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SCALE 6.3 Modeling Strategies for Reactivity, Nuclide Inventory, and Decay Heat of Non-LWRs

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OAK RIDGE National Laboratory

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Nuclear Energy and Fuel Cycle Division

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ABBREVIATIONS

ABTR	Advanced Burner Test Reactor
ARP	automated rapid processing
BWR	boiling water reactor
CE	continuous-energy
CHPOP	columnar hexagonal point-on-point
CRAM	Chebyshev Rational Approximation Method
CSAS	Criticality Safety Analysis Sequence
DEM	discrete element modeling
DNP	delayed neutron precursor
FHR	fluoride salt–cooled high-temperature reactor
HALEU	high-assay low-enriched uranium
HCP	hexagonal close-packing
HPR	heat pipe reactor
HTGR	high-temperature gas-cooled reactor
INL	Idaho National Laboratory
LEU	low-enriched uranium
LWR	light-water reactor
MATREX	hybrid matrix exponential/linear chains method
MG	multigroup
MOX	mixed oxide fuel
MSR	molten salt–fueled reactor
MSRE	Molten Salt Reactor Experiment
MTIHM	metric ton initial heavy metal
NRC	US Nuclear Regulatory Commission
OGS	off-gas system
ORIGEN	Oak Ridge Isotope Generation code
ORNL	Oak Ridge National Laboratory
PBR	pebble-bed reactor
PWR	pressurized water reactor
SFR	sodium-cooled fast reactor
SLICE	SCALE Leap-In method for Cores at Equilibrium
SNL	Sandia National Laboratories
TRISO	tristructural isotropic
TRU	transuranic
TSL	thermal scattering law
U/TRU	uranium/transuranic

ABSTRACT

To assess modeling and simulation capabilities for thermal hydraulics, accident progression, source term, and consequence analysis for non–light-water reactor (LWR) technologies, the US Nuclear Regulatory Commission (NRC) initiated a collaborative project between Oak Ridge National Laboratory (ORNL) and Sandia National Laboratories (SNL) in FY20, which is detailed in "Volume 3: Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis." This project demonstrated the capabilities of the MELCOR and SCALE codes to calculate accident scenarios during operation of relevant non-LWRs. The following five non-LWR concepts were selected for capability demonstration based on recently renewed industry interest in the United States to develop and deploy such reactor technologies: pebble-bed high temperature gas-cooled reactors (HTGRs), pebble-bed fluoride salt-cooled reactors (FHRs), molten salt–fueled reactors (MSRs), heat pipe reactors (HPRs), and sodium-cooled fast reactors (SFRs).

Within this project, the SNL team used and further developed MELCOR to perform thermal hydraulics, accident progression and source term analyses for selected accident scenarios during operation of the five aforementioned non-LWRs. The ORNL team used SCALE to provide MELCOR with initial and boundary conditions including nuclide inventories, decay heat, power profiles, and reactivity coefficients. MELCOR used these SCALE-predicted initial and boundary conditions together the geometry of the reactor facility to simulate accidents.

This report summarizes the SCALE non-LWR modeling strategies and best practices developed in this project. This includes an overview of SCALE methods and tools used for reactivity, power, and inventory calculations, specific recommendations for the use of the various SCALE sequences, and modeling recommendations for the various non-LWRs. This report is intended for SCALE users who are tasked with the modeling and analysis of a non-LWR and who want to benefit from the collective lessons learned by SCALE analysts. Recommendations are based on SCALE version 6.3.1. Future versions of SCALE will include updates based on the lessons learned in this project including minor updates to improve application for non-LWRs and the addition of new capabilities.

ACKNOWLEDGMENTS

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1. INTRODUCTION

To assess modeling and simulation capabilities for thermal hydraulics, accident progression, source term, and consequence analysis for non–light-water reactor (LWR) technologies, the US Nuclear Regulatory Commission (NRC) initiated a collaborative project in FY20 between Sandia National Laboratories (SNL), and Oak Ridge National Laboratory (ORNL), which is detailed in "Volume 3: Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis" (US NRC 2020). This project demonstrated the capabilities of the MELCOR (Humphries et al. 2021) and SCALE (Wieselquist and Lefebvre 2023) codes to simulate accident scenarios for five non-LWRs reference plants that were selected based on recently renewed industry interest in the United States to develop and deploy such reactor technologies (US NRC 2022) and based on the availability publicly accessible design specifications. Within this project, the SNL team used and further developed MELCOR to perform thermal hydraulics, accident progression and source term analyses for selected accident scenarios for the five non-LWRs referece plants. The ORNL team used SCALE to provide MELCOR with initial and boundary conditions including nuclide inventories, decay heat, power profiles, and reactivity coefficients. MELCOR uses these SCALE-predicted initial and boundary conditions together with the geometry of the reactor facility to simulate accidents.

Five representative non-LWR designs were studied in this project, public workshops were held, and the following reports for the SCALE and the MELCOR analyses were published:

- Pebble-bed high-temperature gas-cooled reactor (HTGR) (Skutnik and Wieselquist 2021; Wagner, Beeny, and Luxat 2022) with representative reactor PBMR-400 (NEA 2013),
- Pebble-bed fluoride salt–cooled high-temperature reactor (FHR) (Bostelmann et al. 2022; Wagner, Haskin, et al. 2022) with representative reactor UC Berkeley Mark 1 (UCB Mk. 1) (Andreades et al. 2014),
- Molten salt–fueled reactor (MSR) (Lo et al. 2022; Wagner et al. 2023) with representative reactor Molten Salt Reactor Experiment (MSRE) (Shen et al. 2019),
- Heat pipe reactor (HPR) (Walker et al. 2021; Wagner, Faucett, et al. 2022) with representative reactor Idaho National Laboratory (INL) Design A (Sterbentz et al. 2018), and
- Sodium-cooled fast reactor (SFR) (Shaw et al. 2023; Wagner, Beeny, and Luxat 2023) with representative reactor Advanced Burner Test Reactor (ABTR) (Kim 2020).

This report synthesizes the experience and insights gained from the studies documented in the SCALE-focused reports into a single volume providing modeling strategies and recommended best practices for applying SCALE to predict non-LWR reactivity, nuclide inventory, and decay heat.

Table 1 lists the design characteristics of the selected five non-LWRs concepts in comparison with those of a pressurized water reactor (PWR). Besides the fuel form, the coolant, and the moderator (or the absence of a moderator), a major difference between non-LWRs and LWRs is found in the fuel enrichment range. LWRs operate with low-enriched uranium (LEU) with an enrichment of up to 5 wt.% ^{235}U. In contrast, many of the non-LWRs designs use high-assay low-enriched uranium (HALEU) fuel with an enrichment greater than 5 wt.% and less than 20 wt.% ^{235}U. In the case of SFRs, uranium/transuranic (U/TRU) fuel from reprocessing of spent LWR or spent SFR fuel is additionally considered in some design specifications. Although reprocessing is not currently pursued in the United States, analyses using this type of fuel were performed because of the availability of these design specifications and because reprocessing was performed in the past.

Figure 1 presents visualizations of the developed SCALE models for the five non-LWR reference plants. SCALE input and output files can be found in the public repository for this project: https://code.ornl.gov/scale/analysis/non-lwr-models-vol3

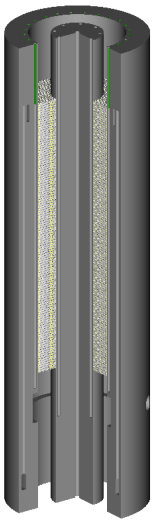
This report is structured as follows. First, an overview of SCALE methods and tools used for reactivity, power, and inventory calculations as well as relevant files are described. Then, the modeling strategies for pebble-bed reactors (PBRs), fast-spectrum SFRs and HPRs, and MSRs are discussed. Finally, specific recommendations for the use of the various SCALE sequences are listed. This report is intended for SCALE users who are tasked with modeling a non-LWR and who want to benefit from collective lessons learned by SCALE analysts. Recommendations are based on applying SCALE version 6.3.1. Additional SCALE capabilities that have been or are being implemented since SCALE version 6.3.1 as a result of experience gained from this project are noted where applicable.

Table 1. Comparison of LWR and non-LWR basic design characteristics

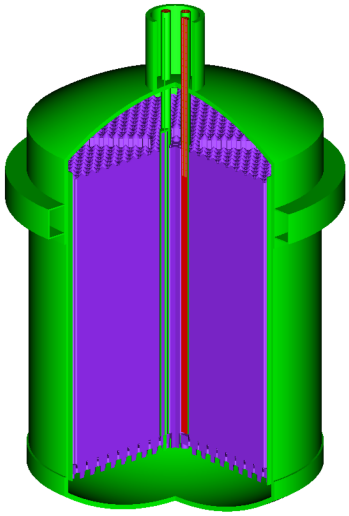
	PWR	Pebble-bed HTGR	HPR	Pebble-bed FHR	MSR	SFR
Fuel Form	Fuel rod	TRISO particles[a]	Fuel rod	TRISO particles[a]	Molten salt	Fuel rod
Fuel Type	LEU	HALEU	HALEU	HALEU	HALEU	HALEU or U/TRU
Coolant	H_2O	He (gas)	K or Na (liq.)	FLiBe salt	Li or Cl salt	Na (liq.)
Primary Moderator	^1H	Graphite	—	Graphite	Graphite/—	—
Neutron Energy Spectrum	thermal	thermal	fast	thermal	thermal/fast	fast
Discharge Burnup (GWd/MTU)	45–60	90–120	2	up to 180.0	continuous	100

Note: The above-listed characteristics are based on concepts available in the public literature and serve here to highlight major differences among the reactor concepts. Characteristics of new advanced reactor designs may differ.

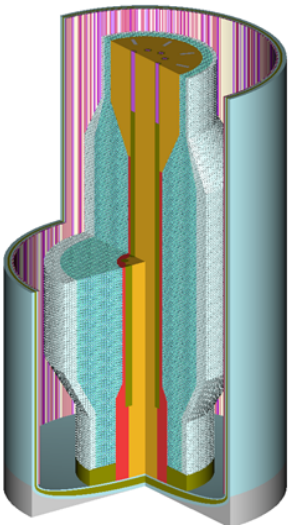
[a] TRISO particles in fuel pebbles



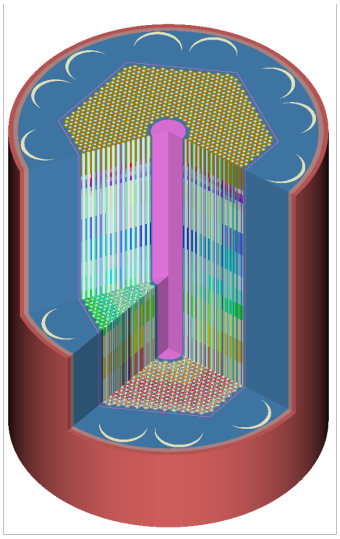
(a) PBMR-400 (HTGR)



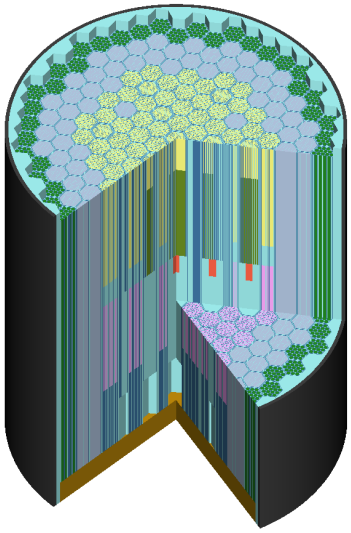
(b) MSRE (MSR)



(c) UCB Mk. 1 (FHR)



(d) INL Design A (HPR)



(e) ABTR (SFR)

Figure 1. SCALE model visualizations.

2. SCALE METHODS AND TOOLS FOR REACTIVITY, POWER, AND INVENTORY CALCULATIONS

This section briefly introduces the relevant modules of the SCALE code system that were used in this project to generate nuclide inventory and to calculate reactivity and power profiles for the individual non-LWR concepts. The section ends with an overview of available and recommended nuclear data libraries for use in the relevant SCALE tools. Details of all described methods and tools can be found in the public SCALE manual: https://scale-manual.ornl.gov/. For the selection of the individual SCALE tools depending on the problem statement and for specific recommendations for the use of the various SCALE tools and libraries, including common pitfalls, see Section 4.

To simplify descriptions in the following subsections, relevant files used across the different SCALE tools for this project are summarized in the following list.

- **Standard output file**: An ASCII output file that is generated during each SCALE calculation. It includes a repetition of the input and views all output that is printed by the applied SCALE tool.
- **3dmap file**: A binary file that stores tallied energy-dependent quantities over a mesh, together with statistical uncertainties and energy-collapsed total values for each mesh element. The data can be visualized with Fulcrum as an overlay over the geometry for which the mesh file was generated.
- **ORIGEN concentration file** (F71): A binary file that stores time-dependent nuclide densities of over 2,000 nuclides. The content of this file can be viewed with various SCALE tools (Fulcrum, OPUS, OBIWAN), and it can be directly used in ORIGEN and ORIGAMI for continued depletion or decay calculations (i.e., restart calculations) without losing precision. The file stores nuclide inventory data for multiple cases. If this file is generated with TRITON, then the case numbers correspond to the mixture identifiers in the TRITON model.
- **ORIGEN *cross section* library** (F33): A binary file that stores the transition coefficient matrix, 1-group removal/loss cross sections, 1-group fission cross sections, relative neutron yields, and problem-independent data (decay constants, molar masses, recoverable energy from decay (Q), recoverable energy from photons, radiotoxicity factors, energy released per fission and per non-fission event) for 1 mixture as a function of burnup.
- **ORIGEN *reactor* library**: A set of ORIGEN cross section libraries for a specific reactor type and fuel assembly configuration, parameterized to, for example, the following: enrichment, moderator density, plutonium content, ^{239}Pu values (MOX fuel). The reactor libraries are defined through a specific file ("arpdata.txt") that lists the individual ORIGEN cross section libraries that together build the reactor library.[1]
- **Inventory interface file** (II.JSON): A JSON-formatted file containing detailed inventory for all nuclides consistent with the ORIGEN concentration file as well as relevant nuclear data. The relevant nuclear data (decay constants, energy release, etc.) are provided to allow downstream operations to calculate decay heat, mass, activity, and other derived quantities. The JSON-formatted inventory interface file was developed as part of this project and facilitates streamlined analysis and data exchange with other codes such as MELCOR, for which the II.JSON file was used in this project to generate MELCOR decay heat input files.

1. An HDF5-formatted ORIGEN reactor library archive format has already been introduced for SCALE 7.0 that will eventually replace the individual cross section library files connected through "arpdata.txt".

2.1 REACTIVITY AND FLUX CALCULATIONS WITH CSAS AND TRITON

Multiple kernels are available in SCALE for neutron transport calculations in 1D, 2D, or 3D. For reactivity calculations of complex 3D models, three Monte Carlo codes can be used both in multigroup (MG) and continuous-energy (CE) mode: KENO-V.a, KENO-VI, and Shift. Shift (T. M. Pandya et al. 2016) is a new Monte Carlo code that has been made available with the SCALE 6.3 release. While KENO-V.a is limited in supported geometry shapes—which allows an improved runtime performance—KENO-VI and Shift were used in this project because they allow more complex geometries, such as hexagonal and dodecahedral lattices, as needed for non-LWR analysis.

Shift has additional capabilities compared to KENO-VI that are relevant for the modeling of double-heterogeneous systems, such as PBRs in which tristructural isotropic (TRISO) particles (first level heterogeneity) are distributed in fuel pebbles (second level heterogeneity). Shift can automatically place TRISO particles at random locations, for example, within an HTGR or FHR pebble. The integration of mesh acceleration in SCALE 7.0 for such geometries results in excellent runtime performance for such complex models (T. M. Pandya et al. 2022; T. Pandya et al. 2023). Furthermore, Shift demonstrates excellent performance when used with massive parallelization, which can reduce runtime.

SCALE's other unique capability for double-heterogeneous systems, which can be applied by both KENO and Shift, is a special cross section self-shielding treatment implemented in SCALE's cross section processing code XSProc for MG calculations (Williams, Choi, and Lee 2015; Bostelmann, Celik, Williams, et al. 2020; Kim et al. 2020). When using this treatment in KENO-VI or Shift MG calculations of PBR systems, the neutron transport calculations are up 25× faster in SCALE 6.3 and about 2× faster in current SCALE 7.0 beta versions (due to the above mentioned mesh acceleration in CE mode) compared to fully detailed CE calculations (Elzohery et al. 2023).

The reactivity calculations performed for this project used Shift or KENO-VI, invoked by SCALE's Criticality Safety Analysis Sequence (CSAS) or SCALE's TRITON depletion sequence. SCALE sequences usually automate execution of other modules or codes in SCALE, i.e. they do the data management including processing of results, but they do not include any physics themselves. In this case, the CSAS and TRITON sequences automatically perform the required nuclear data processing (including the self-shielding for MG calculations), call the requested neutron transport kernel, and collect the results.

Shift and KENO-VI calculate the multiplication factor k_{eff} that can be used to calculate reactivity ρ:

$$\rho = \frac{k - 1}{k}. \tag{1}$$

For the calculation of reactivity coefficients, reactivity differences between two states were compared

$$\Delta\rho = \rho_1 - \rho_2 = \frac{1}{k_2} - \frac{1}{k_1}, \tag{2}$$

or the reactivity was fitted over the perturbed parameter of interest (e.g., a temperature).

The effective delayed neutron fraction β_{eff} was calculated using the k-ratio method (Bretscher 1997) by determining the reactivity difference (via Eq. 2) between a nominal k_{eff} calculation and a k_{eff} calculation with only prompt neutrons (input parameter *pnu=yes*).

CSAS and TRITON also permit the tallying of specific quantities (neutron flux; fission source; fission density as a good proxy for power) on a Cartesian 3D mesh over the geometry[2], resulting in a 3dmap file. This

2. The implementation of other mesh types, such as hexagonal and cylindrical meshes, is planned for the SCALE 7.0 release.

capability was used to investigate energy-dependent flux distributions in specific regions of a reactor core; it was also leveraged to investigate the spatial distribution of fast and thermal neutron flux over the core.

Notes on 3D Monte Carlo calculations

1. Perform calculation of the full 3D core or reduced-symmetry models ($^1/_6$, $^1/_3$, $^1/_2$, etc.) with appropriate boundary conditions to generate k_{eff}, flux and power profiles:
   - Ensure fission source convergence of the Monte Carlo calculation by inspection of the results of all provided convergence tests.
   - Propagate the Monte Carlo statistical error from k_{eff} to the reactivity coefficients to ensure sufficient statistical convergence.

2.2 INVENTORY GENERATION WITH TRITON, ORIGEN, AND ORIGAMI

Radionuclide inventory can be obtained with SCALE in various ways. ORIGEN, the depletion and decay solver in SCALE, can be used as a standalone solver or as part of a SCALE sequence. For inventory calculations based on explicitly defined 1D, 2D, or 3D models, the reactor physics sequence TRITON is used. Rapid inventory calculations based on pre-generated ORIGEN cross section libraries are performed with the ORIGAMI code. All depletion sequences output ORIGEN concentration files that store detailed mixture- and time-dependent nuclide densities.

The reader should note that a second reactor physics sequence, Polaris, is optimized for LWR assembly depletion calculations. This sequence was not applied in this project.

TRITON

The time-dependent transmutation of various materials in 1D, 2D, or 3D models can be calculated with the reactor physics sequence TRITON (De Hart and Bowman 2011). TRITON coordinates the nuclear data processing, the neutron transport calculations for 1D, 2D, and 3D configurations, and the depletion and decay to estimate the isotopic concentrations of depleted mixtures, mixture-wise power and burnup, neutron flux, and other quantities as a function of burnup. The neutron transport calculation results in material-wise collapsed 1-group fission and removal cross sections and energy-dependent flux, which are transferred together with the material compositions to the depletion solver for the depletion or decay calculation. The material compositions are then updated, and the next neutron transport calculation is run. For the cross section processing, TRITON invokes the XSProc module; for depletion and decay, TRITON invokes ORIGEN; and for the neutron transport calculations, TRITON can be used in combination with SCALE's deterministic 1D XSDRN and 2D NEWT solvers and the 3D Monte Carlo codes KENO-V.a, KENO-VI, and Shift.

In this project, TRITON was used in combination with KENO-VI and Shift for depletion of 3D models. In addition to the reactivity and (if requested) the flux, as described in Section 2.1, TRITON outputs an ORIGEN concentration file, one ORIGEN cross section library for each mixture, and an ORIGEN cross section library for a system-average mixture. By analyzing the printed mixture-wise power, a power map over a model can be constructed.[3] Relevant for non-LWR analysis is TRITON's capability to consider material feed and removal during depletion that allows the simulation of refueling and fission gas removal for liquid fuel systems.

TRITON depletion calculations require the knowledge of material volumes. Users can manually specify material volumes, or they can enable automatic volume calculations via a ray tracer or Monte Carlo method that are included in Shift and KENO, respectively.

3. The implementation of a power mesh tally is planned for the SCALE 7.0 release.

TRITON can be used to generate ORIGEN reactor libraries. As mentioned in the introduction to this section, an ORIGEN reactor library is a set of ORIGEN cross section libraries for a specific reactor type and fuel assembly configuration, parameterized to relevant characteristics such as enrichment or moderator density. Each TRITON calculation results in an ORIGEN cross section library for a system-average mixture. By running multiple TRITON calculations for input models in which relevant characteristics were perturbed, a set of ORIGEN cross section libraries can be generated that together build an ORIGEN reactor library for use in, for example, ORIGAMI. The relevant characteristics for which the libraries should be parameterized can be determined through sensitivity calculations by investigating the collapsed 1-group cross sections on the libraries as a function of burnup and their response to a parameter variation.

Notes on TRITON

1. Use TRITON for depletion calculations of detailed 1D, 2D, or 3D models:
   - Specify all volumes and double-check their values with automatic volume calculations.
   - Use MG neutron transport calculations when possible to reduce runtime.
   - Ensure sufficient depletion steps early in the depletion calculation to correctly capture cross section changes and xenon buildup (see Section 4.2).
2. Use TRITON to generate ORIGEN reactor libraries:
   - Run sensitivity calculations to determine relevant system parameters (e.g., enrichment, temperature, spatial expansion, material densities) for cross section parameterization.

ORIGEN

Oak Ridge Isotope Generation code (ORIGEN) solves the Bateman equations to calculate time-dependent concentrations, activities, and radiation source terms for a large number of isotopes considering generation or depletion by neutron transmutation, fission, and radioactive decay (Gauld et al. 2011). ORIGEN includes two solver kernels that can solve the depletion/decay equations: the hybrid matrix exponential/linear chains method (MATREX)[4], and the Chebyshev Rational Approximation Method (CRAM) (Pusa and Leppänen 2010; Pusa 2011). The CRAM solver results in similar runtimes compared to MATREX, but is more accurate and robust on a larger range of problems. Given that CRAM is a relatively new addition, ORIGEN's default in SCALE 6.3.1 is to use MATREX, while all codes that use ORIGEN can manually select CRAM instead of MATREX.

ORIGEN is used within TRITON and ORIGAMI to perform depletion and decay, or it can be used as a standalone SCALE module to perform depletion, decay, and activation calculations and to generate alpha, beta, neutron, and gamma decay emission spectra. Relevant for non-LWR analysis is the continuous nuclide feed and chemical removal capability in ORIGEN, which can be used to model liquid fuel systems.

When used as a standalone SCALE module, ORIGEN relies on a problem-dependent ORIGEN library. ORIGEN can directly use an ORIGEN *cross section* library generated by, for example, TRITON if this library is adequate for the system of interest. It can also rely on the interpolation of an existing ORIGEN *reactor* library through the automated rapid processing (ARP) module to specific conditions covered through the parameterization of the reactor library. And finally, ORIGEN can also use a user-defined spectrum and self-shielded cross sections by employing the COUPLE module in SCALE, which prepares the data in the correct format. For decay-only calculations, a standard decay library such as SCALE's "end7dec" may also be used.

4. https://scale-manual.ornl.gov/origen/origen-theory.html#matrex

Notes on ORIGEN

1. Use ORIGEN for rapid fuel inventory calculations based on existing ORIGEN cross section libraries:
   - Double-check selected position of applied ORIGEN cross section library to match intended burnup step on the library.
   - Assure adequateness of applied ORIGEN cross section library for depletion calculation, i.e. use for short time steps or use for systems in which cross sections only have a small burnup-dependency (e.g., SFRs and HPRs).
2. Use ORIGEN for inventory decay calculations to estimate full core or assembly decay heat after shutdown:
   - Select SCALE's "end7dec" decay library as cross section library for decay-only ORIGEN calculations.
3. Use ORIGEN to generate location-dependent MSR inventory at a specific point in time.

ORIGAMI

ORIGAMI is another module available within SCALE that can be used for rapid depletion calculations based on pre-generated ORIGEN *reactor* libraries (Skutnik, Williams, and Lefebvre 2015). Instead of having to rely on the ARP module to interpolate the 1-group ORIGEN cross section libraries to the desired conditions, ORIGAMI automates this interpolation so that users may directly input their desired fuel assembly characteristics. ORIGAMI in SCALE 6.3.1 supports parameters for fuel enrichment, moderator density, plutonium content, and ^{239}Pu values (for MOX fuel). ORIGAMI in SCALE 7.0 will be extended such that arbitrary user-defined parameters are supported (based on interpolation parameters available on the provided library).

In versions up to the SCALE 6.3 release, the ORIGAMI workflow allows users to compute detailed isotopic compositions for LWR assemblies—PWRs and boiling water reactors (BWRs). For such cases, the fuel can be modeled using either lumped or pin-wise representations with the option of including axial zones. ORIGEN burnup calculations are then performed for each of the specified power regions to obtain the spatial distribution of isotopes in the burned fuel. ORIGAMI also allows for depletion calculations involving multiple cycles with varying depletion times and down times. Even though this capability was developed for LWR analysis, it can also be used for HPR and SFR inventory calculations because these reactors employ static fuel assemblies and operate in cycles as well (or in case of the HPR, just 1 cycle), and they do not require additional interpolation parameters.

Recent work for SCALE 7.0 included the extension of ORIGAMI for PBRs (Skutnik, Bostelmann, and Wieselquist 2022; Skutnik et al. 2024). For PBRs, ORIGAMI models the depletion of a pebble via a series of transits through the core. Axial transit zones are defined to be composed of multiple radial zones, and multiple transit zones are stacked to represent the full core. The relative probability of a pebble being located within one of the radial zones within an axial zone is provided through an input parameter. Once a pebble enters the core, it is assumed that it remains within the radial zone—that is, the pebble axial motion exclusively consists of "streamlines" through the core between axial zones. ORIGAMI calculates the time-dependent inventory of pebbles by following their transit through the stacked axial zones given their radial distribution. Multiple passes through the core can be simulated to model the complete lifetime of fuel pebbles in a given core.

Note that ORIGAMI does not include material feed or removal capabilities and it therefore not well suited for MSR analysis. MSRs are best analyzed with ORIGEN and TRITON, as discussed above.

Notes on ORIGAMI

1. Use ORIGAMI for rapid PBR, HPR, and SFR fuel assembly inventory generation.
   - Assure that the required parameter space is appropriately captured with the available ORIGEN reactor libraries and under consideration of ORIGAMI's supported parameterization.
2. Note ORIGAMI's limitations in SCALE 6.3.1 regarding the supported parameterization and new capabilities in SCALE 7.0.

OBIWAN

SCALE's command-line tool OBIWAN can be used for inventory interrogation and manipulation. The following OBIWAN capabilities were used in this project.

- View and filter content of ORIGEN concentration files
- Blend compositions from ORIGEN concentration files and generate new concentration file
- Generate inventory interface JSON files

Although Fulcrum can also be used to visualize the content of ORIGEN concentration files, OBIWAN permits the display of additional data (for example, total heavy metal content) and can be easily integrated into existing workflows for efficient and consistent data interrogation and manipulation. Additionally, OBIWAN can be used to view data from ORIGEN cross section libraries, which is beneficial for the sensitivity studies needed to prepare ORIGEN reactor libraries.

Notes on OBIWAN

1. Use OBIWAN to view all data from ORIGEN concentration and cross section files.
2. Use OBIWAN to blend data from ORIGEN concentration files without losing precision.
3. Use OBIWAN to generate II.JSON files from ORIGEN concentration files.

2.3 NUCLEAR DATA

Because the selection of the nuclear data library can significantly affect computed results, the available nuclear data libraries are briefly mentioned here.

SCALE 6.3 includes CE and MG cross section libraries based on evaluated nuclear data libraries ENDF/B-VII.1 and ENDF/B-VIII.0. Relevant updates between ENDF/B-VIII.0 compared to ENDF/B-VII.1 for the non-LWR analyses performed in this project concern the cross sections and neutron multiplicity of ^{235}U, ^{238}U, ^{239}Pu, as well as the availability of additional data for graphite. It is noted that a depletion history effect was observed in LWR analyses where a significant reactivity underestimation was obtained with ENDF/B-VIII.0 Kim and Wieselquist 2021. The most influential nuclides for these studies included ^{239}Pu, ^{235}U, and ^{238}U which are relevant for non-LWR studies as well. It is therefore recommended to use ENDF/B-VII.1 cross section data or to use ENDF/B-VIII.0 with caution.

Accurate prediction of the neutron flux in moderated systems requires the use of thermal scattering law (TSL) data for moderator nuclides. While many codes leave it to the user to specify TSL data, SCALE automatically adds TSL data depending on the name of the nuclide used to specify a material composition. The selection of "graphite" in a SCALE composition refers to carbon cross sections combined with graphite TSL data. Up to ENDF/B-VII.1, graphite TSL data were provided for crystalline graphite without porosity. With ENDF/B-VIII.0, additional TSL data were made available corresponding to graphite at 10% and 30% porosity. Depending on the graphite density of a certain material in comparison to the theoretical graphite

density, users can now choose between graphite TSL data of 0%, 10%, and 30% porosity. However, there are concerns related to the new TSL data for 10% and 30% porosity that are being discussed within the nuclear data community (Al-Qasir et al. 2021; Ramic et al. 2023; Al-Qasir 2023; Nakayama, Iwamoto, and Kimura 2024; Ramic et al. 2024). Comparisons of the measured phonon density of states and graphite scattering cross sections to the corresponding calculated data from ENDF/B-VIII.0 suggest inconsistencies for the graphite data at 10% and 30% porosity. Given the scarcity of experimental data from critical or reactor physics benchmarks using graphite moderator, and given that the few benchmarks that do exist do not have high-quality materials characterization required to adequately determine the specific kind of graphite used, it is difficult to draw clear conclusions regarding the impact on calculated results (that is, if calculated results using the new TSL data improve or worsen the agreement to measurements). At this writing, we recommend the use of TSL data for standard crystalline graphite.

It is noteworthy that ENDF/B-VII.1 was the last ENDF/B release to provide elemental data for carbon/graphite. In contrast, ENDF/B-VIII.0 provides isotopic data: data for ^{12}C and ^{13}C. ENDF/B-VIII.0 also provides, for the first time, TSL data for silicon carbide (SiC), the material used for one of the layers in a TRISO fuel particle.

SCALE provides multiple MG cross section libraries with different group structures. The recommended MG library for the analysis of thermal systems has 252 groups.[5] A 56-group library exists that was optimized for LWRs and should, therefore, only be used with caution when analyzing thermal spectrum non-LWR systems. For fast spectrum SFR systems, a 302-group library with many energy groups in the fast energy range may be used. However, fast spectrum systems and systems with irregular geometries should be simulated using CE cross section libraries (see Section 4.5.1 for additional recommendations). In general, all MG calculations must be verified through comparison with corresponding CE calculations to confirm the adequateness of the selected MG library and cross section processing options.

The various depletion sequences in SCALE use additional data, including the following:

- Fission product yields
- Decay data (decay constants, decay mode, branching fractions)
- Recoverable energy from fission and capture
- Additional cross sections to supplement cross section data for missing nuclides on the ENDF/B cross section libraries

Details on these data libraries can be found in the ORIGEN data resource section in the SCALE 6.3 manual.[6]

Notes on the use of the different nuclear data libraries

1. Verify all MG calculations by comparing MG results with corresponding CE calculations to confirm the adequateness of the selected MG library and the MG approach.
2. Use ENDF/B-VII.1 cross section libraries.
3. When using ENDF/B-VIII.0 cross section libraries, always use the standard crystalline graphite TSL data; graphite TSL data for porous graphite must not be applied.

5. A 258-group MG library specifically optimized for HTGR analysis is currently being developed for SCALE 7.0.
6. https://scale-manual.ornl.gov/origen-data-resources/index.html

3. NON-LWR MODELING STRATEGIES WITH SCALE

The development of SCALE non-LWR full core models for calculation of reactivity, flux, and power requires a detailed geometry as well as accurate fuel inventory. While the development of a 3D Monte Carlo full core model is usually straightforward as long as sufficient specifications are available, the determination of accurate time- and/or location-dependent inventory can be more challenging.

For LWR models, rapid generation of time-dependent fuel inventory is performed for the reactor design of interest at various burnups for a provided operating history with ORIGAMI based on pre-generated ORIGEN reactor libraries that are provided as part of the SCALE release. These reactor libraries were generated with TRITON using reflected 2D LWR assembly models (i.e., infinite arrays of assemblies). They are parameterized according to

- ^{235}U enrichments: 0.5–8.5 wt%,
- moderator density / void fraction (BWRs), and
- plutonium content, ^{239}Pu values (mixed oxide fuel (MOX) fuel),

and they cover burnups up to 82.5 GWd/MTU for most BWR and PWR assemblies. This approach is usually adequate for LWRs because the neutron flux within an assembly model is generally representative of the neutron flux in the LWR core due to the short neutron mean free path. The average neutron mean free path is in the range of a few centimeters (a neutron needs on average 16 collisions with hydrogen in water to slow down to a thermal energy).

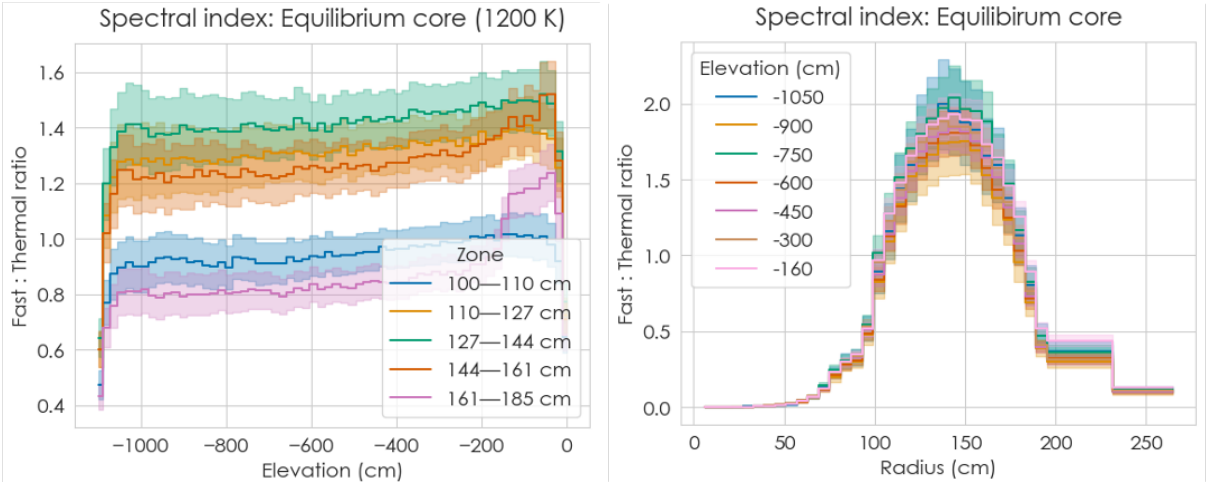
However, in case of non-LWRs, the assumption that one fuel component (fuel assembly, fuel pebble, fuel rod) has a similar neutron flux spectrum to that of the core no longer holds due to the longer neutron mean free path. Systems with graphite as moderator (e.g., HTGRs, FHRs) have a much longer neutron mean free path of tens of centimeters (a neutron needs on average 92 collisions with carbon to slow down to a thermal energy), and the local flux is impacted by core components several centimeters away. Fast spectrum systems (e.g., SFRs, HPRs) are relatively transparent to neutrons (mean free path in the range of meters) so that neutron coupling is found across the reactor.

The following comparison provides a simple example to illustrate this difference.

Depletion of an HTGR fuel pebble in a single reflected pebble model: When depleting a single reflected fuel pebble, the ^{239}Pu buildup causes the neutron flux spectrum in the pebble to harden. Since the discharge burnup of HTGR fuel pebbles can reach 100 GWd/MTU (for FHRs even higher), this spectrum hardening is even more significant. Given the energy dependence of cross sections, changes in the neutron spectrum influence fission and capture in the fuel, which in turn affects the calculation of the burnup-dependent nuclide inventory.

Depletion of a pebble as it travels through an actual HTGR core: When a fuel pebble travels through an HTGR for a number of passes (typically 5–6 times), it experiences a flux that is the result of the surrounding fuel pebbles at various levels of burnups and the graphite structures that surround the core. The surrounding pebbles have a similar impact on the flux, with only small differences between the axial core regions due to the increase of region-average burnup with decreasing axial height. The proximity of a fuel pebble to radial and axial reflectors has a significant impact on the flux level as well as an influence on the thermal vs. fast peak of the flux spectrum (Skutnik and Wieselquist 2021) (Figure 2 and 3). This means that the spectral conditions vary only slightly during a pebble's pass through the core, the major influence on the flux being the radial zone instead of the pebble's own burnup.

Consequently, the depletion of a fuel pebble within an infinite reflected lattice, including large spectral changes over the course of burnup, is inadequate. It does not capture realistic spectral conditions and, ultimately, results in inaccurate fuel inventories.



(a) Axial **(b) Radial**

Figure 2. Radial and axial distribution of the fast-to-thermal flux ratio in an HTGR (Skutnik and Wieselquist 2021). Solid lines indicate axial zone–average flux within the radial zone, and shaded regions indicate the spread of the flux over a radial zone.

In summary, this means that for these non-LWRs, the inventory cannot be generated through simple fuel component depletion calculations. Other adequate surrogate models must be found, and the approach for inventory generation must be revised from what has been used for LWRs.

As a first step in generating inventory for the various non-LWRs in this project, key characteristics and operation details of the non-LWRs were determined, such as the following:

- Fuel type: liquid vs. solid fuel, fresh fuel vs. reprocessed fuel, LEU vs. HALEU fuel
- Operating state: continuous operation at equilibrium state (e.g., PBRs) vs. operation in equilibrium cycles (e.g., SFRs) vs. once-through depletion (e.g., HPRs)
- Reactor-specific peculiarity: continuous batch-wise feed of fuel or fuel components, removal of fuel or fuel components or fission products

Through developing 3D full core Monte Carlo models, understanding of the individual reactor's neutronics and reactor physics behavior was obtained. For example, location-dependent spectral conditions were analyzed by studying spatial flux profiles as well as energy-dependent neutron flux spectra at key core locations.

For the generation of adequate ORIGEN reactor libraries for rapid inventory generation, surrogate models for detailed depletion calculations with TRITON were determined by comparing the spectral conditions and collapsed 1-group cross sections between the surrogate model and the full core model. The parameterization for the reactor libraries was chosen based on spectral conditions and based on performed sensitivity studies for key parameters (such as enrichment and temperature). For some non-LWR concepts, multiple fuel types or compositions were considered to cover potential design choices.

Based on the newly generated ORIGEN reactor libraries, inventory was rapidly calculated with ORIGEN and/or ORIGAMI. This inventory was used to update the Monte Carlo full core models if needed, and it was

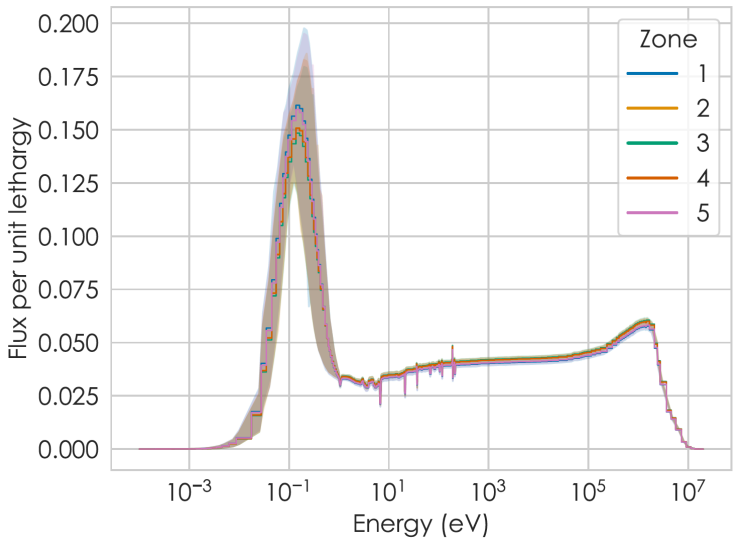


Figure 3. Normalized neutron spectrum by radial zone in an HTGR (numbered innermost to outermost) (Skutnik and Wieselquist 2021). Solid lines indicate axial zone–average flux within the radial zone, and shaded regions indicate the spread of the flux over a radial zone.

used to generate fuel inventory files that included detailed actinide and fission product inventory to provide MELCOR with an accurate nuclide inventory for accident simulations. The rapid inventory calculations also enabled opportunities for additional sensitivity studies on inventory based on varying operating parameters.

The following subsections provide notes on the generation of inventory and the analysis of reactivity coefficients for the different non-LWR systems, along with recommendations on the use of specific modeling tools or options in SCALE. Colored boxes list key recommendations for the discussed non-LWR system up front.

Key steps of inventory generation approach

1. Understand the reactor's neutronics and reactor physics behavior and all relevant phenomena.
2. Generate ORIGEN reactor libraries with an adequate parameterization using an adequate surrogate model.
3. Rapidly generate fuel inventory with ORIGAMI based on the new ORIGEN reactor libraries.

3.1 PEBBLE-BED HTGR AND FHR

Two PBR concepts were studied as part of this NRC project, the helium-cooled HTGR and the salt-cooled FHR. The fuel components of both reactor types are graphite pebbles with embedded TRISO fuel particles (see Figure 4). The pebbles are contained in a cylindrical core that is surrounded by graphite reflector structures. Both reactors are continuously operated at an equilibrium state in which fuel pebbles are continuously added and removed from the core. In an HTGR, the fuel pebbles enter the core from the top and travel down toward the discharge channels. In an FHR, pebbles enter the core from the bottom. Driven by buoyancy in the liquid coolant salt, they travel upward through the core. In both reactors, pebbles that have not reached their target discharge burnup are re-inserted for another pass through the core.

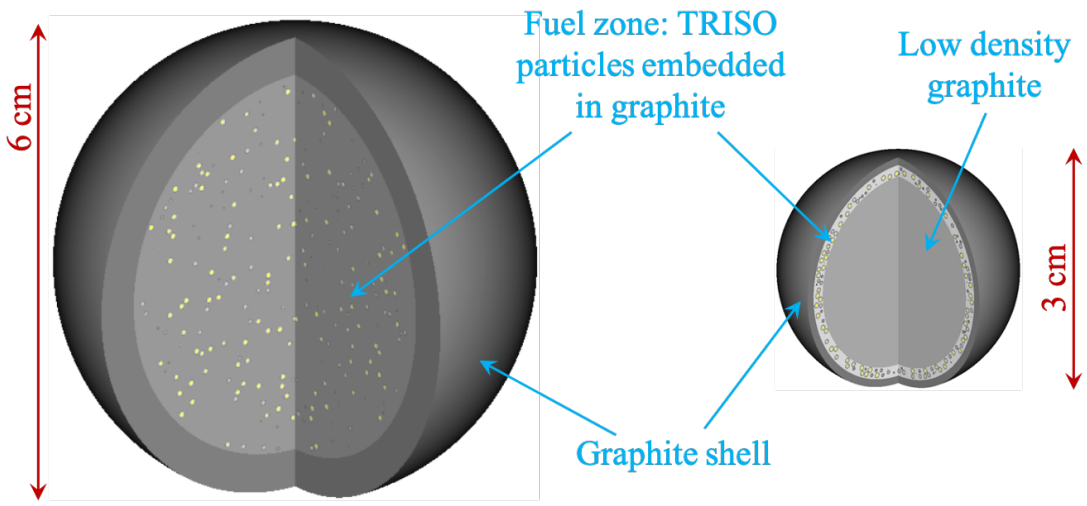


Figure 4. Comparison of an HTGR (left) and FHR (right) fuel pebble.

Key PBR modeling recommendations

1. TRISO particle modeling:
   - Use SCALE's unique MG approach for double-heterogeneous systems to obtain accurate results using lower modeling efforts and short runtimes.
   - For CE fuel pebble models, use Shift's *randommix* feature for automatic placement of TRISO particles at random positions in the fuel zone for packing fractions up to 20%.
   - If modeling TRISO fuel particles in a regular lattice, then avoid clipping.
2. Fuel pebble modeling:
   - Model fuel pebbles in regular arrays that may be clipped.
3. Generate zone-wise fuel pebble compositions for a full core model with the SCALE Leap-In method for Cores at Equilibrium (SLICE) method.
4. Rapidly generate individual fuel pebble inventory with ORIGAMI.
5. Estimate the tritium generation rate in salt-cooled reactors with ORIGEN.

3.1.1 Monte Carlo Model Development

Assuming the fuel compositions in the individual zones of the reactor are known, the development of 3D Monte Carlo PBR models for CSAS and TRITON comes with two major challenges:

1. The modeling of fuel pebbles in the cylindrical core, and
2. The modeling of the TRISO fuel particles in the fuel pebbles.

Although the most accurate modeling approach for fuel pebbles would be an explicit placement of pebbles at coordinates determined from a discrete element modeling (DEM) solver that considers the explicit core geometry, the pebble velocities in the various core regions, the coolant properties, etc., it was found that an adequate model can be developed by modeling the fuel pebbles in a regular lattice. Dodecahedral hexagonal close-packing (HCP) fuel pebble lattices defined to match a target packing fraction were used in this work because they have shown the best performance over other lattices such as columnar hexagonal point-on-point (CHPOP) lattices (Skutnik and Wieselquist 2021). To further simplify the modeling process, infinite pebble lattices were used that allowed the outermost pebbles to be clipped by the surrounding cylindrical surface

that defines the outer boundary of the core and the beginning of the reflector models. Clipping of fuel pebbles has been shown to have a small impact on reactivity, while the impact on nuclide inventory estimates is assumed to be negligible. Given the long mean free path of the neutrons in these graphite-moderated reactors, matching the correct fuel-to-moderator ratio and the correct heavy metal mass in the core was a key modeling goal, whereas details on the local arrangement of fuel pebbles were of minor relevance for the calculation of quantities such as inventory and power distributions in this project.

The approach to modeling TRISO fuel particles (Figure 5) in the fuel pebbles differs for CE and MG models.

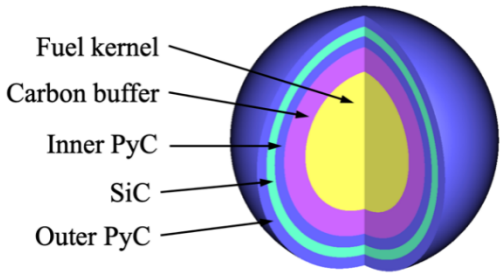


Figure 5. SCALE TRISO particle model.

For MG models, SCALE offers a unique self-shielding calculation specifically for double-heterogeneous models. Based on the information of the TRISO particles' dimensions and packing fraction in the fuel component, SCALE's cross section processing engine XSProc prepares flux-weighted homogenized cross sections for the fuel zone. These cross sections can then be placed via a corresponding mixture number into the fuel zone, avoiding any explicit modeling of the TRISO particles (Figure 6). An MG model is fast and straightforward to develop, the runtime of such an MG model can be many times faster compared to a corresponding CE model, and the accuracy of a calculation with an MG model compared to a CE model has been demonstrated many times for k_{eff} and nuclide inventory (Bostelmann, Celik, Williams, et al. 2020; Bostelmann et al. 2022).

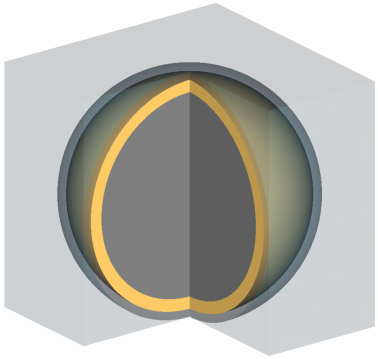


Figure 6. SCALE FHR pebble model for MG calculations: the double-heterogeneous mixture (i.e., problem-dependent cross sections) are placed in the fuel region (orange)(Bostelmann et al. 2022).

CE calculations require explicit modeling of TRISO particles within the fuel pebble. Volume homogenization of the TRISO particles within the graphite matrix has been shown many times to be inadequate and to result in incorrect results; for example, the ^{238}U being distributed across the pebble's fuel zone in such a model results in a higher probability of the neutrons to be absorbed and, consequently, a lower k_{eff}, whereas in reality there is spatial self-shielding of the TRISO particle. The explicit modeling of TRISO particles is

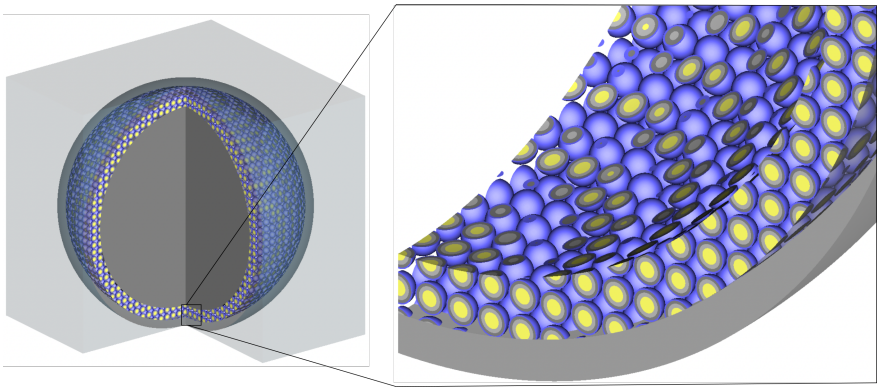
required and can be approached via a regular lattice or random distribution as discussed below. For both options, the correct amount of fuel mass must be included in the fuel pebble.

- **Regular lattice of TRISO particles:** When choosing the option of a regular lattice, the clipping of TRISO particles by surfaces defining the fuel zone must be avoided. In contrast to the clipping of pebbles, the clipping of TRISO particles can produce a non-negligible bias on results. By clipping TRISO particles, one is basically introducing a larger number of smaller particles (Figure 7a). With additional smaller particles, there is more absorption in ^{238}U, which is causing a reduction in k_{eff}. For example, for an FHR fuel pebble with a fuel zone of a spherical shell, reactivity biases of up to 500 pcm during a sample burnup calculation were observed (Bostelmann et al. 2022). Additionally, the calculation of the fuel volume, and thus the fuel mass, introduces additional approximations because fuel volumes in a pebble with clipped TRISO particles can usually only be achieved with numerical computations with limited precision. The definition of a regular lattice without clipping involves the placement of TRISO particles at specific lattice positions, which can be time-consuming and which requires some scripting (Figure 7b).
- **Random TRISO particle distribution:** Explicitly placing TRISO particles at a random distribution in the fuel pebble avoids unnecessary approximations and is the preferred approach (Figure 7c). The Shift Monte Carlo code offers an automatic random placement based on simple user input with input parameters like the packing fraction. Although this capability in SCALE 6.3.1 is limited to packing fractions of approximately 20% and to the placement of spheres into spheres, cylinders and cuboids, work began in 2023 to reduce these limitations. At this writing, packing fractions of 55% can be achieved, and TRISO particles can be placed into additional shapes such as spherical shells, as relevant for FHR modeling. Coordinates for a random distribution generated outside of SCALE can also be leveraged by placing the TRISO particle as holes into the fuel zone at these coordinates. The runtime for models with explicit particle placement can be very long. However, in 2023, a mesh acceleration was implemented into Shift for geometries that are defined with the automatic random placement or that use a specific input block that reads a list of particle coordinates. This acceleration has resulted in dramatic runtime improvements. For example, for a container filled with fuel pebbles, the runtime of a CE calculation was only a factor of 2 slower than the corresponding MG calculation, whereas in SCALE 6.3.1 the CE calculation was a factor of 20 slower (Elzohery et al. 2023).

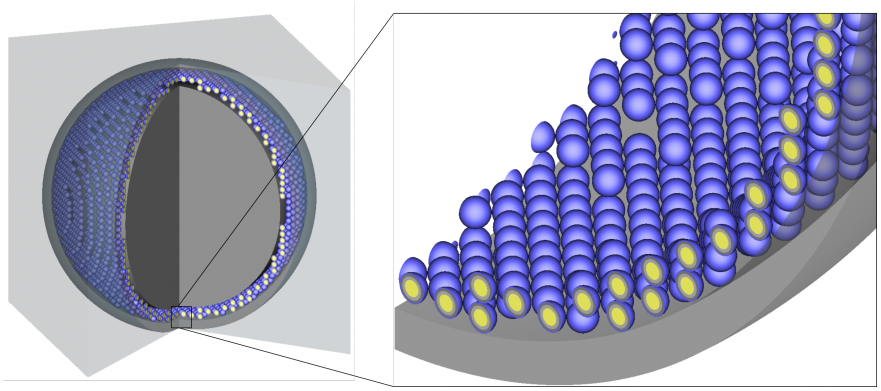
3.1.2 Equilibrium Core Generation

The startup core of a PBR contains a mixture of fresh fuel pebbles and unfueled graphite pebbles. During the running-in phase, the unfueled graphite pebbles are slowly removed and replaced with fresh fuel pebbles until only fuel pebbles are contained in the core. Also, fuel pebbles that have reached their target burnup are replaced by fresh fuel pebbles. (Note that the fuel pebbles of the initial startup core and the fuel pebbles that are used for refueling may have different levels of enrichment.) For most of their lifetime, PBRs operate at an equilibrium state in which the core is filled with only fuel pebbles at various levels of burnup. Approximately speaking, if pebbles travel on average N times through the core (i.e., N passes) before reaching their target burnup, each region in the core contains a mixture of N "pebble types" corresponding to the different passes. The region-average burnup is increasing from top to bottom in an HTGR, and it is increasing from bottom to top in an FHR given the travel direction of the pebbles. From the perspective of inventory of nuclides available to be released during an accident, the equilibrium core provides the most limiting condition because the average burnup, and therefore the fission product inventory, is higher here than during any stage of the running-in phase.

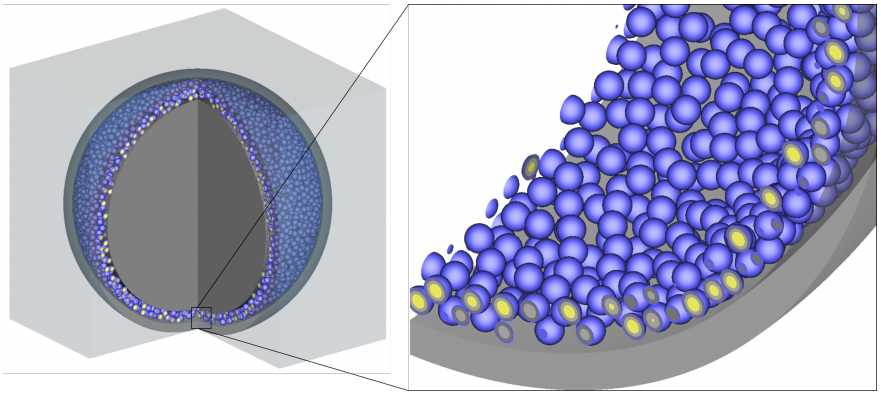
For the generation of fuel compositions for pebbles within an equilibrium core, various methods and tools have been developed over time. Within this project, an iterative approach using TRITON and ORIGEN was



(a) TRISO particles arranged in a square lattice, clipped by the surrounding surfaces.



(b) TRISO particles arranged in a square lattice without clipping.



(c) TRISO particles randomly distributed.

Figure 7. SCALE FHR fuel pebble modeling options for CE calculations (Bostelmann et al. 2022).

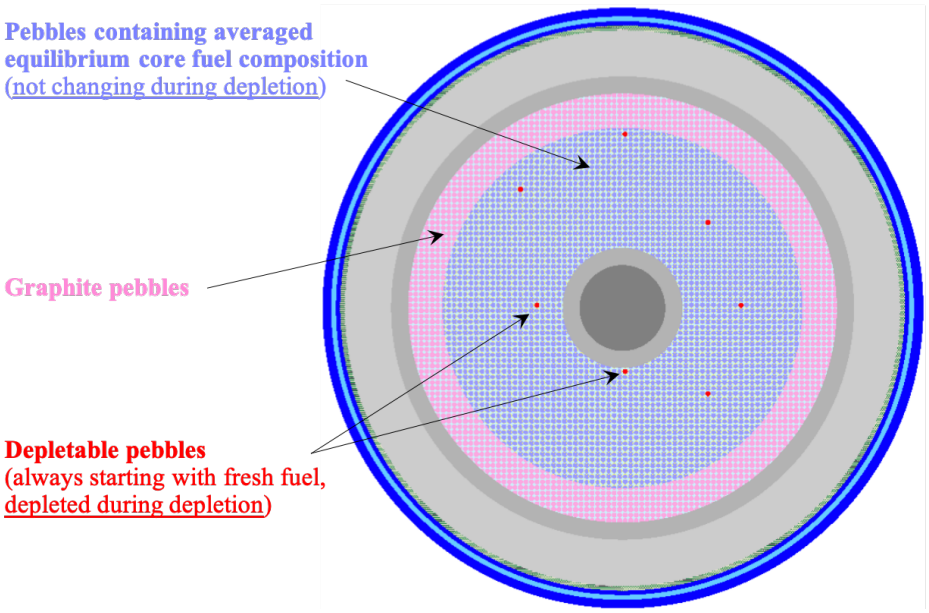


Figure 8. SCALE quasi-2D slice model for an FHR (Bostelmann et al. 2022).

developed to generate *region-average* fuel compositions, i.e. an approximate *average inventory* in pebbles within a specific reactor region. This iterative approach has been further developed over the course of this project and is now named SLICE. Details are discussed in (Bostelmann et al. 2022; Skutnik, Bostelmann, and Wieselquist 2022; Skutnik et al. 2024). The key repeating steps of this approach are as follows:

1. Generate burnup-dependent ORIGEN cross section libraries with a TRITON depletion calculation of a surrogate model.
2. Generate fuel pebble pass- and zone-dependent inventory with ORIGEN using the ORIGEN cross section libraries generated in Step 1.
3. Generate region-average and core-average inventory by blending inventory from Step 2.

For large PBRs, a quasi-2D slice model through the PBR center was found to adequately capture spectral conditions of the corresponding full core model (Skutnik and Wieselquist 2021). Given the large axial height of these reactors, the thermal and fast neutron flux is approximately constant over the axial core regions. In contrast, the fast and thermal flux differ significantly between the different radial zones in the core because of the surrounding (and potentially central) graphite reflector structures and radial leakage. A quasi-2D slice model captures the important radial effects, and detailed Monte Carlo calculations of such a model can be achieved with a reasonable computation time.

Consequently, a TRITON depletion model of a quasi-2D slice model is used as surrogate model in Step 1 of the SLICE method (Figure 8). This slice model contains two types of pebbles: (1) "non-depletable" fuel pebbles that contain core-average fuel compositions and that are updated during the iterations and (2) "depletable" fresh fuel pebbles. The non-depletable fuel pebbles provide the majority of the pebbles, while a number of fresh depletable fuel pebbles are distributed over the model (for example, 5% of the pebbles in the model) to adequately capture the important spectral conditions.

In the very first iteration, both the depletable and the non-depletable pebbles include fresh fuel. The depletable fuel pebbles are depleted with TRITON to generate burnup-dependent ORIGEN cross section libraries. These libraries are then used by ORIGEN to generate detailed fuel pebble inventory while the pebble travels multiple

times via the various axial zones through the core, thereby slowly increasing burnup up to the target discharge burnup (Step 2). By appropriately averaging this inventory, a core-average inventory is obtained that is used to update the fuel composition in the non-depletable pebbles of the slice model. For the second iteration, the TRITON depletion calculation is repeated by depleting fresh depletable fuel pebbles surrounded by the non-depletable pebbles that contain now a first approximation of core-average fuel compositions and therefore improve the spectral condition under which the depletion calculation is performed. These iterations continue until the nuclide inventory is converged.

Using the ORIGEN-generated inventory from Step 2 of the last iteration, region-average fuel compositions can be determined and placed into the corresponding regions of a full PBR model that can then be used for flux, power, and reactivity analyses. To improve the obtained inventory further, the above iterations can be repeated under consideration of an updated axial power profile. Additionally, the SLICE method can be used to determine inventory for both individual axial zones and for multiple radial zones.

The SLICE method involves various assumptions and approximations, but good agreement was found when comparing results to publicly available results generated with other codes (Kile et al. 2022; Berens, Bostelmann, and Brown 2024). Various sensitivity studies have been performed and are still ongoing to investigate the impact of modeling assumptions. Assumptions of the initial SLICE method that are worth highlighting are as follows:

1. Pebbles in all radial zones are assumed to travel with the same velocities through the core, although, in reality, pebble velocities can be reduced in areas next to the reflector.
2. Pebbles travel within a unique radial zone through the core during a given pass, i.e. they do not change their radial zone during one specific path.
3. Because the actual travel path of a pebble cannot be known and a pebble might travel through different radial zones during its passes, the inventory of the individual radial zones is averaged and serves as starting inventory for the respective next pass.
4. The initial implementation considered a target discharge burnup as the limiting condition, whereas a radial zone-dependent target residence time for each pass may be more adequate (specification of target residence times are enabled in SLICE implementations following this work).
5. Control rods and control rod movements in the reflector are neglected.

The SLICE method was realized through Python scripts that perform the inventory management and the input file updates. These scripts are currently prepared to be released in the public SCALE repository[7], and an automatic user-friendly capability is planned as part of SCALE's new Titan reactor physics sequence.

3.1.3 Rapid Pebble Inventory Generation

The rapid fuel inventory generation with ORIGAMI requires reactor-specific ORIGEN reactor libraries with an adequate parameterization to the most important model parameters. For large PBRs, these ORIGEN reactor libraries can be generated using TRITON depletion calculations of a quasi-2D slice model because such a model captures the most relevant spectral effects (see Section 3.1.2). Sensitivity calculations revealed that PBRs require parameterization to at least the following parameters:

- Fuel temperature
- Reflector temperature
- Radial zones

7. Public SCALE repository: https://code.ornl.gov/scale/

- Axial zones for core geometries with varying axial zone conditions (such as upper and lower cones and (de)fueling chutes)

For the rapid generation of fuel pebble inventory, ORIGAMI's latest enhancements for PBRs in SCALE 7.0 can be applied (see Section 2.2). In this way, pass-wise fuel pebble inventory can be rapidly generated for different conditions such as different radial zones, residence times, and temperatures. Additionally, this capability of ORIGAMI can be used for integration into the SLICE method to avoid manual generation (through Python) of inputs for ORIGEN cross section library interpolation and ORIGEN calculations.

3.1.4 Reactivity Coefficients

Reactivity coefficient calculations can be performed using full PBR Monte Carlo models by perturbing individual parameters. In this project, isothermal temperature coefficients were determined for the following materials:

- Fuel
- Graphite moderator (graphite in fuel pebbles and potentially moderator pebbles)
- Reflector
- Coolant (for FHRs)

For this purpose, multiple criticality calculations were performed with varying material temperatures over a range of several hundred degrees Kelvin. Temperatures were assumed to be constant within the selected materials. The reactivity (Eq. 1) for most material temperature perturbations was found not to follow a strictly linear behavior, in particular for the graphite temperature reactivity (Bostelmann et al. 2022) (Figure 9a). Although reactivity differences with small temperature variations would likely be adequate to calculate the reactivity coefficient at specific temperatures, this work performed fits with second-order polynomials. The gradient of a fit at a specific temperature point corresponds to the reactivity coefficient at this temperature.

For salt-cooled FHRs, but not for gas-cooled HTGRs, the calculation of coolant temperature feedback is relevant. For the calculation of the salt temperature coefficient, it must be considered that the salt density changes as a function of temperature. Thus, the reactivity coefficient is a combined temperature and density coefficient (Figure 9b). For the considered FHR, the reactivity was found to follow an approximately linear curve as a function of temperature.

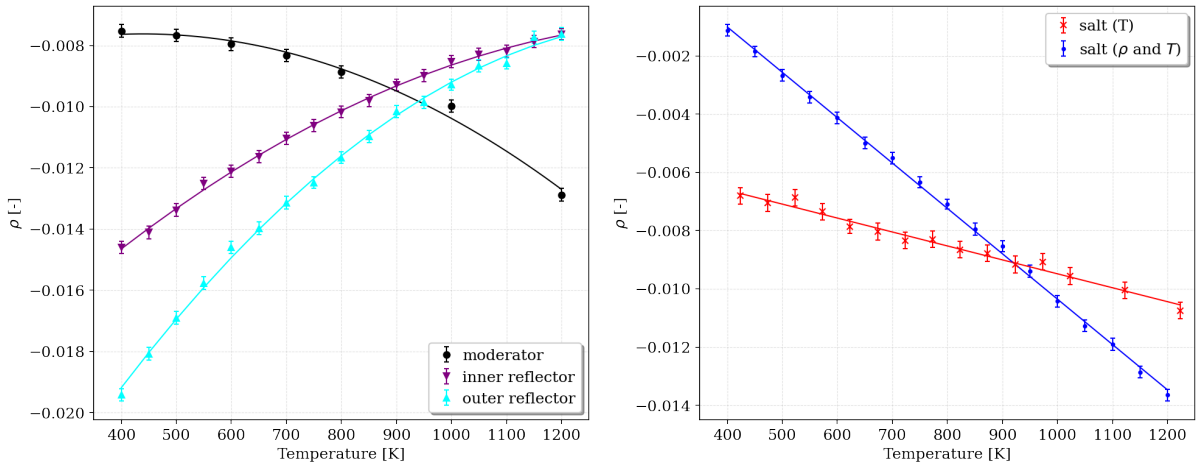
Sensitivity studies showed that the obtained reactivity coefficients were approximately the same when using constant material temperatures everywhere compared to considering temperature distributions over the model.

3.2 FAST SPECTRUM SFR AND HPR

A U/transuranic (TRU) fueled SFR and a potassium-cooled HALEU-fueled HPR were studied as part of this project. An SFR is operated in so-called equilibrium cycles, in which fuel assemblies are reshuffled or replaced after each cycle. The HPR is operated in a once-through mode, in which the reactor is operated for years at low power until it is eventually shut down and replaced.

Key SFR and HPR modeling recommendations

1. Use CE calculations of detailed 3D Monte Carlo models to determine reactivity, flux, and power.
2. Rapidly generate inventory of individual fuel assemblies with ORIGAMI.



(a) Graphite temperature

(b) Salt temperature and combined salt temperature and density effect

Figure 9. Temperature reactivity feedback of an FHR (Bostelmann et al. 2022).

3.2.1 Monte Carlo Model Development

For the SFRs and HPRs, detailed full core Monte Carlo models were developed for reactivity calculations with CSAS and ORIGEN library generation with TRITON calculations. Only CE calculations were performed because SCALE's self-shielding calculation for the preparation of problem-dependent cross sections for MG calculations is currently limited to consideration of representative 1D unit cells (for example, fuel pins in an infinite lattice). However, given the very long mean free path of the neutrons in fast spectrum SFR and HPR systems, problem-dependent cross sections must be prepared using a flux that adequately captures the conditions—which, in these fast flux cases, requires consideration of the geometry and materials in the whole core, and the large neutron leakage. It should be noted that previous work focusing on uncertainty and sensitivity calculations using MG SFR calculations resulted in a 302-group library, which is provided with SCALE, that has a fine energy group structure in the fast energy range to capture resonances at higher energies (Bostelmann, Rearden, et al. 2020). This library and the current self-shielding calculation were sufficient for the calculations intended for uncertainty and sensitivity calculations. However, to avoid unnecessary assumptions and MG biases, this project used only CE calculations.

3.2.2 Rapid Assembly Inventory Generation

The rapid fuel inventory generation with ORIGAMI requires reactor-specific ORIGEN reactor libraries with an adequate parameterization to the most important model parameters. For large SFRs, these ORIGEN reactor libraries can be generated using TRITON depletion calculations with a quasi-2D axial slice model because such a model captures the most relevant spectral effects (Shaw et al. 2023). For smaller HPRs, the libraries must be generated using depletion of full 3D Monte Carlo models to correctly capture axial leakage.

SFRs and HPRs require parameterization to the fuel type:

- TRU fraction in U/TRU fuel
- ^{235}U enrichments in HALEU fuel

SFR concepts have been proposed with metallic fresh HALEU fuel and with U/TRU fuel from reprocessed fuel (reprocessed from LWRs or SFRs), and some designs consider weapons-grade plutonium as startup

fuel. HPR concepts have been proposed with fresh HALEU fuel. Therefore, parameterization is required for details of the fuel composition.

Once ORIGEN reactor libraries are generated, they can be used with ORIGAMI to rapidly generate fuel assembly inventory over the course of an assembly lifetime.

Note that SFRs are operated with equilibrium cycles in which fuel assemblies are reshuffled or replaced after a cycle. SCALE does not yet include a capability for a SFR core simulation that can consider fuel assembly shuffling[8]. However, ORIGAMI calculations based on ORIGEN reactor libraries generated under adequate spectral conditions are suitable for the generation of assembly-wise inventory in support of severe accident calculations or other analyses.

3.2.3 Reactivity Coefficients

The calculation of reactivity coefficients of SFRs and HPRs using full core Monte Carlo calculation is challenging because it requires large numbers of neutron histories to converge reactivity differences caused by temperature, density, or geometry changes. For reactivities such as those for coolant density changes, the reactivity differences are so small that results from multiple calculations with different random seeds were averaged to statistically resolve the reactivity coefficient. Relevant reactivity effects are:

- Fuel temperature
- Fuel axial and radial expansion
- Coolant temperature
- Coolant density and coolant void
- Assembly duct temperature
- Assembly duct expansion
- Radial grid plate expansion
- Control rod driveline expansion

For the fuel temperature coefficient (i.e., the Doppler coefficient), it is worth noting that reactivity as a function of the temperature follows a non-linear curve that was best fitted with a logarithmic function.

For SFRs cores, reactivity coefficients can have a spatial dependence because they are often the result of a combination of spectrum hardening and leakage effects. Calculations of assembly-wise reactivity effects revealed that they are almost impossible to converge with Monte Carlo methods. With large cluster usage, it was possible to resolve radial effects of sodium voiding and axial fuel expansion. However, other effects cause even smaller reactivity differences and are therefore even more challenging to resolve. For such a calculation, a deterministic SFR core solver is needed, which is currently under development for SCALE.

3.3 MSR

The thermal spectrum MSR studied in this project was a graphite-moderated reactor in which a mixture of LiF-BeF_2-ZrF_4-UF_4 fuel salt and LiF-BeF_2 carrier salt was circulated that served simultaneously as fuel and coolant. The MSR is continuously operated, and online refueling is performed through the addition of fresh fuel salt. Gaseous fission products are continuously removed through the off-gas system (OGS). A

8. An SFR core simulator is under development for SCALE 7.0. The SFR core simulator will accurately calculate MG cross sections for fast full core transport calculations and allow fuel assembly shuffling

relevant phenomenon for inventory generation is the plating out of noble metals at components such as the heat exchanger and structural components, such as the pipes.

The reader should note that a fast-spectrum chloride salt MSR was not studied in this project.

Key MSR modeling recommendations

1. Use CE calculations of detailed 3D Monte Carlo models to calculate reactivity, flux, and power.
2. Use TRITON to generate time-dependent system-average fuel salt inventory using the feed and removal capabilities.
3. Use ORIGEN to calculate location-dependent fuel inventory for a single point in time:
   - Simulate a fuel slug flow by creating a chain of ORIGEN cases with each ORIGEN case corresponding to an individual MSR loop segment with an appropriate time step, flux level, and ORIGEN cross section library.
   - Simulate a number of transits through the loop to reach convergence of short-lived fission products.
   - Use one ORIGEN input for each transit, with multiple cases for the individual segments in the loop, to avoid memory issues when using too many cases per ORIGEN input.

3.3.1 Monte Carlo Model Development

For the MSR, detailed full core Monte Carlo models were developed for CSAS and TRITON calculations. Only CE calculations were performed because SCALE's self-shielding calculation for the preparation of problem-dependent cross sections for MG calculations is currently limited to consideration of regular lattices (for example, lattices of fuel pins). However, the structure in the MSR does not follow a standard pin cell design; rather, the salt flows through channels in the graphite structure. Such a repeating pattern requires the determination of an appropriate self-shielding cell, which can be challenging and requires several verification calculations. Additionally, the spectrum of an MSR has resonances in the fast energy range from the salt components (e.g., fluorine and lithium) that might not be adequately captured with SCALE's standard MG libraries, which were originally optimized for water-cooled and -moderated systems. To avoid unnecessary assumptions and MG biases, only CE calculations were used in this project.

3.3.2 Salt Inventory Generation

The generation of salt inventory was divided into two separate considerations: (1) the generation of system-average salt compositions as a function of time and (2) the generation of inventory as a function of the location in the system for a specific point in time.

Time-dependent system-average inventory

TRITON's FLOW block allows users to simulate continuous material feed and material removal (Section 2.2). Users may provide feed rates in units g/s and removal fraction in 1/s, the list of elements or nuclides that are being fed or removed, and potential changes in the rates over time. This allows for the consideration of refueling, fission gas removal in the OGS, and phenomena such as plating-out of noble metals.

A TRITON calculation of a model that uses one fuel salt mixture can be used to calculate the system-average fuel salt composition over time under consideration of feed and removal mechanisms. Similar to the findings for PBRs, it was found that a quasi-2D slice through the center of the moderated MSR core provides an adequate surrogate model. Therefore, the TRITON depletion calculations in this project were performed with this model instead of a full core model. Because the total salt volume is distributed across the core, the pipes, and several loop components (salt pump, heat exchanger, OGS), the power applied in the TRITON

calculation was adjusted to accurately account for the fraction of the salt volume outside the active region of the core.

Location-dependent inventory at a point in time

In addition to the analysis of system-average fuel salt inventory, the spatial distribution of nuclides across the MSR loop can be studied. In this project, the spatial distribution was analyzed with ORIGEN using the ORIGEN concentration file and the ORIGEN cross section library from the TRITON calculation. ORIGEN permits feed and removal of nuclides such that consistent settings with TRITON can be applied. However, in contrast to TRITON, ORIGEN can be used to simulate a batch of fuel (a fuel slug) as it travels through the whole loop. For this purpose, the loop was divided into a number of regions following the major components of the loop (core, off-gas system, fuel salt pump, heat exchanger, piping between components); for each region, an ORIGEN depletion or decay calculation was consecutively performed. Residence times in the individual regions were set considering the different region volumes. Regions outside of the core applied zero power, such that ORIGEN ran decay calculations on the inventory. The core was subdivided into multiple regions, and power for ORIGEN depletion calculations was applied according to an axial power profile obtained from a TRITON full core calculation.

Using the TRITON fuel inventory at a specific point in time as a starting point, ORIGEN was used to calculate region-wise inventory for several fuel salt transits through the core. After fewer than 10 transits, an equilibrium of nuclide concentrations in the individual regions was established. While the density of long-lived fission products remained approximately constant over the various regions, short-lived fission products accumulated while the salt traveled through the reactor and decayed quickly after leaving the reactor. Given a very short loop transit time in the considered system (25 seconds in MSRE), location dependence of the inventory was found not to be relevant for the purpose of severe accident simulation in this project. Depending on the transit times in other MSRs, such location-dependent inventory calculation may still be useful for analyses in which a most accurate calculation of a region-specific inventory is relevant.

3.3.3 Reactivity Coefficients

Reactivity coefficient calculations can be performed using full MSR Monte Carlo models by perturbing individual parameters. In this project, isothermal temperature coefficients were determined for the following materials:

- Fuel salt
- Graphite moderator

For this purpose, multiple criticality calculations were performed with varying material temperatures over a range of several hundred degrees Kelvin. Temperatures were assumed to be constant within the selected materials. For the calculation of the salt temperature coefficient, the salt density change as a function of temperature was considered. Thus, the fuel salt reactivity coefficient is a combined temperature and density coefficient. The reactivity (Eq. 1) for the fuel and the graphite perturbations was found to follow an approximate linear behavior (Lo et al. 2022). The gradient of a linear fit corresponds to the reactivity coefficient.

For the calculation of the effective delayed neutron fraction β_{eff}, it must be mentioned that SCALE does currently not have the capability to consider delayed neutron precursor (DNP) drift. Precursor drift occurs in systems with flowing fuel where decaying fission products that release neutrons (i.e., DNPs) move away from their birth location. DNPs may decay once they have moved outside of the core, thus yielding neutrons that do not contribute to the sustained critical condition of the reactor. Since SCALE assumes that all neutrons are born inside the core, the calculated β_{eff} is overestimated. The addition of a capability to address this limitation in SCALE is planned for a future release.

4. SCALE NON-LWR MODELING FAQ

This section includes specific recommendations for the use of the various SCALE tools and libraries, including common pitfalls.

4.1 WHICH TOOL TO CHOOSE FOR WHICH ANALYSIS

Reactivity, flux, and power profiles

The analysis of the reactivity—including k_{eff} and reactivity coefficients—as well as flux profiles for 3D full core models of non-LWRs in SCALE require Monte Carlo calculations. Since these require individual neutron transport calculations for specific states, CSAS can be used for calculations with the Monte Carlo code KENO or Shift. If a TRITON model is used, a neutron transport calculation without any depletion can be requested through the appropriate setting in TRITON's *BURNDATA* block (Section 4.5.3).

The selection of the specific Monte Carlo code—KENO-V.a, KENO-VI, or Shift—depends on the type of non-LWR studied. KENO-V.a performs calculations in a shorter time compared to KENO-VI and Shift. However, KENO-V.a is limited in supported geometry shapes. Most non-LWR involve complex geometries, such as hexagonal and dodecahedral lattices, and therefore require the use of KENO-VI or Shift. In the case of CE calculations of PBRs, Shift allows automatic placement of TRISO particles at random locations in fuel pebbles and can therefore be the preferred code. Additional capabilities for PBR modeling will continue to be added to Shift in SCALE 7.0. For other non-LWRs, such as SFRs, HPRs, and MSRs, either KENO-VI or Shift can be used.

If power profiles are needed, then TRITON can be used to obtain mixture-specific power to construct a power map over the core; a power tally is still under development. For the analysis of flux profiles, either CSAS or TRITON can be used to generate results on a 3D mesh.

Depletion

ORIGEN[9] is used for the depletion of one of a few fuel regions with complex irradiation histories. Any fuel type, including MOX fuel, can be considered. The COUPLE module can be provided with a flux spectrum to collapse cross sections for use in ORIGEN. Alternatively, ORIGEN can directly read cross sections from an ORIGEN cross section library. The **ARP** module can be used to interpolate cross sections from an ORIGEN cross section library to the desired burnup. The runtime of ORIGEN is in the range of seconds to minutes.

ORIGAMI[10] is used for depletion of many regions or many compositions at once based on pre-generated ORIGEN reactor libraries. Cross section interpolation is automatically performed corresponding to user-provided irradiation histories. ORIGAMI provides output for follow-on analysis with CSAS, MAVRIC, or MCNP. The standard implementation supports uranium oxide fuel, and a new capability for PBRs is available. The runtime of ORIGAMI is in the range of seconds to minutes.

TRITON[11] is used for simultaneous depletion of any number of mixtures in detailed 1D, 2D, 3D models using accurate cross sections based on mixture-wise fluxes obtained in neutron transport calculations. TRITON supports density and temperature perturbations during depletion as well as time-dependent material feed and removal. TRITON generates ORIGEN cross section libraries for all mixtures and for a system average. The runtime depends primarily on the individual neutron transport method used. For 3D depletion problems, the runtime is in the range of hours to days, depending on the available computational resources for parallel code execution.

9. ORIGEN section in the SCALE manual: https://scale-manual.ornl.gov/origen/index.html
10. ORIGAMI section in the SCALE manual: https://scale-manual.ornl.gov/origen/origami.html
11. TRITON section in the SCALE manual: https://scale-manual.ornl.gov/TRITON.html

4.2 TIPS FOR ACCURATE DEPLETION AND DECAY CALCULATIONS

This section summarizes best practices and recommendations for accurate depletion and decay calculations that are applicable to ORIGEN, ORIGAMI, and TRITON.

Depletion calculations require 1-group cross sections, which vary as a function of burnup. Cross section sensitivity to burnup can be greatest at lower burnups, as visible in Figure 10, where the cross sections change the most significantly at the beginning of depletion. Users can specify depletion over a time step with a constant flux or a constant power. Recommendations for depletion calculations are as follows:

- Avoid large time steps during depletion:
  - Use sub-steps or sub-cycles
  - Use at least one cross section library update per reactor cycle
- Avoid large swings in flux within a time step:
  - Verify that the provided power corresponds to the chosen mass basis
  - Use smaller time intervals for large power changes

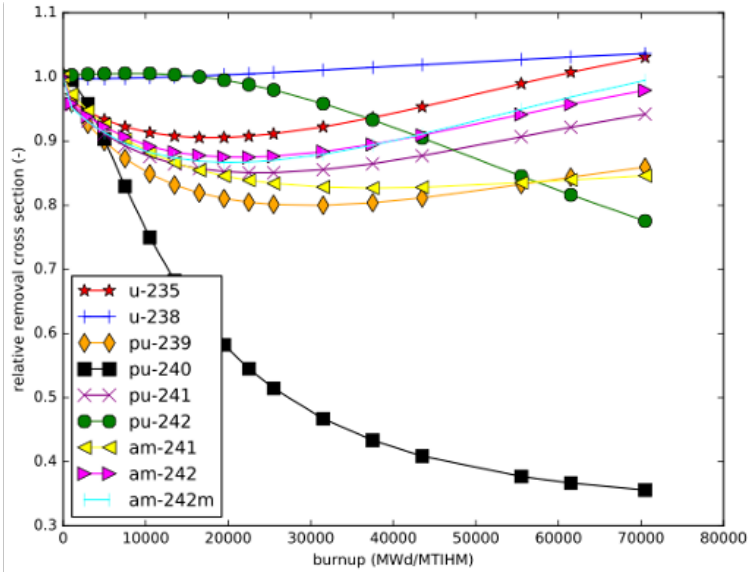


Figure 10. Relative change of 1-group microscopic cross sections as a function of burnup for typical UOX fuel.

While TRITON and ORIGAMI support only the specification of a total decay time after a cycle, ORIGEN can be used to determine detailed decay histories, also based on ORIGEN concentration files generated with TRITON and ORIGAMI. Recommendations for decay calculations with ORIGEN are as follows:

- Use sufficiently granular time steps to capture phenomena of interest (e.g., xenon buildup with initial time steps in the order of hours)
- When using the MATREX solver (default solver in ORIGEN in SCALE 6.3.1), follow the rule of 3s: $\Delta t_i \leq 3\Delta t_{i-1}$
- When using the CRAM solver, use logarithmically spaced steps
- Split up very long decay intervals across multiple cases

4.3 ORIGEN

ORIGEN allows for the most flexible specification of irradiation history information for rapid depletion problems when the user has an existing ORIGEN cross-section library (typically obtained by interpolating an ORIGEN reactor library using ARP).

What are some of the most common pitfalls?

One of the most common mistakes users make when using ORIGEN is failing to ensure that their cross section library is consistent with the problem being evaluated in ORIGEN. Put another way: the process of *interpolating* an ORIGEN reactor library to problem-specific conditions (initial enrichment, moderator density, and mid-cycle burnup) occurs independently of the problem specification in ORIGEN. Thus, a common pitfall is that a user specifies a library interpolation for one set of initial conditions (e.g., 5% initial ^{235}U enrichment) that are inconsistent with the starting materials used by the ORIGEN depletion calculation; ORIGEN has no way of "knowing" whether a cross section library is physically consistent with the problem being evaluated. Similarly, when performing depletion calculations over multiple cycles, it is important to ensure that the ORIGEN cross section library is similarly updated for burnup, as illustrated in Listing 1.

Listing 1. Using multiple burnup positions with an ORIGEN cross-section library across multiple cycles

```
=origen
case(cycle1)
{
  lib{file="my_lib.f33" pos=1}
  mat{ iso=[u235=50000 u238=950000 o=118518] units=GRAMS }
  power=[ 10R 35.0 ]
  time=[ 8I 40.0 400.0 ]
}
case(cycle2)
{
  lib{ pos=2 }
  power=[ 10R 30.0 ]
  time=[ 8I 440.0 800.0 ]
}
end
```

What are the limitations to ARP for interpolating ORIGEN reactor libraries?

The ARP module used to interpolate ORIGEN reactor libraries is limited to pre-defined interpolation parameters (initial ^{235}U enrichment (%), average moderator density, and mid-cycle burnup for UO_2-based fuels; plutonium fraction of heavy metal content (%), ^{239}Pu fraction of plutonium content (%), moderator density, and burnup for MOX fuel). In general, these parameters have been found to be sufficient to cover most LWR modeling cases.

For *non*-LWRs, the required interpolation parameters can be highly problem-specific. As noted previously, fast-spectrum systems such as HPRs and SFRs do not generally require interpolation parameters beyond those provided by ARP (i.e., initial enrichment can be used as-is or as a proxy for parameters such as the initial fissile loading of an assembly). However, pebble-based systems such as HTGRs and FHRs introduce new parameters that must be explicitly accounted for, such as the pebble location relative to reflector regions, the reflector temperature, and potentially the fuel temperature itself. For these cases, OBIWAN's reactor library interpolation capabilities can be used in place of ARP, using user-defined "tag" metadata on the individual cross section libraries (i.e., wherein each cross section library contains metadata corresponding to its individual state parameters, such as the relative fuel pebble location, and reflector temperature.).

Starting in SCALE 7.0, a new HDF5-based ORIGEN library "archive" format will beintroduced with the intention of deprecating ARP in favor of fully "self-characterized" libraries containing their metadata that can then be interpolated inline using ORIGEN and ORIGAMI. ORIGAMI in SCALE 7.0 already relies upon this new "archive" format for library interpolation, and similar support is expected to be added to ORIGEN's *lib* block prior to the 7.0 public release.

4.4 ORIGAMI

ORIGAMI allows users to control the number of library interpolations per cycle using parameter *nlib* (default: *nlib=4*). Users should test a second, higher *nlib* to ensure that the interpolated cross section grid is sufficient.

For higher burnups or later cycles, fewer interpolations are needed to obtain accurate results because the 1-group cross sections vary less at higher burnups. Reducing the number of interpolations for these cycles will provide some speedup with minimal loss of accuracy.

Are ORIGAMI and ORIGEN calculations equivalent?

Yes, assuming the user is specifying the same problem in ORIGEN and ORIGAMI. Specifically, this assumes that the user is specifying the same initial material compositions, ORIGEN reactor library, and (sub-)cycle burnups. Through SCALE 6.3, ORIGAMI internally calls ARP to perform library interpolation based on the initial fuel composition and moderator density for each axial zone; it similarly calculates the mid-cycle burnups for each cycle. ORIGAMI internally calls ORIGEN to solve for depleted material inventories.

How does ORIGAMI perform interpolation in SCALE 7.0?

In SCALE 7.0, ORIGAMI uses an ORIGEN reactor "archive," which is a consolidated data format consisting of all of the individual reactor cross section libraries corresponding to a reactor data library. Each cross section library is stored on the archive with its own problem-specific metadata; what this means is that users can now define their own problem-specific parameters for library interpolation rather than being constrained to hard-coded dimensions. ORIGAMI then queries the (HDF5-formatted) archive file at run time to ensure that the requested dimensions are present and that the user-provided bounds fall within the range available on the archive.

An example of how custom interpolation parameters are specified in ORIGAMI in SCALE 7.0 is presented as Listing 2. Here, interpolation information is *directly* specified via the `state` block within each `transit_zone`; additionally, information about the fuel initial enrichment would be implicitly interpolated from the initial fuel composition (not shown).

Listing 2. Example of ORIGAMI input for SCALE 7.0; interpolation dimensions are specified via the `state` block.

```
=origami
mode=fold
libs=[ "pbmr400.h5" ]

axial_configs=[
  transit_zone(top)={ rpower=[1.1 0.9 1.05] state{
      spectral_zone=[ INNER_REFLECTOR CENTER OUTER_REFLECTOR ]
      fuel_temp=[800.0] reflector_temp=[1000.0] } }
  transit_zone(middle)={ rpower=[1.2 0.9 1.1] state{
      spectral_zone=[ INNER_REFLECTOR CENTER OUTER_REFLECTOR ]
      fuel_temp=[750.0] reflector_temp=[1200.0] } }
  transit_zone(bottom)={ rpower=[1.0] state{
      spectral_zone=[ INNER_REFLECTOR CENTER OUTER_REFLECTOR ]
      fuel_temp=[600.0] reflector_temp=[900.0] } }
```

```
]
...
end
```

4.5 TRITON

A TRITON model consists of several parts for the cross section preparation, the neutron transport model, and depletion settings. These are discussed in separate subsections.

4.5.1 XSProc: Multi-Group Cross Section Processing

When running a calculation in MG mode, SCALE's cross section processing engine XSProc[12] prepares problem-dependent shielded MG cross sections for the neutron transport calculation. XSProc relies on the *CELLDATA* input block that defines the representative unit cells used to generate adequate cross sections for the model.

How do I select the right cross section library?

In addition to CE libraries, SCALE provides several MG cross section libraries with different group structures that can be selected according to the spectral conditions of the problem (for example, thermal vs. fast neutron flux spectrum) and depending on the desired solution accuracy vs. available computation time.

- Best library for analysis of thermal systems:[13] 252-group library (*v7.1-252*)
- Best library for quick solutions, to be used with caution as it was optimized for LWR applications: 56-group library (*v7.1-56*)
- Best library for quick solutions for fast spectrum systems that have a negligible amount of neutrons in the thermal energy range: 302-group library (*fine_fast_e7.1*, to be used with caution as it was optimized for SFRs applications)
- Generally applicable library with energy group boundaries from the 252-group library and a very fine group structure in the fast energy range: 1597-group library (*vfine_e7.1*)
- Generally applicable library: CE (*ce_v7.1_endf*)

Results of an MG calculation must always be verified with a corresponding CE calculation to assess the bias due to MG cross section processing and the choice of the MG cross section library. This is especially valid when developing a new reactor model that has different characteristics (spectral conditions, geometry, materials) compared to previously verified models. For an initial assessment, results of the neutron transport calculation (k_{eff}, neutron flux, etc.) can be compared between MG and CE. Once results are satisfactory, comparisons of fuel compositions as a function of burnup can be performed between MG and CE for depletion calculations.

Which MG cross section processing options should be used?

The most accurate MG solution is obtained using the CENTRM code (default) within XSProc and a fine-group cross section library. Unit cells should be defined for all fuel components and important non-fuel components. Multiple unit cell types are supported:

- *Latticecell*: sufficient for most unit cells; assumes that the fuel pin is located in an infinite lattice of other fuel pins

12. XSProc section in the SCALE manual: https://scale-manual.ornl.gov/XSProc.html
13. A 258-group MG library specifically optimized for HTGR analysis is currently being developed for SCALE 7.0.

- *Multiregion*: to be used if a unit cell needs to be divided in multiple rings or more complex scenarios
- *Doublehet*: to be used for double-heterogeneous systems with fuel particles dispersed in a fuel component
- *Infhommedium*: to be used for infinite homogeneous media; the default cell type, usually only used for non-fuel materials

If the approximation of an infinite lattice of fuel pins is insufficient (for example, if the fuel pin lattice is irregular or if strong absorbers are present in the lattice), then the Dancoff factor for that fuel pin can be modified. Dancoff factors can be calculated with SCALE's tool MCDancoff and applied through the *CENTRMDATA* option below each defined unit cell within the *CELLDATA* block.

If a unit cell geometry is widely different from a repeated fuel lattice, then a *Multiregion* unit cell with representative radii that preserve material areas can be created, and Dancoff factors may be additionally applied. In such a case, especially thorough verification with CE calculations is required. An example for the need to create a corresponding *Multiregion* is an MSR model for which the repeating pattern consists of a graphite stringer with fuel salt channels. For this case, the cross section areas of the graphite and the fuel salt can be calculated, and a *Multiregion* cell with corresponding radii can be set up.

What are common input errors?

Because SCALE's input validation does not require all materials to be included in unit cells inside the CELLDATA block, and because it does not verify whether geometric details are consistent with the neutron transport model (e.g., radii), the input of the CELLDATA block should be thoroughly checked. The following lists some collected notes and recommendations:

- Check that all necessary cell parameters are included: all radii, pitches, and heights; but remove optional parameters that may have been added by Fulcrum's auto-completion feature.
- Check that boundary conditions are correct, in particular for *Multiregion* cells (e.g., the default boundary *right_bdy=vacuum* is most likely incorrect for approximations of regular lattices).
- Note the different options to specify geometrical dimensions: regular lattice pitch (*pitch*) vs. half pitches (*hpitch*); fuel radius (*fuelr*) vs. fuel diameter (*fueld*); etc.
- Triple-check that the material IDs in the cell specifications correspond to the target materials defined in the composition block and that they are consistent with their use in the neutron transport model (especially after a copy/paste from an old input).
- Note that options specified in the *MORE DATA* and the *CENTRMDATA* block apply only to the cell specified immediately above. If options should be applied to multiple unit cells, then these blocks must be repeated below each unit cell as applicable.
- For *Doublehet* cells (see Listing 3):
  - Note that coatings can be specified via radius, diameter, or thickness: *coat**r***, *coat**d***, *coat**t***.
  - Specify either volume fraction of fuel particles (*vf*) or number of particles (*numpar*), and delete the corresponding unused option that is inserted by SCALE's input auto-completion.
  - A *Doublehet* cell requires the definition of a *Doublehet* mixture ID. This new ID must not be confused with the fuel mixture ID from a possible CE model. The *Doublehet* mixture must be filled into the fuel zone—for example, into the zone in which TRISO fuel particles are dispersed in the graphite matrix.

Listing 3. CELLDATA block with a doublehet fuel pebble cell

```
read celldata
 doublehet fuelmix=10 end
   gfr=0.025    11
   coatt=0.0095 12
   coatt=0.0040 13
   coatt=0.0035 14
   coatt=0.0040 15
   matrix=16
   numpar=15000 end grain
  pebble sphtriangp right_bdy=white
   hpitch=3.2   100
   fuelr=2.5
   cladr=3.0    17 end
end celldata
```

4.5.2 KENO/Shift 3D Neutron Transport

Given the complexity of the considered non-LWR designs, the neutron transport calculations in this project were performed almost exclusively with the 3D Monte Carlo codes KENO and Shift.[14] Though the development of a 3D model is in most cases straightforward, the following compiles recommendations based on modeling experience gained in this project.

What options should I use in Monte Carlo calculations?

Depending on the size of the model and the investigated output quantity, different settings for the Monte Carlo calculation are recommended. An example of a *PARAMETERS* block for a KENO or Shift calculation is provided in Listing 4.

- *NPG*: Ensure a sufficient *number of particles per generation* is used; ≥ 50,000 for reactor physics models; ≥ 10,000 for criticality safety models
- *NSK*: Check convergence of specific output quantities as well as convergence tests reported in the output file to ensure that the *number of inactive cycles* is large enough; ≥ 100 for reactor physics models; ≥ 25 for simple criticality safety models
- Larger numbers of bodies and larger separations require larger *NPG*, *NSK*, and *GEN*
- *SIG*: Use *SIG* parameter to converge k_{eff} result to specific level; for this option, also set the number of generations (*GEN*) to a large number (10,000+)
- *RND*: For spatially dependent output quantities (e.g., power profile), run multiple calculations with different random seeds (parameter *RND*) and average obtained results

Listing 4. PARAMETERS block

```
read parameters
 gen=10000 nsk=200 npg=50000 sig=0.00010 rnd=12345
end parameters
```

14. Multiple sections in the SCALE manual are relevant for Monte Carlo calculations: the Monte Carlo section for KENO-specific descriptions and input parameters https://scale-manual.ornl.gov/Monte-Carlo-Transport-Overview.html, the CSAS section for the general input structure and relevant output https://scale-manual.ornl.gov/Criticality-Safety-Overview.html, and the description of supported shapes for both KENO and Shift https://scale-manual.ornl.gov/KenoB.html.

How do I use the new capability for automatic random placement of TRISO fuel particles?

Listing 5 provides an example of a *RANDOMGEOM* input block in which a random particle distribution is defined, and it demonstrates how to place the created *randommix* into a unit.[15]

Listing 5. CSAS-Shift *randommix* input for an HTGR fuel pebble (simplified for display).

```
=csas6-shift
HTGR
ce_v7.1_endf
read composition
' fuel kernel: UO2
    u-235       100 0 3.99198e-03 300   end
    u-238       100 0 1.92441e-02 300   end
    o-16        100 0 4.64720e-02 300   end
' coatings: buffer/101, iPyC/102, SiC/103, oPyC/105
' graphite pebble shell/106
' saturated air/300
end composition

read parameter
 gen=250 npg=10000 nsk=50
end parameter

read geometry
unit 1
 com='TRISO particle'
 sphere 1    2.50e-02
 sphere 2    3.40e-02
 sphere 3    3.80e-02
 sphere 4    4.15e-02
 sphere 5    4.55e-02
 media  100 1    1
 media  101 1    2  -1
 media  102 1    3  -2
 media  103 1    4  -3
 media  104 1    5  -4
 boundary 5

global unit 10
 com='pebble'
 sphere 1    2.5
 sphere 2    3.0
 cuboid 3    6p3.0
 media  105 1    1  randommix='trisos'
 media  106 1    2  -1
 media  300 1    3  -2
 boundary 3
end geometry

read randomgeom
 randommix = 'trisos'
  type=random
  units=1 end
  pfs=0.05054954 end
  clip=no
```

15. Description of the *RANDOMGEOM* block in the manual: https://scale-manual.ornl.gov/CSAS-Shift.html#random-geometry. Note that the *RANDOMGEOM* input block will slightly change in SCALE 7.0.

```
  seed=1111
 end randommix
end randomgeom

read bounds all=refl end bounds
end data
end
```

What are some common KENO and Shift input errors?

- Incorrect array definition or array placement:
  - Incorrect number of units listed in array fill statement
  - Array placement leads to undefined region in a unit
  - Units used in array do not have the same outer boundaries (e.g., not the same axial expansion)
- Overlapping holes
- Undefined or doubly defined space
- Missing *end data* at the end of the neutron transport input before the final *end* statement

Developing an input with Fulcrum greatly helps with detecting input errors. Fulcrum's validation points to various problems early on, and the geometry visualization helps detect problems such as undefined spaces in the geometry. If this does not help, then it can be easier to check a model by running SCALE with the sequence-level parameter *parm=(check)* or to study KENO or Shift's error message by running the problem with a very small number of neutron histories. The latter can be especially helpful in the case of problems with arrays, as KENO and Shift will point to multiply defined space or lost neutrons due to undefined space.

4.5.3 Depletion

Although the specification of the input needed for a TRITON depletion calculation is in most cases straightforward, the following highlights relevant aspects and provides recommendations based on experience collected in this project.

How many nuclides are tracked with ORIGEN vs. during the neutron transport calculation?

TRITON permits the selection of nuclide sets to be considered in the neutron transport calculation. While ORIGEN tracks >2,000 nuclides for the depletion calculation, the neutron transport calculation requires only a subset of nuclides that significantly influence the calculation of the neutron flux. While nuclides specified in the composition block are always tracked in the neutron transport calculation, the sequence-level parameter *ADDNUX* is used with TRITON to control the set of additional nuclides: *parm=(ADDNUX=N)* with *N=0,1,2,3,4*. The default is *ADDNUX=2*, which adds 95 nuclides. This is adequate for most cases, especially LWR systems. Higher *ADDNUX* levels improve the accuracy of the neutron transport calculation but also require longer run times. *ADDNUX=4*, which adds 388 nuclides, is desired for best-estimate benchmark models and when simulating non-LWR models. *ADDNUX=0* adds no nuclides and should be used only for single state-point calculations—never for any actual depletion problem.

How can I simplify my input when I have many repeating material definitions?

TRITON permits the definition of an *ALIAS* block in which a material name can be assigned to a list of mixture IDs. The specified material block can be used in the *COMPOSITION* block to specify the composition of this material once instead of specifying individual compositions for each of the mixture IDs. The use of an *ALIAS* block is recommended in complex models to make the input files shorter and easier to read. For

example, doing so is useful when depleting a number of fuel components that all start with the same initial fuel compositions, but which shall be tracked separately during depletion. Another example is a model with different fuel pebbles: although the fuel composition may differ between the individual pebbles, the different particle layers, the graphite matrix, and the shell have the same composition, so the compositions of these parts can be simplified using aliases (see Listing 6). Finally, because TRITON does not yet include a power tally and a reactor power map can be estimated through the analysis of mixture-specific powers, aliases can be used to subdivide fuel regions to obtain a more detailed power map.

Fulcrum offers an alias expansion so that the fully expanded input can be double-checked. Additionally, the expanded input is also printed in TRITON's output file. The reader should note that CSAS does not permit an *ALIAS* block. When converting a TRITON input to a CSAS input, the fully expanded input must be used. Alternatively, TRITON can be run with parameter *burn=0* in the *BURNDATA* block to enable a transport-only calculation without depletion (see below).

Listing 6. TRITON ALIAS and COMPOSITION block for 10 PBR fuel pebbles

```
read alias
 $fuel    10-19 end
 $buffer  20-29 end
 $ipyc    30-39 end
 $sic     40-49 end
 $opyc    50-59 end
 $matrix  60-67 68 69 end
 $shell   70 71 72 73 74 75 76 77 78 79 end
end alias
read composition
 uo2          $fuel    den=10.4 1.0 1136.45 92234 0.051 92235 5.768 92238 94.181 end
 c-graphite   $buffer  den=1.05 1.0 1136.45 end
 c-graphite   $ipyc    den=1.90 1.0 1136.45 end
 atomSiC      $sic      3.18 2  6000 1 14000 1 1.0 1136.45 end
 c-graphite   $opyc    den=1.90 1.0 1136.45 end
 c-graphite   $matrix  den=1.74 1.0 1136.45 end
 c-graphite   $shell   den=1.74 1.0 1136.45 end
end composition
```

How do I determine the specific power for depletion?

TRITON's BURNDATA block is used to define the power history of the depletion, with the specific power in MW/metric ton initial heavy metal (MTIHM), the depletion time in days, optionally a sub-division of the depletion time into sub-intervals, and optionally the subsequent decay time (see Listing 7). The DEPLETION block lists all mixtures to be depleted—that is, those mixtures for which the compositions will change over the course of the depletion. Power normalization to specific mixtures and depletion by power vs. by flux can be controlled in this block (see Listing 7).

The specific power can be derived by dividing the total reactor power by the *initial* heavy metal mass. The "initial" referring to the start of the depletion calculation with TRITON, but it does not necessarily imply a fresh fuel state. For reactors that start with fresh uranium fuel, the initial heavy metal (initial uranium) mass is often easy to determine from fuel specifications. For reactors that start with used or reprocessed fuel, it can be more tedious to determine the heavy metal mass from nuclide densities of a range of actinides. In such a case, it is recommended to simply take the initial heavy metal mass from TRITON's output that is printed in the mass normalization block (Listing 9).

Listing 7. TRITON BURNDATA block for a PBR surrogate model depletion

```
read burndata
```

```
 power=98.431 burn=177.79  nlib=3          end
 power=98.431 burn=888.95  nlib=6 down=100 end
end burndata
read depletion
 $fuel
end depletion
```

How should I subdivide the depletion steps?

The division of a depletion period into sub-intervals via parameter *nlib* is desirable to control the number of cross section updates during depletion. TRITON follows a predictor–corrector scheme, in which cross sections for the depletion calculation are updated through the neutron transport calculation in the middle of an interval. The first depletion step should be very small (~ 100 hours) in order to correctly consider the xenon and samarium equilibrium buildup and to capture larger cross section changes at low burnups (see Section 4.2. For new models, the determination of adequate depletion intervals should be determined with simple sensitivity studies. Also see the previous section, Section 4.2, for guidance on depletion.

Why do I get k_{eff} results for different points in time compared to the nuclide inventory?

The above-mentioned predictor–corrector scheme results in the neutron transport calculation (i.e., k_{eff} output) always being provided in the middle of a depletion step, whereas nuclide densities are provided at the end of a depletion step. If additional neutron transport calculations are desired, then users can add very short (*burn=1e-5*) time steps to force additional neutron transport calculations at the desired time during depletion (usually at the very end).

Can I run a transport-only calculation with TRITON?

In some cases, it can be desirable to only run the initial neutron transport calculation in TRITON instead of a depletion problem. This can be achieved by setting the depletion time to zero (see Listing 8). Because the regular TRITON output is still provided, it can serve to determine specific output quantities for the initial transport calculation that is not available with CSAS, but only with TRITON. In this project, this option was used to determine mixture-specific powers to allow the generation of a reactor power map through adequate mixture discretization. If only a transport calculation is desired, users can set sequence-level parameter "ADDNUX=0" to avoid adding additional nuclides to the fuel compositions.

Listing 8. TRITON BURNDATA block for a transport-only calculation

```
read burndata
 power=98.431 burn=0  end
end burndata
read depletion
 10 11 12 13 14 15 16 17 18 19
end depletion
```

What is the impact of TRITON's mass normalization?

Because TRITON was initially developed for 2D problems only, it performs a mass normalization before initializing materials in ORIGEN.[16] Before the first depletion calculation is initiated, the model's total heavy metal content is determined. A scaling factor (printed in the normalization block; see Listing 9) is then determined to scale the total heavy metal mass to 1 MTIHM, and the scaling factor is applied to all depletable mixtures (mixtures listed in the *DEPLETION* block) before they are initialized in ORIGEN. This normalization does not have any impact on the neutron transport calculation—only on the material masses

16. Users will be able to disable this normalization in SCALE 7.0.

that ORIGEN is tracking. Because the output ORIGEN concentration file collects ORIGEN output, this file contains nuclide inventory of the scaled materials. When nuclide densities (e.g., atoms/b-cm) are read from the ORIGEN concentration file, there is no impact of the normalization. However, if the absolute amounts of a nuclide are needed, then the absolute amount must be scaled back to the original model with the scaling factor.

Example 1: A model contains multiple fuel mixtures, and the depletion block lists all these fuel mixtures. Then, the sum of the initial heavy metal masses of all these materials is 1 MTIHM. The ORIGEN concentration file shows an initial heavy metal mass of 1 MTIHM for case=0, the case that contains the sum of all materials. The cases with the TRITON material numbers show initial heavy metal masses that are scaled using the scaling factor.

Example 2: A model contains multiple fuel mixtures, but only a few of these fuel mixtures are depleted. Then, the ORIGEN concentration file shows less than 1 MTIHM for case=0. The cases with the TRITON material numbers still show initial heavy metal masses that are scaled using the scaling factor.

OBIWAN can be used to show an overview of the content of an ORIGEN concentration file to check the initial heavy metal masses (see Listing 10).

Listing 9. TRITON normalization block

```
*******************************************************************************
** System total mass is  7.8419e+03 grams heavy metal.                       **
** Masses will be normalized by a factor of  1.2752e+02 to obtain a total    **
** system mass of  1.0000e+06 g of heavy metal                                **
*******************************************************************************
```

Listing 10. OBIWAN viewing the content of a TRITON-generated ORIGEN concentration file

```
# View F71 file for a model in which all fuel was contained in mixture 10 and mixture 10 was depleted
# --> initial heavy metal of all depletable mixtures (case 0) = 1 MTIHM
obiwan view my_triton_file.f71

   pos         time        power         flux      fluence       energy    initialhm       volume libpos   case   step DCGNAB
   (-)          (s)         (MW)   (n/cm^2-s)     (n/cm^2)        (MWd)      (MTIHM)      (cm^3)    (-)    (-)    (-)    (-)
     1  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00  1.00000e+00  9.55865e+06      1     10      0 DC----
     2  4.32000e+05  3.66970e+01  1.84624e+13  7.97574e+18  1.83485e+02  1.00000e+00  9.55865e+06      2     10      1 DC----
     3  8.64000e+05  3.66970e+01  1.84690e+13  1.59544e+19  3.66970e+02  1.00000e+00  9.55865e+06      3     10      2 DC----
     4  3.45600e+06  3.66970e+01  1.85051e+13  6.39195e+19  1.46788e+03  1.00000e+00  9.55865e+06      4     10      3 DC----
     5  6.04800e+06  3.66970e+01  1.85608e+13  1.12029e+20  2.56879e+03  1.00000e+00  9.55865e+06      5     10      4 DC----
     6  8.64000e+06  3.66970e+01  1.85996e+13  1.60239e+20  3.66970e+03  1.00000e+00  9.55865e+06      6     10      5 DC----
     7  2.41920e+07  3.66970e+01  1.87194e+13  4.51363e+20  1.02752e+04  1.00000e+00  9.55865e+06      7     10      6 DC----
     8  3.24000e+07  3.66970e+01  1.88599e+13  6.06165e+20  1.37614e+04  1.00000e+00  9.55865e+06      8     10      7 DC----
...
    49  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00  1.00000e+00  9.55866e+06      1      0      0 DC----
    50  4.32000e+05  3.66970e+01  1.84624e+13  7.97574e+18  1.83485e+02  1.00000e+00  9.55866e+06      2      0      1 DC----
    51  8.64000e+05  3.66970e+01  1.84690e+13  1.59544e+19  3.66970e+02  1.00000e+00  9.55866e+06      3      0      2 DC----
    52  3.45600e+06  3.66970e+01  1.85051e+13  6.39195e+19  1.46788e+03  1.00000e+00  9.55866e+06      4      0      3 DC----
    53  6.04800e+06  3.66970e+01  1.85607e+13  1.12029e+20  2.56879e+03  1.00000e+00  9.55866e+06      5      0      4 DC----
    54  8.64000e+06  3.66970e+01  1.85996e+13  1.60239e+20  3.66970e+03  1.00000e+00  9.55866e+06      6      0      5 DC----
    55  2.41920e+07  3.66970e+01  1.87194e+13  4.51363e+20  1.02752e+04  1.00000e+00  9.55866e+06      7      0      6 DC----
    56  3.24000e+07  3.66970e+01  1.88599e+13  6.06165e+20  1.37614e+04  1.00000e+00  9.55866e+06      8      0      7 DC----
...


# View F71 file for a model that contains two fuel mixtures, but only one fuel mixture (mixture 150) was depleted
# --> initial heavy metal of all depletable mixtures (case 0) < 1 MTIHM
obiwan view my_triton_file.f71

   pos         time        power         flux      fluence       energy    initialhm       volume libpos   case   step DCGNAB
   (-)          (s)         (MW)   (n/cm^2-s)     (n/cm^2)        (MWd)      (MTIHM)      (cm^3)    (-)    (-)    (-)    (-)
     1  0.00000e+00  5.98611e-01  3.90300e+14  0.00000e+00  0.00000e+00  1.45853e-03  1.56461e+02      1    150      0 DC----
     2  6.35418e+06  5.98611e-01  3.90300e+14  2.48003e+21  4.40241e+01  1.45853e-03  1.56461e+02      2    150      1 DC----
     3  1.27084e+07  5.63772e-01  3.97133e+14  5.00349e+21  8.54860e+01  1.45853e-03  1.56461e+02      3    150      2 DC----
     4  1.90625e+07  5.13398e-01  4.00123e+14  7.54594e+21  1.23243e+02  1.45853e-03  1.56461e+02      4    150      3 DC----
     5  2.54167e+07  4.58982e-01  3.98832e+14  1.00802e+22  1.56999e+02  1.45853e-03  1.56461e+02      5    150      4 DC----
     6  3.17709e+07  4.14377e-01  3.98631e+14  1.26132e+22  1.87473e+02  1.45853e-03  1.56461e+02      6    150      5 DC----
     7  3.81251e+07  3.73137e-01  3.96898e+14  1.51351e+22  2.14915e+02  1.45853e-03  1.56461e+02      7    150      6 DC----
     8  4.44793e+07  3.36810e-01  3.95598e+14  1.76488e+22  2.39686e+02  1.45853e-03  1.56461e+02      8    150      7 DC----
     9  5.08334e+07  3.07507e-01  3.93136e+14  2.01469e+22  2.62301e+02  1.45853e-03  1.56461e+02      9    150      8 DC----
    10  0.00000e+00  5.98611e-01  3.90300e+14  0.00000e+00  0.00000e+00  1.45853e-03  1.56461e+02      1      0      0 DC----
    11  6.35418e+06  5.98611e-01  3.90300e+14  2.48003e+21  4.40241e+01  1.45853e-03  1.56461e+02      2      0      1 DC----
    12  1.27084e+07  5.63772e-01  3.97133e+14  5.00349e+21  8.54860e+01  1.45853e-03  1.56461e+02      3      0      2 DC----
```

```
    13  1.90625e+07  5.13398e-01  4.00123e+14  7.54594e+21  1.23243e+02  1.45853e-03  1.56461e+02      4      0      3 DC----
    14  2.54167e+07  4.58982e-01  3.98832e+14  1.00802e+22  1.56999e+02  1.45853e-03  1.56461e+02      5      0      4 DC----
    15  3.17709e+07  4.14377e-01  3.98631e+14  1.26132e+22  1.87473e+02  1.45853e-03  1.56461e+02      6      0      5 DC----
    16  3.81251e+07  3.73137e-01  3.96898e+14  1.51351e+22  2.14915e+02  1.45853e-03  1.56461e+02      7      0      6 DC----
    17  4.44793e+07  3.36810e-01  3.95598e+14  1.76488e+22  2.39686e+02  1.45853e-03  1.56461e+02      8      0      7 DC----
    18  5.08334e+07  3.07507e-01  3.93136e+14  2.01469e+22  2.62301e+02  1.45853e-03  1.56461e+02      9      0      8 DC----
...
```

How do I best calculate the material volumes for a complex geometry?

It is a best practice to explicitly specify all material volumes, or at least all fuel volumes, based on analytical calculations in the TRITON input. An alternative is the addition of a *VOLUME* block to enable an automatic volume calculation with given settings. When using KENO, a Monte Carlo and a trapezoidal integration method can be enabled. When using Shift, a parallelized ray tracer can rapidly calculate volumes.[17] The settings should be chosen to result in very small statistical errors for the determined volumes.

Furthermore, it is a best practice to confirm analytically determined volumes by using Fulcrum or by using a *VOLUME* block. Fulcrum can generate an updated input file with volumes specified for all media records as determined through a ray tracer calculation that works for most geometries. Since these values are not provided with statistical errors, they should only be used to confirm analytically determined values. When using a *VOLUME* block to confirm volumes, users can set the sequence-level parameter to *parm=(check)*, which enables only the volume calculation in addition to input checks. The determined volumes, together with corresponding statistical errors, can then be found in the output file.

If any material volume is not specified in the input, TRITON's current implementation enables a volume calculation with default settings for each neutron transport calculation, i.e., one volume calculation per depletion step. Depending on the complexity of the model and the chosen settings for an automatic volume calculation, this can take a considerable amount of time.

Listing 11. TRITON VOLUME block to enable a volume calculation via Shift's ray tracer

```
=t6-depl-shift parm=(check)
...
read volume
 type=trace nrays=1000000
end volume
end
```

What are some common mistakes or issues?

- Material volumes are incorrect, lead to incorrect mixture powers, and therefore lead to an accumulating bias in the depletion calculation. This applies most often to volumes specified for units that are used multiple times in an array: volumes specified for materials in a unit refer to the total material volumes in the whole model.
- Typos in a shell block immediately before or after the TRITON input lead to injection files[18] not being found or files not being copied back from the temporary working directory.
- When converting a CSAS input to a TRITON input, TRITON lines *read model* and *end model* are missing, or KENO/Shift's *end data* is accidentally deleted.
- TRITON's mass normalization was not considered when analyzing masses from the ORIGEN concentration file.

17. Note that when using the *randommix* feature with Shift in SCALE 6.3.1, the ray tracer does not provide a volume for the region into which the particles are filled. This issue was fixed in SCALE 7.0.

18. Users can write a part of their SCALE input in a separate file. In their main SCALE input file, they can then "inject" their files into the corresponding input block by writing "<filename.inj". Injection files must be found in the temporary working directory. When using injection files, Fulcrum cannot perform input validation.

5. CONCLUSIONS

This report summarizes the collected non-LWR modeling strategies with SCALE based on extensive SCALE modeling and simulation work performed for five representative non-LWR designs within the scope of NRC project "Volume 3: Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis." Given the project goal to demonstrate the capabilities of the MELCOR and SCALE codes for the simulation of accident scenarios, the focus with SCALE was to provide MELCOR with initial and boundary conditions including nuclide inventories, decay heat, power profiles, and reactivity coefficients.

This document provides an overview of SCALE methods and tools used for non-LWR reactivity, power, and inventory calculations. Specific recommendations are given for the use of the various SCALE sequences, and modeling recommendations for the various non-LWRs are discussed.

This report is intended for SCALE users who are tasked with the modeling and analysis of a non-LWR and who want to benefit from collected lessons learned of SCALE analysts. Recommendations are based on SCALE version 6.3.1. Upcoming relevant capabilities for SCALE 7.0 are mentioned as well. SCALE input and output files developed in this project can be found in the public repository: https://code.ornl.gov/scale/analysis/non-lwr-models-vol3

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