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August 2023

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Nuclear Energy and Fuel Cycle Division

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ACRONYMS

ANL	Argonne National Laboratory
ARDP	Advanced Reactor Demonstration Program
ARP	Automated Rapid Processing
BWR	boiling water reactor
CE	continuous-energy
DOE	Department of Energy
DOE-NE	DOE Office of Nuclear Energy
EFPD	effective full power days
HTGR	high-temperature gas-cooled reactor
LWR	light-water reactor
MeV	Modeling, Experimentation, and Validation
MG	multi-group
ORIGEN	Oak Ridge Isotopic Generation
ORNL	Oak Ridge National Laboratory
PBMR	pebble bed modular reactor
PWR	pressurized water reactor
SA&I	Systems Analysis and Integration
UIUC	University of Illinois Urbana-Champaign

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ABSTRACT

The US Department of Energy (DOE) announced the Advanced Reactor Demonstration Program (ARDP) to accelerate the deployment of advanced reactor concepts. Awardees of ARDP funds are expected to demonstrate the operation of an advanced reactor within 7 years of receiving the award [1]. X-Energy's advanced reactor concept, the Xe-100, was selected as one of two advanced reactor concepts to receive funding to demonstrate the operation of its high-temperature gas-cooled pebble-bed reactor before the end of this decade. As a result of this push to bring advanced reactors to maturation and commercialization, transition and deployment scenario studies are being performed under the Systems Analysis and Integration (SA&I) campaign within the DOE Office of Nuclear Energy (DOE-NE) to evaluate the transition of the current US commercial fleet of light-water reactors (LWRs) to a future fleet of advanced reactors consisting of a mix of ARDP type reactor concepts and advanced LWRs [2]. To accurately evaluate the front- and back-end resource requirements, it is important to perform reactor physics calculations to determine the discharge burnup and isotopic content, fuel residence time, as well as other parameters. For this purpose, a summer project funded by the SA&I campaign allowed for the setup of SCALE models for full-core Xe-100 type high-temperature gas-cooled pebble-bed reactor and a Xe-100 type slice using publicly available information [3]. The core-averaged equilibrium compositions and zone-wise equilibrium compositions for the slice and 3D models, respectively, were obtained following an iterative depletion method developed by Bostelmann et al. using SCALE's [4] reactor physics sequence TRITON [5]. The slice model was used with TRITON to generate burnup-dependent cross section libraries at different temperatures which can be used with SCALE's ORIGAMI code to rapidly determine fuel inventory and therefore to perform quick sensitivity studies on parameters such as the pebble location in the core. The SCALE/TRITON transport and depletion calculation for the Xe-100 type slice model indicates that the isotopic concentrations are in good agreement at 1,300 effective full power days (EFPD) for ^{235}U. An analysis of ^{236}U results match ^{239}Pu results would seem to indicate a typographical error in Mulder and Boyes [3] wherein the reported results of ^{236}U and ^{239}Pu are reversed. In addition to SCALE/TRITON calculations, a new capability within SCALE/ORIGAMI for the simulation of pebble-bed reactors was used to study the burnup sensitivity with respect to the pebble pathway through the core. The SCALE/ORIGAMI results show that pebbles that travel closer to the reflector for the entire depletion history have a higher burnup than pebbles that travel through the middle of the core because of the higher thermal to fast flux ratio near the reflector. Consequently, a pebble's burnup is strongly affected by the pebble's pathway for each pass. Additional phenomena such as temperature distributions in the core and different travel times of the pebbles in the individual radial zones further affect the burnup distribution. The sensitivity of the discharge vector to the pebble pathways taken during each pass can be evaluated in the future using SCALE/ORIGAMI now that the SCALE inputs have been established.

1. INTRODUCTION

The US Department of Energy (DOE) started an Advanced Reactor Demonstration Program (ARDP) to accelerate the commercialization of advanced reactor concepts. This program involves cost-sharing the demonstration of advanced reactor concepts with the private nuclear industry. In 2020, DOE identified two advanced reactor concepts, one of which is X-Energy's Xe-100, to receive funding for demonstrating their advanced reactor concept within 5 to 7 years of receiving funding. As a result of this push to bring ARDP reactors to a path of maturation, transition and deployment scenario studies are being performed under the Systems Analysis and Integration (SA&I) campaign within the DOE Office of Nuclear Energy (DOE-NE). These studies evaluate the transition of the current US commercial fleet of light-water reactors (LWRs) to a future fleet of advanced reactors consisting of a mix of ARDP type reactor concepts and advanced LWRs [2]. To accurately evaluate the front- and back-end resource requirements, it is important to perform reactor physics calculations to determine the discharge burnup and isotopic content, fuel residence time, and other important parameters. Xe-100 type pebble-bed reactor models were developed for calculations with the SCALE code system [4] to perform confirmatory analyses on the isotopic inventory reported in the literature [3].

The Xe-100 is a 165 MWth pebble-bed high-temperature gas-cooled reactor (HTGR). The primary objectives of the work documented herein were to:

- create a Xe-100 type pebble-bed reactor SCALE models based on publicly available literature,
- determine the fuel compositions for an equilibrium core,
- generate cross section libraries at different temperatures,
- perform sensitivity studies on discharge isotopic vectors, and
- determine the discharge isotopic vectors.

In the context of this report and similar studies, the term "equilibrium core" is used to describe the asymptotic steady-state condition following "running in" (i.e., operations starting from a fresh core) for which the isotopic vector for pebbles at any given point in space are invariant with respect to time. Similarly, the makeup of fresh pebbles and their rate of introduction is held constant. As such, the neutron flux distribution within the core is likewise presume to have converged upon equilibrium state with respect to time.

Section 2 of this report discusses the codes used to set up the models and to perform the analysis. SCALE/TRITON was used to model the Xe-100 type reactor and to generate cross section libraries for different temperatures. SCALE/ORIGEN was used to perform depletion calculations to determine the isotopic content in each axial zone in the Xe-100 type model after each pass. In an iterative scheme, python scripts were used to determine the zone- and core-averaged compositions for an equilibrium core based on the SCALE/ORIGEN results. Finally, SCALE/ORIGAMI was used to perform quick sensitivity studies. Section 3 describes the 2D and 3D Xe-100 type SCALE models as well as the assumptions and design parameters used to set them up. Section 4 describes the iterative process of generating the equilibrium core isotopics. Section 5 discusses the inputs set up to perform sensitivity studies using SCALE/ORIGAMI. Section 6 discusses the results generated by SCALE/TRITON and SCALE/ORIGAMI. Section 7 summarizes the work performed for this project, the results, and potential future work.

The analyses documented herein are part of a summer student project in which the student was tasked with learning SCALE to set up the models and to perform all the required simulations.

2. CODE DESCRIPTIONS

SCALE was used to perform all the analyses for this work. Various sequences and modules within SCALE were used and are described briefly below.

2.1 REACTOR PHYSICS AND DEPLETION METHODS IN SCALE

The SCALE code system is structured as a series of discrete modules designed to handle specific tasks within a reactor analysis workflow. For example, ORIGEN (Oak Ridge Isotopic Generation) [6] solves the Bateman equations for calculated time-dependent nuclide inventories provided a “transition matrix” that defines the relative nuclide transition rates between species based upon flux-weighted one-group cross sections (derived from multi-group transport calculations).

SCALE provides for both deterministic 2D neutron transport for fuel assembly lattices via NEWT and both continuous-energy (CE) and multi-group (MG) transport via KENO [7] and, as of SCALE 6.3, the new massively-parallel Shift module [8]. The TRITON reactor physics control module coordinates the execution and data passing between modules, including calling the neutron transport code (for example, KENO) to calculate the neutron flux and cross sections of the model, COUPLE to perform the one-group collapse of cross sections based on the calculated fine-group flux and to generate an updated “transition matrix,” and ORIGEN to calculate the updated isotopic inventories over the depletion step [6].

A frequent workflow for rapid, follow-on depletion calculations is to interpolate one-group cross sections generated at each burnup interval for a fuel assembly lattice for varying problem configurations (e.g., initial enrichment, average moderator density). For each depletion step performed within TRITON, the one-group transition matrix is saved to a binary ORIGEN reactor data library (commonly referred to as a `.f33` file), which can then be employed in subsequent standalone depletion calculations by ORIGEN. By generating such libraries for different fuel assembly state points, the user can use SCALE’s ARP module to interpolate them to problem-specific conditions and then perform rapid depletion calculations with ORIGEN (on the order of seconds), avoiding the need for a computationally expensive transport calculation and resulting in minimal loss of fidelity [6]. This workflow is commonly used in the form of the ORIGEN-ARP [6] and ORIGAMI [9] sequences in SCALE for rapid depletion calculations using assembly-averaged cross section libraries.

For the purposes of this analysis, all neutron transport calculations were performed using SCALE’s built-in 252-group ENDF/B-VII.1 cross section library with KENO; one-group cross section libraries generated from these transport calculations were used with ORIGEN and ORIGAMI to calculate time-dependent isotopic inventories.

2.2 FLOWING-PEBBLE DEPLETION ANALYSIS USING ORIGAMI

ORIGAMI was first introduced in SCALE 6.2 for multi-dimensional LWR assembly depletion [9]. In recent development versions of SCALE 7, ORIGEN was extended to analyze both static fuel assemblies (e.g., pressurized water reactor (PWR) and boiling water reactor (BWR) assemblies) and flowing pebble-bed systems [10], [11]. It provides a simple, fast, and lightweight way to perform sensitivity and uncertainty analysis as well as to determine zone-wise isotopic inventories and discharge pebble characteristics.

The new enhancement in ORIGAMI for pebble-bed reactors models core depletion via a series of axial zones; for flowing-pebble systems, the fundamental unit is a “transit zone.” Each transit zone can contain multiple radial nodes, each with unique parameters defining cross section data library interpolation characteristics such as fuel temperature, moderator temperature, or power. Multiple transit zones are stacked together to represent the path of the pebble through the core, allowing one to capture effects such as axial and radial power variations as well as features that influence the local neutron spectrum (e.g., reflector temperature). Within a transit, the relative probability of a pebble being located within one of the radial zones is defined by the `rpop` keyword. For each transit, the problem mass and total zone power are apportioned based on the radial population within each node.

During the depletion calculation, it is assumed that the pebble moves straight down (i.e., it stays in one radial zone during transit). This agrees with real-world observations of pebble-bed flow, which in general is dominated by axial flow [12]–[15], where differences in axial velocity are driven strongly by wall-to-pebble friction interactions [13], [14].

After completing one pass through the core, the masses in the radial zones are summed, the depleting material is decayed for a user-defined downtime, and then the material masses are redistributed according to the radial mass distributions in the next transit zone. Multiple passes through the core can be simulated to model the complete lifetime of fuel pebbles in a given core. Figure 1 shows a flowchart of the ORIGAMI depletion method.

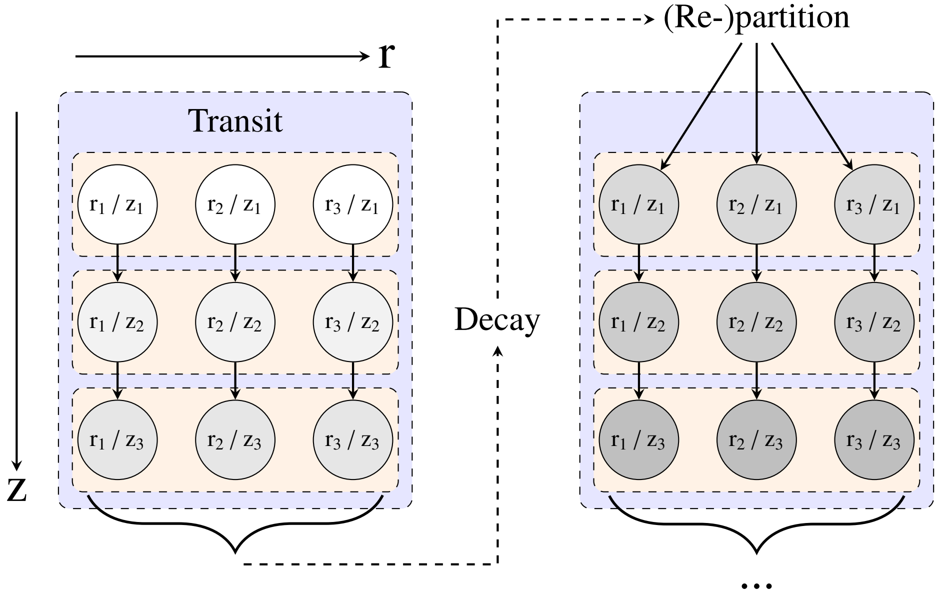


Figure 1. Flowchart of the ORIGAMI depletion method for pebble-bed reactors, from [10]. Pebbles are represented as radial nodes within a "transit zone" (light orange), which are grouped together to represent a pass (transit) through the core (light blue).

3. SCALE MODELS

This section discusses the SCALE/TRITON Xe-100 type pebble-bed model and provides a description. The Xe-100 is a 165 MWth pebble-bed HTGR as described in [3]. The reactor specifications published by Mulder and Boyes [3] were used to gather input parameters for setting up the SCALE Xe-100 type model. When it was not possible to determine the dimensions of the Xe-100 from Mulder and Boyes [3], an assumption was made using information for the pebble bed modular reactor (PBMR-400) [16], [17]. As a result, the SCALE model is referred to as an ”Xe-100 type” pebble-bed reactor model. Two types of models were created in SCALE: (1) a slice model and (2) a full-core model. The slice model is a 10 cm axial cross section of the active fuel region of the full-core model. Both these models were built using the following assumptions:

- The material temperatures are constant throughout the model at each depletion step and in each region (i.e., an isothermal model is assumed), unless otherwise stated.
- The specific power is also assumed to be a constant value based on the discharge burnup provided in Mulder and Boyes [3].
- The spacings between helium risers and their total number are not available in [3]. Therefore, it was assumed that the arc length from the center of one helium riser to the next riser in the Xe-100 type model is the same as it is in PBMR-400 [18]. Using this arc length, and the distance from the center of a riser to the center of the reactor, the angle of separation between the riser channels is determined.
- Only 5 of the 9 main control rods are inserted in the model; these rods are inserted to their full depth. The remaining four main control rod channels, and the nine emergency control rod channels are simply modeled as empty channels through the graphite reflector.
- Each pebble makes six passes through the core for all the depletion analyses.
- Pebbes transit in each axial zone for the same amount of time and therefore, assumes that the pebble speed remains constant through each region.
- Uniform axial pebble velocity is assumed for all radial regions (i.e., wall friction effects near the reflector are neglected)

Furthermore, general reactor dimensions and parameters are given in Table 1.

3.1 FULL-CORE

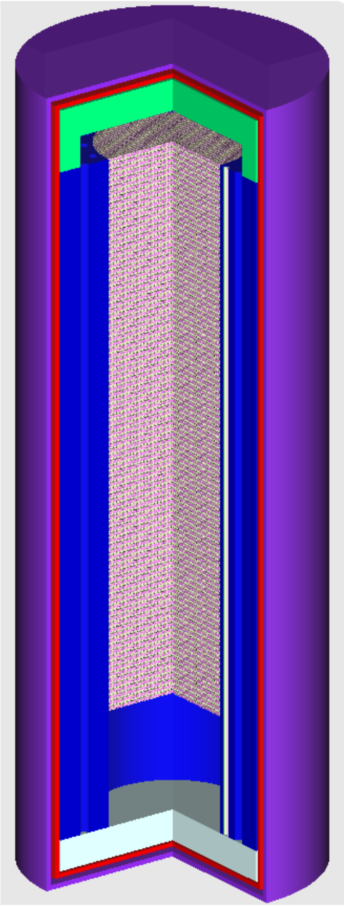
The full-core model’s main features consist of a graphite reflector surrounding an active fuel zone, a core barrel, and an outer reactor pressure vessel. In an Xe-100 reactor, the pebbles flow from the top to the bottom of the core. The reactor core has a conical region at the bottom to funnel pebbles into the discharge chute. However, because of the complexity of this region, the effective full-core height was used to model the active fuel region. In the SCALE/TRITON model, however, the core is assumed to be a cylinder with a flat bottom. The lower discharge pipe and helium outlet is not explicitly modeled and is replaced with a helium-filled void. The reactor pressure vessel and core barrel are made of 304 stainless steel, whereas the graphite is A3-3 [3]. Figure 2a shows the 3D view of the full-core model with a quarter taken out to show the inside. Finally, the fuel region is split into six axial regions with equal pebble volumes. Once the equilibrium compositions are determined for each zone, they are used to generate the power profiles using the full-core model.

3.2 SLICE MODEL

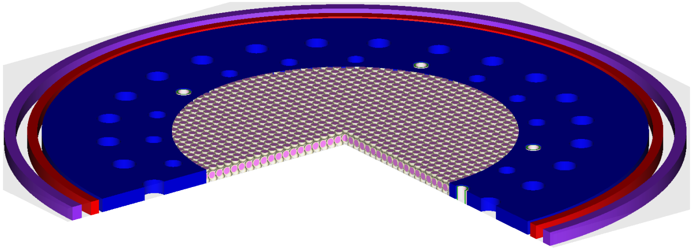
For calculations discussed in the next section, a “slice” model is used instead of the full-core model for the sake of reducing computational load to determine the equilibrium fuel compositions. This “slice” model is a 10 cm thick cross section through the center of the active fuel region. As the pebbles are 6.0 cm in diameter, and as the pebble packing lattice is dodecahedral, this 10 cm slice captures slightly more than two complete layers of pebbles. Figures 2b and 2c show the geometry of the slice model, providing a clearer view of the control rod and helium riser layout.

Table 1. Xe-100 type fuel pebble and reactor design parameters assumed for this study—adapted from [3], [16], [17]

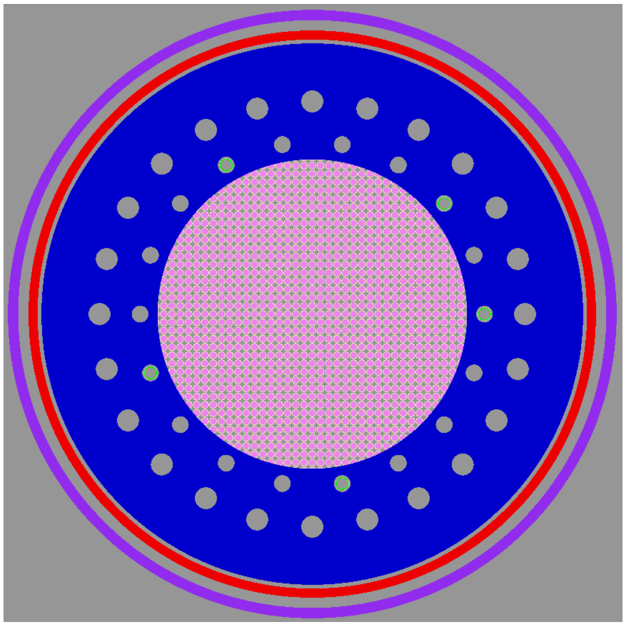
Parameter	**Value**
Pebble characteristics	
Inner (fueled) zone radius [cm]	2.5
Outer (fuel-free) zone thickness [cm]	0.5
Initial uranium loading [g]	7.0
Uranium chemical form	UCO
Initial enrichment [wt. % ^{235}U]	15.5
TRISO particles per pebble	19,000
Core characteristics	
Rated thermal power [MWth]	165
Helium inlet temperature [K]	533.15
Helium outlet temperature [K]	1023.15
Average helium pressure [MPa]	6.0
Active (fuel-bearing) core radius [cm]	120
Effective core height [cm]	893
Graphite reflector thickness [cm]	90
Number of RCS rods	9
Number of RSS rods	9
Number of helium riser channels	24
Core barrel gap thickness [cm]	3.0
Core barrel thickness [cm]	7.0
Reactor pressure vessel gap thickness [cm]	8.0
Reactor pressure vessel thickness [cm]	8.0
Pebble packing density $\left[\frac{\text{pebbles}}{\text{m}^3}\right]$	
3.2 cm radius unit cell	5458
3.213 cm radius unit cell	5397



(a) Full-core model with a quarter cut removed



(b) Axial "slice" 3-D view with a quarter cut removed



(c) Top-down view

Figure 2. Three-dimensional full-core model (with one axial zone), and axial slice model used for library generation. Helium is shown at reduced opacity in the 3D models for clarity.

4. GENERATION OF ONE-GROUP CROSS SECTIONS FOR DEPLETION CALCULATIONS

This section discusses the method used to determine the core equilibrium isotopic compositions and cross section libraries.

4.1 FUEL EQUILIBRIUM COMPOSITION GENERATION

Information on the exact equilibrium composition of fuel in the Xe-100 is not publicly available. The equilibrium composition is required to simulate the representative "average" spectral condition of the full core under steady state operating conditions. Therefore, to determine the equilibrium compositions (used to subsequently generate the cross section libraries for this analysis), an iterative depletion method was employed using the "slice" model. Full details regarding this iterative method are described in Bostelmann et al. [5], but the following steps outline the process (further illustrated as Figure 3):

1. An initial core of all fresh pebbles is assumed in the "slice" model.
2. Five "representative" pebbles are selected for depletion and are spaced radially throughout the slice (see Figure 4).
3. These pebbles are depleted using SCALE/TRITON for the full lifetime of the pebble—that is, 1,561.2 days—the time required to achieve a discharge burnup of 165 $\frac{\mathrm{GWd}}{\mathrm{tHM}}$. This step determines the fuel composition and the one-group cross section libraries at the beginning and end of each pass. It is assumed that the pebbles make six passes through the core.
4. SCALE/ARP is used to interpolate the one-group cross section libraries using the burnup-dependent specific power (from step 3) for depletion substeps at the beginning/end of user-specified axial zones and passes. As mentioned earlier, each pebble makes six passes through the core, and there are six equi-volume axial fuel regions in the full-core model.
5. SCALE/ORIGEN then determines the zone- and pass-wise isotopic compositions in each user-specified axial zone.
6. The pass-wise isotopic compositions are averaged to determine the zone-wise compositions for the reactor, and these zone-wise compositions are averaged to determine the core-averaged isotopic composition.
7. This new core-averaged composition replaces the fresh fuel composition in all the pebbles except the five representative pebbles in the SCALE/TRITON "slice" model. The representative pebbles still have fresh fuel compositions to allow for depletion from 0 to 165 $\frac{\mathrm{GWd}}{\mathrm{tHM}}$ while being surrounded by pebbles that include the new core-averaged composition calculated in step 6. Updating the core-average compositions in the non-depletable pebbles update the spectral conditions under which the pebbles that initially contain fresh fuel compositions are depleted. The process repeats (from step 3 onward) until the isotopes of interest (i.e., ^{235}U, ^{239}Pu) converge.

All these steps required Python scripts that aided in the creation of SCALE/ORIGEN-ARP input files for the sub-depletion steps, averaging of isotopic compositions, and creation of SCALE/TRITON material compositions with the newly determined equilibrium isotopic compositions. These Python scripts were generated by Bostelmann [5] and were modified for the Xe-100 type reactor analyses.

Table 2 shows the k_{eff} for the "slice" model during the iterative process described above as well as the core-averaged isotopic concentrations obtained at the end of all the iterations. Iteration 0 is the first case with all fresh fuel pebbles, which is the reason for the very high k_{eff}. As the isotopic compositions approach an equilibrium, the k_{eff} for the "slice" model converges to ~1.205.

The results show that after five iterations, the ^{235}U content is converged and varies by less than 0.01% between iteration 4 and 5. Therefore, the equilibrium fuel compositions determined at iteration 5 are used to update the compositions in the six axial zones of the full-core model to generate the axial power profile (see Figure 6), and in the "slice" model to generate temperature-dependent cross section libraries for this Xe-100 type reactor (see Figure 5).

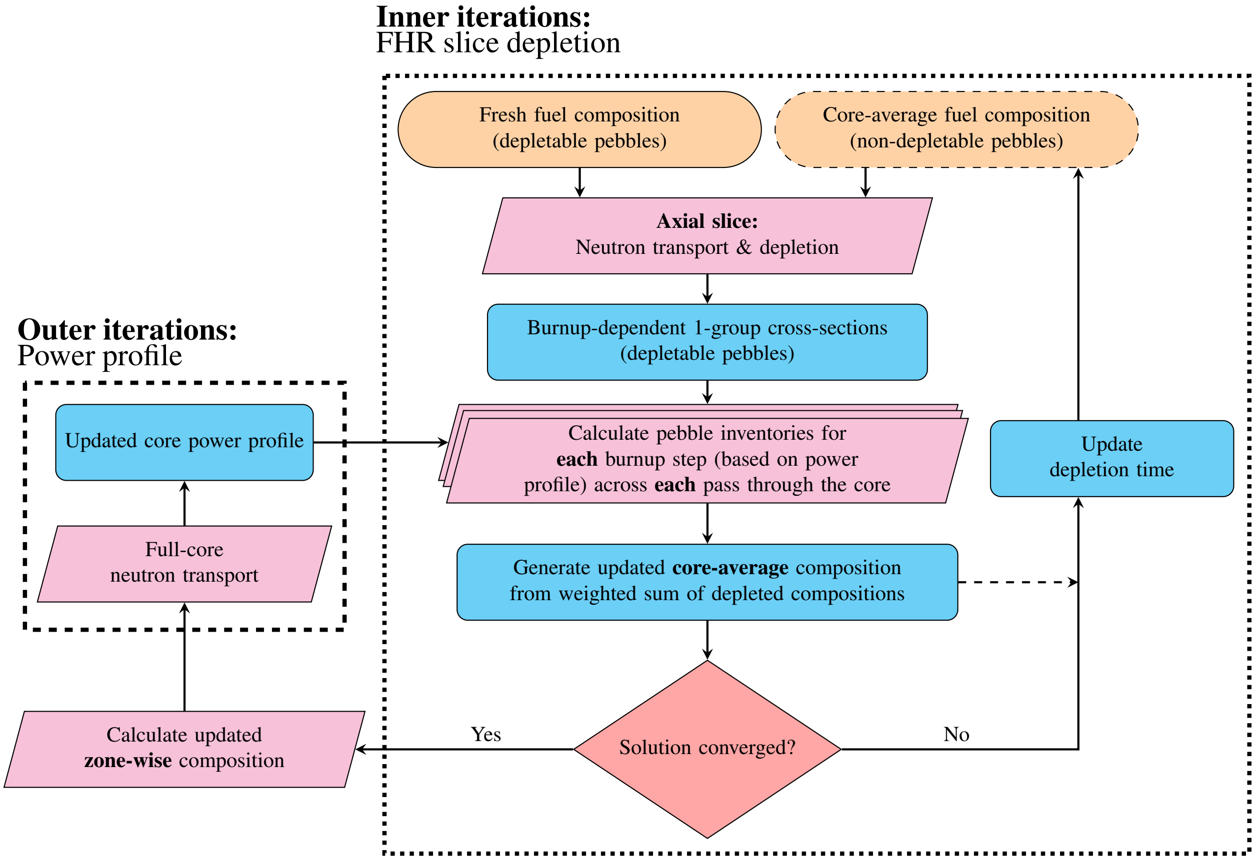


Figure 3. Iterative solution procedure for equilibrium core composition estimation [5].

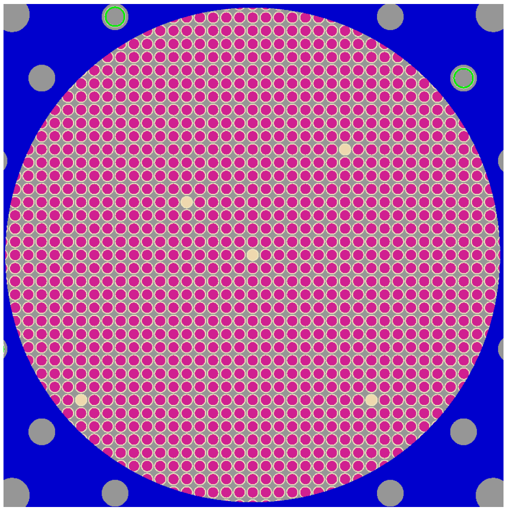


Figure 4. Close-up view of the surrogate pebble layout. Pebbles in pink are non-depleting, whereas pebbles in yellow are the surrogate, depleting pebbles.

4.2 TEMPERATURE-DEPENDENT CROSS SECTION LIBRARY GENERATION

Before performing SCALE/ORIGAMI sensitivity analyses, the temperature-dependent HDF5 libraries must be created for the simulations. For SCALE users familiar with binary f33 files, a large number of these cross section sets in the form of binary f33 files are combined into an HDF5 archive for use in ORIGAMI. To do this, the slice model is

Table 2. Convergence history for eigenvalue and isotopic concentrations $\left[\frac{\text{g}}{\text{cm}^3}\right]$ over each iteration used to estimate the equilibrium core composition

Iteration	k_{eff} (slice)	^{235}**U**	^{236}**U**	^{238}**U**	^{239}**Pu**
0	1.54027	—	—	—	—
1	1.21385	1.6473×10^{-3}	3.2221×10^{-4}	1.9244×10^{-2}	1.6238×10^{-4}
2	1.20577	1.6029×10^{-3}	3.2283×10^{-4}	1.9324×10^{-2}	1.3835×10^{-4}
3	1.20548	1.5996×10^{-3}	3.2217×10^{-4}	1.9332×10^{-2}	1.3581×10^{-4}
4	1.20537	1.5992×10^{-3}	3.2213×10^{-4}	1.9333×10^{-2}	1.3578×10^{-4}
5	1.20521	1.5991×10^{-3}	3.2218×10^{-4}	1.9333×10^{-2}	1.3565×10^{-4}

used once again. However, the slice is split into three radial zones to create cross sections that would capture differences in the cross sections due to differences in the radial flux. These three radial zones are defined such that they have equal volumes. Fresh surrogate pebbles, as in the iterative equilibrium composition generation method, are placed in each zone. The depleting pebbles are composed of the core-averaged equilibrium composition determined in iteration 5 from the previous section. Both depleting and non-depleting pebbles are uniquely defined in the radial zones, resulting in six separate sets of materials in the slice model (3 depleting and 3 non-depleting sets of materials). SCALE/TRITON inputs for the "slice" model with material compositions for fuel and moderator temperatures of 600, 750, and 900 K were created to make a series of slice model variations. Table 3 provides a full enumeration of the fuel and moderator temperature permutations used for the cross section library generation.

Table 3. Fuel and moderator temperatures used to generate the SCALE/ORIGEN HDF5 1G cross-section archive

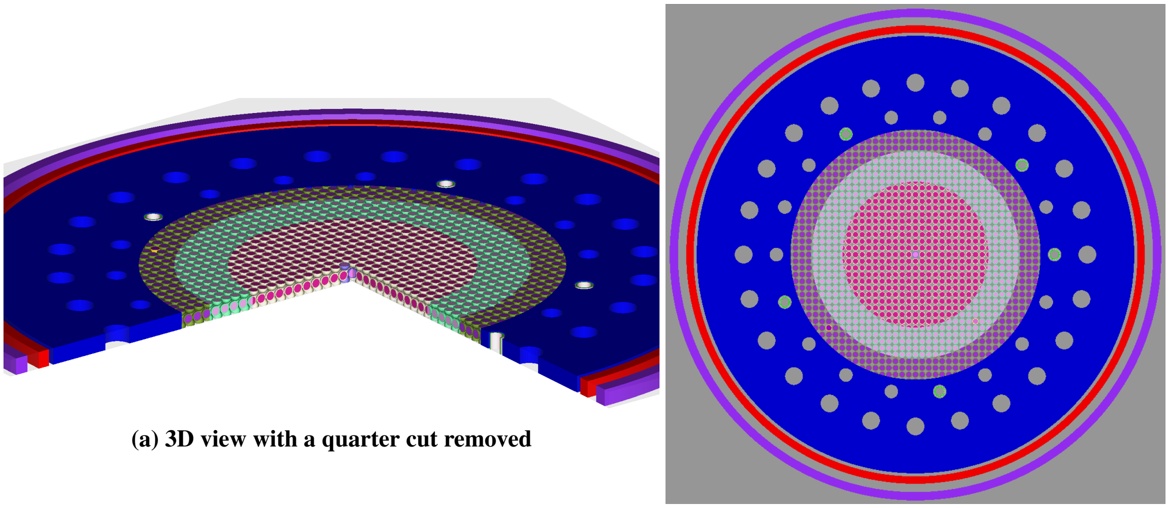
Fuel Temperature [K]	Moderator Temperature [K]
600	600
600	750
600	900
750	600
750	750
750	900
900	600
900	750
900	900

Figure 5 shows the three-zone layout for the slice models, including the radial zone boundaries and the locations of the surrogate pebbles.

Each SCALE/TRITON calculation results in one-group cross section file (`*.f33`). In preparation of ORIGAMI calculations, these files are tagged and compiled into an HDF5 library archive. Since this approach is based on new developments in SCALE/ORIGAMI, the individual commands executed with `obiwan` are described in the following for documentation purposes. `obiwan` is a command line utility that allows the user to easily manipulate SCALE output files.

- `obiwan tag *.f33 -idtags='fuel_type=pebble'`
  - This will tag all f33 files with the id tag:

    `"fuel_type=pebble"`
  - A wildcard is used here to tag all f33 files, but this command can be used for individual files as well.
  - `idtags` are strings, and non-iterable values, such as the `fuel_type` in the example above, or the radial zone that the material is associated with, etc.
  - These `idtags` are set by the user to help identify the problem type.
- `obiwan tag *m1200K* -interptags='reflector_temp=1200.0'`


(a) 3D view with a quarter cut removed

(b) Top-down view

Figure 5. Slice model with three radial zones. The helium coolant is shown with reduced opacity in the 3D model to aid visibility.

  - This example would tag the associated files with the `interptag`

    `"reflector_temp=1200.0"`
  - `interptags` are floats, which can be used to perform interpolations during the sensitivity studies in SCALE/ORIGAMI for fuel and moderator temperatures.

- `obiwan convert -format=hdf5 *.f33`
  - This command converts the .f33 files after they have been tagged into one HDF5 file.
  - The HDF5 file output will automatically be named after the first .f33 file it was fed. This HDF5 file can be renamed to any user-specified cross section library file.

5. SENSITIVITY STUDIES USING SCALE/ORIGAMI

5.1 DETERMINING RADIAL AND AXIAL POWER PROFILES

The radial and axial power profiles in the Xe-100 type reactor are required to provide the shape of the power in SCALE/ORIGAMI. The radial power profile can be determined using the output files generated during the SCALE/TRITON slice simulations to make the HDF5 cross section library. These output files were used to determine the radial power profile in the three separate radial zones.

The axial power profile is determined by creating and running a SCALE/TRITON full-core model with six axial fuel regions of equal volume (see Figure 6). The material compositions for each of these six zones are extracted from the zone-wise compositions generated from the converged iteration 5 in Section 4.1. The resulting zone-wise powers in the SCALE/TRITON output is used to determine the axial power shape for SCALE/ORIGAMI. The ratio of the power profile from the nominal power in each of the six zones is shown below, where Zone 1 is the first axial zone at the top and Zone 6 is the last axial zone at the bottom of the core:

Table 4. Zone-wise axial power profile and reflector temperatures

Axial zone	Normalized power profile	Reflector temperature [K]
1	1.16	623.15
2	1.74	623.15
3	1.50	623.15
4	0.95	623.15
5	0.47	648.15
6	0.16	723.15

The power profile shows that the power peaks toward the top of the core because the pebbles flow from the top of the reactor to the bottom. For this full-core model with equilibrium compositions, the k_{eff} is 0.95821 ± 0.00014. The eigenvalue (k_{eff}) is less than one because the goal of this work was not to optimize for this global parameter. This can be achieved by using radial and axial power profiles when determining the equilibrium fuel composition, accounting for different pebble speeds in each of the different radial zones, and adjusting the control rods or material impurities in the reflector or other regions of the core. However, optimizing for the eigenvalue could be included in future work, but was outside the scope of this study. For the purposes of this work, the depletion calculations are performed such that only the specific power used to normalize the flux is required.

Table 5. Radial power profile & temperatures by axial zone

Axial zone	Normalized radial power profile			Fuel temperature (K)		
	Outer	Middle	Inner	Outer	Middle	Inner
1	0.21141[1]	0.33199[1]	0.44535[1]	623.15	823.15	873.15
2				773.15	823.15	873.15
3				900.0[2]	900.0[2]	900.0[2]
4				900.0[2]	900.0[2]	900.0[2]
5				900.0[2]	900.0[2]	900.0[2]
6				900.0[2]	900.0[2]	900.0[2]

[1] The same radial power distribution is used for all axial nodes.

[2] Separate analysis indicated a higher fuel temperature for these regions; however, the maximum fuel temperature permutation used for library generation in this study was 900 K. Thus, the upper limiting value was used for the fuel temperature in these zones.

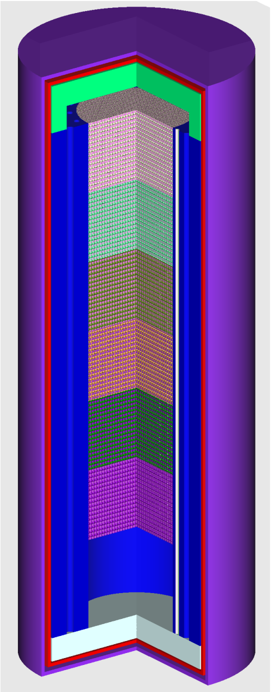


Figure 6. 3D view of full-core model with 6 axial zones. The helium coolant is shown with lower opacity.

5.2 ORIGAMI INPUT DESCRIPTION AND SENSITIVITY STUDY

The ORIGAMI input builds on the results obtained from the SCALE/TRITON models and uses the one-group cross section data generated using these models. Therefore, the assumptions used in the ORIGAMI analysis is provided last, alongside a few brief examples from an ORIGAMI input.

ORIGAMI input is relatively short compared to TRITON input. Only a few key parts of the input file are described here, as the new capabilities in ORIGAMI for pebble-bed reactor analysis are still under development at the time of this writing.

Example 1 illustrates the definition of a `transit_zone` block, which is the basic unit for defining spectral and power characteristics of different axial segments of the core.

```
transit_zone(ax1)={
  rpower=[0.21141 0.33199 0.44535]
  state{
    spectral_zone=[ outer middle inner ]
    fuel_temp=[773.15 823.15 873.15]
    reflector_temp=[623.15 623.15 623.15]
  }
}
```

Example 1. A “transit zone” definition in ORIGAMI. For each transit zone, a (relative) radial power shape is specified (`rpower`) along with corresponding interpolation parameters for each radial zone (`state`)

Multiple transit zones can be defined to capture the characteristics of the entire reactor. Reflector and fuel temperatures were estimated using the work by Mulder [19]. The `rpower` term describes the shape of the radial power profile and is normalized to the `rpop` parameter given in the `history` block, described below.

Example 2 demonstrates the definition of a `transit`, a unit representing the history of the pebble over a single pass through the core. The `burn` keyword takes the burnup length in days, and the `down` keyword gives the downtime, in days, after the burn time, during which the fuel material decays. The power given is the specific power, in $\frac{\text{MWd}}{\text{tHM}}$. The `rpop` keyword describes the mass distribution between the radial zones. Moving into the transit path descriptor, the

```
transit(first){
    burn=260
    down=5.0
    power=105.7
    rpop=[ 1.0 1.0 1.0 ]
    dump_steps=zone print_steps=ALL
    transit_path=[
        ax1={ frac=0.16 pz=1.16 }
        ax2={ frac=0.16 pz=1.74 }
        ax3={ frac=0.16 pz=1.50 }
        ax4={ frac=0.16 pz=0.949 }
        ax5={ frac=0.16 pz=0.469 }
        ax6={ frac=0.16 pz=0.158 }
    ]
  }
```

Example 2. A `transit` definition in ORIGAMI, defining the irradiation history characteristics of a single pass through the core. Multiple `transit_zone` objects are linked together to form a `transit_path` representing the axial history of the pebble. Each label in `transit_path` corresponds to a `transit_zone` defined previously.

order of axial zones listed (`ax1`, `ax2`, `ax3`, etc.) is the order in which the pebble will "move through" the zones. The `frac` keyword is for the fraction of time that the pebble spends in that particular transit zone, making it possible to simulate a velocity that changes in the axial direction. At this time, it is not yet possible to specify differential radial velocities; however, this is a feature planned for inclusion in a future beta release. The `pz` keyword is for the relative power in that axial zone and is used to shape the axial power profile.

Four SCALE/ORIGAMI simulations were created to perform a sensitivity study on the discharge isotopic inventory: "Control", "Inner", "Middle", and "Outer". Each of the latter three of these radial zone definitions represents the relative spectral characteristics of the core across the three regions modeled using SCALE/TRITON. Given the strong impact of the relative location of the pebble in proximity to the graphite reflector regions on the observed neutron flux profile [11], [18], these categorical variables thus represent differences in the relative shape of the neutron spectra radially.

These zone definitions were then used to assess the bounding conditions for the possible pebble transit histories to determine the isotopic vector of the pebble upon discharge. The "control" condition represents an "average" condition in which the pebble has an equal probability of flowing through one of these three zones per transit. Meanwhile, separate cases were investigated for the pebble exclusively traveling through one of the three radial zones over its entire history. For example, the "outer" case represents the most "pathological" condition in which the pebble is always situated in the region closest to the reflector—thus observing the most thermalized spectrum and achieving the highest burnup for a fixed number of passes. Conversely, pebbles in the "inner" case would observe the least thermalized neutron spectrum shape, resulting in a lower ratio of thermal to fast neutrons.

A more thorough sensitivity analysis could not be performed because of time constraints, but such an analysis can be performed in the future because the inputs have now been created to do so more easily. The SCALE/ORIGAMI runs identified for this project have some universal qualities and assumptions, which are listed in Table 6.

Within the SCALE/TRITON model, the boundaries of the radial zones used for the cross section library generation were set such that volumes for each zone were equal. Within the ORIGAMI calculation, the "control" (baseline) case distributed pebbles uniformly across each radial node (i.e., assuming an equal probability of pebbles landing within each radial zone at each transit, averaging the discharge compositions and re-apportioning after each transit). Within each radial node, it was assumed that there was a radial dependence on fuel temperature but that the reflector temperature was constant (i.e., the same reflector temperature was used for all radial nodes within a given axial zone).

The sensitivity studies thus focused on evaluating the discharge characteristics of a pebble transiting through *exclusively* one of the three radial zones for each core transit: inner, middle, and outer. The library interpolation characteristics were held consistent with the respective values for each of these zones used in the "control" case. In other words, each of the three sensitivity cases effectively assigns the radial population distribution to only one of the three zones defined in the "control" case, thus allowing for a specific evaluation of the bounding conditions for discharge isotopic inventories based on the pebble location history.

Table 6. Modeling assumptions used for SCALE/ORIGAMI common to each case considered

Axial zones (per transit)	6
Radial nodes	3 (inner, middle, outer)
Irradiation time per transit	260 days
Specific power	105.7 $\frac{\text{MWd}}{\text{tHM}}$
Decay time between transits	5 days
Number of core transits	6
Axial power shape Reflector temperature distribution	Table 4
Radial power shape Pebble fuel temperature distribution	Table 5

6. RESULTS

This section summarizes the results obtained from SCALE/TRITON as well as SCALE/ORIGAMI.

6.1 SCALE/TRITON CORE ISOTOPICS

From the results of the equilibrium composition study in 4.1, the isotopic composition of ^{235}U, ^{236}U, and ^{239}Pu in a pebble as a function of burnup can be extracted. The isotopic compositions for these isotopes were extracted from the SCALE/TRITON output file and compared to the publicly available Xe-100 results in [3]. Figure 7 compares them side by side, whereas Table 7 provides the values and compares the isotopic vectors of zones 1 and 6 for ^{235}U, ^{236}U, and ^{239}Pu.

Figure 7 shows that the discharge ^{235}U content (at 1,300 EFPD) is about 0.12 $\frac{\text{grams}}{\text{pebble}}$, whereas it is about 0.1 $\frac{\text{grams}}{\text{pebble}}$ as reported in Mulder and Boyes [3]. The ^{235}U depletion rate in SCALE/TRITON has a linear profile, whereas the work documented in the paper published by X-Energy [3] lacks this profile. This difference is most likely caused by the methods and assumptions used in the models. For example, within the SCALE models, a constant pebble power is used throughout each core transit, which is an unrealistic assumption given the depletion of fissile material within the pebble. That is, the pebble specific power will be higher than the average at the beginning of life and below the average power as it approaches its discharge burnup.

However, when comparing the ^{236}U and ^{239}Pu isotopic compositions, SCALE/TRITON and X-Energy results in Mulder and Boyes [3] are reversed. A closer inspection of the line labeled "^{239}Pu Without Depletion" at low burnup shows that it matches the line labeled ^{236}U, but is under the line labeled ^{239}Pu. Once this discrepancy was identified, a new reference was found. It was a presentation made by the same author in Mulder and Boyes [3] to the Modeling, Experimentation, and Validation (MeV) school at Argonne National Laboratory (ANL) in 2021 on Xe-100 reactor physics calculations [19]. In this presentation, the ^{236}U and ^{239}Pu results are reversed from what was presented previously [3] and are in agreement with the SCALE/TRITON results. Therefore, the authors of this report believe that there is a typographical error in Mulder and Boyes [3] in the reported ^{236}U and ^{239}Pu results.

Table 7 shows the ^{235}U, ^{236}U and ^{239}Pu isotopic content in Zones 1 and 6 after each pass throughout the core. The label "mid" signifies the average isotopic content in the middle of each axial zone, and "discharge" signifies the average isotopic content at discharge from Zone 6. A note at the bottom of the table indicates the burnup associated with each of the regions and passes. The table shows that at time of discharge, the average ^{235}U, ^{236}U, and ^{239}Pu compositions in a pebble after six passes through the core are ~0.04, 0.15 and 0.048 $\frac{\text{grams}}{\text{pebble}}$, respectively, with a burnup of 165.27 $\frac{\text{GWd}}{\text{tHM}}$. The ^{239}Pu isotopic content peaks after the pebble is discharged from the fourth pass through the core, and then this content subsequently burns down slightly as ^{239}Pu fissions increase. The ^{236}U isotopic content increases slowly as the pebble burnup increases.

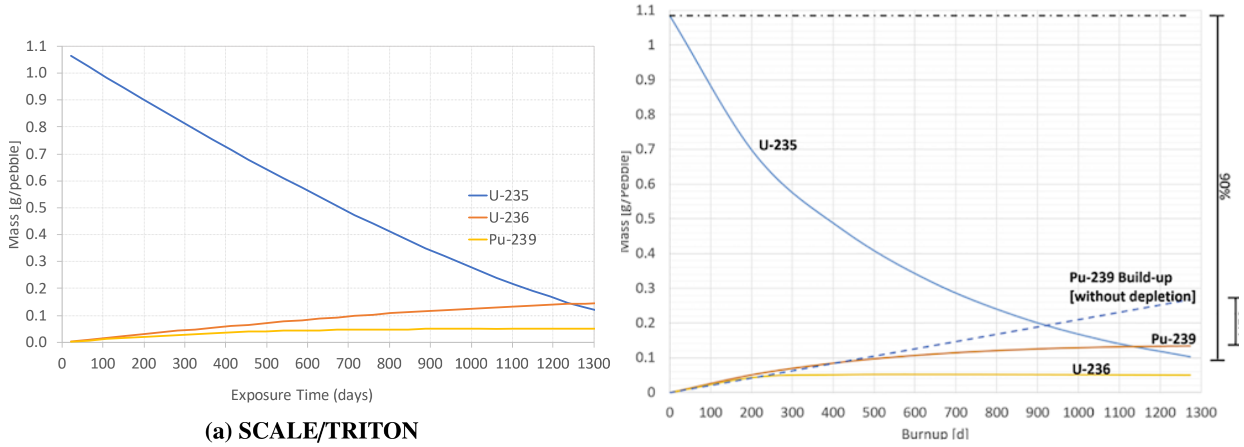
Table 7. SCALE/TRITON isotopic compositions per pass

Isotope	Axial zone	Pass 1	Pass 2	Pass 3	Pass 4	Pass 5	Pass 6
^{235}U	Zone 1 (mid)[1]	1.06	0.83	0.61	0.41	0.24	0.11
	Zone 6 (mid)[2]	0.87	0.64	0.44	0.27	0.13	0.04
	Zone 6 (discharge)[3]	0.85	0.63	0.43	0.25	0.12	0.04
^{236}U	Zone 6 (discharge)[3]	0.01	0.05	0.08	0.11	0.13	0.15
^{239}Pu	Zone 6 (discharge)[3]	0.027	0.042	0.048	0.05	0.049	0.048

[1] Zone 1 (mid) for passes 1, 2, 3, 4, 5, and 6 are associated with 21.7, 281.9, 542.0, 802.2, 1,062.4, and 1,322.5 EFPD or 2.3, 29.85, 57.3, 84.8, 112.3, and 139.8 $\frac{\text{GWd}}{\text{tHM}}$.

[2] Zone 6 (mid) for passes 1, 2, 3, 4, 5, and 6 are associated with 238.5, 498.7, 780.5, 1,019.0, 1,279.2, and 1,539.34 acefpd, or 25.2, 52.7, 80.2, 107.7, 135.2 and 162.7 $\frac{\text{GWd}}{\text{tHM}}$.

[3] Zone 6 (discharge) for passes 1, 2, 3, 4, 5, and 6 are associated with 260.2, 520.3, 780.5, 1,040.7, 1,300.9, and 1,561.0 EFPD, or 27.5, 55.0, 82.5, 110.0, 137.5, and 165.0 $\frac{\text{GWd}}{\text{tHM}}$.



(a) SCALE/TRITON

(b) X-Energy [3]

Figure 7. Select isotopic compositions as a function of exposure time (days), as calculated using SCALE/TRITON and those reported by X-Energy [3]. Results are reported in mass per 7 gHM pebble.

6.2 SCALE/ORIGAMI RESULTS

Previously, SCALE/TRITON results were extracted and presented. In this section, SCALE/ORIGAMI results are discussed for the four scenarios discussed in Section 5.2. SCALE/ORIGAMI allows the user to generate discharge isotopic compositions quickly for varying parameters such as power profiles, burnup, and temperatures. Due to time constraints, a detailed sensitivity study could not be performed. As discussed, four cases were set up: “Control”, “Inner”, “Middle”, and “Outer”. The SCALE/ORIGAMI output was studied and compared with the SCALE/TRITON results for the baseline case to ensure consistency in the discharge isotopic content. Figure 9 below gives the concentrations of select isotopes as a function of burnup in $\frac{\text{MWd}}{\text{tHM}}$, alongside a graph of ^{235}U, ^{236}U, and ^{239}Pu versus burnup in days. Tables 8, 9, 10, and 11 list the isotopic content as a function of burnup for each case. Additionally, they also show the concentrations of ^{238}U, ^{238}Pu, ^{240}Pu, and ^{241}Pu.

For the “Control” case in SCALE/ORIGAMI, there is an equal probability that the pebble will flow through one of the three radial regions (shown in Figure 5). The SCALE/ORIGAMI results for the “Control” case indicates that the isotopic inventory is similar to that was generated with SCALE/TRITON. The ^{235}U, ^{236}U and ^{239}Pu at discharge at 1590 days in SCALE/ORIGAMI is approximately 0.05, 0.15, and 0.049 $\frac{\text{grams}}{\text{pebble}}$ whereas with TRITON at 1561 days, the corresponding results were 0.04, 0.15, and 0.048 $\frac{\text{grams}}{\text{pebble}}$. The SCALE/ORIGAMI allowed the analysis to be extended to three additional cases, where the pebble would experience the flux spectra associated with being in the inner zone (“Inner” case), the middle zone (“Middle” case), or the outer zone (“Outer” case) for the entire burn history. This is evident in the spectral change associated with being in the “Inner” vs. the “Middle” vs. the “Outer” radial zones, as illustrated in Figure 8.

Skutnik previously identified observed differences in the PBMR-400 pebble discharge vectors driven by shifts in the neutron spectrum relative to the pebble’s proximity to reflector regions [18]. As explained in Section 5.2, the “Outer” zone near the reflector sees a relatively higher ratio of thermal to fast neutrons compared to the “Inner” zone, thereby achieving a higher fission rate (and thus higher burnup). This is evident when evaluating the SCALE/ORIGAMI results in Tables 9 to 11. The “Inner” and “Middle” zones have similar discharge ^{235}U content of 0.048 and 0.046 $\frac{\text{grams}}{\text{pebble}}$, respectively. However, for the “Outer” zone, which experiences a higher thermal to fast ratio (near the reflector), the ^{235}U content is 0.0296 $\frac{\text{grams}}{\text{pebble}}$. Therefore, the longer a pebble stays near the reflector, the higher the burnup; the nearer it stays to the center of the core, the lower the burnup. These sensitivity studies using SCALE/ORIGAMI are valuable, and additional analyses can be performed now that the inputs have been established for the Xe-100 models.

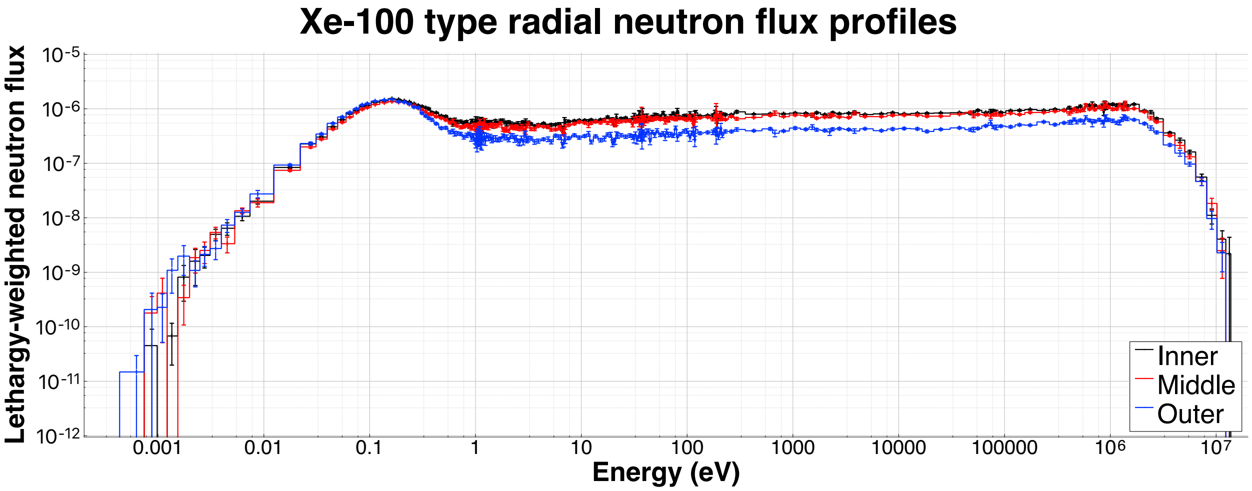


Figure 8. 252-group neutron flux for the three radial zones modeled. Note the relatively higher ratio of thermal to fast neutrons in the outer region (closest to the reflector).

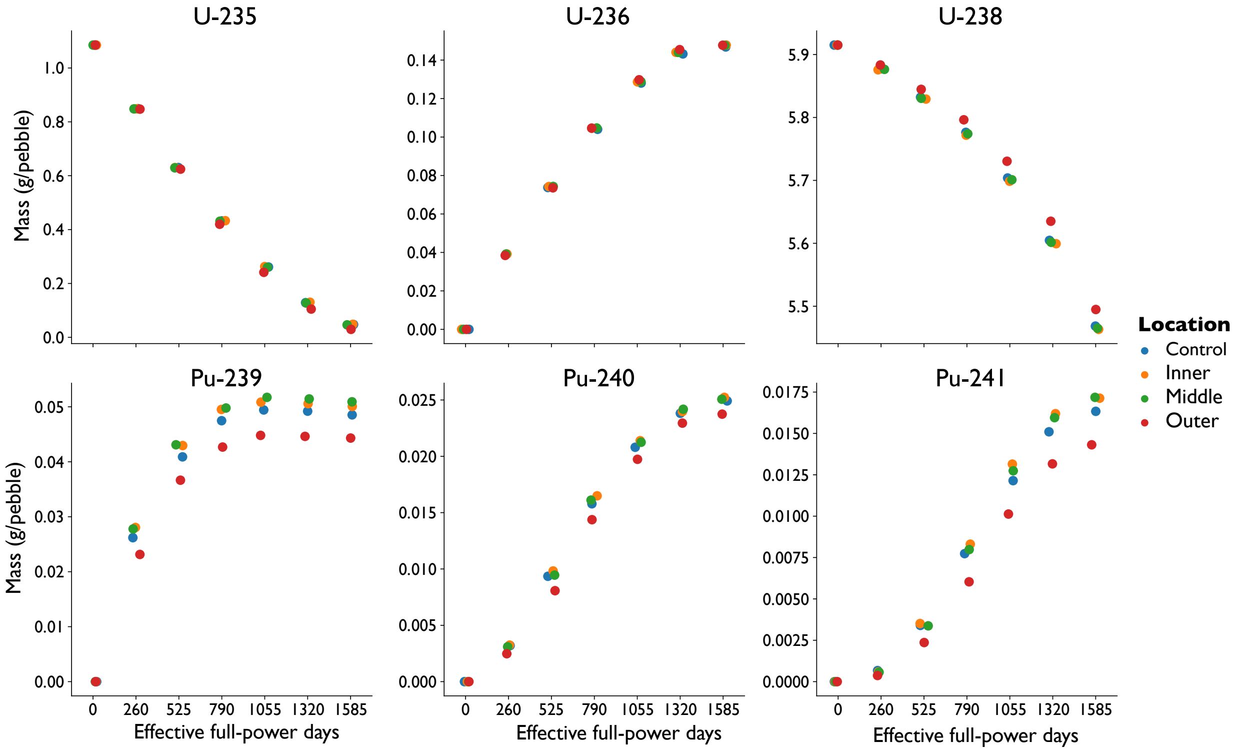


Figure 9. Isotopic concentrations of selected uranium and plutonium isotopes (in $\frac{\text{grams}}{\text{pebble}}$, y-axis) from SCALE/ORIGAMI analysis as a function of exposure time (in EFPD, x-axis). Notably, the ORIGAMI results extend to a longer exposure time than the Xe-100 and SCALE/TRITON results

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Table 8. Isotopic inventories over time $\left[\frac{\text{grams}}{\text{pebble}}\right]$: Control case

Exposure Time (EFPD)	^{235}U	^{236}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu
0	1.085	0	5.915	0	0	0	0
260	0.849	0.0388	5.877	1.692×10^{-5}	2.619×10^{-2}	3.12×10^{-3}	6.689×10^{-4}
525	0.630	0.0737	5.832	1.426×10^{-4}	4.090×10^{-2}	9.352×10^{-3}	3.397×10^{-3}
790	0.432	0.104	5.776	5.444×10^{-4}	4.747×10^{-2}	1.579×10^{-2}	7.736×10^{-3}
1060	0.261	0.128	5.704	1.501×10^{-3}	4.943×10^{-2}	2.080×10^{-2}	1.215×10^{-2}
1320	0.129	0.143	5.605	3.368×10^{-3}	4.921×10^{-2}	2.382×10^{-2}	1.510×10^{-2}
1590	0.0475	0.147	5.468	6.240×10^{-3}	4.854×10^{-2}	2.492×10^{-2}	1.634×10^{-2}

Table 9. Isotopic inventories over time $\left[\frac{\text{grams}}{\text{pebble}}\right]$: Inner case

Exposure Time (EFPD)	^{235}U	^{236}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu
0	1.085	0	5.915	0	0	0	0
260	0.848	0.0392	5.876	1.346×10^{-5}	2.805×10^{-2}	3.243×10^{-3}	5.900×10^{-4}
525	0.630	0.0743	5.829	1.306×10^{-4}	4.296×10^{-2}	9.825×10^{-3}	3.512×10^{-3}
790	0.433	0.105	5.772	5.274×10^{-4}	4.952×10^{-2}	1.649×10^{-2}	8.308×10^{-3}
1060	0.263	0.129	5.699	1.488×10^{-3}	5.085×10^{-2}	2.139×10^{-2}	1.3146×10^{-2}
1320	0.130	0.144	5.599	3.387×10^{-3}	5.057×10^{-2}	2.397×10^{-2}	1.619×10^{-2}
1590	0.0483	0.148	5.463	6.396×10^{-3}	5.008×10^{-2}	2.523×10^{-2}	1.713×10^{-2}

Table 10. Isotopic inventories over time in $\left[\frac{\text{grams}}{\text{pebble}}\right]$: Middle case

Exposure Time (EFPD)	^{235}U	^{236}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu
0	1.085	0	5.915	0	0	0	0
260	0.848	0.0392	5.876	1.356×10^{-5}	2.778×10^{-2}	3.094×10^{-3}	5.688×10^{-4}
525	0.629	0.0743	5.830	1.291×10^{-4}	4.310×10^{-2}	9.456×10^{-3}	3.372×10^{-3}
790	0.431	0.105	5.774	5.165×10^{-4}	4.979×10^{-2}	1.611×10^{-2}	7.982×10^{-3}
1060	0.260	0.129	5.701	1.468×10^{-3}	5.172×10^{-2}	2.125×10^{-2}	1.274×10^{-2}
1320	0.127	0.145	5.602	3.379×10^{-3}	5.144×10^{-2}	2.418×10^{-2}	1.595×10^{-2}
1590	0.0463	0.148	5.465	6.380×10^{-3}	5.092×10^{-2}	2.507×10^{-2}	1.718×10^{-2}

Table 11. Isotopic inventories over time in $\left[\frac{\text{grams}}{\text{pebble}}\right]$: Outer case

Exposure Time (EFPD)	^{235}U	^{236}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu
0	1.085	0	5.915	0	0	0	0
260	0.847	0.0384	5.883	9.981×10^{-6}	2.314×10^{-2}	2.478×10^{-3}	3.714×10^{-4}
525	0.624	0.0736	5.845	9.680×10^{-5}	3.665×10^{-2}	8.074×10^{-3}	2.363×10^{-3}
790	0.420	0.105	5.796	4.025×10^{-4}	4.268×10^{-2}	1.438×10^{-2}	6.033×10^{-3}
1060	0.241	0.130	5.730	1.193×10^{-3}	4.481×10^{-2}	1.974×10^{-2}	1.013×10^{-2}
1320	0.105	0.145	5.635	2.889×10^{-3}	4.462×10^{-2}	2.295×10^{-2}	1.316×10^{-2}
1590	0.0296	0.148	5.495	5.650×10^{-3}	4.432×10^{-2}	2.374×10^{-2}	1.431×10^{-2}

7. CONCLUSION AND FUTURE WORK

Full-core and slice models of an Xe-100 type pebble-bed reactor were created in SCALE. SCALE/TRITON and SCALE/ORIGEN were used to generate zone-wise compositions for an equilibrium core. The SCALE/TRITON results at 1,300 EFPD are consistent with the results in a presentation made at the MeV school at ANL [19]. The ^{235}U isotopic composition from SCALE/TRITON has a linear trendline over the exposure time, which alludes to differences in the models and methods between SCALE/TRITON and those used by X-Energy to generate their results [3], [19]. A discrepancy was identified in a figure presented in Mulder and Boyes [3] in which the results for ^{236}U and ^{239}Pu are reversed from the corresponding set of results generated from SCALE/TRITON. The authors believe this to be a typographical error in Mulder and Boyes [3], as those results are reversed in the presentation those same authors made at the MeV school in 2021 [19], which documents results that are in agreement with the SCALE/TRITON results.

Once the equilibrium core compositions were generated, they were used in the slice models for varying fuel and moderator temperatures to generate a set of temperature-dependent one-group cross sections. These cross sections were compiled to generate temperature-dependent cross section libraries that can be used to perform quick sensitivity calculations with a recent enhancement to SCALE's ORIGAMI module that allows the rapid generation of inventories for pebbles in pebble-bed reactors (to be included in the SCALE 7.0 release).

SCALE/ORIGAMI inputs were run for four cases: a "control" model in which pebbles are distributed across three radial zones during each pass through the core with equal probability, and then three separate runs (i.e., "inner", "mid", and "outer") in which pebbles travel exclusively through one of the three radial zones throughout each pass through the core. The purpose of this analysis was to provide a bounding sensitivity analysis elucidating the effects of the pebble location history within the core, as the neutron spectrum shape has been shown to be highly sensitive to the pebble's radial proximity to the graphite reflector. During this work, user testing and feedback were provided to the development team to aid in the software development of SCALE/ORIGAMI. The implementation of user feedback allowed for the completion of the analyses for this report.

The results generated in this report from SCALE Xe-100 type pebble-bed models indicate that the methods and models presented are consistent with those reported in Mulder and Boyes [3] and Mulder [19]. Therefore, these models can be used to perform other scoping studies with SCALE. Future work could include expanding the cross section library to include a wider range of temperature-dependent cross sections since the HDF5 library archive currently goes up to only 900 K. Using the steps detailed in Section 4, the temperature range can be expanded to include data points at 1050 and 1200 K, which would cover the entire operating temperature range in the Xe-100. Additionally, although the four ORIGAMI runs described here cover the most basic cases, there is still room to analyze a series of cases that perturb the axial and radial power profiles, fuel and reflector temperatures, and the pebble radial distributions; such an analysis would produce a full sensitivity profile of the discharged isotopic inventories. These sensitivity studies would be more easily performed since the models and inputs are now established in SCALE using publicly available information.

REFERENCES

[1] *Advanced Reactor Demonstration Program*, https://www.energy.gov/ne/advanced-reactor-demonstration-program, Accessed: 2022-30-8.

[2] T. K. Kim, S. Richards, A. Cuadra, R. Hays, J. W. Bae, and E. Davidson, “Report on Fuel Cycle Facility Requirements for Deployment of Demonstration Reactors and Potential Evolutionary Fuel Cycle Scenarios,” Argonne National Laboratory, Tech. Rep. ANL/NSE-22/39, Jul. 2022.

[3] E. Mulder and W. Boyes, “Neutronics characteristics of a 165 MWth Xe-100 reactor,” *Nuclear Engineering and Design*, vol. 357, p. 110 415, Feb. 2020, ISSN: 0029-5493. DOI: 10.1016/j.nucengdes.2019.110415.

[4] “SCALE Code System,” Oak Ridge National Laboratory, Oak Ridge, TN, Tech. Rep. ORNL/TM-2005/39, Version 6.2.4, Apr. 2020.

[5] F. Bostelmann, C. Celik, R. F. Kile, and W. A. Wieselquist, “SCALE Analysis of a Fluoride Salt-Cooled High-Temperature Reactor in Support of Severe Accident Analysis,” Oak Ridge National Laboratory, Tech. Rep. ORNL/TM-2021/2273, Mar. 2022.

[6] I. C. Gauld, G. Radulescu, G. Ilas, B. Murphy, M. Williams, and D. Wiarda, “Isotopic Depletion and Decay Methods and Analysis Capabilities in SCALE,” *Nuclear Technology*, vol. 174, no. 2, pp. 169–195, May 2011. DOI: 10.13182/NT11-3.

[7] S. Goluoglu, J. Lester M. Petrie, M. E. Dunn, D. F. Hollenbach, and B. T. Rearden, “Monte carlo criticality methods and analysis capabilities in scale,” *Nuclear Technology*, vol. 174, no. 2, pp. 214–235, May 2011. DOI: 10.13182/NT10-124.

[8] G. G. Davidson, T. M. Pandya, S. R. Johnson, T. M. Evans, A. E. Isotalo, C. A. Gentry, and W. A. Wieselquist, “Nuclide depletion capabilities in the shift monte carlo code,” *Annals of Nuclear Energy*, vol. 114, Dec. 2017, ISSN: 0306-4549. DOI: 10.1016/j.anucene.2017.11.042. [Online]. Available: https://www.osti.gov/biblio/1429205.

[9] S. Skutnik, M. Williams, and R. Lefebvre, “ORIGAMI: A New Interface for Fuel Assembly Characterization with ORIGEN,” in *2015 International High-Level Radioactive Waste Management Conference (IHLRWM 2015)*. Charleston, SC, Apr. 2015, pp. 418–425.

[10] S. Skutnik, *Extending ORIGAMI capabilities to flowing-fuel systems*, Presentation at NRC Program Review, Oak Ridge National Laboratory, Aug. 2022.

[11] S. Skutnik, F. Bostelmann, and W. Wieselquist, “Rapid Depletion Analysis of Flowing-Pebble Reactor Systems at Equilibrium using SCALE,” in *International Conference on Physics of Reactors 2022 (PHYSOR 2022)*. May 2022.

[12] H. D. Gougar, F. Reitsma, and W. Joubert, “A comparison of pebble mixing and depletion algorithms used in pebble-bed reactor equilibrium cycle simulation,” in *International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)*, Saratoga Springs, NY, May 2009.

[13] Y. Tang, L. Zhang, Q. Guo, B. Xia, Z. Yin, J. Cao, J. Tong, and C. H. Rycroft, “Analysis of the pebble burnup profile in a pebble-bed nuclear reactor,” *Nuclear Engineering and Design*, vol. 345, pp. 233–251, 2019, ISSN: 0029-5493. DOI: 10.1016/j.nucengdes.2019.01.030.

[14] H. D. Gougar, A. M. Ougouag, W. K. Terry, and K. N. Ivanov, “Automated Design and Optimization of Pebble-Bed Reactor Cores,” *Nuclear Science and Engineering*, vol. 165, no. 3, pp. 245–269, DOI: 10.13182/NSE08-89.

[15] S. Sen, “HTGR Methods and Simulation,” Idaho National Laboratory, Idaho Falls, ID, Tech. Rep. INL/MIS-19-56948-Revision-0, Dec. 2019.

[16] International Atomic Energy Agency (IAEA), *Evaluation of High Temperature Gas Cooled Reactor Performance: Benchmark Analysis Related to the PBMR-400, PBMM, GT-MHR, HTR-10 and the ASTRA Critical Facility*, IAEA-TECDOC-1694. Vienna, Austria: IAEA, Apr. 2013, ISBN: 978-92-0-137610-7.

[17] Nuclear Science Committee, Nuclear Energy Agency (NEA), *PBMR Coupled Neutronics / Thermal-hydraulics Transient Benchmark The PBMR-400 Core Design*, NEA/NSC/DOC(2013)10. Paris, France: OECD/NEA, Jul. 2013, vol. 1: The Benchmark Definition.

[18] S. E. Skutnik and W. A. Wieselquist, “Assessment of ORIGEN Reactor Library Development for Pebble-bed reactors based on the PBMR-400 benchmark,” Oak Ridge National Laboratory, Oak Ridge, TN, Tech. Rep. ORNL/TM-2020/1886, Jul. 2021.

[19] E. Mulder, *Xe 100: Aspects of Multi Scale, Multi Physics Modeling*, Presentation at MeV School, Jul. 2021.