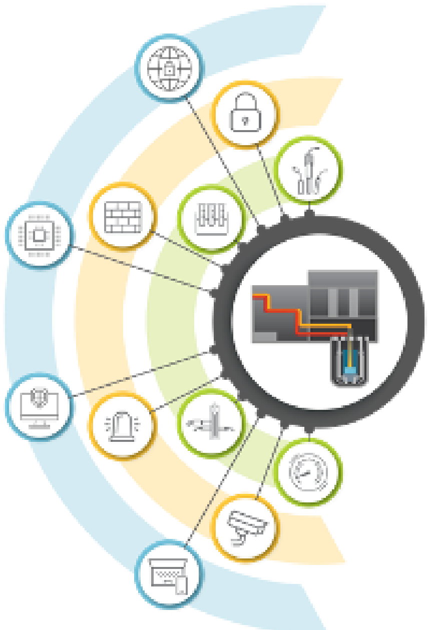

Uncertainty Quantification of the Discharge Burnup and Isotopic Inventory for an Individual Pebble using a Correlation Matrix

Prepared for
US Department of Energy

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Oak Ridge National Laboratory

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Nuclear Nonproliferation Division

UNCERTAINTY QUANTIFICATION OF THE DISCHARGE BURNUP AND ISOTOPIC INVENTORY FOR AN INDIVIDUAL PEBBLE USING A CORRELATION MATRIX

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August 2024

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ABBREVIATIONS

BCC	body-centered cubic
GWd/tHM	gigawatt-days per metric tonne of heavy metal
MC&A	Material Control and Accounting
MCNP	Monte Carlo N-Particle radiation transport code
MWth/tHM	Mega-Watt thermal per metric tonne of heavy metal
NRC	The U.S. Nulcear Regulatory Commission
PBR	pebble bed reactor
PBMR	Pebble Bed Modular Reactor
SCALE	Standardized Computer-Analysis for Licensing Evaluation
TRISO	tri-structural isotropic
VSOP	Very Superior Old Programs

EXECUTIVE SUMMARY

A computational study was conducted to explore the sensitivity of fuel burnup, plutonium buildup, and residual uranium-235 (^{235}U) enrichment in a fuel pebble to various pebble bed reactor (PBR) operating parameters, such as neutron flux, neutron energy spectra, pebble residence time, pebble power, fuel temperature, and initial ^{235}U enrichment. The requisite fuel burnup simulations were conducted using Monte Carlo N-Particle (MCNP) 6.2 code and SCALE/ORIGAMI by developing the fuel pebble model of a publicly available PBR design: a 400 MW pebble bed modular reactor (PBMR-400). Initial fuel depletion comparisons using a body-centered cubic (BCC) lattice pebble configuration showed strong agreement between MCNP and SCALE/TRITON predictions for key quantities, including infinite neutron multiplication factor (k_{inf}), fuel burnup, and residual fissile content. Detailed fuel burnup simulations using SCALE/ORIGAMI were conducted by simulating the random transit history of 20,000 pebbles through the axial meshes within radial channels in the reactor core model. Accurate definitions of radial channels and axial meshes, potentially guided by experiments or discrete element modeling, are crucial for precise simulations. These simulations indicated that parameters such as pebble transit/residence time, radial channel neutron energy spectrum, and pebble power significantly affect fuel burnup, the residual ^{235}U, ^{239}Pu buildup, and total Pu content. The most sensitive parameters were pebble transit time and the radial channel neutron energy spectrum. Conversely, fuel temperature and ^{235}U enrichment changes had negligible effects within the chosen perturbation range. Unique correlations between perturbed parameters and responses were also observed in each pass of an individual pebble through the reactor core as a result of varying pebble flow channels. Finally, sensitivity of residual ^{239}Pu to nuclear data perturbations were also analyzed, which showed that the highest contributor was ^{238}U (n,γ) reaction. Detailed SCALE/ORIGAMI simulations on various parametric sensitivities showed a maximum variation of approximately ±10 mg Pu per discharged pebble considering one standard deviation (σ). MCNP results were found to be conservative compared with the detailed SCALE/ORIGAMI simulations with respect to Material Control and Accounting (MC&A), especially for the MCNP simulations performed using averaged initial ^{235}U enrichment and other reactor parameters (fuel temperature, residence time, neutron flux, neutron energy spectrum).

The differences in Pu masses caused by variability in operational parameters and the resulting fuel burnup and fissile content in pebbles could manifest themselves to impact MC&A and nuclear safeguards, specifically in shipper/receiver difference or difference between the declared mass value and measured mass value during verification. Differences in Pu and the corresponding masses of residual fission products can also impact radiation dose calculations and, therefore, nuclear safety and security. An important outcome of this work is that the initial fuel burnup simulations can be improved when experience is gained from reactor operation by focusing on the most sensitive parameters identified that affect fuel burnup and residual fissile content in the discharged pebbles. This understanding of parametric uncertainties and their effects can inform PBR modelers and designers on targeted improvements to obtain more accurate values for the quantities of interest in the discharged pebbles. Uncertainty estimation can support MC&A of discharged pebbles stored in used fuel canisters.

1. PURPOSE AND SCOPE OF WORK

1.1 PURPOSE

The U.S. Nuclear Regulatory Commission (NRC) is eganged in pre-application activities with the X Energy, LLC (X-energy), the designer of the Xe-100 Pebble Bed Reactor (PBR)[1]. Such an engagement is considered as an indication that the PBR is a promising advanced nuclear reactor design geared towards licensing and operation in the near term. The PBR uses tri-structural isotropic (TRISO) microspheres consisting of a high-assay low enriched uranium-based fuel kernel encapsulated by three layers of carbon- and ceramic-based materials that prevent the release of radioactive fission products[2]. Several thousands of TRISO microspheres are dispersed in a spherical graphite pebble, and hundreds of thousands of these pebbles are used as fuel in a PBR (see Figure 1). The pebbles travel from the top to the bottom of the PBR core during each pass, and the uranium fissions produce heat that is removed by either gaseous helium or molten salt coolant. The neutron-irradiated fuel pebbles that reach the bottom of the reactor core undamaged and have not achieved the desired fuel burnup are re-inserted at the top of the reactor core to maximize the use of its fissile material content and achieve high fuel burnup. After achieving the desired fuel burnup, the fuel pebbles are permanently discharged for disposal. The re-inserted fuel pebbles can travel from the top to the bottom of the reactor core through a different radial zone than that traveled during preceding passes. Hence, the isotopic compositions of plutonium (Pu) and U in the discharged fuel pebbles vary as a function of fuel burnup. The isotopic composition depends on the pebbles' residence time (flow velocity varies in each radial zone) in the reactor vessel, as well as their location (neutron flux and energy spectrum vary from location to location), even though the number of passes through the reactor vessel is the same. Other factors affecting Pu and U composition in an irradiated pebble are the initial ^{235}U enrichment and the temperature to which the pebble is exposed passing through different axial and radial zones in the reactor core. Therefore, a range of fuel burnup and nuclide inventories is expected in pebbles upon their discharge. These variations have been quantified in prior work using the SCALE/ORIGAMI code [1].

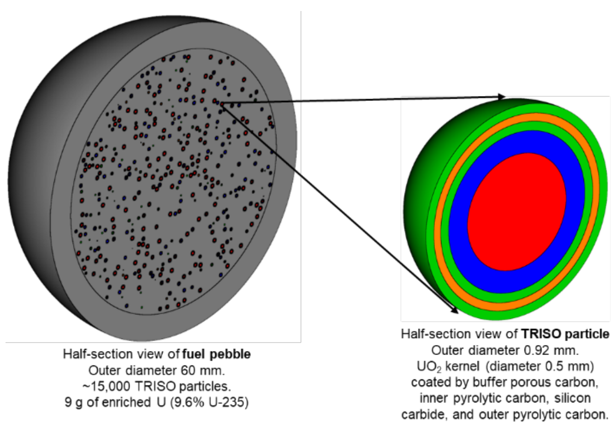

Figure 1. A PBMR-400 fuel pebble containing thousands of TRISO particles [2].

The purpose of this study is to expand on prior work to investigate how minor perturbation of parameters such as fuel temperature, neutron flux (or specific power), initial ^{235}U enrichment, and residence time will affect the quantities of interest for the material control and accounting (MC&A) aspects of nuclear security and safeguards of PBRs. The quantities of interest are fuel burnup and residual masses of ^{235}U,

[1]https://www.nrc.gov/reactors/new-reactors/advanced/who-were-working-with/licensing-activities/pre-application-activities/xe-100.html (accessed on August 2, 2024)
[2]https://www.energy.gov/ne/articles/triso-particles-most-robust-nuclear-fuel-earth

^{239}Pu, and total Pu in the discharged fuel pebbles. The initial estimates of fissile mass in the discharged pebbles, as determined by both the neutronics code and fuel burnup measurements, are expected to be reasonable. However, there will be opportunities to improve these estimations on fuel burnup and residual fissile mass with a better understanding of the most sensitive parameters and assumptions for the permanently discharged pebbles. Such an understanding of parametric uncertainties and their effects can inform PBR modelers and designers on targeted improvements to obtain more accurate values for the quantities of interest in the discharged pebbles. Uncertainty estimation can support MC&A of discharged pebbles stored in used fuel canisters.

1.2 SCOPE AND STRUCTURE OF REPORT

In this work, the fuel pebble model of a publicly available PBR design: a 440 MW pebble bed modular reactor (PBMR)-400, [2, 3, 4] was chosen as the reference PBR. This PBMR-400 pebble model was used in performing minor perturbation studies on fuel temperature, neutron flux (or specific power), initial ^{235}U enrichment, and residence time to quantify the effects of these factors on fuel burnup and masses of ^{235}U, ^{239}Pu, and total Pu of permanently discharged pebbles. Two modeling and neutronics simulation codes—MCNP version 6.2 [5] and SCALE/ORIGAMI [6]—were used in this study. Section 2 describes the modeling and simulation aspects of PBMR-400. Results from the simulations and interpretation of those results are provided in Section 3. Salient conclusions of the study are provided in Section 4.

2. PBMR-400 AND SIMULATION METHODOLOGIES

The PBMR-400 data required for the neutronics simulations are publicly available. The PBMR-400 features an annular cylindrical core with an inner radius of 1 m and an outer radius of 1.85 m (see Figure 2). Within the core, one fixed graphite reflector is positioned at the center, and the other is located outside the core. The reactor is loaded with approximately 452,000 pebbles, each containing 15,000 TRISO particles enriched to 9.6 wt.% ^{235}U. Operating on a multi-pass scheme, the pebbles circulate through the core an average of six times before their permanent discharge, achieving an average discharged fuel burnup target of 90 GWd/tHM with an average specific power of 98.431 MWth/tHM. The fuel depletion calculations of the pebbles were conducted using MCNP and SCALE/ORIGAMI, as described in Subsections 2.1 and 2.2. The perturbation parameters and the range of perturbations used in the fuel burnup simulations with MCNP and SCALE/ORIGAMI codes are shown in Table 1.

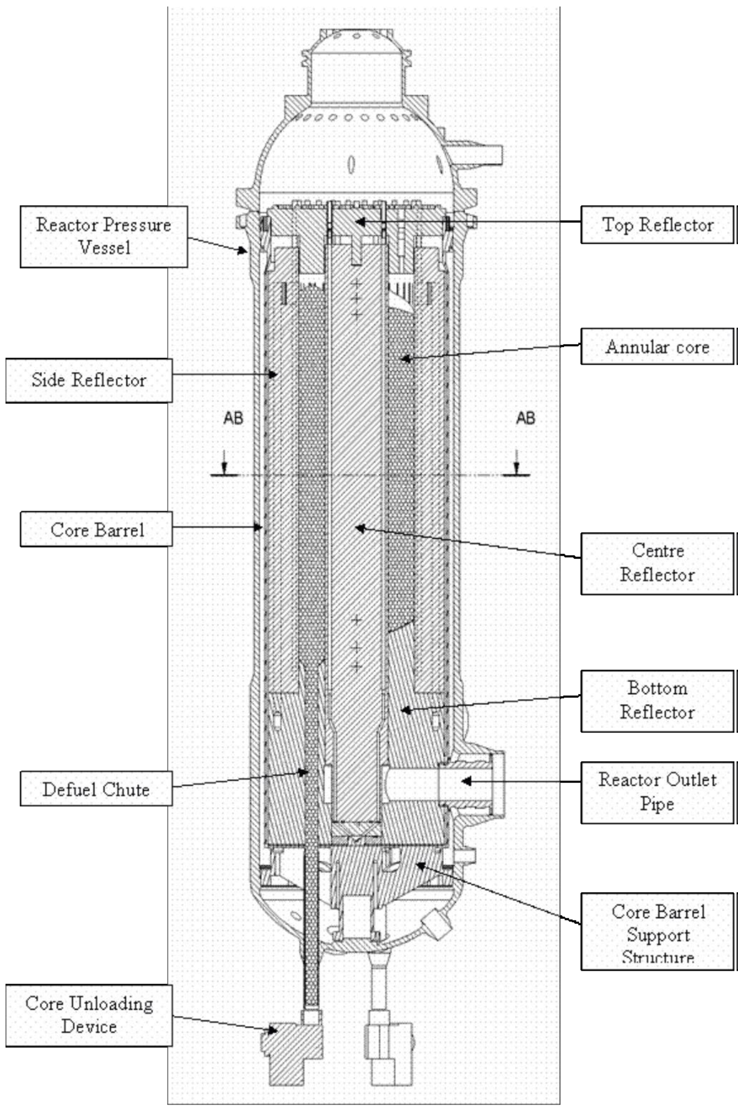

Figure 2. PBMR-400 core layout [2].

Table 1. Perturbation parameters of the fuel pebble and their ranges as selected for fuel depletion sensitivity studies using MCNP and SCALE

Parameter	Range	Distribution
Radial zone neutron energy spectrum	Following radial flow probability	Radial zone 1 is fast; radial zone 5 is thermal
Transit time	± 2 days	Uniform
Pebble power[+]	± 2%	Uniform
Temperature	± 10 K	Uniform
Initial ^{235}U enrichment[*]	± 0.1%	Uniform

[*] Variability in the initial ^{235}U enrichment was assumed to be consistent with that of the AGR5/6/7 fabrication [7].
[+] The power and temperature uncertainties were derived from the PBMR-400 accident analysis study [8].

2.1 MCNP FUEL BURNUP SIMULATIONS

In the MCNP model, a body-centered cubic (BCC) lattice with a pebble packing fraction of 61% was employed as illustrated in Figure 3. The TRISO microspheres were explicitly modeled and arranged using a rectangular lattice. The URAN feature of MCNP was activated to simulate the randomness of the TRISO locations in the pebble even though they were arranged in a rectangular lattice. Reflective boundary condition is used at all the six outer surfaces in this model. Fuel depletion calculations in MCNP were carried out at a temperature of 1,200 K for the base case using a core average specific power of 98.431 MWth/tHM, an average transit time of 152.4 days per pass, and a cooling time of 4.5 days between each pass. Even though only an infinite lattice model of the pebble was used in the simulation, the average axial core power distribution was incorporated in the model by varying the pebble power (kWth) per axial zone with a residence time 6.9269 days per axial zone. The average core axial power distribution considered to account for the varying power experienced by the pebble during its movement from the top to the bottom of the core is shown in Table 2. Multiple fuel depletion calculations were then performed by step variations of fuel temperature, neutron flux (power), ^{235}U enrichment, and pebble residence time to determine the variations in fuel burnup and residual content of U and Pu in the discharged pebbles. The number of starting neutron histories per neutron generation cycle was 10,000, and the total number of neutron generation cycles simulated was 250, with a skip of 50 cycles for stabilization, thus obtaining equilibrium of the infinite neutron multiplication factor, k_{inf}. The stochastic uncertainty in k_{inf} was less than 0.0005 in every simulation. The results of these MCNP simulations are presented in section 3.1.

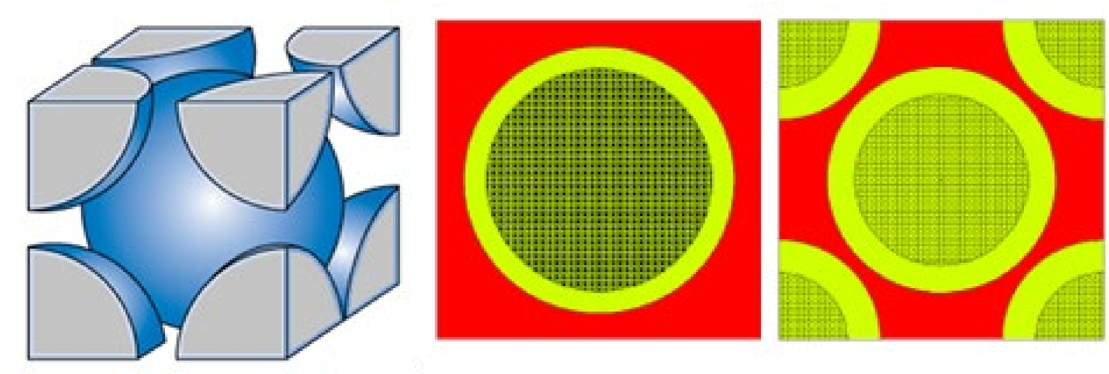

Figure 3. BCC pebble lattice model.

Table 2. Average core fuel pebble power (kWth) per axial zone; axial zone residence time 6.9269 days [4].

Axial Zone No.	Power (kWth)
1	0.6572
2	1.0742
3	1.6724
4	2.4480
5	3.0583
6	3.3824
7	3.4619
8	3.3564
9	3.1265
10	2.8251
11	2.4937
12	2.1619
13	1.8487
14	1.5644
15	1.3128
16	1.0941
17	0.9059
18	0.7447
19	0.6064
20	0.4868
21	0.3828
22	0.3140

2.2 SCALE/ORIGAMI FUEL BURNUP SIMULATIONS

The ORIGAMI sequence in SCALE 7.0 (beta version 8) was developed to rapidly model the depletion of flowing pebbles [9, 10]. Pebble depletion is conducted through axial (transit) zones, with each zone's radial characteristics considered, using the radial power shape, the radial pebble population distribution, and the radial zone library. Multiple passes can be simulated, with each pass defined by a transit history consisting of pebble power, residence time, cooling time, and a series of sequential transit zones, including the fractional irradiation time and the axial power factor. Therefore, SCALE/ORIGAMI can obtain the core average fuel composition by defining several radial channels in a transit history. Alternatively, it can evaluate the burnup and inventory of pebbles flowing through different channels, and other operating uncertainties can be analyzed by selecting a single radial channel in each transit history as applied in this and previous work [1].

Using the VSOP (Very Superior Old Programs) approach [3, 4], five radial flow zones (see Figure 4) were also considered in the SCALE/ORIGAMI simulation. Each channel has a unique neutron energy spectrum according to its temperature profiles and proximity to the graphite reflectors, as illustrated in Figure 5. The variations in neutron energy spectra are larger in the radial direction than in the axial direction. These variations are due to the typical radial reflector design and the slow movement of pebbles near the radial periphery of the core. The neutron energy spectra are softer in radial zones 1 and 5, which are next to the graphite reflectors, compared to the neutron energy spectra in channels 2, 3, and 4. Therefore, the ORIGEN library (in HDF5 format) for SCALE/ORIGAMI was produced using TRITON for each radial channel using an axial slice of the core model, depleting the fresh pebbles surrounded by the nondepleting pebbles at their average equilibrium compositions [9, 10, 11]. The nondepleting pebbles were defined in the model to obtain a representative neutron spectrum so as to generate spectrum dependent neutron cross sections. The library covers pebble and reflector temperatures of 700 K, 900 K, and 1,200 K and burnup ranging up to 100 GWd/tHM.

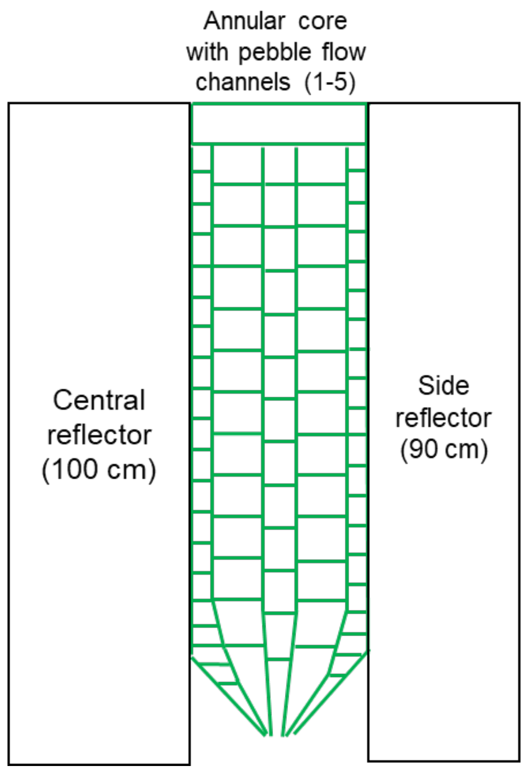

Figure 4. PBMR-400 VSOP model [3].

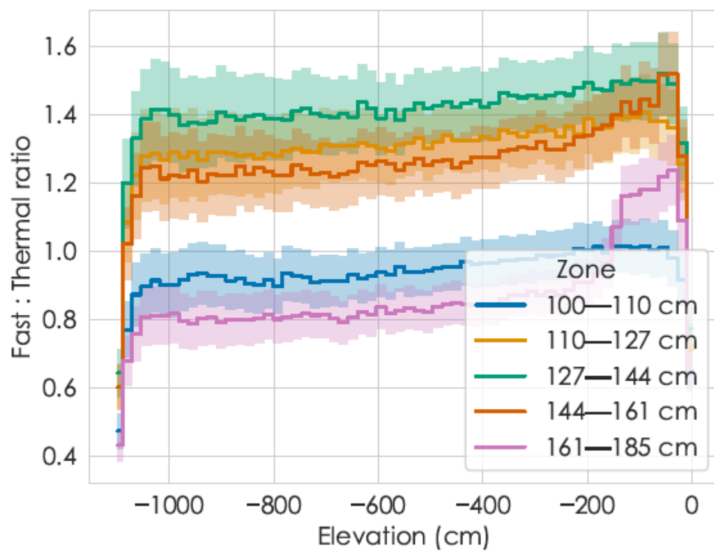

Figure 5. Fast-to-thermal neutron ratio in the five radial zones of PBMR-400 as a function of elevation for each channel [9].

A total of 20,000 pebble depletion calculations were performed using SCALE/ORIGAMI. It has to be noted that no differences were noticed on the quantities of interest between a 10,000 or 20,000 pebble depletion calculations. The VSOP approach for the residence time was also adopted in SCALE/ORIGAMI. The residence time of pebbles in the radial zones varies (143,751 days up to 221.156 days); for example, transit time in radial zones 1 and 5 (see Figure 4) is 54% longer than in channels 2, 3, and 4. The pebble passed through a random channel in each pass, and the probability of a pebble entering a radial channel was determined based on the volume fraction and velocity in the radial zone. The temperature distribution in each channel, as well as the axial and radial power profiles [3] used in the SCALE/ORIGAMI simulations, are shown in Figure 6. Additionally, a 4.5-day cooling time was considered after the end of each pass. Figure 7 illustrates a pebble's power history in each pass, to which perturbations (see Table 1) were added for the simulations conducted in this work.

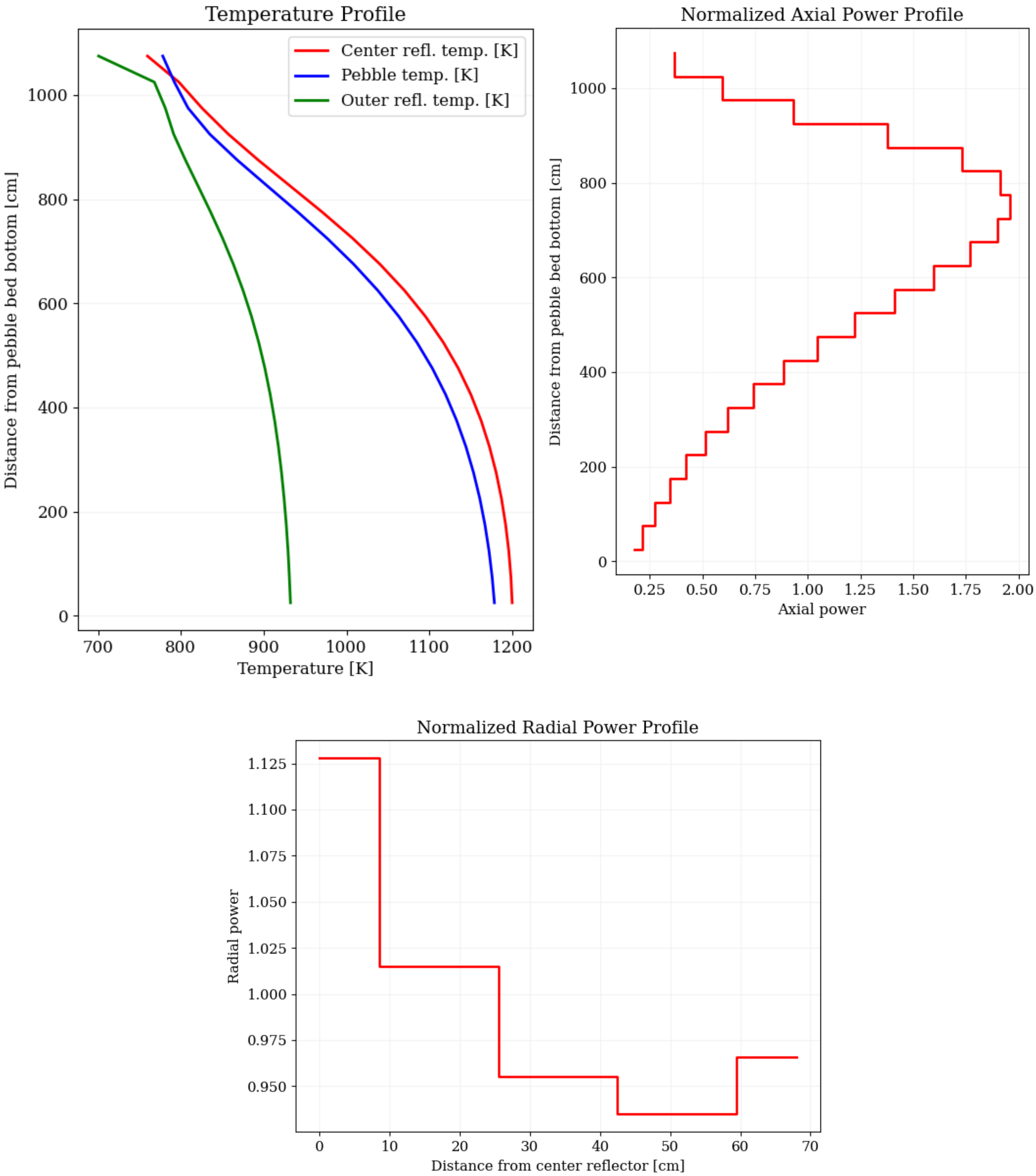

Figure 6. (a) Temperature distributions, (b) axial power profile, and (c) radial power profile used in SCALE/ORIGAMI.

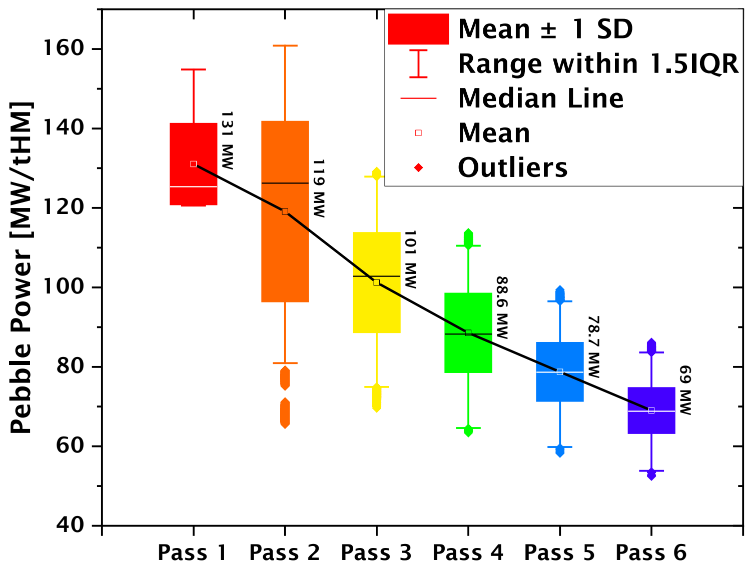

Figure 7. Simulated irradiation histories for all pebbles. ***IQR is interquartile range.***

3. RESULTS AND DISCUSSION

3.1 MCNP FUEL DEPLETION SIMULATION RESULTS WITH BCC PEBBLE LATTICE

Table 3 summarizes the sensitivity studies conducted using MCNP fuel depletion of the BCC pebble lattice model. The results demonstrate that the operating parameters have an effect on both ^{235}U consumption and the total Pu buildup. The step temperature perturbation in the MCNP depletion covers a wide range of temperatures, resulting in relatively large differences compared to those of the other perturbation cases.

The MCNP depletion results at a fuel temperature of 1,200 K, and with other nominal parameters of uranium enrichment (9.6 wt.% ^{235}U), transit time (152.3918 d/pass), and reactor power (100%), the results were also compared with those of the SCALE/TRITON-Shift [6] and Serpent 2.2 [12] BCC pebble lattice model with explicit TRISO microspheres. Figure 8 compares the k_{inf} among the three codes, showing an excellent agreement at 0 days. It should be noted that the reactivity control methods were not included in the simulation to maintain the neutron multiplication factor at 1.0. However, SCALE and Serpent agreed more than SCALE and MCNP in the burnup calculation. It is noted that SCALE did not calculate the k_{inf} value during cooling down between each pass. Meanwhile, the residual ^{235}U and total Pu content per pebble and fuel burnup at the last depletion time step are summarized in Table 4, indicating good agreement between the three codes.

Table 3. Residual masses of ^{235}U, total Pu, k_{inf}, and fuel burnup from MCNP BCC pebble lattice simulations

Parameter perturbed		k_{inf}	Residual ^{235}U per pebble (wt. %)	Pu content per pebble (mg)	Fuel burnup (GWD/tHM)
Fuel temperature					
	900 K (100% power)	1.00057	2.6	169.82	89.96
	1,200 K (100% power)	0.98394	3.0	175.19	89.96
Fuel temperature, 1,200 K					
Power	102%	0.97993	2.9	176.58	91.76
	98%	0.99010	3.1	173.79	88.16
Fuel temperature, 1,200 K					
Transit time	-2 days per pass	0.98188	3.0	176.11	91.14
	+2 days per pass	0.98816	3.1	174.33	88.78
Fuel temperature, 1,200 K					
Initial ^{235}U	9.7 wt.%	0.98694	3.1	175.69	89.96
enrichment	9.5 wt.%	0.98163	2.9	174.55	89.96
Average		**0.98664**	**3.0**	**174.55**	**89.96**
% Std. Dev.		**0.7%**	**5.7%**	**1.2%**	**1.3%**

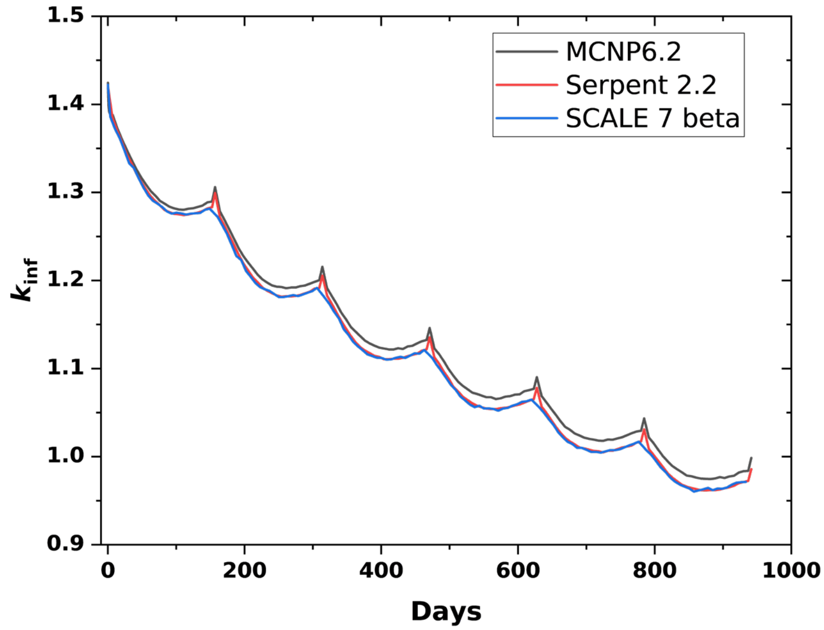

Figure 8. Comparison of k_{inf} from different codes for BCC pebble lattice at a fuel temperature of 1,200 K and 100% power.

Table 4. Residual masses of ^{235}U and total Pu from different codes for BCC pebble lattice simulations at the last depletion step

Codes	Residual ^{235}U per pebble (wt. %)	Pu content per pebble (mg)	Fuel burnup (GWD/tHM)
MCNP 6.2	3.0	175.19	89.96
Serpent 2.2	3.03	179.19	89.93
SCALE 7 beta	3.01	179.51	89.92

3.2 SCALE/ORIGAMI FUEL BURNUP SIMULATION RESULTS

3.2.1 Fuel Burnup and Pu Estimations

Discharge burnup distributions and the isotopic compositions of pebbles were evaluated using all simulated cases. After each pass, pebbles were filtered based on a burnup limit of 85.5 GWd/tHM in the fuel burnup monitoring system. Pebbles reaching this limit were retired or permanently discharged, whereas those below the limit were recirculated. Consequently, although the average number of passes is six, some pebbles may have been retired earlier if their fuel burnup exceeded the set point, as shown in Figure 9(a), in which a very small fraction (0.03%) of the pebbles were retired after four passes. However, 2.7% of the pebbles had to go through seven passes to reach the set burnup because of their respective flowing paths. This approach yielded an average fuel burnup of the retired pebbles at 90.048 ± 3.266 GWd/tHM. Distribution of cumulative burnup after each pass with the perturbations given above is shown in Figure 9(b).

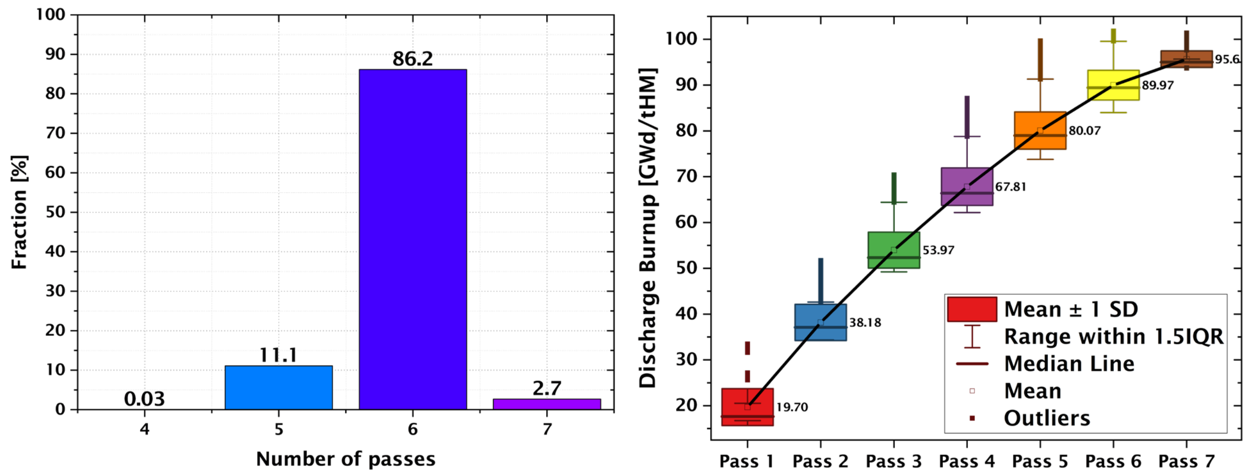

Figure 9. (a) Fraction of retired pebbles, (b) pebble discharge burnup distribution.

Table 5 and Figure 10 summarize the average and maximum mass values of ^{239}Pu and total Pu in the pebbles for each pass and at discharge. The retired pebbles only include those after passes 4, 5, 6, and 7 that had reached the burnup set point.

Table 5. Average and maximum mass values of ^{239}Pu and total Pu in a pebble as a function of fuel pass

Pass	Avg. ^{239}Pu Mass (mg)	Max. ^{239}Pu Mass (mg)	Avg Pu Mass (mg)	Max. Pu Mass (mg)
1	34.7 ± 1.8	37.9	43.5 ± 2.6	49.7
2	45.4 ± 3.6	49.7	71.2 ± 2.8	76.6
3	48.1 ± 4.3	52.6	89.5 ± 3.3	95.1
4	48.4 ± 4.7	53.2	102.6 ± 4.0	108.8
5	48.2 ± 4.6	53.1	112.7 ± 4.2	119.5
6	48.0 ± 4.5	52.8	120.5 ± 4.2	127.7
7	48.1 ± 4.6	52.5	126.1 ± 4.4	131.7
Retired	47.3 ± 5.0	53.0	119.3 ± 6.0	131.7

When MCNP result of the residual total mass of total Pu (175 mg) is compared with the detailed SCALE/ORIGAMI result (125 mg, average of 20,000 pebbles tracked), it can be inferred that the MCNP results is conservative from an MC&A perspective. This conservative value was obtained from the MCNP simulations that was performed using average values of initial ^{235}U enrichment and other reactor parameters (temperature, pebble residence time, neutron flux, neutron energy spectrum). This discrepancy stemmed from the neutron energy spectrum difference to obtain the one-group depletion cross section. SCALE/ORIGAMI used the neutron energy spectrum at the average core composition of each channel. In contrast, MCNP used the depleted pebbles' neutron energy spectrum to collapse the one-group cross section. In addition, the minor differences in modeling approaches between MCNP and SCALE also contributed to this discrepancy, for e.g., depletion in non-critical condition vs. critical depletion, with and without the use of equilibrium isotopics in the "other" pebbles.

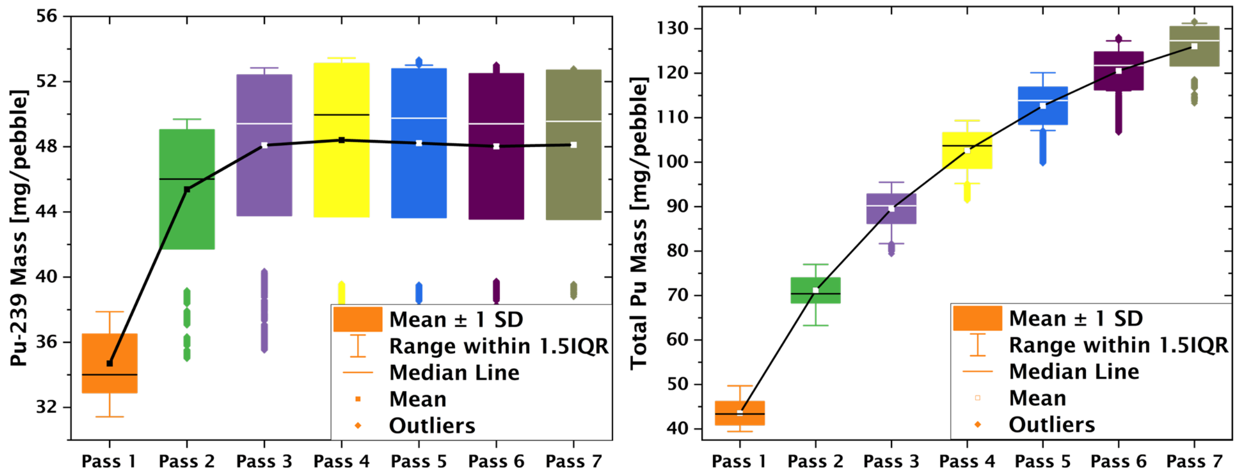

Figure 10. Average and maximum mass of (a) ^{239}Pu and (b) total Pu in a pebble as a function of fuel pass.

3.2.2 ^{239}Pu Mass Change Caused by Nuclear Data Uncertainty

The *sensitivity coefficient*, defined as the relative change in the mass of isotope (^{239}Pu) caused by a variation in nuclear data, was calculated using ORIGEN based on the depletion perturbation theory. This method allows for the evaluation of how sensitive the mass of ^{239}Pu is to changes in specific nuclear reactions. Table 6 presents the sensitivity coefficients for ^{239}Pu in a PBMR-400 pebble across five distinct radial zones. The results of this perturbation study led to the following conclusions.

- The buildup of ^{239}Pu increases by 0.94% if the ^{238}U (n,γ) neutron cross section increases by 1%
- The buildup of ^{239}Pu decreases by 0.37% if the ^{239}Pu (n,γ) neutron cross section increases by 1%
- The buildup of ^{239}Pu decreases by 0.60% if the ^{239}Pu (n,f) neutron cross section increases by 1%

Table 6. Sensitivity coefficients of ^{239}Pu in PBMR-400 Pebble for each nuclear reaction of interest.

Isotope	Reaction	Radial Channel 1	Radial Channel 2	Radial Channel 3	Radial Channel 4	Radial Channel 5
^{238}U	**(n,γ)**	**9.44** × 10^{-1}	**9.37** × 10^{-1}	**9.35** × 10^{-1}	**9.38** × 10^{-1}	**9.46** × 10^{-1}
^{238}Pu	(n,γ)	1.12 × 10^{-3}	8.74 × 10^{-4}	8.15 × 10^{-4}	8.81 × 10^{-4}	1.11 × 10^{-3}
^{236}U	(n,γ)	1.00 × 10^{-3}	7.27 × 10^{-4}	6.67 × 10^{-4}	7.37 × 10^{-4}	1.00 × 10^{-3}
^{235}U	(n,γ)	9.80 × 10^{-4}	7.17 × 10^{-4}	6.60 × 10^{-4}	7.26 × 10^{-4}	9.81 × 10^{-4}
^{237}Np	(n,γ)	8.52 × 10^{-4}	6.29 × 10^{-4}	5.80 × 10^{-4}	6.39 × 10^{-4}	8.57 × 10^{-4}
^{241}Pu	β^-	2.95 × 10^{-4}	2.52 × 10^{-4}	2.39 × 10^{-4}	2.52 × 10^{-4}	2.89 × 10^{-4}
^{240}Pu	(n,γ)	1.90 × 10^{-4}	1.59 × 10^{-4}	1.50 × 10^{-4}	1.61 × 10^{-4}	1.89 × 10^{-4}
^{242}Cm	α	1.66 × 10^{-4}	1.42 × 10^{-4}	1.35 × 10^{-4}	1.42 × 10^{-4}	1.64 × 10^{-4}
^{241}Am	(n,γ)	1.62 × 10^{-4}	1.50 × 10^{-4}	1.46 × 10^{-4}	1.50 × 10^{-4}	1.62 × 10^{-4}
^{238}U	(n,f)	-2.06 × 10^{-4}	-2.28 × 10^{-4}	-2.31 × 10^{-4}	-2.26 × 10^{-4}	-1.80 × 10^{-4}
^{235}U	(n,f)	-2.18 × 10^{-4}	-1.38 × 10^{-4}	-1.22 × 10^{-4}	-1.42 × 10^{-4}	-2.25 × 10^{-4}
^{239}U	β^-	-2.30 × 10^{-4}	-1.85 × 10^{-4}	-1.75 × 10^{-4}	-1.90 × 10^{-4}	-2.38 × 10^{-4}
^{239}Np	(n,γ)	-1.44 × 10^{-3}	-1.34 × 10^{-3}	-1.33 × 10^{-3}	-1.36 × 10^{-3}	-1.49 × 10^{-3}
^{239}Np	β^-	-3.11 × 10^{-2}	-2.48 × 10^{-2}	-2.33 × 10^{-2}	-2.55 × 10^{-2}	-3.21 × 10^{-2}
^{239}Pu	**(n,γ)**	**-3.66** × 10^{-1}	**-3.67** × 10^{-1}	**-3.66** × 10^{-1}	**-3.66** × 10^{-1}	**-3.64** × 10^{-1}
^{239}Pu	**(n,f)**	**-6.02E-01**	**-6.00E-01**	**-5.99E-01**	**-6.01E-01**	**-6.03E-01**

3.2.3 Correlation Matrices

The Pearson correlation matrices between the operating parameters and the responses were constructed using the 20,000 depletion samples. These matrices include fuel burnup, ^{235}U consumption, ^{239}Pu, and total Pu buildup at each pass.

The residence time demonstrates a strong positive correlation with fuel burnup (see Figure 11) and a strong negative correlation with the ^{235}U consumption (see Figure 12). As defined herein, fuel burnup increased linearly with residence time, leading to higher ^{235}U consumption. The correlation between residence time and fuel burnup weakened from the second to the sixth pass, as did the correlation with ^{235}U consumption in these passes. These observations are attributed to pebbles flowing through different radial channels during each pass; only 15% of the pebbles traveled through the channels adjacent to the reflector (radial channels 1 and 5), which have about 54% longer residence time than the other radial channels. However, in the seventh pass, residence time showed a strong positive correlation with fuel burnup and a strong negative correlation with ^{235}U consumption because most pebbles have a uniform fuel burnup range of 80.0 to 85.5 GWd/tHM.

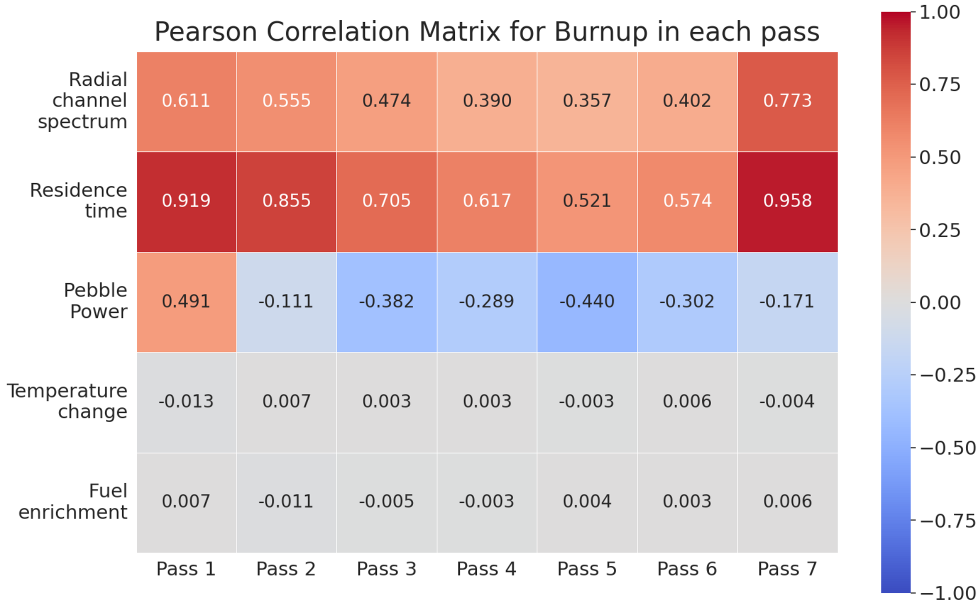

Figure 11. Correlation between perturbed parameters and fuel burnup at each pass.

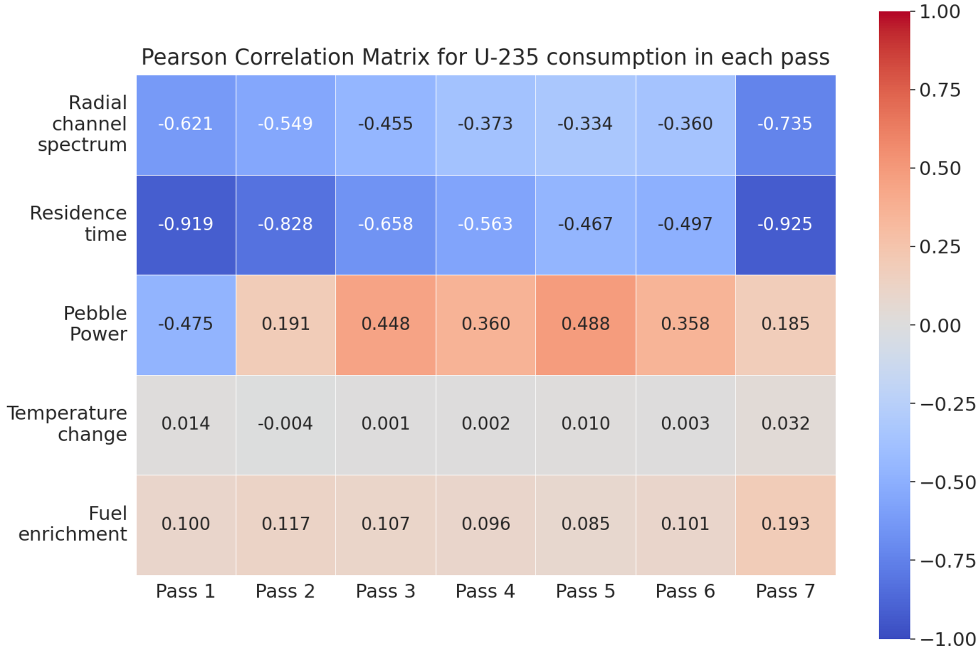

Figure 12. Correlation between perturbed parameters and ^{235}U consumption at each pass.

The radial channel neutron energy spectrum depicted in the plots (Figs. 5 and 6) characterizes the thermal neutron energy spectrum of the radial channel. This thermal neutron energy spectrum indirectly impacts fuel burnup and ^{235}U consumption because most thermal channels are situated near the reflector wall, which has a longer residence time. Additionally, a thermalized channel increases the neutron reaction rate of ^{235}U. Interestingly, pebble power showed a positive correlation with fuel burnup in the first pass but shifted to a negative correlation in subsequent passes, whereas the correlation with ^{235}U consumption exhibited the opposite trend. This shift is attributed to the decreasing power of the pebble at each pass as fissile material is consumed.

The buildup of ^{239}Pu demonstrates a strong negative correlation with the residence time, with the next strongest correlation being the radial channel spectrum, as shown in Figure 13. These correlations increased with each pass and eventually reached saturation, mirroring a similar trend observed in the ^{239}Pu buildup, as illustrated in Figure 10(a). A longer residence time and a softer neutron energy spectrum reduce the buildup of ^{239}Pu. However, concurrently, ^{239}Pu is continuously produced through the absorption of ^{238}U, ultimately leading to its saturation. The pebble power showed a positive correlation in the first pass, but it decreased in subsequent passes because of the decreasing power.

Figure 14 and Figure 10(b) illustrate the relationship between operating parameters and total Pu buildup, as well as the Pu buildup at the end of each pass, respectively. Initially, residence time and pebble power exhibit positive correlations during the first pass resulting from the absence of Pu in the reactor. However, in subsequent passes, residence time shows negative correlations, indicating that longer residence times reduce total Pu buildup. Meanwhile, the correlation of pebble power becomes less pronounced in the subsequent passes for reasons similar to those observed in the ^{239}Pu buildup. Conversely, the thermal neutron energy spectrum consistently shows negative correlations in each pass, suggesting that a softer neutron energy spectrum consumes more Pu.

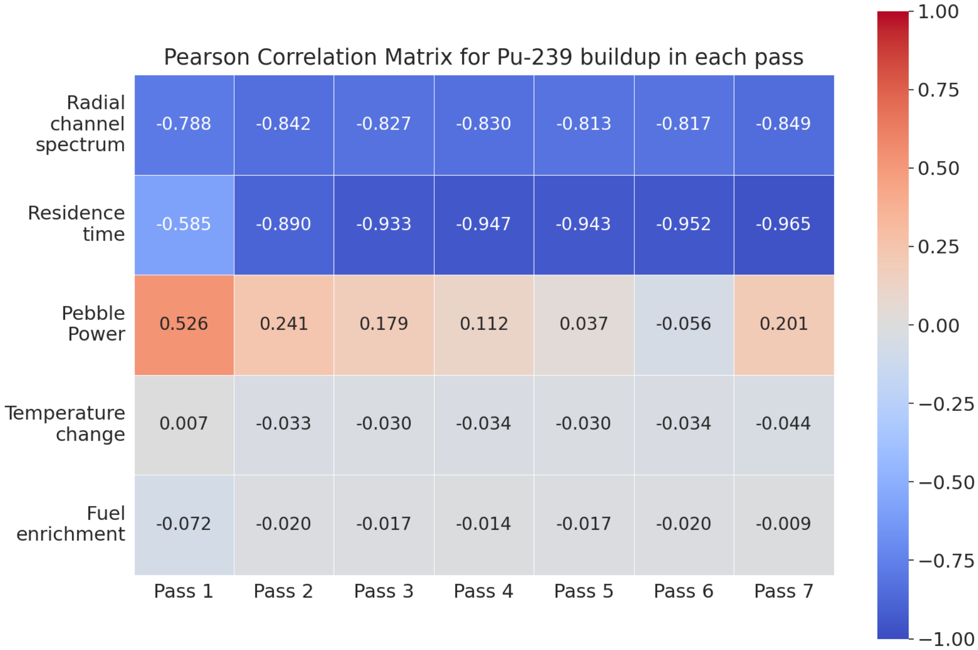

Figure 13. Correlation between perturbed parameters and ^{239}Pu buildup at each pass.

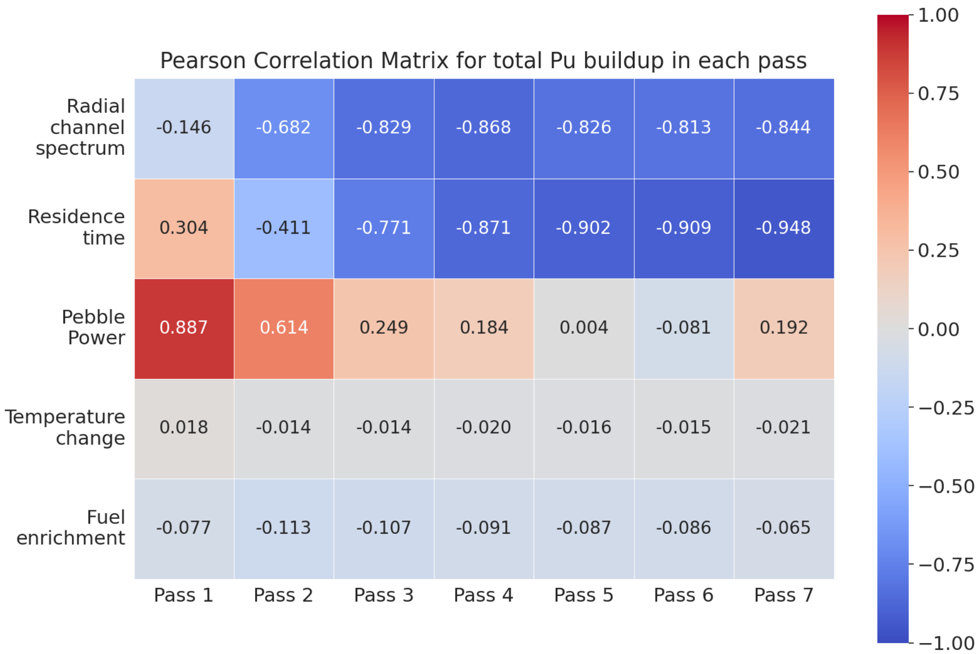

Figure 14. Correlation between perturbed parameters and total Pu buildup at each pass.

Temperature change and fuel enrichment exhibited the least influence on the responses among the perturbed operating parameters. Additionally, Figures 15 through 20 show the Pearson correlation matrices for pebbles in all six passes.

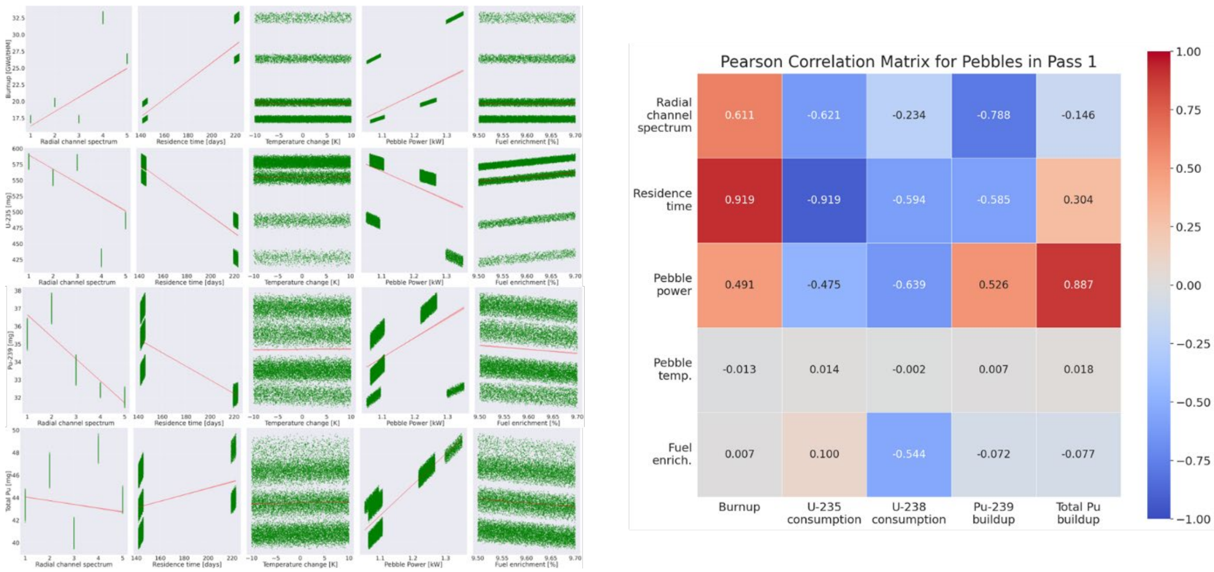

Figure 15. Data points and correlation matrix for pebbles in pass 1.

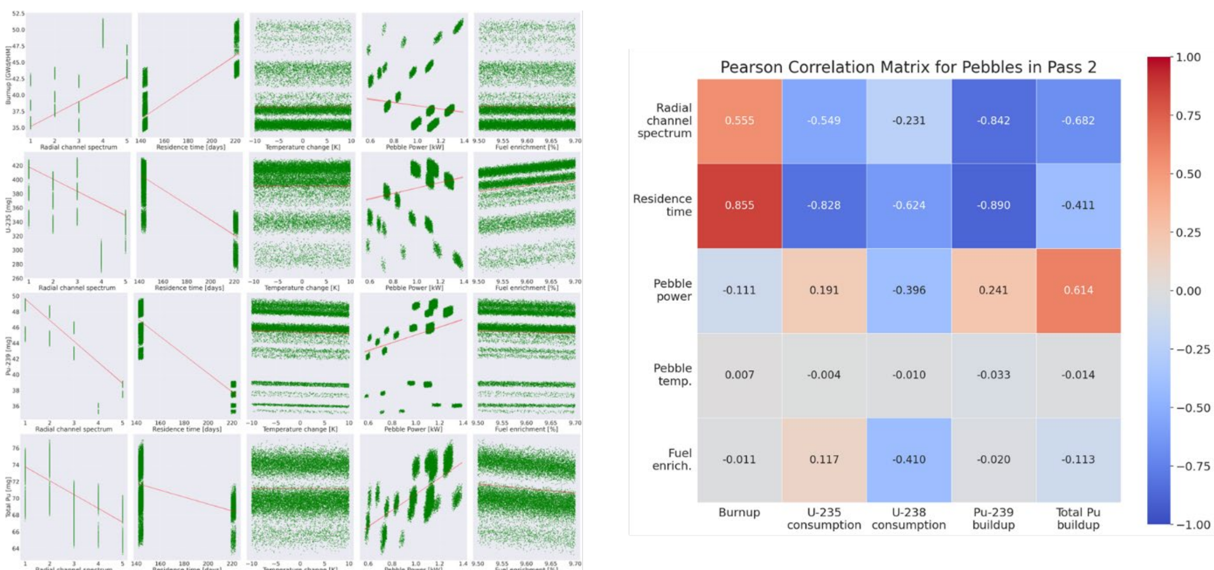

Figure 16. Data points and correlation matrix for pebbles in pass 2.

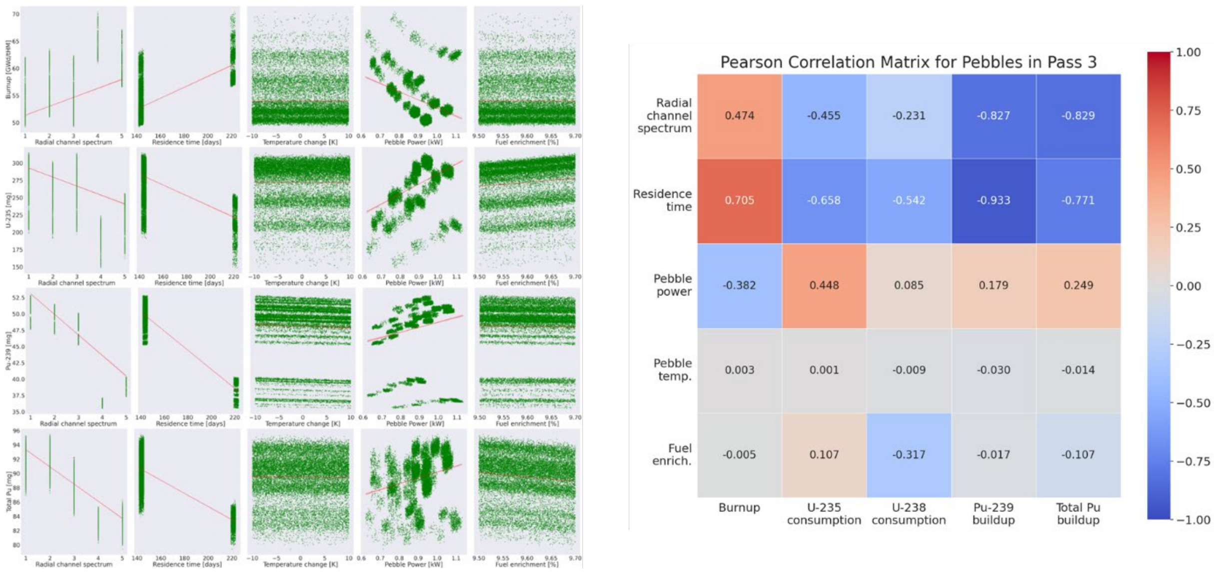

Figure 17. Data points and correlation matrix for pebbles in pass 3.

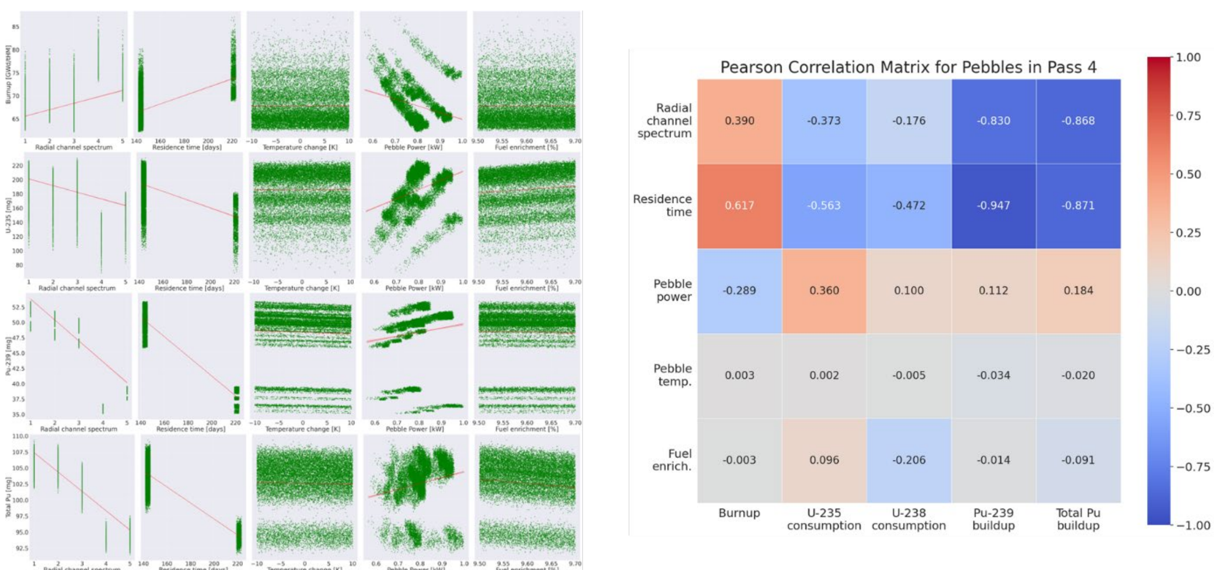

Figure 18. Data points and correlation matrix for pebbles in pass 4.

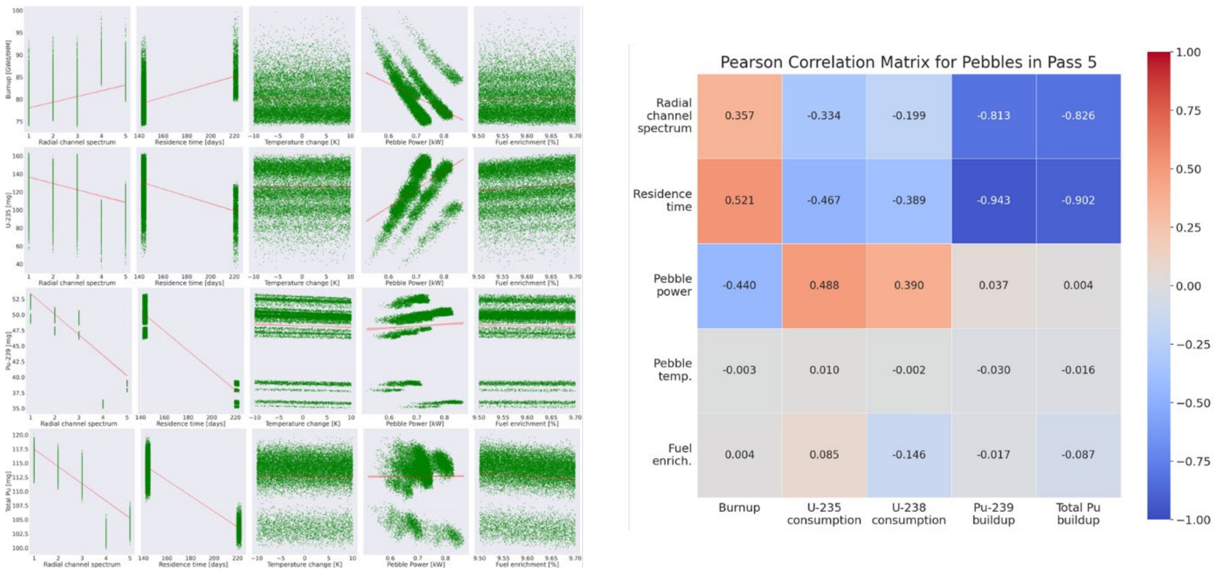

Figure 19. Data points and correlation matrix for pebbles in pass 5.

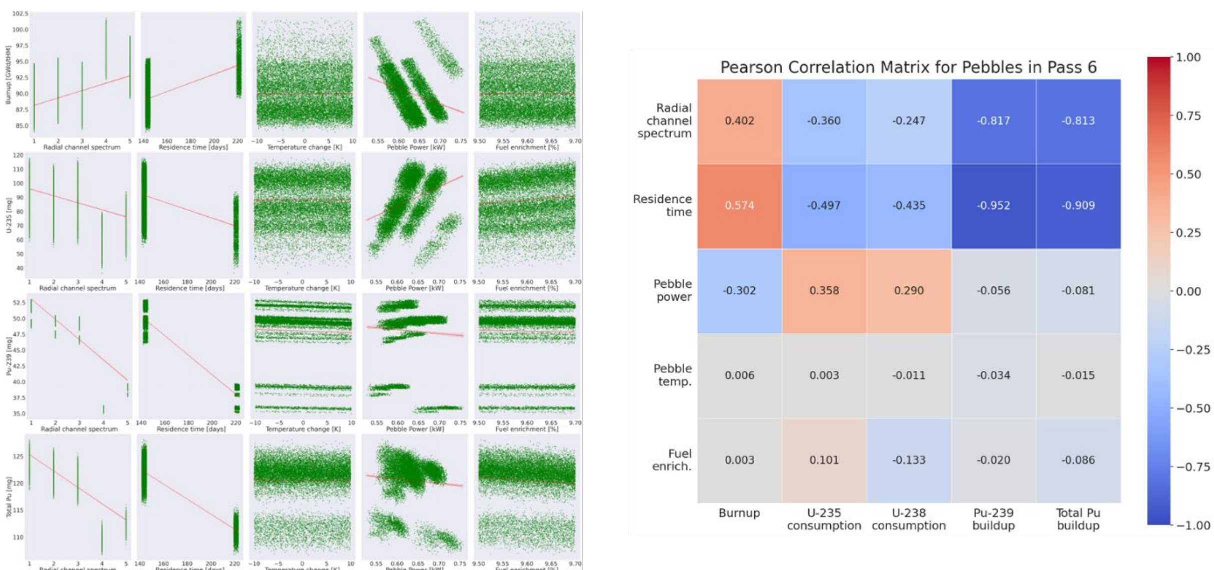

Figure 20. Data points and correlation matrix for pebbles in pass 6.

4. CONCLUSIONS

Fuel burnup simulations of a representative PBR fuel pebble (PBMR-400 fuel pebble) were performed using neutronics codes. This study used MCNP6.2 and SCALE/ORIGAMI to perform fuel burnup simulations to explore the sensitivity of a set of PBR operating parameters (neutron flux and neutron energy spectra, pebble residence or transit time, pebble power, fuel temperature, and initial ^{235}U enrichment) on fuel burnup, the buildup of Pu (total Pu and ^{239}Pu), and residual ^{235}U enrichment in a PBMR-400. The initial comparison using a BCC lattice pebble configuration showed strong agreement between the MCNP and SCALE/TRITON predicted quantities—k_{inf}, fuel burnup, and residual fissile content for the parametric study conducted. The residual enrichment of ^{235}U predicted by both MCNP and SCALE/TRITON codes was found to be similar. Detailed SCALE/ORIGAMI simulations on various parametric sensitivities showed a maximum variation of about ±10 mg Pu per pebble when considering one standard deviation (σ).

MCNP results were found to be conservative compared with the detailed SCALE/ORIGAMI simulations with respect to MC&A, especially for the MCNP simulations performed using average values of initial ^{235}U enrichment and other reactor parameters (temperature, pebble residence time, neutron flux, neutron energy spectrum). For example, as predicted by MCNP using the average reactor parameters and considering only one pebble in the simulation, the mass of total Pu is 175 mg compared to the 125 mg predicted by the detailed SCALE/ORIGAMI simulations, which tracked 20,000 pebbles. This discrepancy stemmed from the neutron energy spectrum difference to obtain the one-group depletion cross section. SCALE/ORIGAMI used the neutron energy spectrum at the average core composition of each channel. In contrast, MCNP used a dynamic neutron energy spectrum for each burnup time step to collapse the cross-section using 63 groups used in its depletion module CINDER90.

Based on the SCALE/ORIGAMI simulations, it was found that parameters such as pebble residence time, radial channel neutron energy spectrum, and pebble power exhibited correlations with responses such as fuel burnup, ^{235}U consumption, buildup of ^{239}Pu, and total Pu. The most sensitive parameters to fuel burnup and Pu production are the pebble residence or transit time and the neutron energy spectrum in the radial channel. These two parameters are applied in the simulations by grouping the pebbles into several radial flow channels and axial meshes of each radial channel, stressing the need for an accurate definition of the radial channels and axial meshes. These definitions can be guided by using experiments or discrete element modeling and simulation. However, fuel temperature and fuel enrichment perturbations in the range of ± 10 K and ± 0.1%, respetively had negligible influences on the responses such as, residual ^{235}U enrichment and total residual Pu mass in the permanently discharge pebble. Furthermore, the correlation of perturbed parameters with the response is unique in each pass because the pebbles flow through different (random) channels at each pass.

The differences in Pu masses caused by variability in operational parameters and the resulting fuel burnup and residual fissile content in pebbles manifest themselves to impact MC&A and nuclear safeguards, specifically in shipper/receiver difference or the difference between the declared mass value and the measured mass value during verification. Differences in Pu and the corresponding masses of residual fission products can also impact radiation dose calculations and, therefore, nuclear safety and security.

At the beginning of the reactor's life, fissile content is estimated based mostly on fuel burnup simulations and a few fuel burnup measurements, which are expected to be reasonable. However, these estimations can be improved when experience is gained from reactor operation and when attention is paid to the most sensitive parameters identified that affect fuel burnup and residual fissile content in the discharged pebbles. This type of understanding of parametric uncertainties and their effects can inform PBR modelers and designers regarding where improvements should be targeted to obtain more accurate values for the parameters of interest in the discharged pebbles. Uncertainty estimation can support MC&A of discharged pebbles stored in used fuel canisters.

Future work could involve conducting similar analyses for the PBRs considered in the Advanced Reactor Demonstration Program, such as the Xe-100 [12]. Other future work to be considered includes adding more perturbed parameters, such as the number of TRISO particles in a pebble or exploring the variability in fuel and graphite densities of pebbles. The utility of modern data science approaches could also be explored for this application.

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