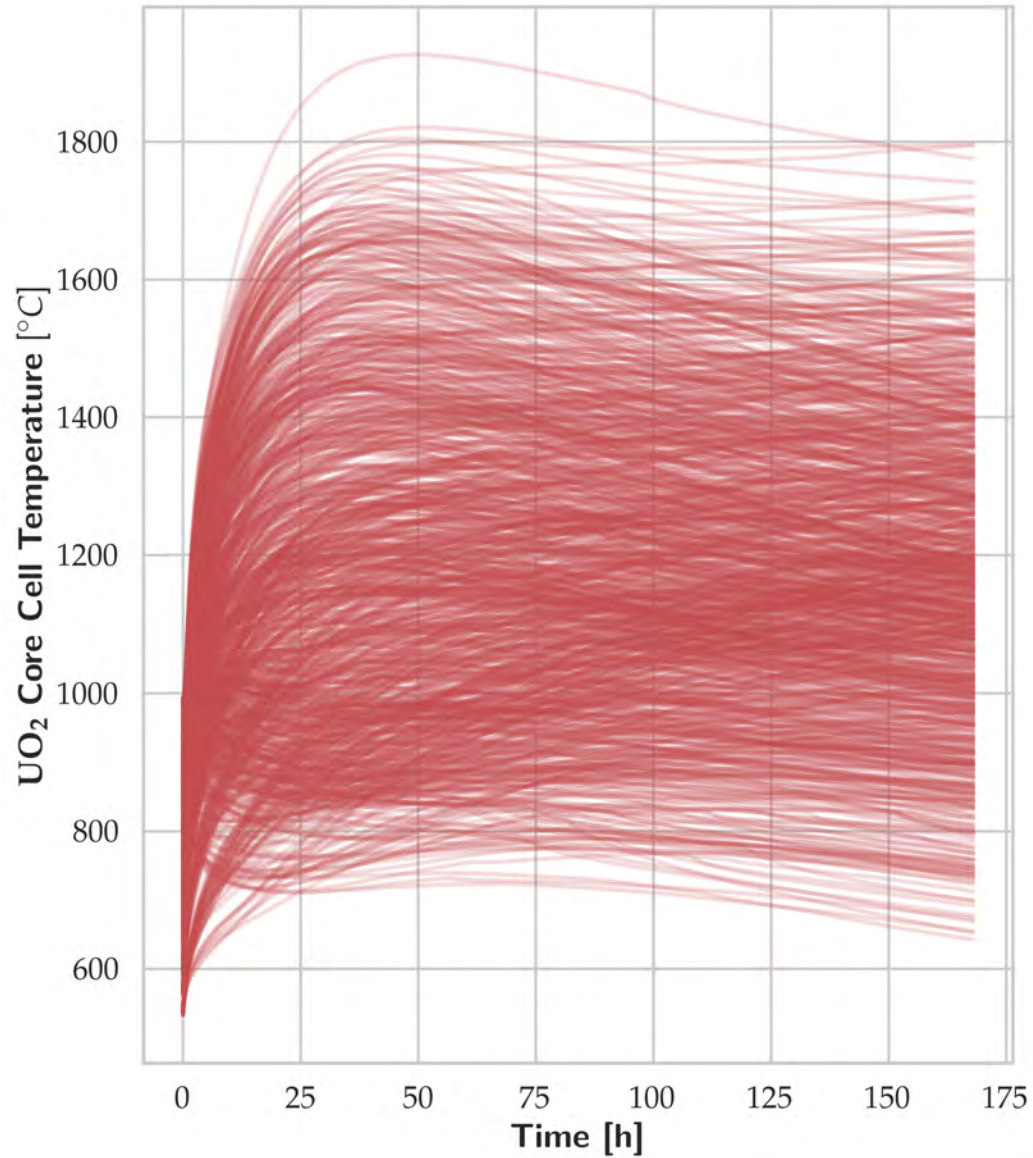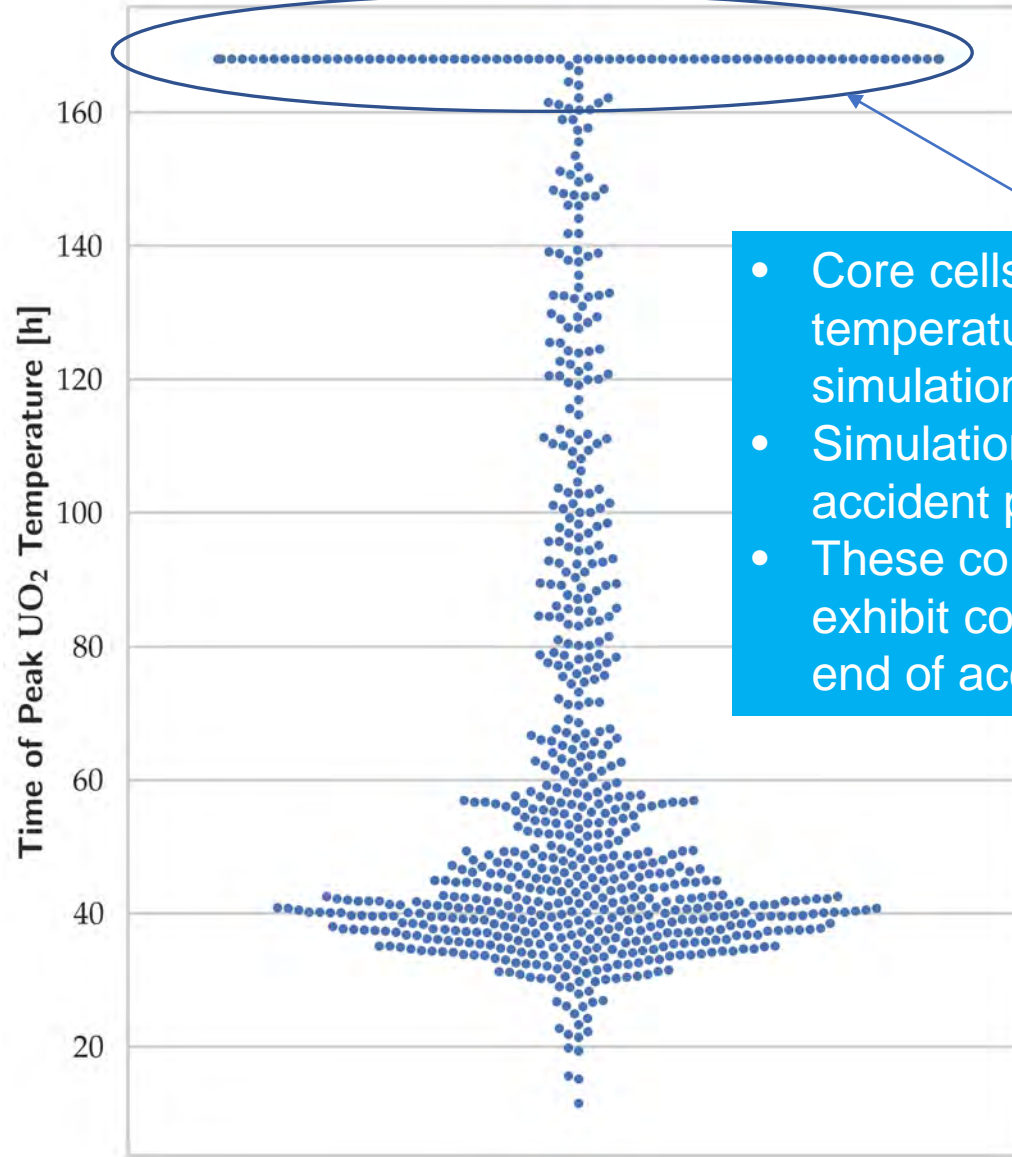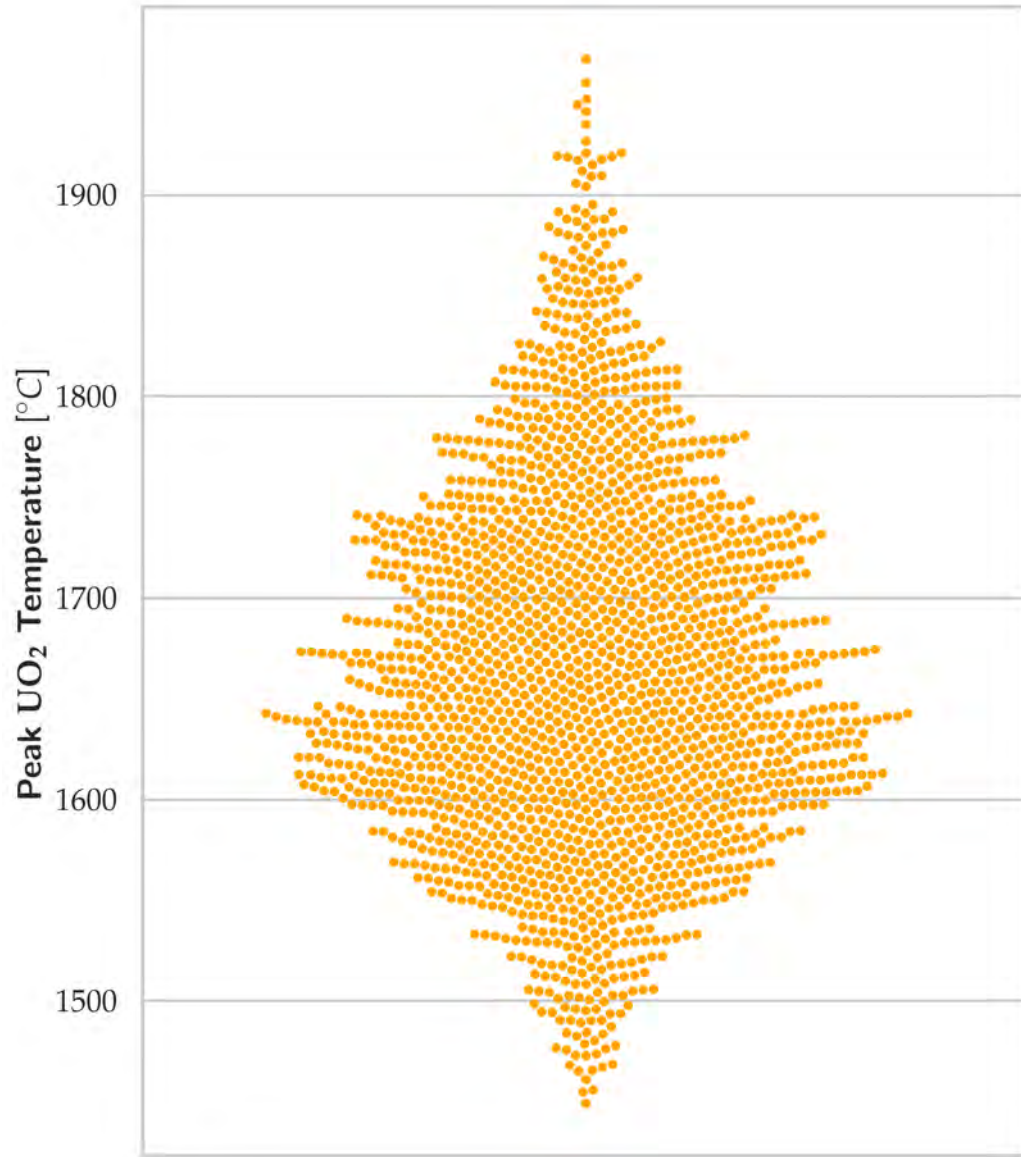
- Core cells with peak fuel temperatures at end of simulation
- Simulation time denoted as accident phase
- These core cells do not exhibit cooldown prior to end of accident phase

TRISO Particle Failure

Long-term TRISO particle failure possible for core cells exhibiting prolonged over-temperatures
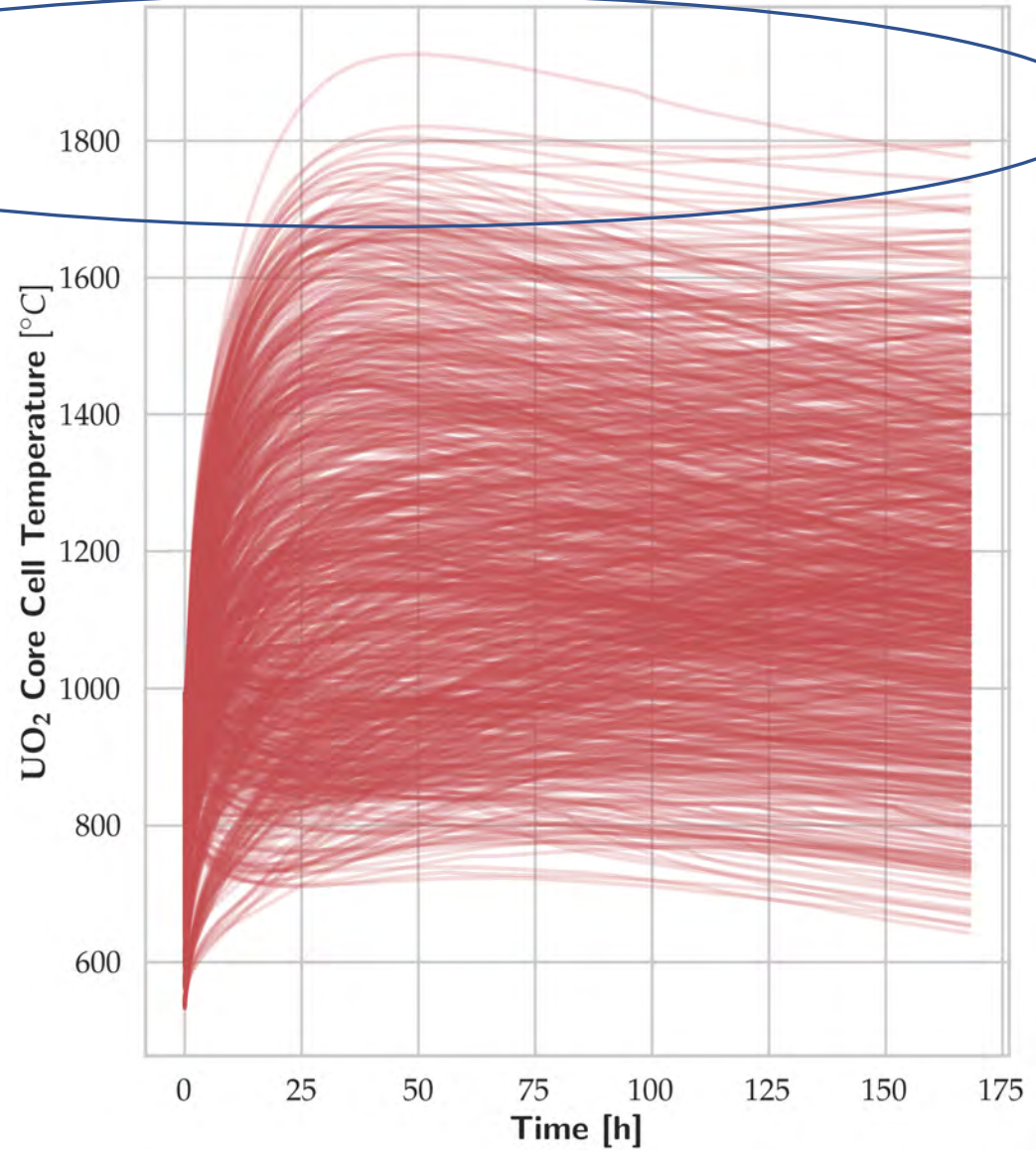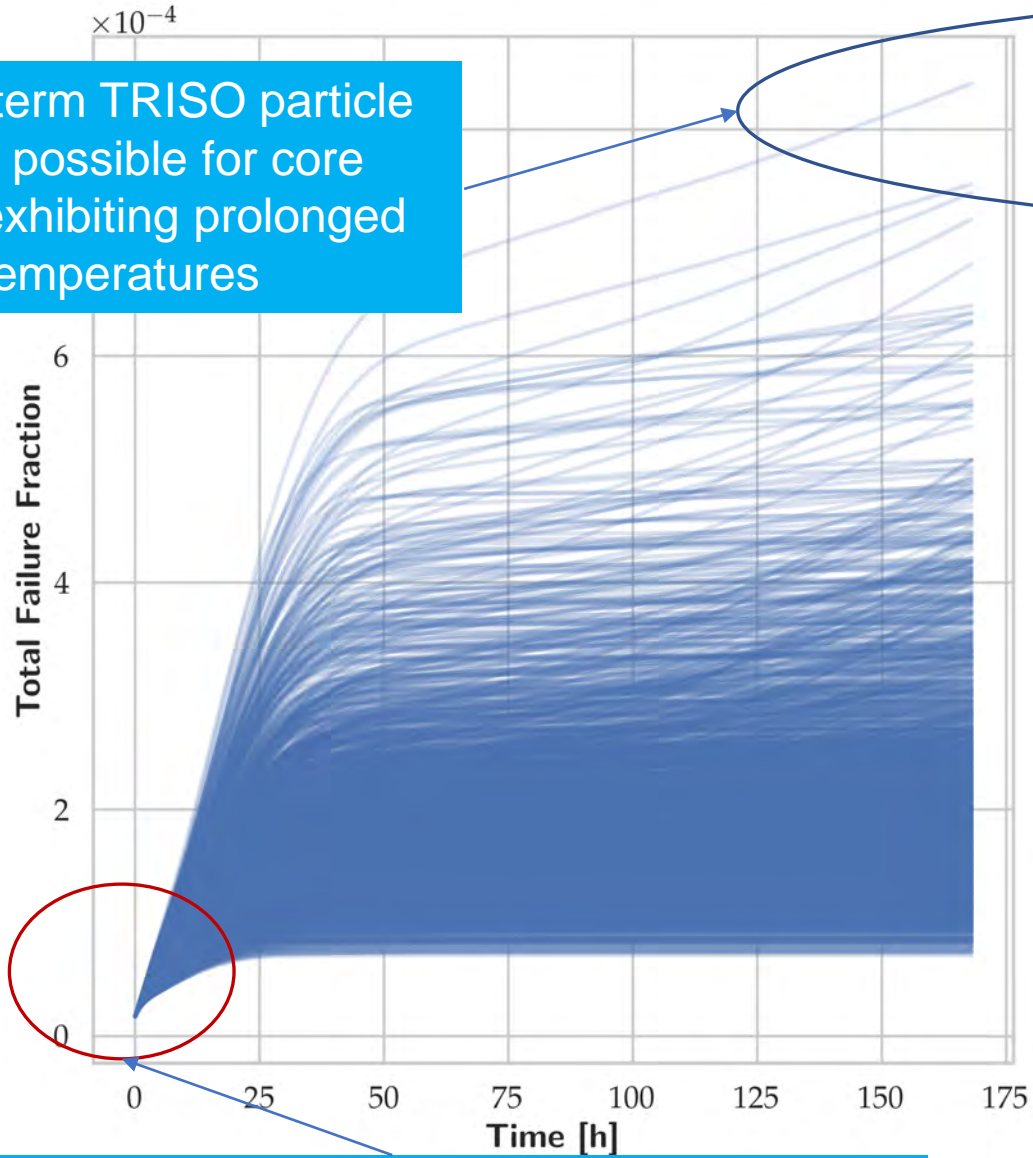
Initial distribution of failed TRISO particles

Evolution of TRISO Particle Failures

Long-term failures of TRISO particles at lower rate but driven by prolonged period of elevated fuel temperature

Tails of realizations contributing to longer term growth of TRISO particle failures

50th percentile reasonably stable in the long-term

Rapid growth in failure fraction driven by the early temperature excursion

Lower rates of failure entirely driven by early temperature excursion
Variability in peak fuel temperature and cooldown transient dominates higher failure rate realizations
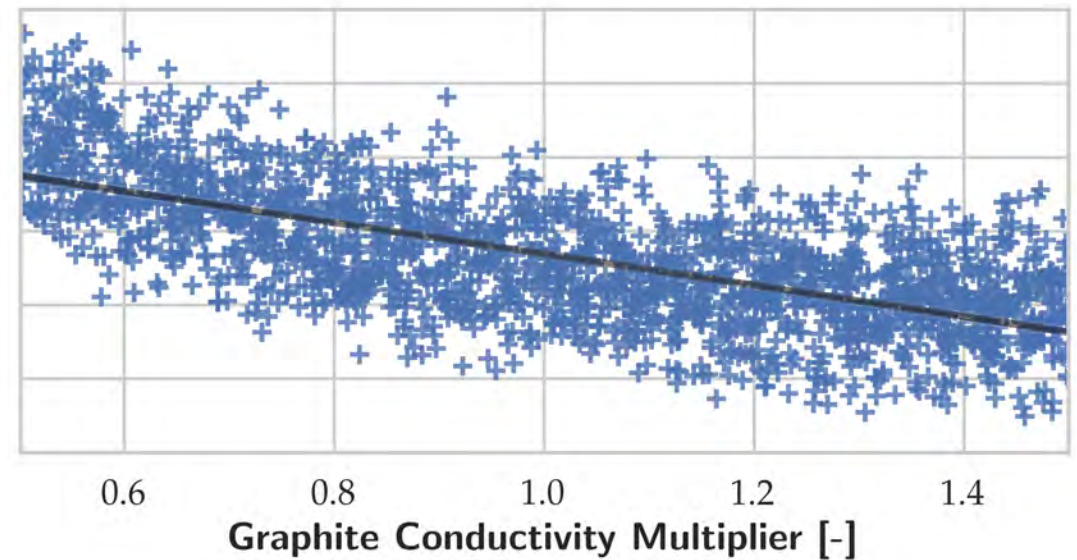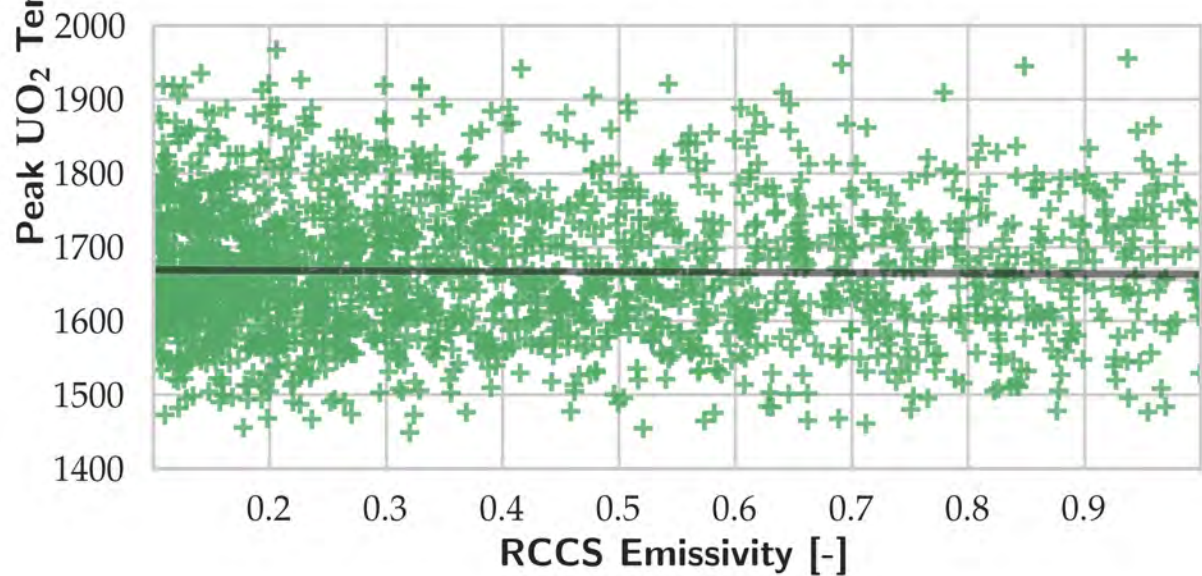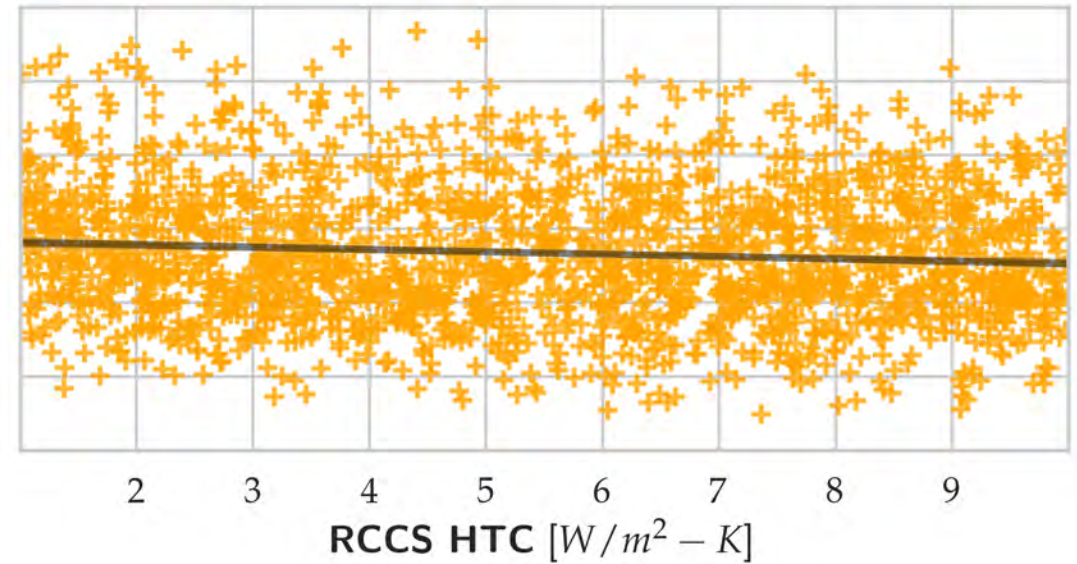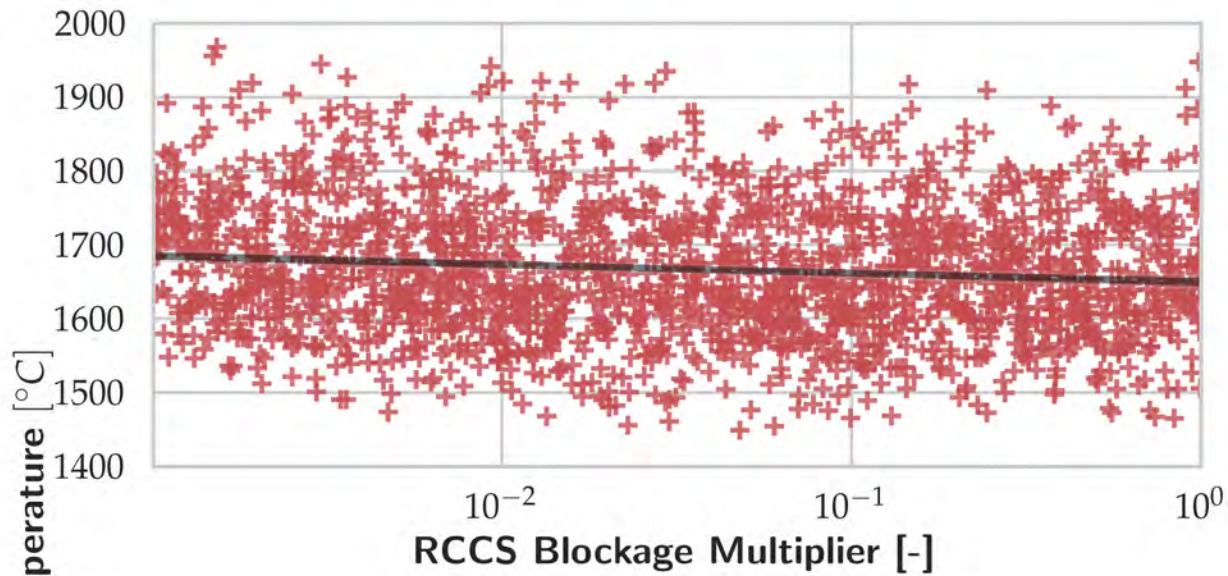
Conclusions

Added HTGR modeling capabilities to SCALE & MELCOR for HTGR source term analysis to show code readiness

Modeling demonstrated for a DLOFC Scenario
- Input of detailed ORIGEN radionuclide inventory data from ORNL
- Input radial and axial power distributions from ORNL neutronic analysis
- Develop MELCOR input model for exploratory analysis
- Fast-running calculations facilitate sensitivity evaluations

Developed an understanding of non-LWR beyond-design-basis-accident behavior and overall plant response

SCALE Overview

SCALE Development for Regulatory Applications

Left column (blue boxes and light blue labels):

- CLAB (Sweden)
- HTC CRITICALS (France)
- FP CRITICALS (France)
- MALIBU/REBUS ARIANE CSN TAKAHAMA Domestic Programs
- St. Laurent MALIBU/REBUS
- IRPhEB/OECD: HTTR (Japan) HTR10 (China) PROTEUS (Switzerland) PBMR400

- Spent fuel calorimeter measurements
- Actinides reactivity worth in spent fuel
- Fission products reactivity worth in spent fuel
- Radiochemical isotopic assays of HI BU SNF
- MOX cycle exposure data
- HTGR criticality – neutronics operating and safety parameters

Center (SCALE (ORNL)):

Nuclear data | Reactor physics
Criticality safety | Radiation shielding
Sensitivity and uncertainty | Hybrid methods
Verification and validation | User interfaces

PARCS (Univ. of Michigan)
- Reactor Kinetics
- Core Design/Follow
- Flow Distribution
- Peaking Factors
- Reactivity Coefficients

Isotopic Composition/Decay Heat | Power Distributions/Limiting Operating Conditions

MELCOR | TRACE | FAST

Regulatory labels (red): 10CFR72, 10CFR71 10CFR72, 10CFR50.68

Right column (green/blue boxes):

- NMSS/SFST Technical Basis for Decay Heat R.G. 3.54
- NMSS/SFST Technical Basis for PWR BUC Interim Staff guidance ISG-8 & BWR BUC
- NRR Catawba MOX Lead Test Assembly
- NRR/NRO Technical Basis for BUC for Spent Fuel Pool Criticality Safety
- NRR Licensing Amendments (i.e., MELLLA+)
- NMSS/FCSS Fuel Cycle Analysis
- NMSS/SFST HBU Fuel for Storage and Transportation Casks Criticality and Decay Heat
- NRO Non-LWR reactors
- NRO New Reactor Design (ESBWR, AP1000, APR1400, NuScale, …)

What Is It?
The SCALE code system is a modeling and simulation suite for nuclear safety analysis and design. It is a modernized code with a long history of application in the regulatory process.

How Is It Used?
SCALE is used to support licensing activities in NRR (e.g., analysis of spent fuel pool criticality, generating nuclear physics and decay heat parameters for design basis accident analysis) and NMSS (e.g., review of consolidated interim storage facilities, burnup credit).

Who Uses It?
SCALE is used by the U.S. Nuclear Regulatory Commission (NRC) and in 61 countries (about 10,000 users and 33 regulatory bodies).

Map Legend
Country with SCALE
Country without SCALE
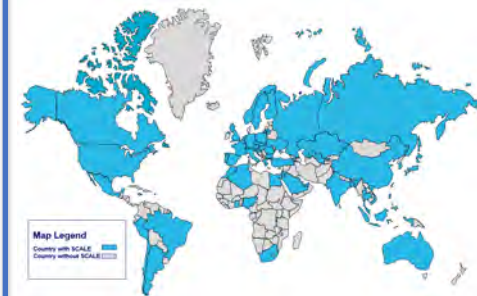
How Has It Been Assessed?
SCALE has been validated against criticality benchmarks (>1000), destructive assay of fuel and decay heat for PWRs and BWRs (>200)

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Data to generate for MELCOR: QOIs

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

VSOP Backup Slides

VSOP workflow shares several features of conventional 2-step LWR core analyses

Core inventories

Single-element / assembly flux solution

Simplified transport / diffusion
- Homogenized material regions with few-group cross-sections

Fuel shuffling / pebble recycle

Depletion update (pin / pebble)

Updated material inventories

Few-group cross-sections (critical spectrum)

Region-wise flux solution

Spatial flux / power distribution across the core
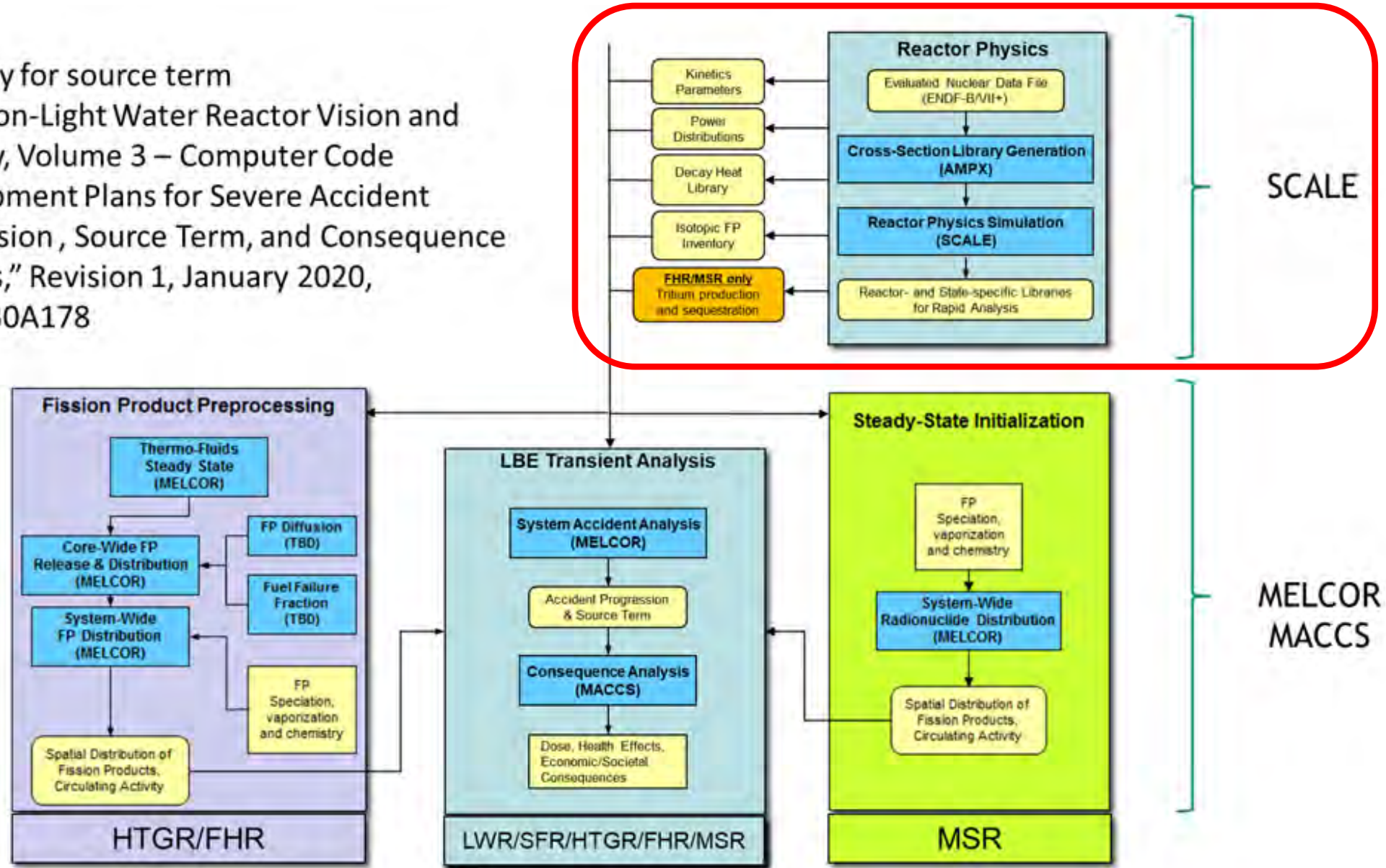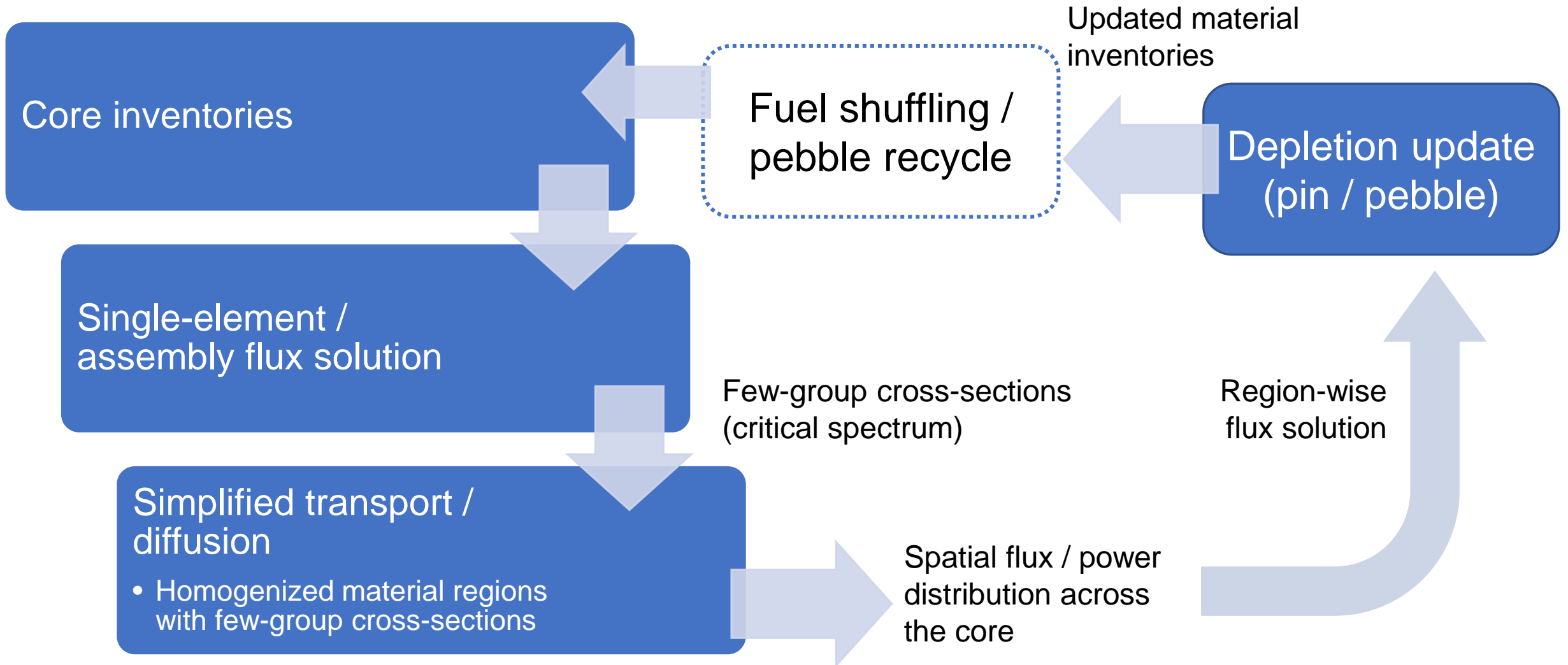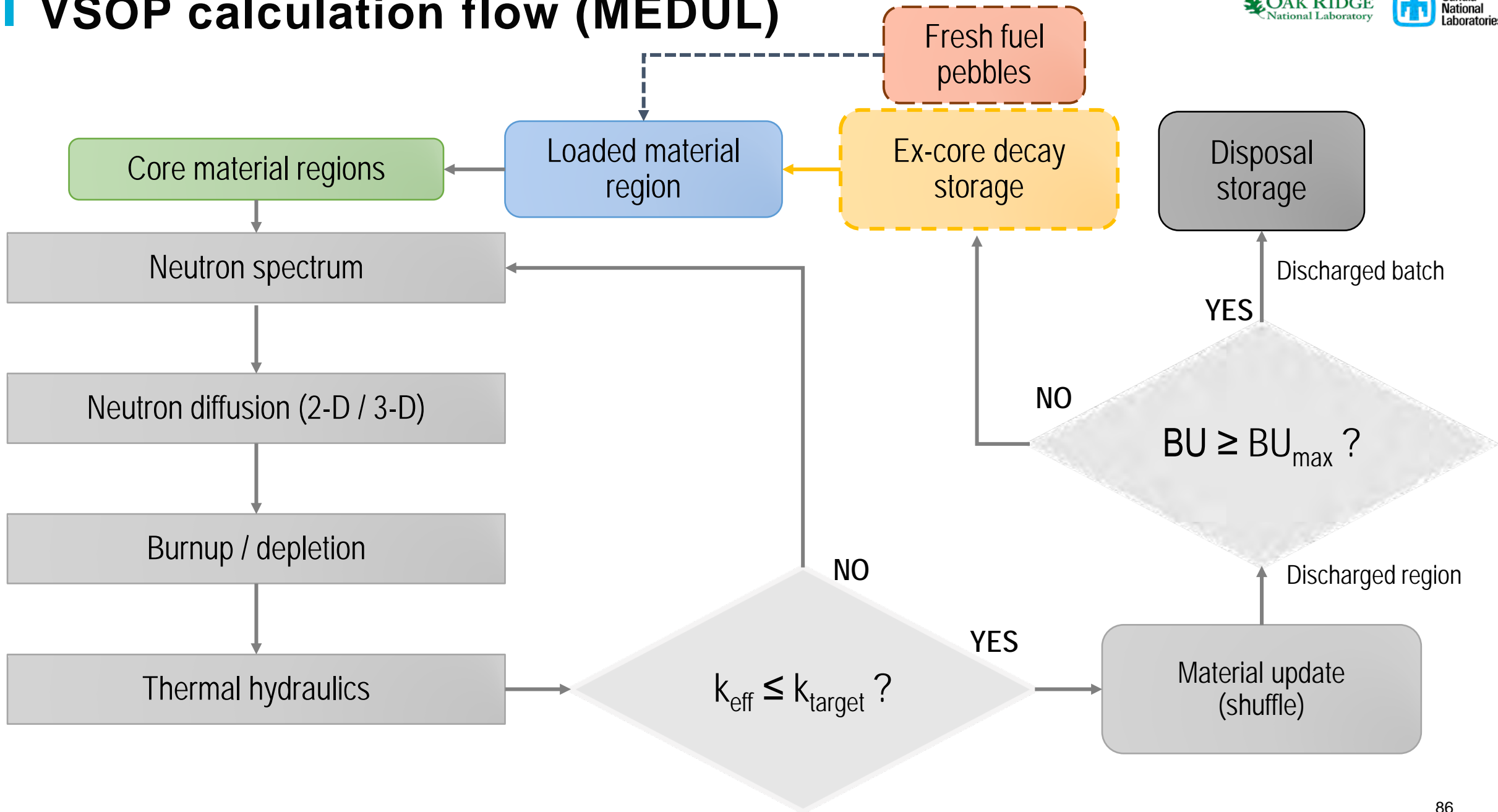
VSOP calculation flow (MEDUL)

VSOP calculation flow (MEDUL)

Fresh fuel pebbles

Loaded material region

Ex-core decay storage

Disposal storage

Core material regions

Neutron spectrum

Neutron diffusion (2-D / 3-D)

Burnup / depletion

Thermal hydraulics

This is just two-step neutronics (Polaris+PARCS)

$k_{eff} \leq k_{target}$?

NO

YES

Material update (shuffle)

Discharged region

$BU \geq BU_{max}$?

YES

NO

Discharged batch

VSOP calculation flow (MEDUL)

Fresh fuel pebbles

Loaded material region

Ex-core decay storage

Disposal storage

Core material regions

Neutron spectrum

Neutron diffusion (2-D / 3-D)

Burnup / depletion

Thermal hydraulics

At equilibrium, spatial distributions are **static**: power, neutron spectrum, isotopics!

We use Monte Carlo to generate the high-fidelity spatial flux spectrum and one-group cross sections

$BU \geq BU_{max}$?

YES — Discharged batch

NO

$k_{eff} \leq k_{target}$?

NO

YES

Material update (shuffle)

Discharged region

VSOP calculation flow (MEDUL)

We simulate a pebble[*] moving through the equilibrium core with a time-dependent power and flux spectrum **based on its position**.

This pebble[*] can be used to reconstruct the detailed core composition or iterate on the equilibrium core.

Fresh fuel pebbles

Core material regions

Loaded material region

Ex-core decay storage

Disposal storage

Neutron spectrum

Neutron diffusion (2-D / 3-D)

Burnup / depletion

Thermal hydraulics

Discharged batch

YES

NO

$BU \geq BU_{max}$?

Discharged region

$k_{eff} \leq k_{target}$?

YES

Material update (shuffle)

*equivalent to a batch of pebbles with same history

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Iterative procedure for developing equilibrium core compositions

Determine **average burnup** of each pebble batch within a zone (axial / radial)

Deplete each **batch** within zone to its respective burnup
- Origen library based on region-wise flux from core transport

Average zone compositions
- Weighted sum of batches

Calculate core power distribution & flux shape by zone
- Generate ORIGEN library for each zone

Repeat on initial guess inventories until k_{eff} converges; depleted compositions represent approximate "equilibrium"

Why use an iterative approach to equilibrium core compositions (instead of 2-step?)

- We're interested in determining equilibrium **compositions** and **flux shape** by region
  - Not trying to perform dynamics or reload analysis; just need equilibrium in-core inventories

- At-equilibrium assumption simplifies analysis
  - Conservative and bounding: i.e., converged upon highest core-averaged burnup (and thus highest fission product inventories)
  - 2-step analysis requires many repeated calculations
    - e.g., 22 axial zones x 5 passes through core => 110 calculations to perform **one** complete cycle! (Still not at equilibrium)
    - Feasible with few-group diffusion, **costly** for MG transport!

ORIGEN Library
Interpolation Backup Slides

Aspects of the ORNL methodology for fuel inventory

- Rapid answers to common questions such as
  What I/Cs/Pu content could I expect in a PBMR-400 pebble at 90 GWd/MTU?
  - a. assuming constant power?
  - b. pass-dependent power?
  - c. during a power maneuver?
  - d. after 4 days of decay?
  - e. after 40 days of decay?
  - f. after 40 years of decay?
  - g. at 80 GWd/MTU?
  - h. in a pebble with +1% enrichment?

Each answer requires a <10 second calc. on a single CPU

Why is speed important? This approach is not just for seeding MELCOR nodalizations. **All back-end analysis** can use this approach: dry storage casks, on-site storage, discharge inventory analysis, transportation packages.

- Up-front work required
  - **Sensitivity analysis** of the reactor system to understand the state changes that impact neutron flux spectrum in the fuel (e.g. moderator density in BWR)
  - Running many CPU-hours of TRITON coupled transport+depletion cases to generate a database of 1-group cross sections σ which can be interpolated to a specific state (ORIGEN reactor library)
  - Those libraries can then be used later (in ORIGAMI) to regenerate inventory and reaction rates:
    $$RR(t) = \sigma(t)\, N(t)\, \phi(t)$$

Why do it this way?
If σ is insensitive to decay time, power level, then b through h can be answered from a single TRITON pre-calculation!

Strategy for LWRs

- What level of TRITON model fidelity is required to generate a reasonable 1-group xs database (ORIGEN reactor library) for rapid **LWR** inventory calculations?

  Increasing fidelity ↑

  a. 3D full-core with plant-specific loading pattern → Requires plant-specific knowledge

  b. 3D full-core with equilibrium loading pattern

  c. 3D core subset

  d. 3D single assembly

  e. 2D core subset

  Assembly position matters → Imposes additional assumptions or requires too much information!

  f. 2D single assembly

  g. 2D single pin

  Has trouble with local variations (control elements, water holes, channel box)

  h. 0D infinitely homogeneous mixture → Has trouble if **any** geometry is important

- For LWRs, using 2D single assembly models to generate the 1-group xs database appears sufficient!

  - **verification** confirms ORIGAMI reproduces TRITON results with same (simple) operating history

  - **validation** against spent fuel inventory and decay heat measurements confirms the overall approach is adequate

    - code results generally within experimental uncertainty bands

   - <1% error in decay heat, <5% error in important nuclides, <15% error in others

Strategy for HTGRs

- What level of TRITON model fidelity is required to generate a reasonable 1-group xs database for rapid **HTGR** inventory calculations?

  a. 3D full-core with plant-specific pebble loading & discharge strategy → Requires plant-specific knowledge

  b. 3D full-core with equilibrium pebble distribution → Computationally expensive

  c. 2D core slice with equilibrium pebble distribution

  d. 1D single pebble with "buffer" for neighbor effects → Previously investigated in other work; difficult to optimize buffer

  e. 1D single pebble → Does not account for reflectors

  f. 0D infinitely homogeneous mixture

  Used in this study to understand sensitivity to model fidelity

- Using at SCALE/TRITON 3D full-core at equilibrium (b) is equivalent to VSOP but with:
  - ENDF/B-VII.1+ modern nuclear data
  - SCALE complete ORIGEN nuclide set instead of VSOP limited set
  - SCALE high-fidelity full-core Monte Carlo transport instead of VSOP diffusion

Our focus for the PBMR-400

- First, understand the state changes that influence the neutron flux spectrum in a pebble as it flows through an <u>equilibrium core:</u>

  a. pebble power history

  b. pebble burnup

  c. axial position in the core

  d. radial position in the core (proximity to radial reflector)

  e. pebble neighbors (burnup/temperature/inventory)

  f. temperature

- Next, **generalize** the SCALE concept of the ORIGEN reactor library for HTGR / PBMR-400
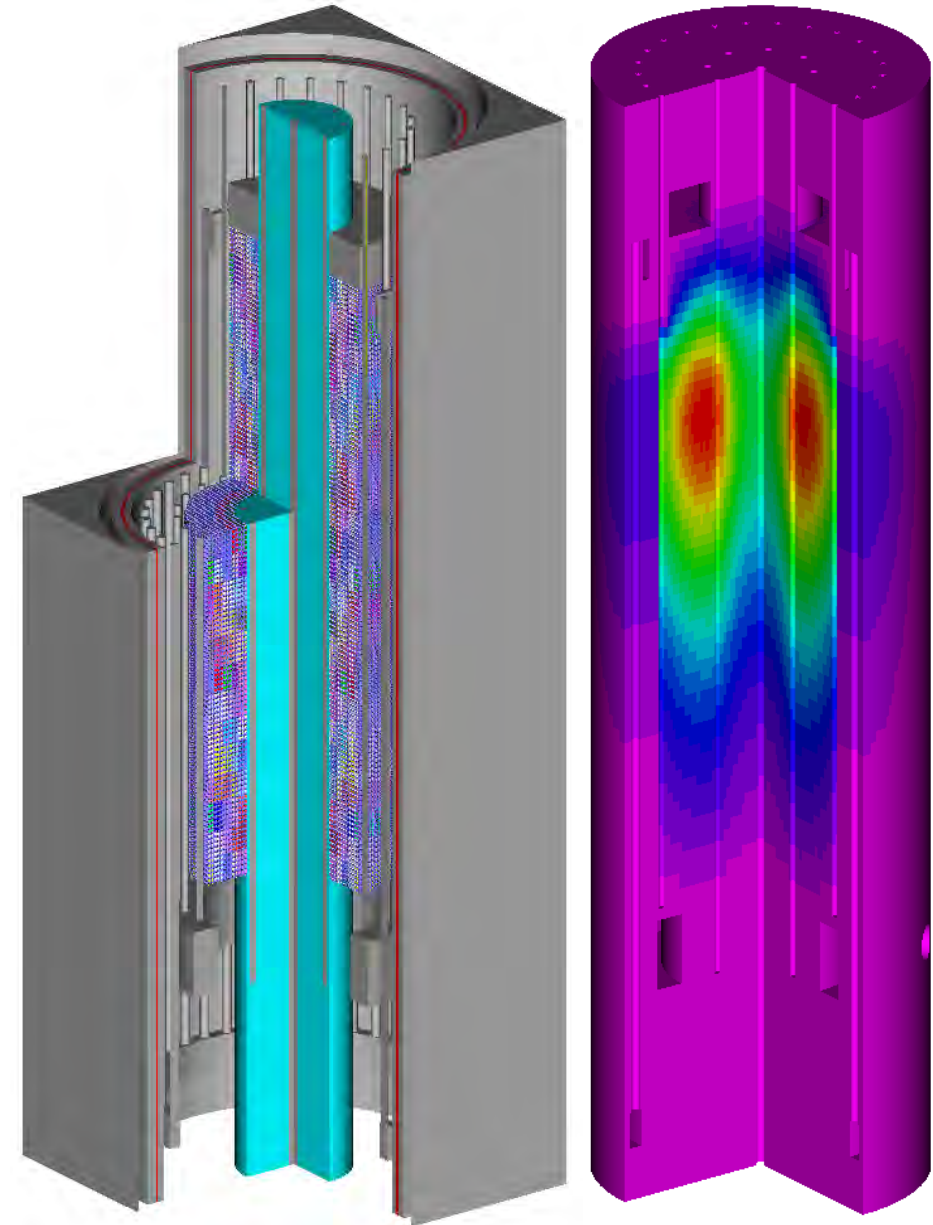
Prototype ORIGAMI input for multi-pass pebble inventory calculations (SCALE 7.0)

radial power shape

axial power shape

(relative) **residence time** in each axial zone

Example history: 3-pass pebble history, each pass moves through declared axial zones

power: average MWd/MTU for that pass
burn: days at power
down: days decay
rzone: radial zone

ORIGAMI operating history input

```
pr = [ p_{r1} p_{r2} ... p_r ]
pz = [ p_1 p_2 ... p_n ]
ztime = [ rt_1 rt_2 ... rt_n ]


hist[

    pass{ power=180  burn=64 down=7 rzone=ANY }
    pass{ power=160  burn=62 down=6 rzone=ANY }
    pass{ power=140  burn=64 down=7 rzone=3 }
]
```

Enhancing ORIGEN library interpolation capabilities to accommodate non-LWR systems

- Legacy ORIGEN library interpolation (via ARP) optimized for LWR analysis
  - Interpolation dimensions of initial enrichment, average moderator density, burnup

- Diverse physics characteristics of non-LWR cores require new dimensions for reactor library interpolation
  - e.g., **PBMR:** radial distance from reflector, initial pebble enrichment, reflector temperature

- To address this, we have developed a new HDF5-based format for **self-describing** ORIGEN libraries capable of accommodating arbitrary dimensions for interpolation

Legacy ORIGEN reactor data library interpolation relies on an ASCII database with hard-coded interpolation dimensions

Pre-defined dimensions:
- ^{235}U Enrichment
- Moderator density

Individual permutations on interpolation dimensions
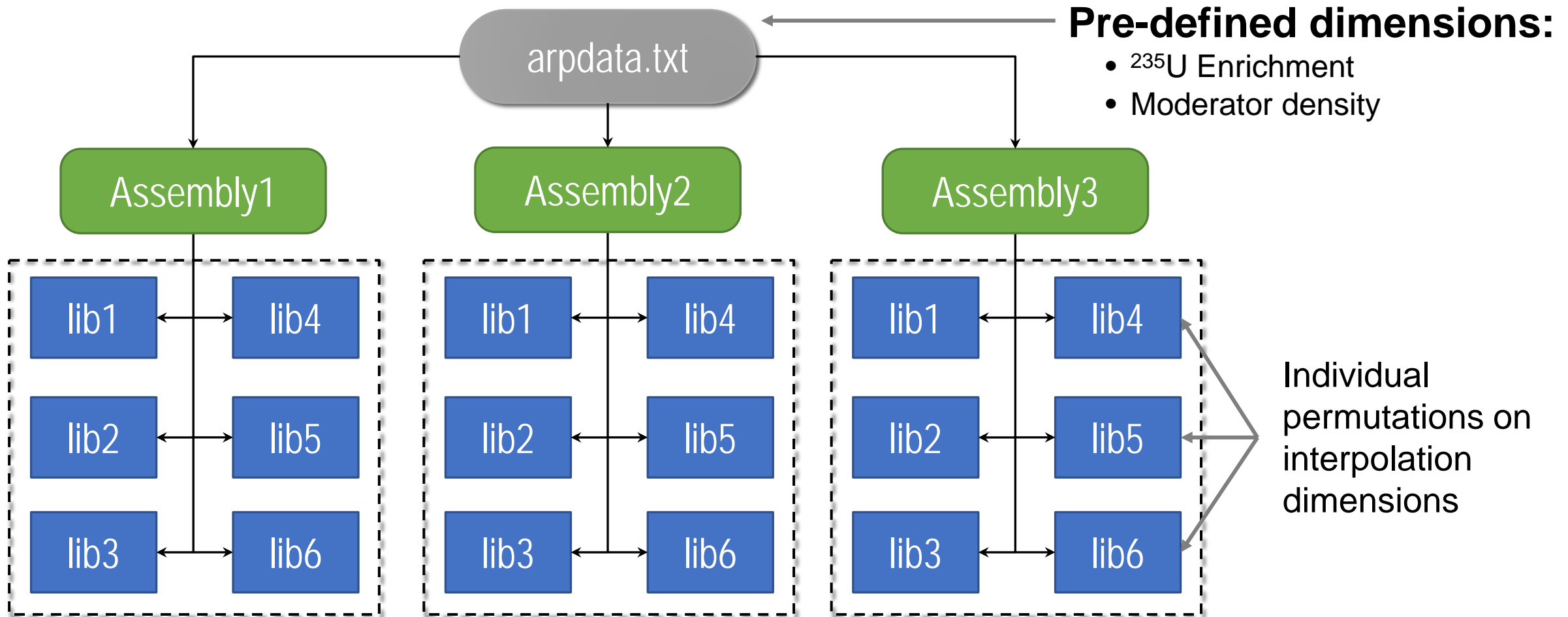
New HDF5-based "Archive" format designed to accommodate arbitrary interpolation dimensions
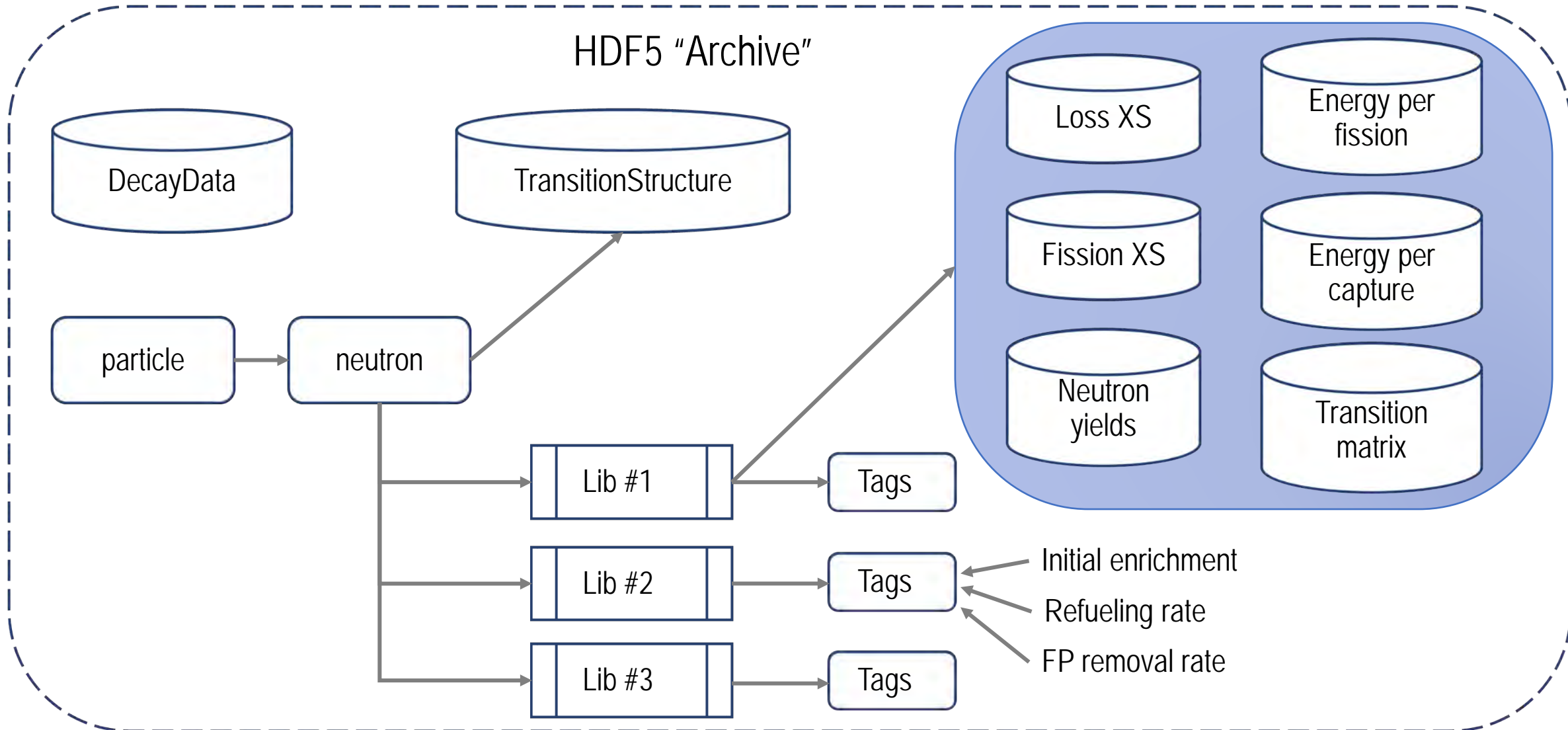
MELCOR Development for Regulatory Applications
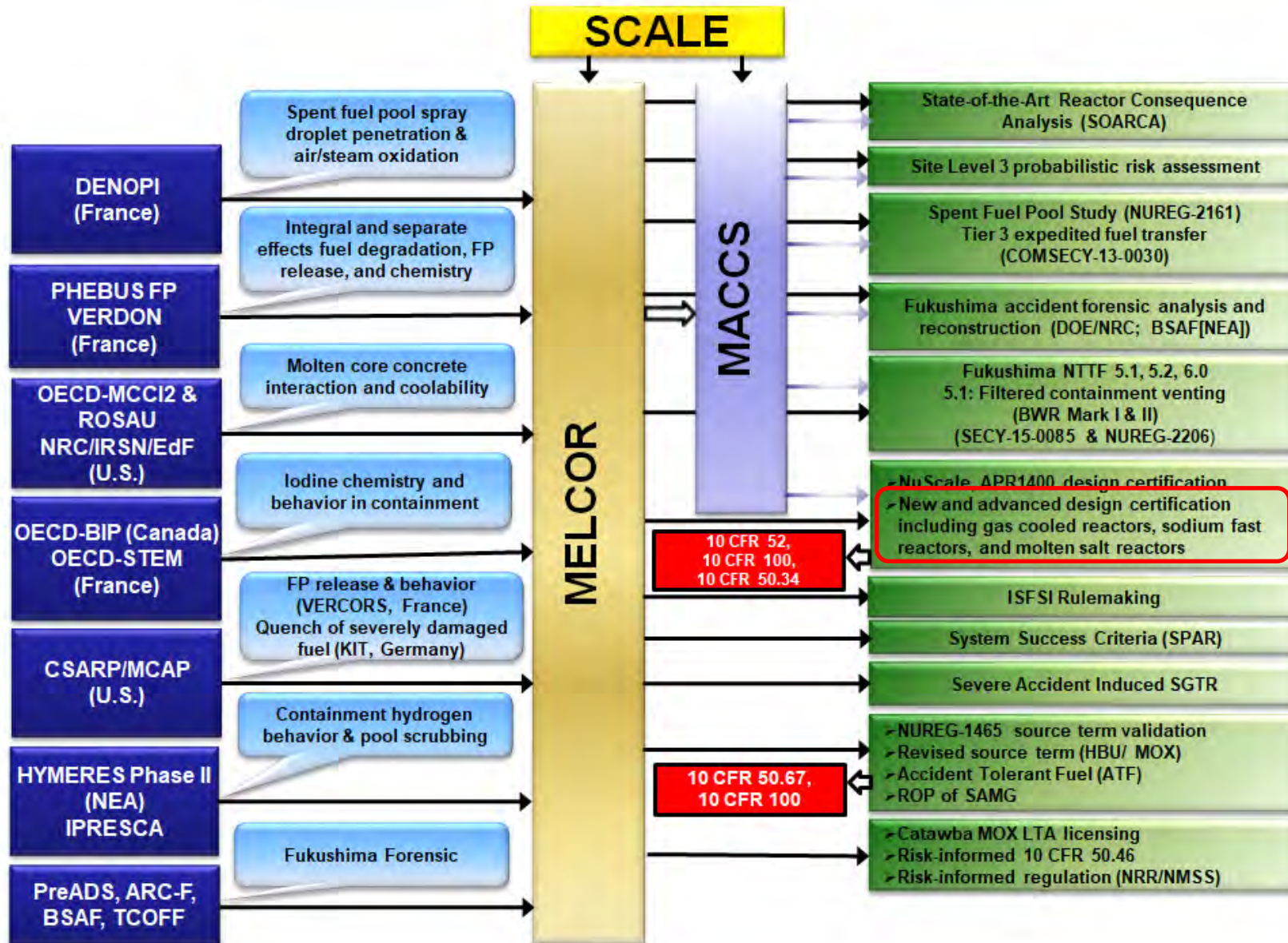
What Is It?
MELCOR is an engineering-level code that simulates the response of the reactor core, primary coolant system, containment, and surrounding buildings to a severe accident.

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
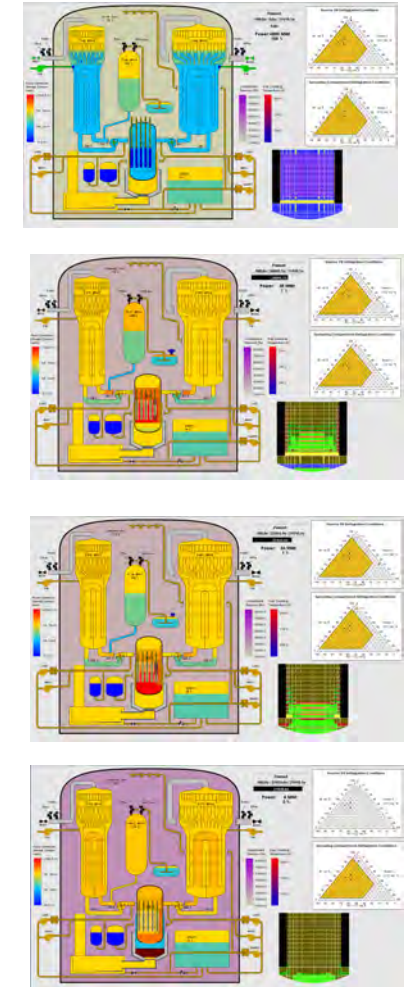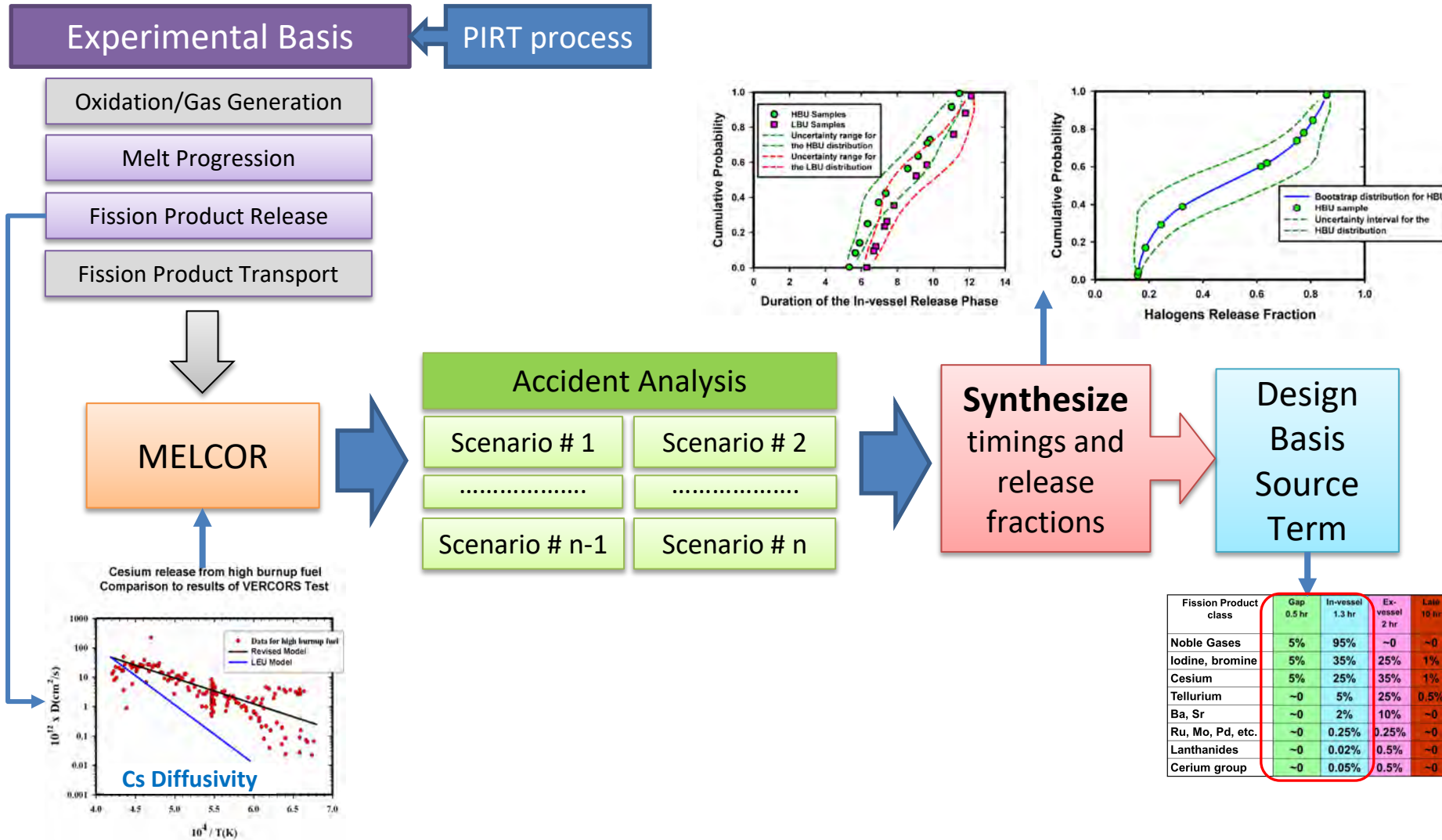
SCALE/MELCOR/MACCS

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	Regulatory	Design/Operational Support	Fusion	Spent Fuel	Facility Safety

• Technology-neutral
  o Experimental
  o Naval
  o Advanced LWRs
  o Advanced Non-LWRs
• Accident forensics (Fukushima, TMI)
• Probabilistic risk assessment
	• License amendments
	• Risk-informed regulation
	• Design certification (e.g., NuScale)
	• Vulnerability studies
	• Emergency preparedness
	• Emergency Planning Zone Analysis
		• Design analysis scoping calculations
		• Training simulators
			• Neutron beam injectors
			• Li loop LOFA transient analysis
			• ITER cryostat modeling
			• He-cooled pebble test blanket (H^3)
				• Risk studies
				• Multi-unit accidents
				• Dry storage
				• Spent fuel transport/package applications
					• Leak path factor calculations
					• DOE safety toolbox codes
					• DOE nuclear facilities (Pantex, Hanford, Los Alamos, Savannah River Site)

MELCOR Attributes
Foundations of MELCOR Development

**Fully integrated, engineering-level code**

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

Level of physics modeling consistent with

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

Traditional application

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

Phenomena modeled
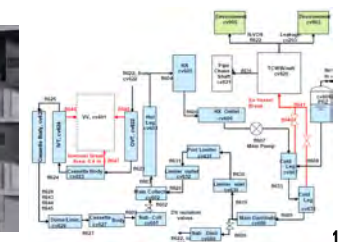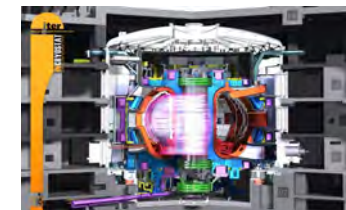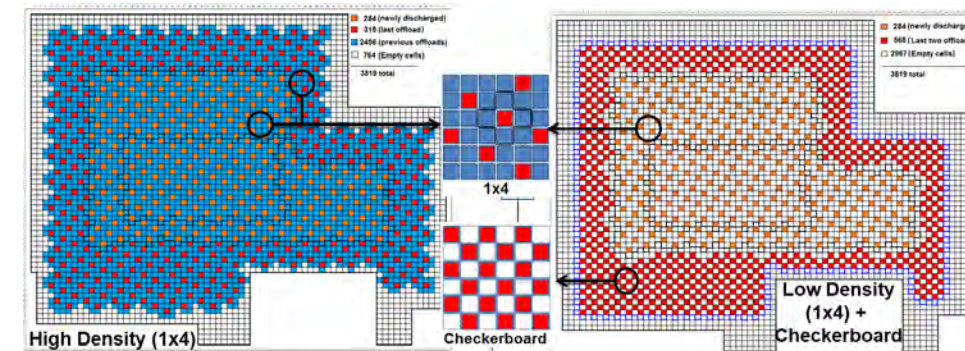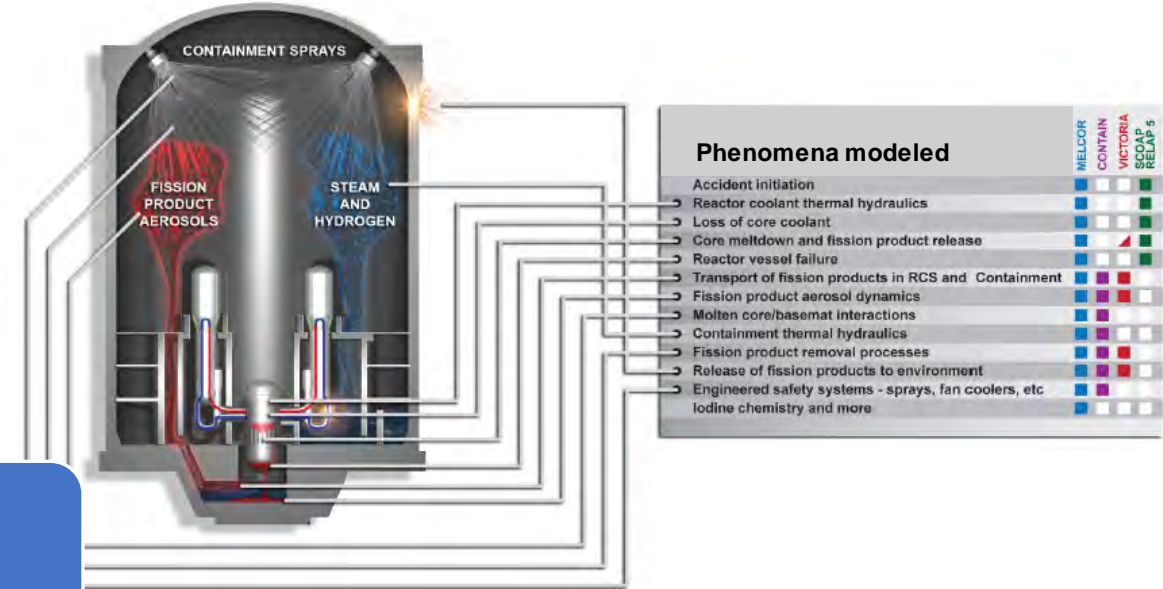
MELCOR Attributes
MELCOR Pedigree

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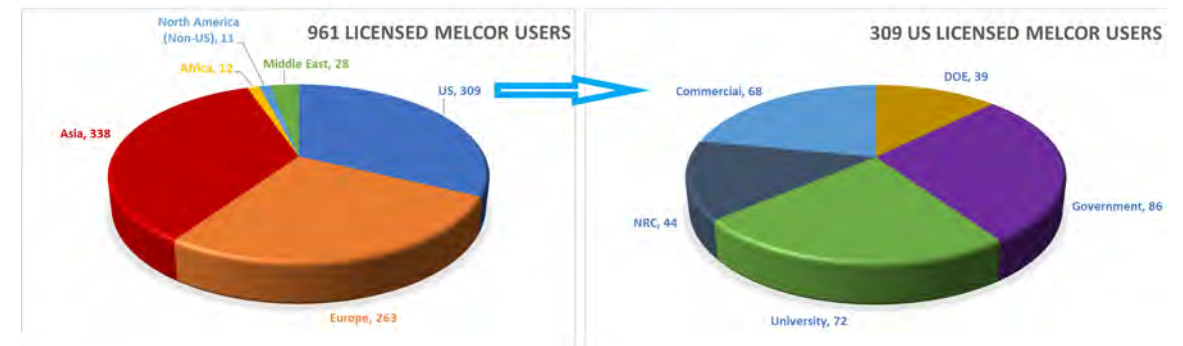
International LWR fleet relies on safety assessments performed with the MELCOR code

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

961 LICENSED MELCOR USERS

North America (Non-US), 11
Africa, 12
Middle East, 28
US, 309
Asia, 338
Europe, 263

309 US LICENSED MELCOR USERS

Commercial, 68
DOE, 39
Government, 86
University, 72
NRC, 44

Common Phenomenology
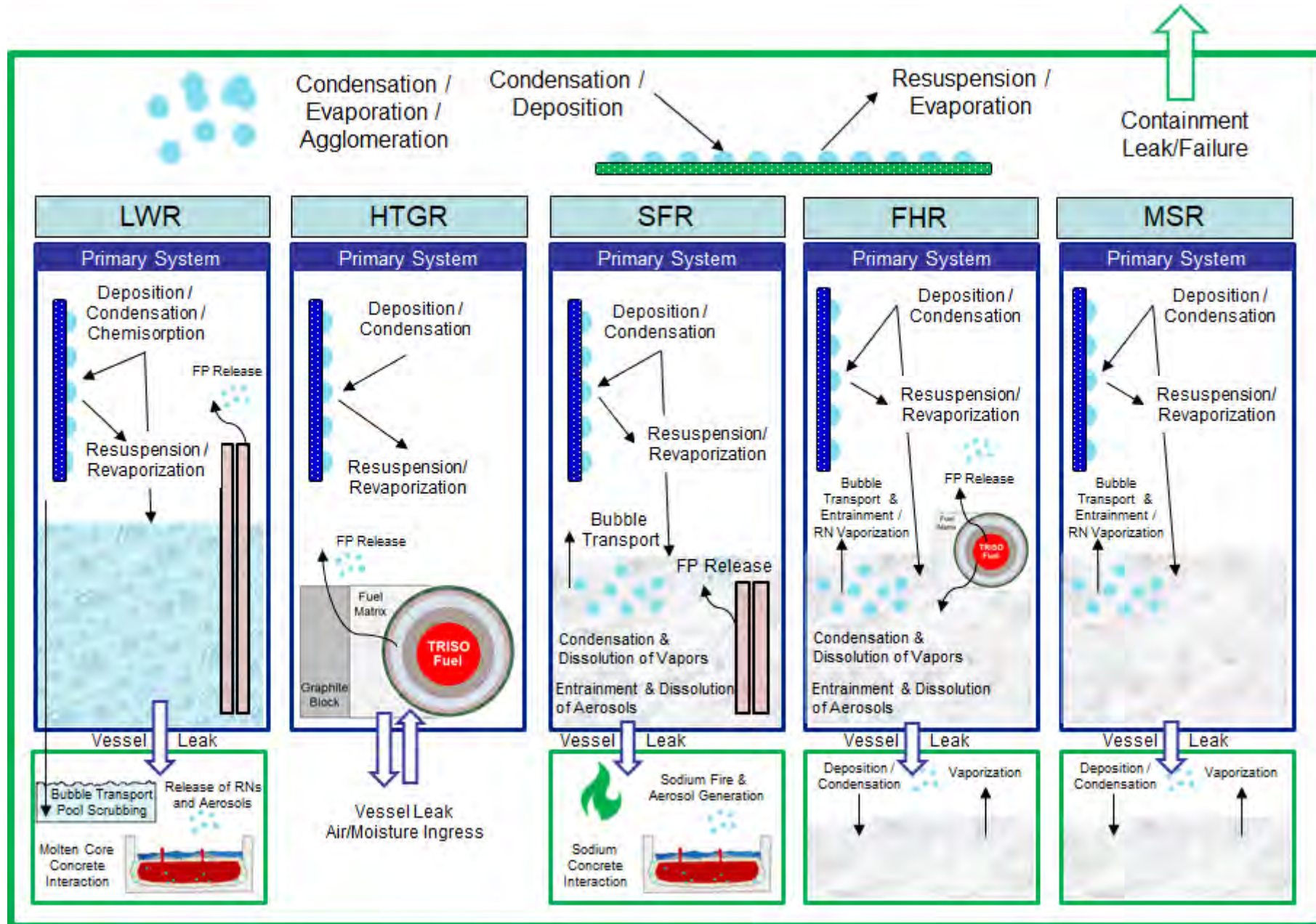
MELCOR Modeling Approach

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

Parametric models enable uncertainties to be characterized

- Majority of modeling parameters can be varied

- Properties of materials, correlation coefficients, numerical controls/tolerances, etc.
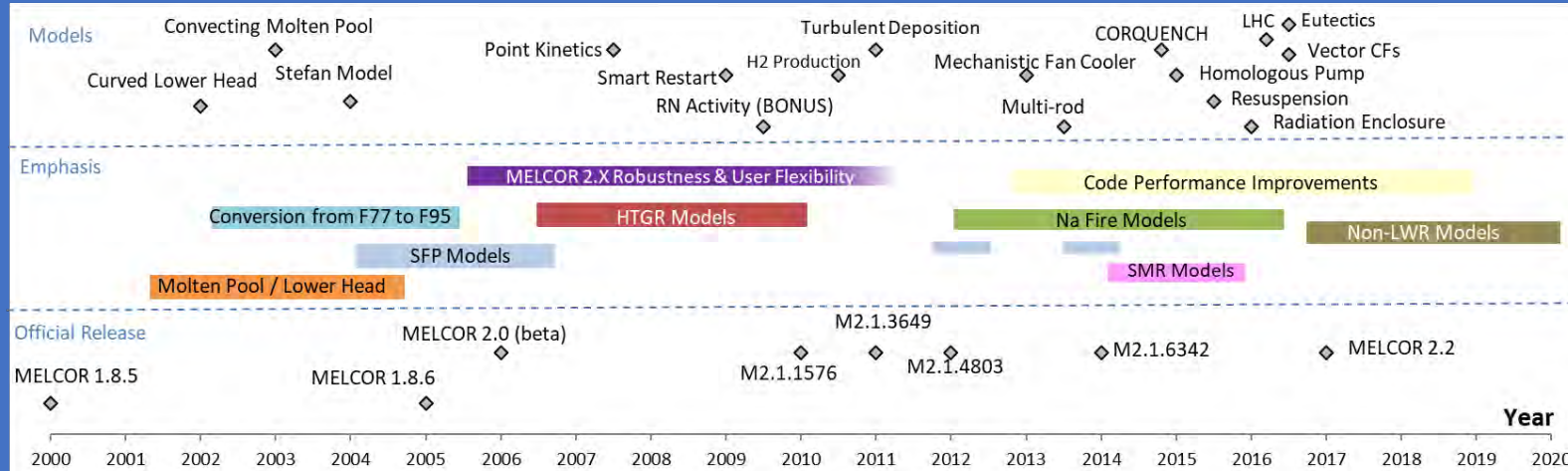
Code models are general and flexible

- Relatively easy to model novel designs

- All-purpose thermal hydraulic and aerosol transport code
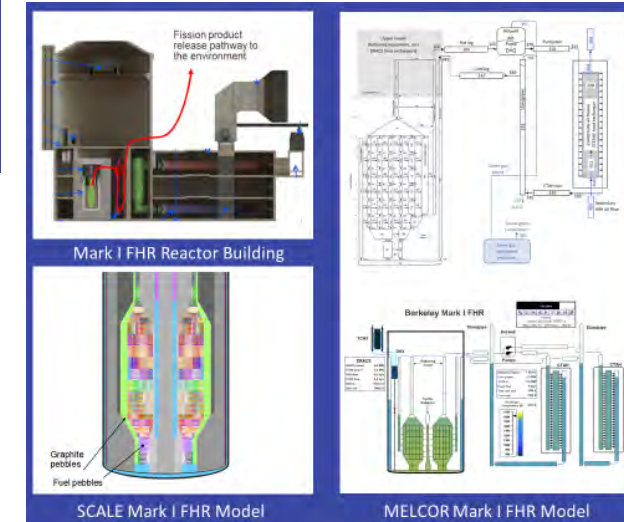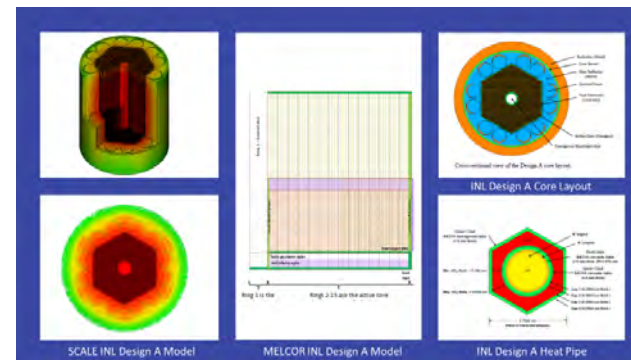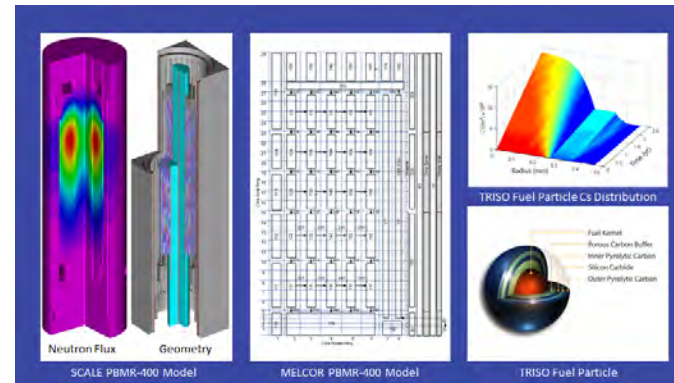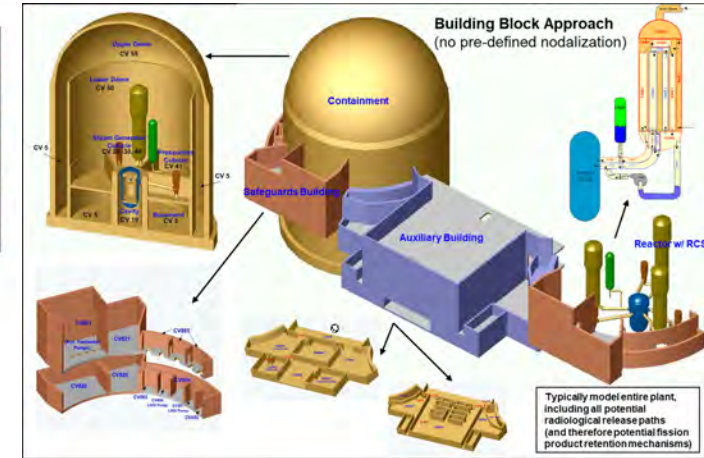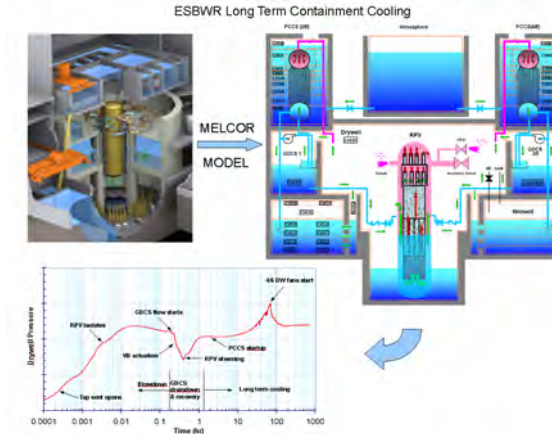
MELCOR State-of-the-Art

MELCOR Code Development

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

M2x Official Code Releases

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)

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			
Test 1new	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
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
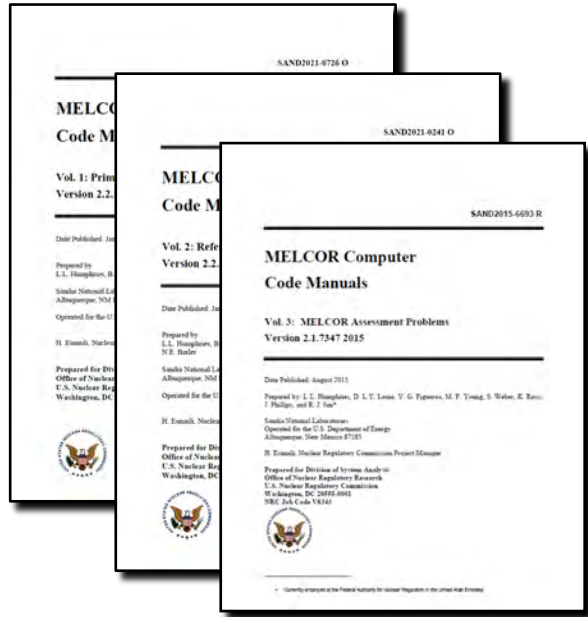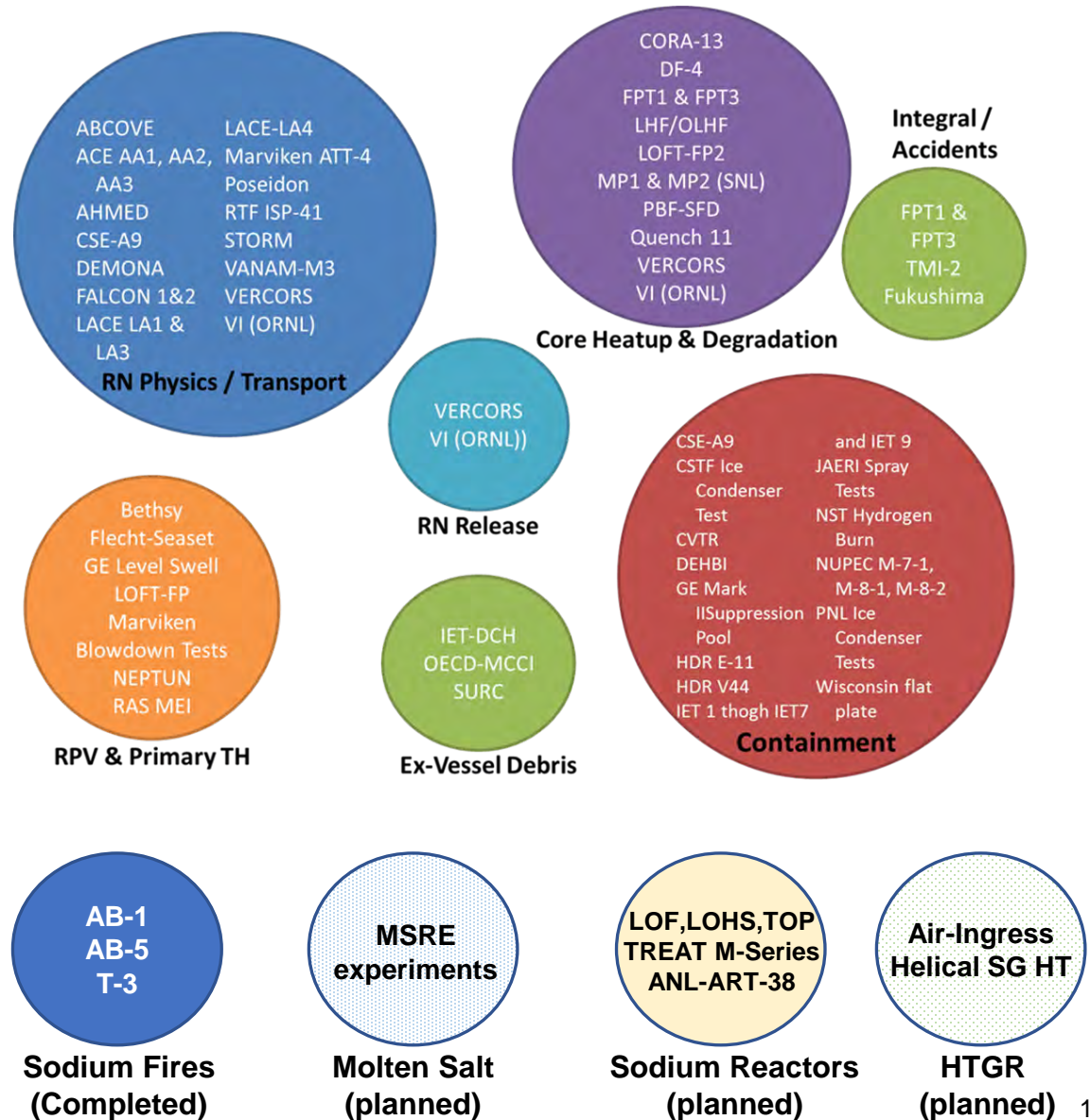

Volume 1: Primer & User Guide
Volume 2: Reference Manual
Volume 3: MELCOR Assessment Problems
    [SAND2015-6693 R]

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

RN Physics / Transport
- ABCOVE
- ACE AA1, AA2, AA3
- AHMED
- CSE-A9
- DEMONA
- FALCON 1&2
- LACE LA1 & LA3
- LACE-LA4
- Marviken ATT-4
- Poseidon
- RTF ISP-41
- STORM
- VANAM-M3
- VERCORS VI (ORNL)

Core Heatup & Degradation / Integral / Accidents
- CORA-13
- DF-4
- FPT1 & FPT3
- LHF/OLHF
- LOFT-FP2
- MP1 & MP2 (SNL)
- PBF-SFD
- Quench 11
- VERCORS VI (ORNL)

- FPT1 & FPT3
- TMI-2
- Fukushima

RN Release
- VERCORS VI (ORNL))

RPV & Primary TH
- Bethsy
- Flecht-Seaset
- GE Level Swell
- LOFT-FP
- Marviken
- Blowdown Tests
- NEPTUN
- RAS MEI

Ex-Vessel Debris
- IET-DCH
- OECD-MCCI
- SURC

Containment
- CSE-A9
- CSTF Ice Condenser Test
- CVTR
- DEHBI
- GE Mark IISuppression Pool
- HDR E-11
- HDR V44
- IET 1 thogh IET7
- and IET 9
- JAERI Spray Tests
- NST Hydrogen Burn
- NUPEC M-7-1, M-8-1, M-8-2
- PNL Ice Condenser Tests
- Wisconsin flat plate

Sodium Fires (Completed)
- AB-1
- AB-5
- T-3

Molten Salt (planned)
- MSRE experiments

Sodium Reactors (planned)
- LOF,LOHS,TOP TREAT M-Series ANL-ART-38

HTGR (planned)
- Air-Ingress Helical SG HT

111

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

ABCOVE AB5

DEMONA-B3

Turbulent Deposition

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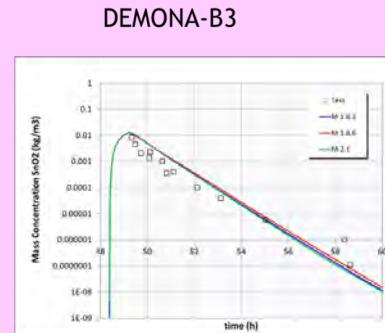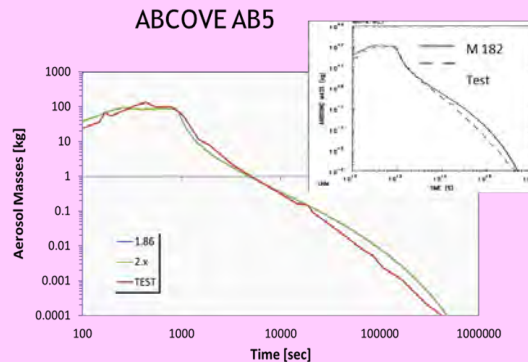
Resuspension

STORM (Simplified Test of Resuspension Mechanism) test facility
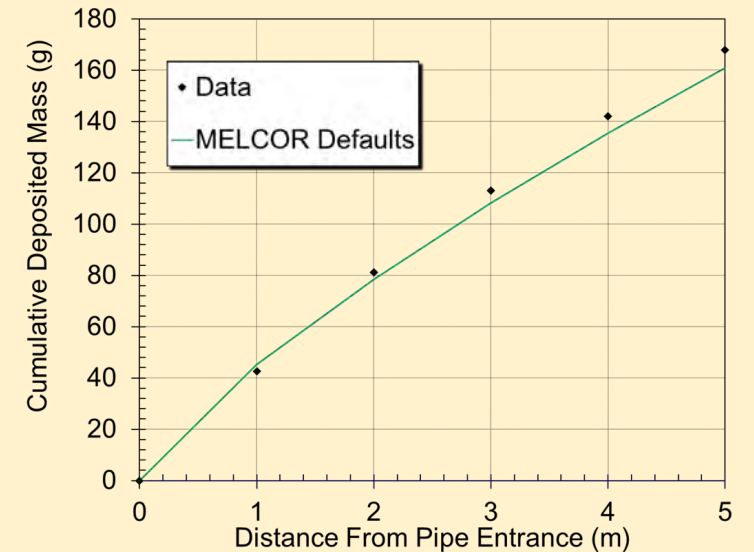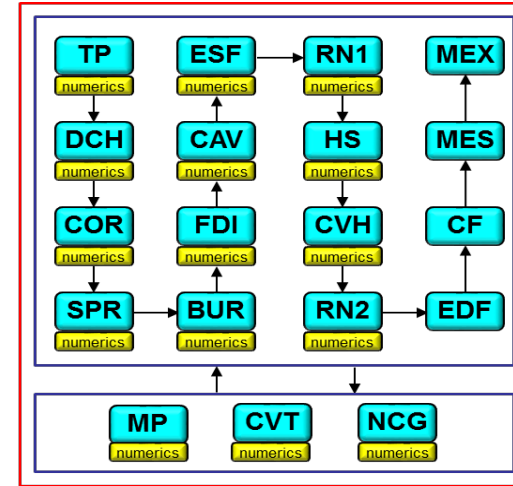
MELCOR Modernization

Generalized numerical solution engine

Hydrodynamics

In-vessel damage progression

Ex-vessel damage progression

Fission product release and transport

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

RN = Radionuclide
HS = Heat Structure
CVH = CV Hydrodynamics
EDF = External Data File
CF = Control Function
MES = Special Messages
MEX = Executive
CVT = CV Thermodynamics
NCG = Non Condensible Gas
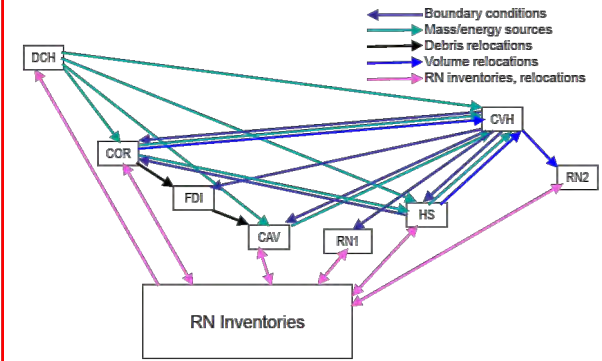
Separate Physics & Numerics
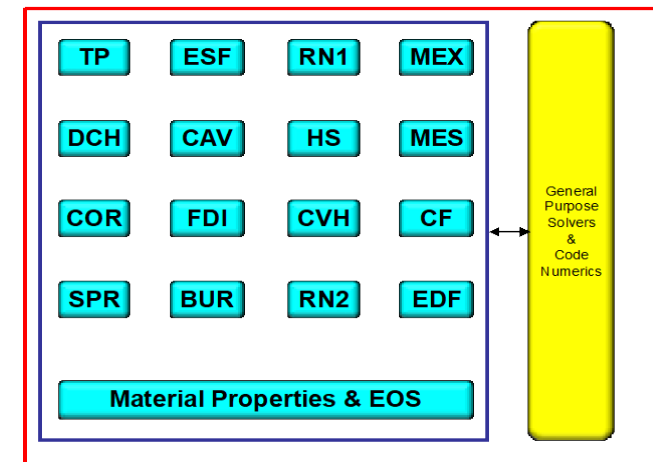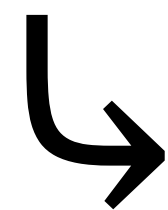
MELCOR default radionuclide classes

MELCOR default radionuclide classes

Class	Class Name	Chemical Group	Representative	Member Elements
1	XE	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	CS	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	BA	Alkaline Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	I2	Halogens	I_2	F, Cl, Br, I, At
5	TE	Chalcogens	Te	O, S, Se, Te, Po
6	RU	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	MO	Early Transition Elements	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	CE	Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	LA	Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10	UO2	Uranium	UO_2	U
11	CD	More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
12	AG	Less Volatile Main Group	Ag	Ga, Ge, In, Sn, Ag