

Modeling and Simulation of Fuel Burnup in Pebble Bed Reactors

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Abstract

Modeling and simulation of fuel burnup plays important roles in reactor design, operation, safety, and security as well as nuclear material control and accounting (MC&A) [1]. This task is uniquely challenging for pebble bed reactors (PBR) because the pebbles are continuously added and recycled into the reactor core, and their paths through the core are random. To address this problem, we present two simulation models in this paper. Brookhaven National Laboratory (BNL) developed a simple lattice model of a PBR in Serpent software to generate used pebble isotopic concentrations. The benefit of using Serpent software in this specific application is that it helps streamline the data generation process without having to use too many independent software codes in combination to achieve a simple task. For example, transport, burnup and zero power decay can be implemented in a single pass. Three-dimensional core models were developed using Serpent to simulate the burnup process of five subject pebbles starting from fresh till they reach nearly target burnup, with each pebble placed in one of the five artificially designated radial channels to capture the changing neutron spectra along the core radius. Equilibrium isotopic concentrations were assumed in all other pebbles in the core. To provide a verification for the Serpent isotope transmutation and decay results, Oak Ridge National Laboratory (ORNL) performed simple SCALE/ORIGEN calculations using the average neutron spectra calculated by Serpent for each of the five pebbles. The 252-group neutron spectra from Serpent were then used by ORIGEN to produce the one-group library for depletion and decay calculations. The isotopic concentrations of a few nuclides of interest and neutron and gamma source terms produced from the ORIGEN calculations were compared with the ones from the Serpent calculations. The model simulated in this work was based on the Pebble Bed Modular Reactor (PBMR)-400 design because many data needed for the simulation such as core power profiles, fuel and reflector temperatures, and equilibrium core composition are publicly available. In this paper, we will compare the results between these two approaches and benchmark the results against a set of well-established simulation results for PBMR-400.

Introduction

The PBMR-400 is a generation IV advanced nuclear reactor which operates on pebble-type fissile fuels. The annular core of the reactor is filled with these pebbles which are progressively burnt to generate power and are later discharged from the core. On average a pebble might get recycled 5 – 8 times back into the core over the reactor’s operational lifetime (each cycle takes about 100 - 200 days depending on the pebble’s path and location in the core). At the end of each cycle the pebbles are typically measured using Non-Destructive Assay (NDA) techniques to determine how much burnup the pebble has accrued and if the pebble should be recycled or considered as spent fuel. This process can be time consuming and inaccurate owing to the limited time of ejection of the pebbles from and operating core the combined high background environments and shielding effects of an operating core. BNL attempted to study the potential of using a machine learning (ML) algorithm to do this and had seen some promising outcomes [2]. However, the Serpent model which was used to facilitate the generation of the spectra data was highly simplistic and basically provided a means to generate unique spectra for specific burn levels. These spectra were not true to any region or location of the core and hence may not be a fair representation of operational reactor or experimental data. Regardless, Serpent still provides functionality to model more realistic and complete reactor systems with the potential of automation of various features using patch scripts. The SCALE/ORIGEN code, developed and maintained by ORNL, has been extensively used to perform burnup calculations for light water reactor (LWR) fuels and non-LWR fuels. [3] For this reason, BNL partnered with ORNL to benchmark the burnup results of the newly developed full core model of the PBMR-400 in Serpent.

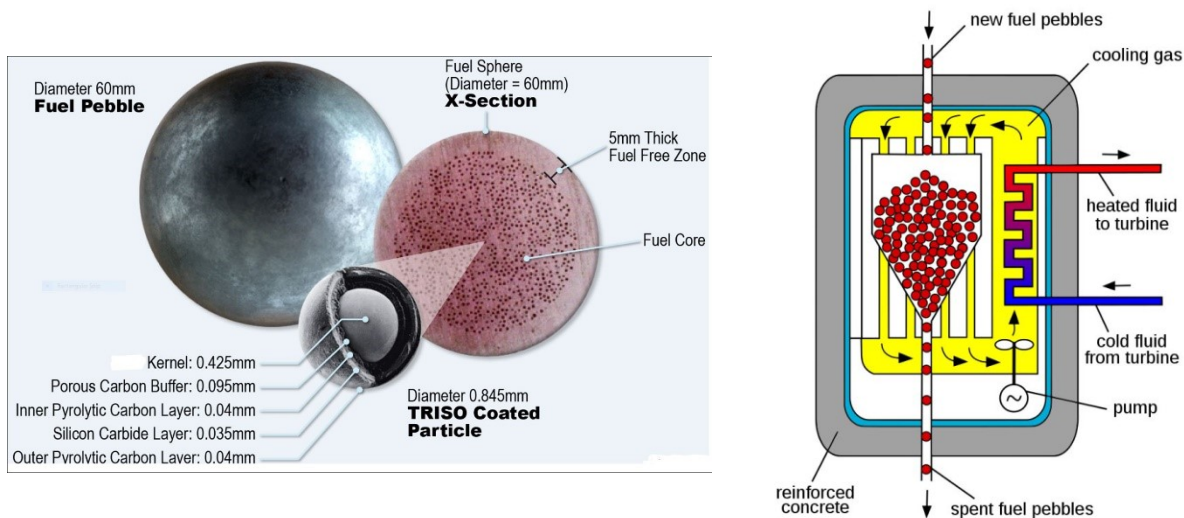


Figure 1: (a) Description of the pebble internals, (b) A generic pebble bed reactor

Methodology

To compare the results obtained in the two codes, BNL and ORNL established a few reactor metrics over which the comparison would be made. First, a depletion and decay stepping were agreed on which would be comparable between both codes. Table 2 shows the cumulative depletion steps and decay steps used for the simulation.

The parameters used in both models are based on the data described in Table 1 below.

Table 1: Parameter used for developing Serpent model.

	Parameter	Value	Units
	Fissile material	UO ₂	-
	Fuel pebble diameter	6.0	cm
	Outer pebble shell	0.5	cm
	Radius of fissile region	0.0025	cm
	Heavy metal content per pebble	9.0	g
	Fuel enrichment	9.6	%
	Number of TRISO particles	15,000	-
	Number of pebbles	451,527	-
	TRISO layer dimensions	0.0095/0.0040/0.0035/0.004	cm
	TRISO layer densities	1.05/1.90/3.18/1.90	g/cm ³
	Control rod material	B ₄ C	-

Table 2: Depletion and cooling times used for simulations.

	Depletion	Units	Cooling (cum)	Units	Cooling(abs)	Units
	1.00	day	931.554174	days	15.00	seconds
	5.00	days	931.554868	days	75.00	seconds
	10.00	days	931.561812	days	11.25	minutes
	30.00	days	931.582625	days	41.25	minutes
	60.00	days	931.624310	days	1.69	hour
	90.00	days	931.832640	days	6.69	hours
	120.00	days	932.249310	days	16.69	hours
	155.259	days	933.249310	days	1.70	day
	310.518	days	937.449300	days	5.90	days
	465.777	days	943.699310	days	12.15	days
	621.036	days	973.699310	days	42.15	days
	776.295	days	1338.69930	days	407.15	days
	931.554	days				

A total of 13 depletion steps and 12 decay steps were used for the simulation. The cooling steps of the simulation were defined as decay only to save the unnecessary time used by Serpent in performing transport after each cooling step. Five special pebbles which would be in each of the five artificially designated but commonly used radial channels of the core were selected. The boundaries of these five radial channels were defined as 100, 109, 135, 150, 176 and 185 cm radii. The simulation in Serpent was performed to achieve a core average burnup of about 90 GWd/MTU. When this is done, the average neutron spectra and power in each of the five pebbles were extracted from the Serpent results and provided to ORIGEN. The 252-group neutron spectra from Serpent were then used by ORIGEN to produce the one-group library needed for depletion and decay calculations. This approach aimed to verify Serpent's isotopic transmutations and decay results. This approach also eliminated the need to build a 3D core model in SCALE and is consistent with the Serpent model and the potential discrepancies in neutron spectra between the Serpent and SCALE results, although 3D SCALE models exist for PBMR-400 [4]. The isotopic concentrations of a few nuclides of interest and neutron and gamma source terms produced from the ORIGEN calculations were compared with the ones from the Serpent calculations.

There are two stages of simulation in Serpent; the burnup and decay phase is where the transient compositions, spatial and local power as well as 252 group fluxes are tallied. The second phase uses the reactor state at the steps corresponding to cooling times in Table 2 to start a source transport simulation which is used to determine the 25-group gamma and 21-group neutron emission spectra after the specified cooling period elapses. Both phases of the Serpent simulation were performed with about 5 million neutron histories (this is possible because Serpent provides functionality to resume a simulation based on a previous run using pre-generated binary files). The highest uncertainty in all result was recorded in the pebble fluxes. The bin uncertainties were in the order of 10 - 20 %.

Results

Three sets of results were obtained in this work; they are the neutron and gamma emission rate and the composition of specific isotopes known to contribute strongly to the neutron and gamma rates.

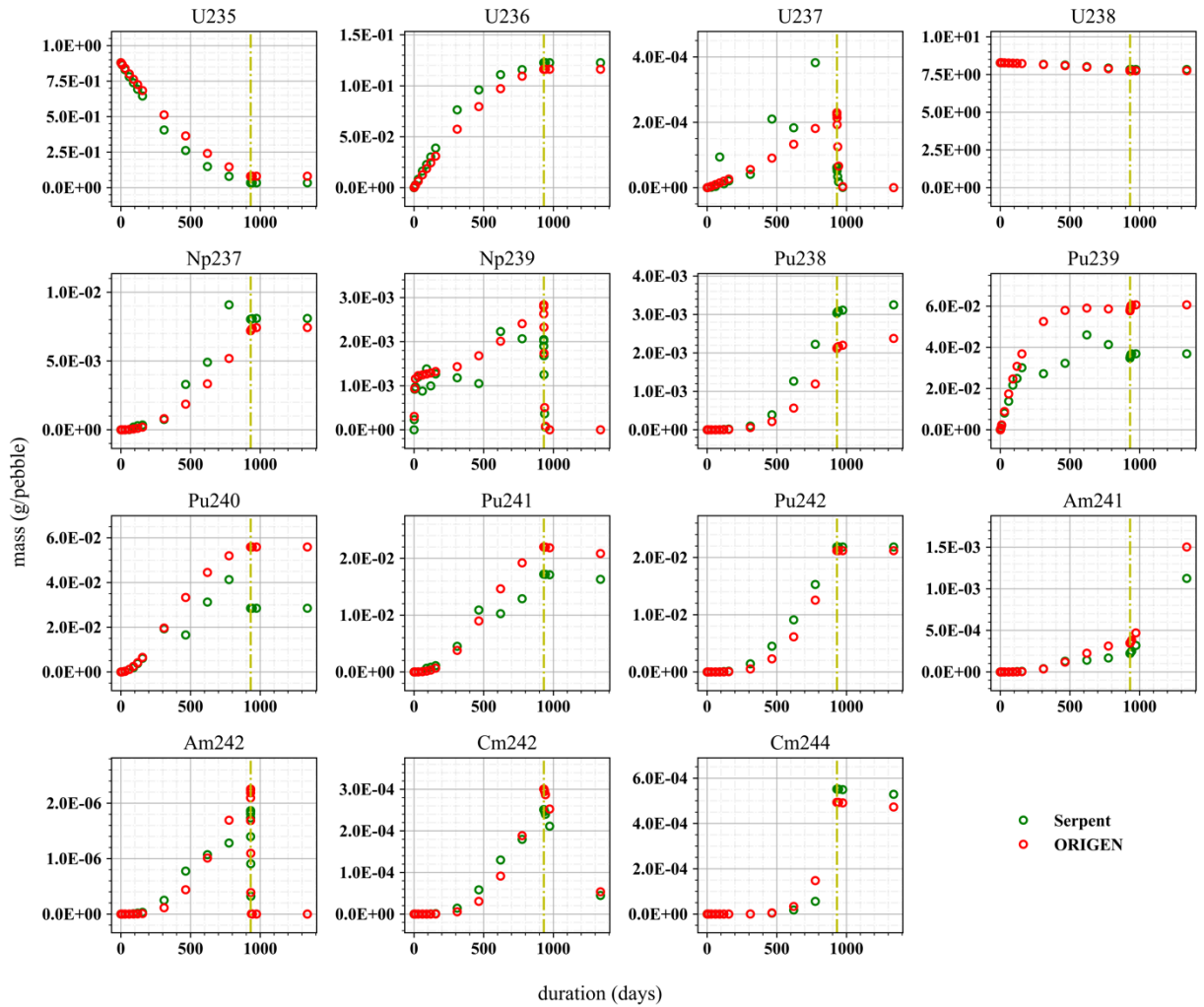


Figure 2: Fission product comparison between ORIGEN (SCALE) and Serpent in radial zone 2

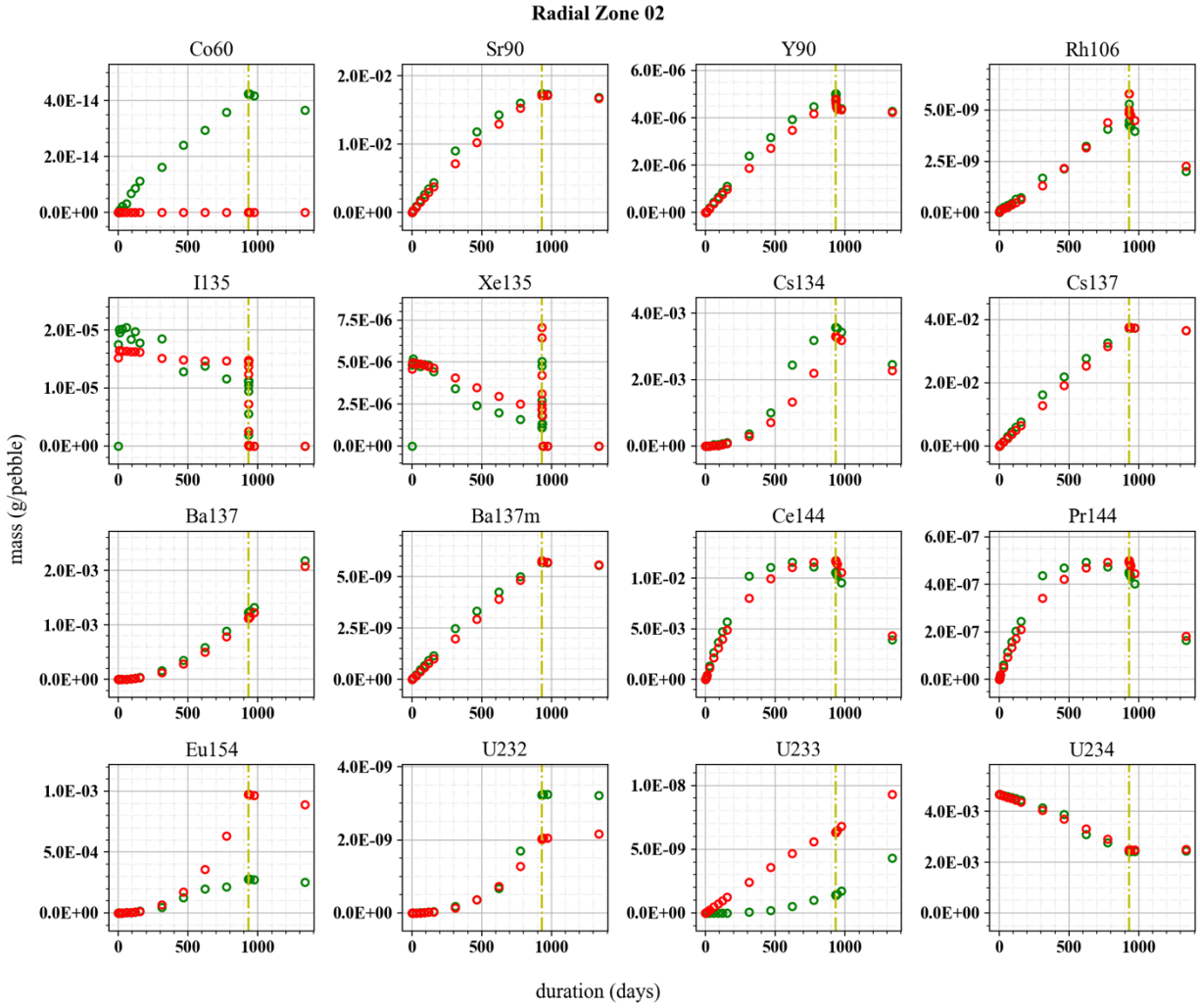


Figure 3: Fission product comparison between ORIGEN (SCALE) and Serpent in radial zone 2 (Cont'd)

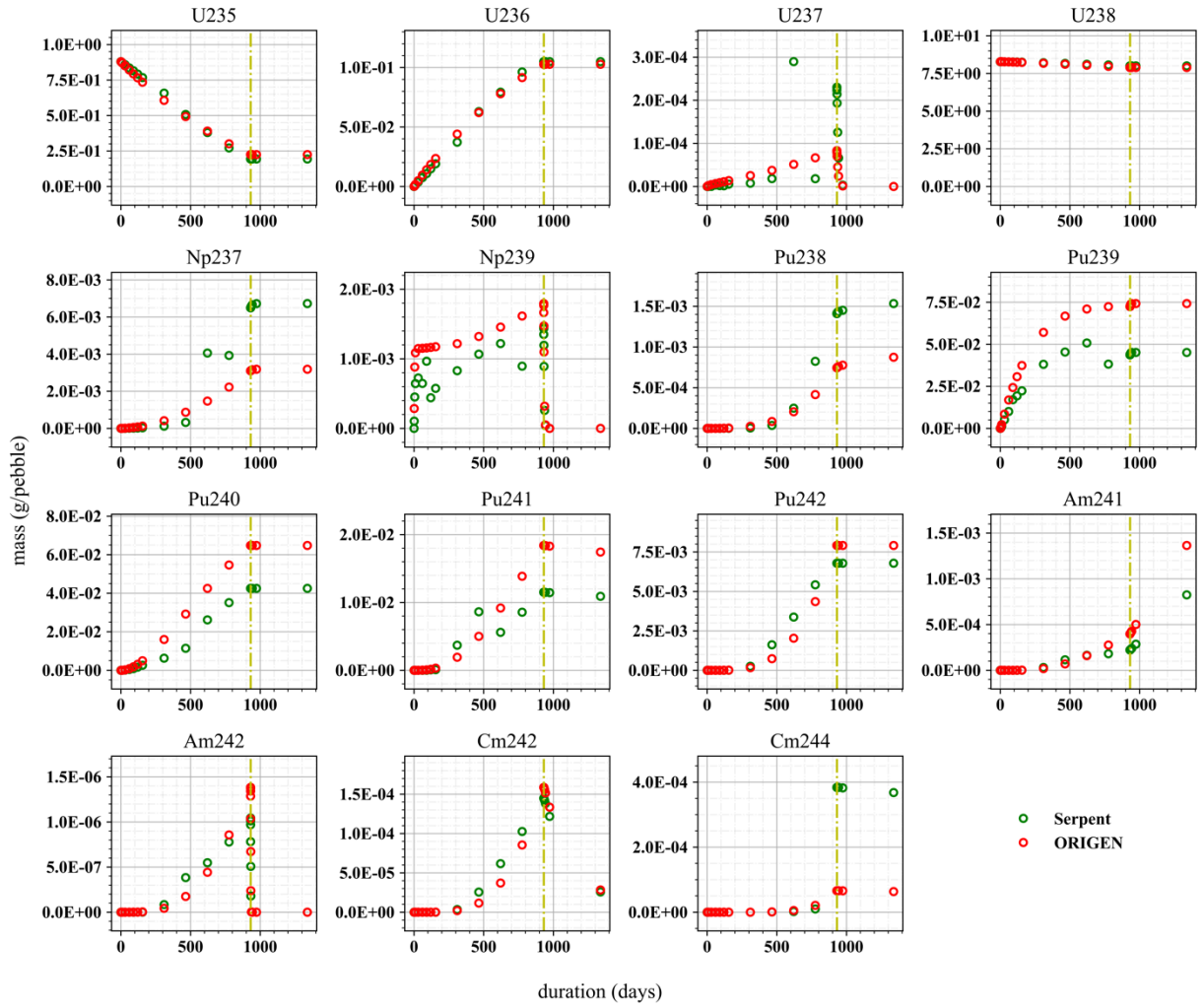


Figure 4: Fission product comparison between ORIGEN (SCALE) and Serpent in radial zone 4

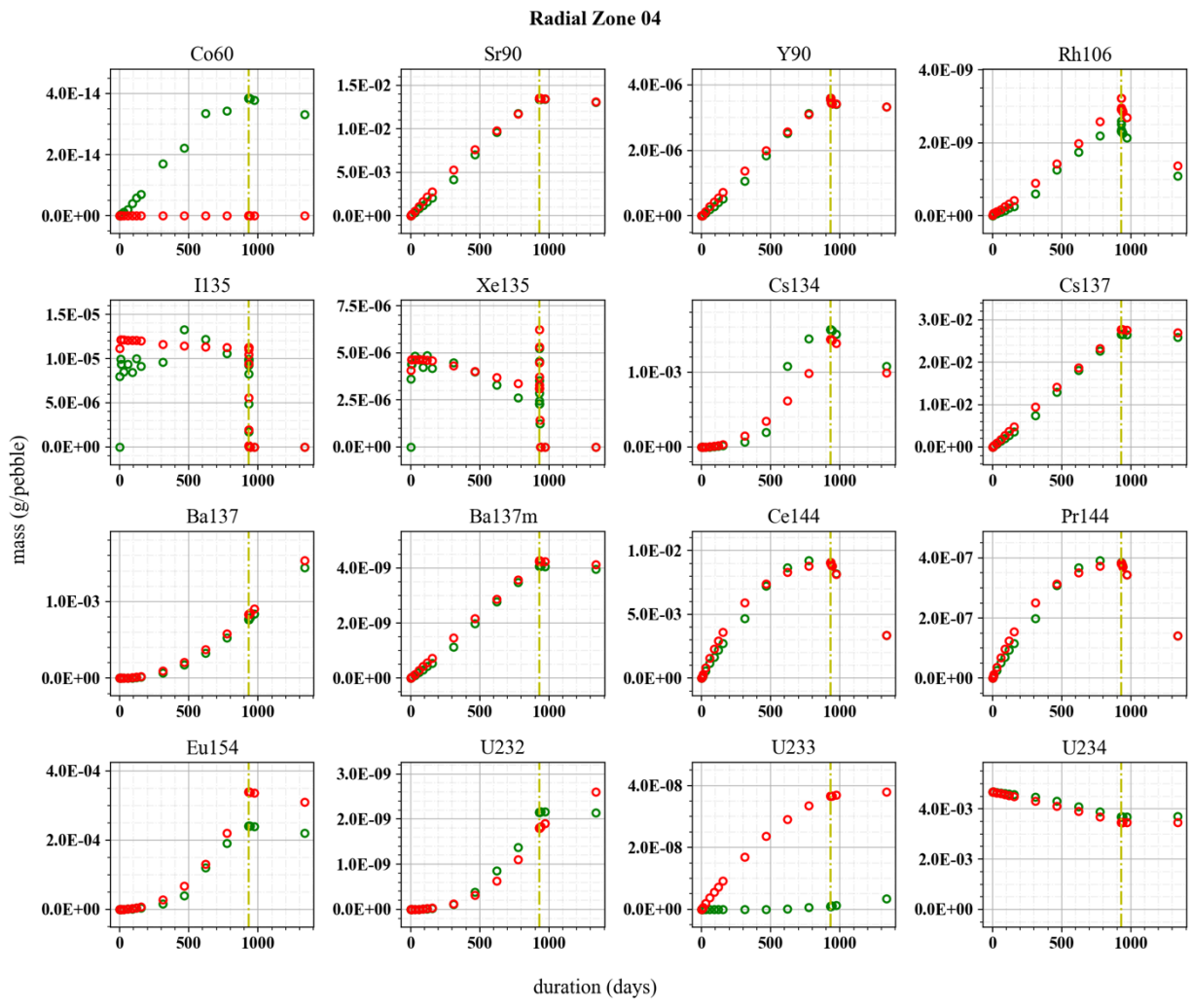


Figure 5: Fission product comparison between ORIGEN (SCALE) and Serpent in radial zone 4 (Cont'd)

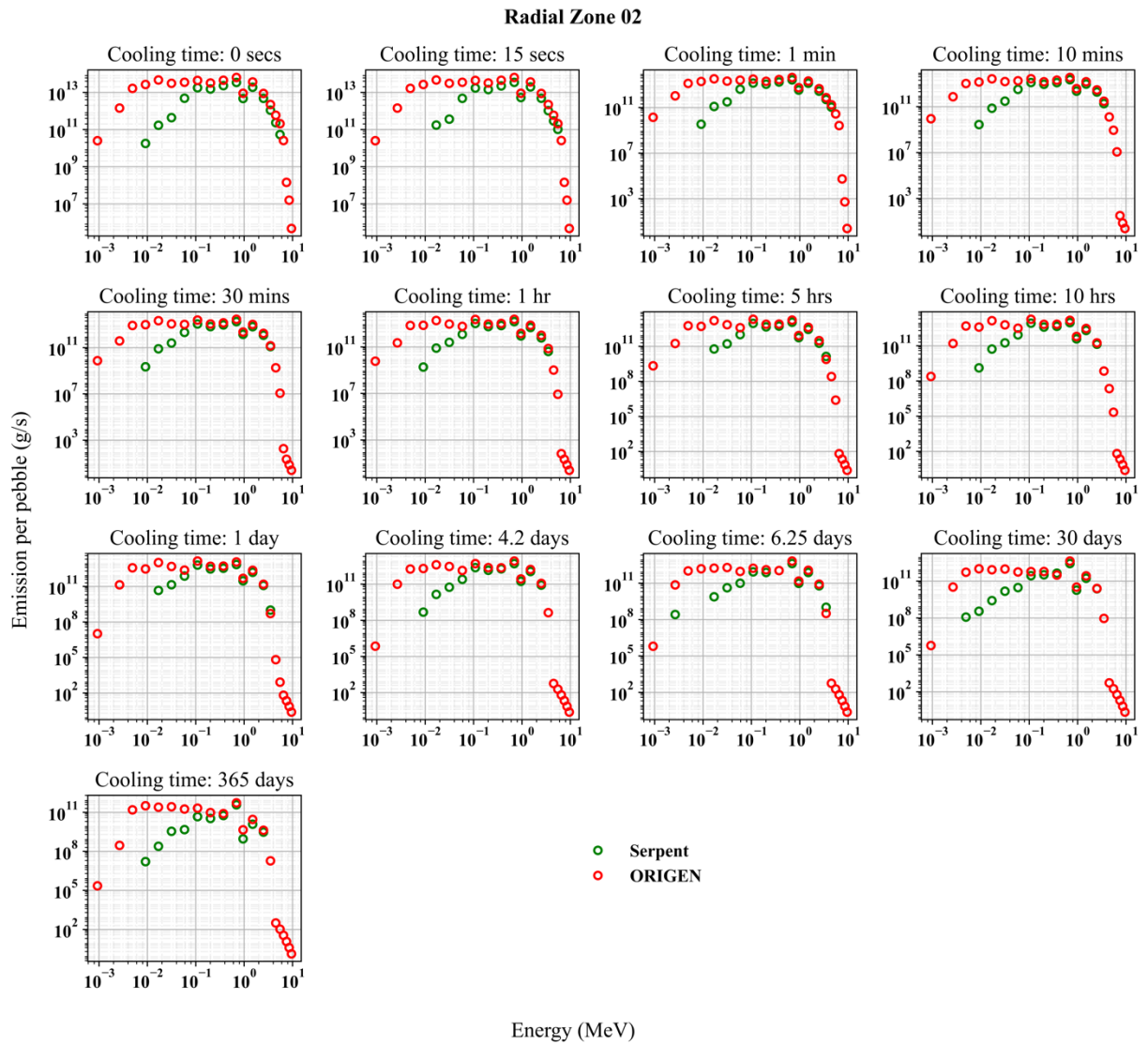


Figure 6: Gamma emission spectra for radial zone 2

Radial Zone 04

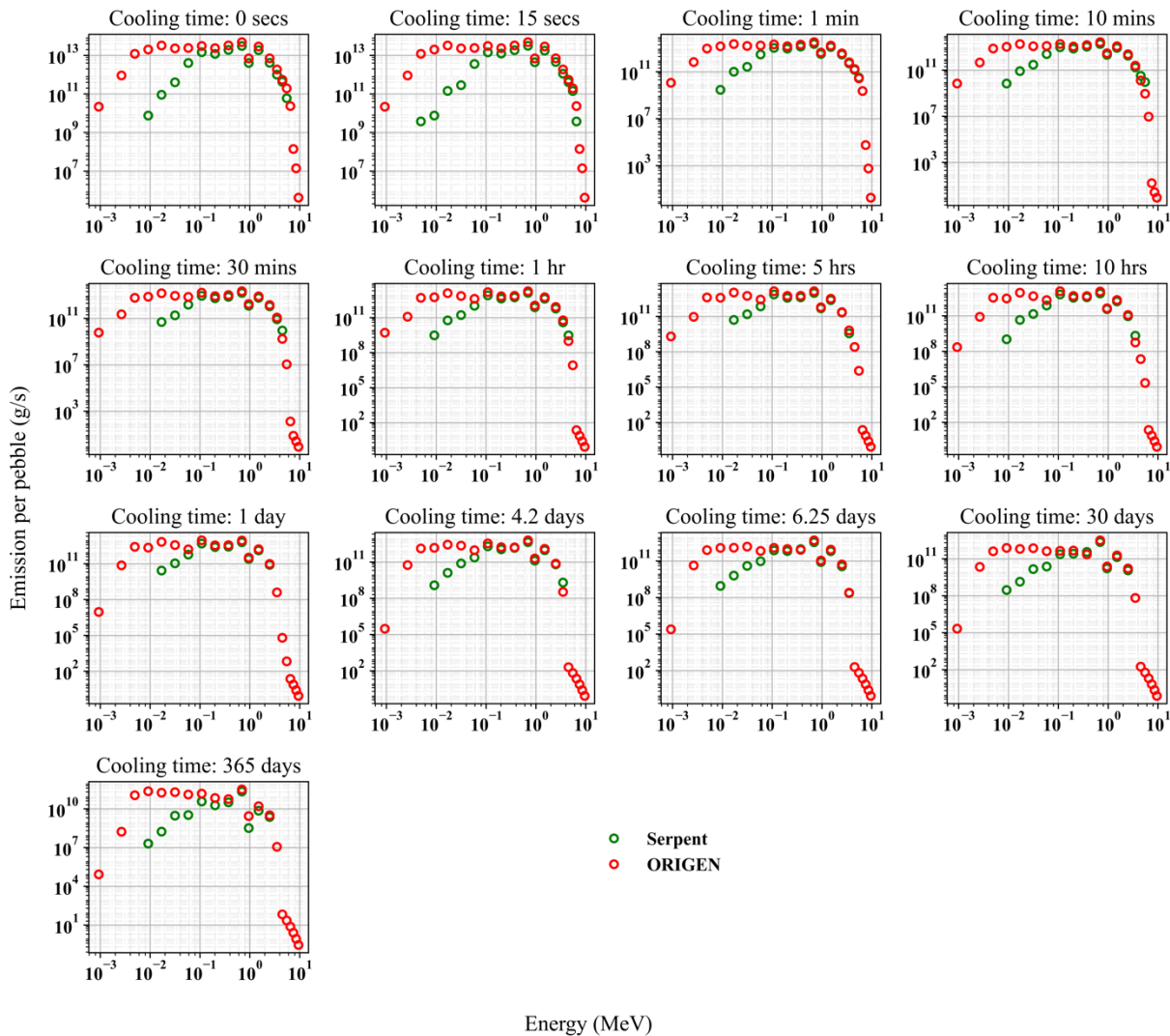


Figure 7: Gamma emission spectra for radial zone 4

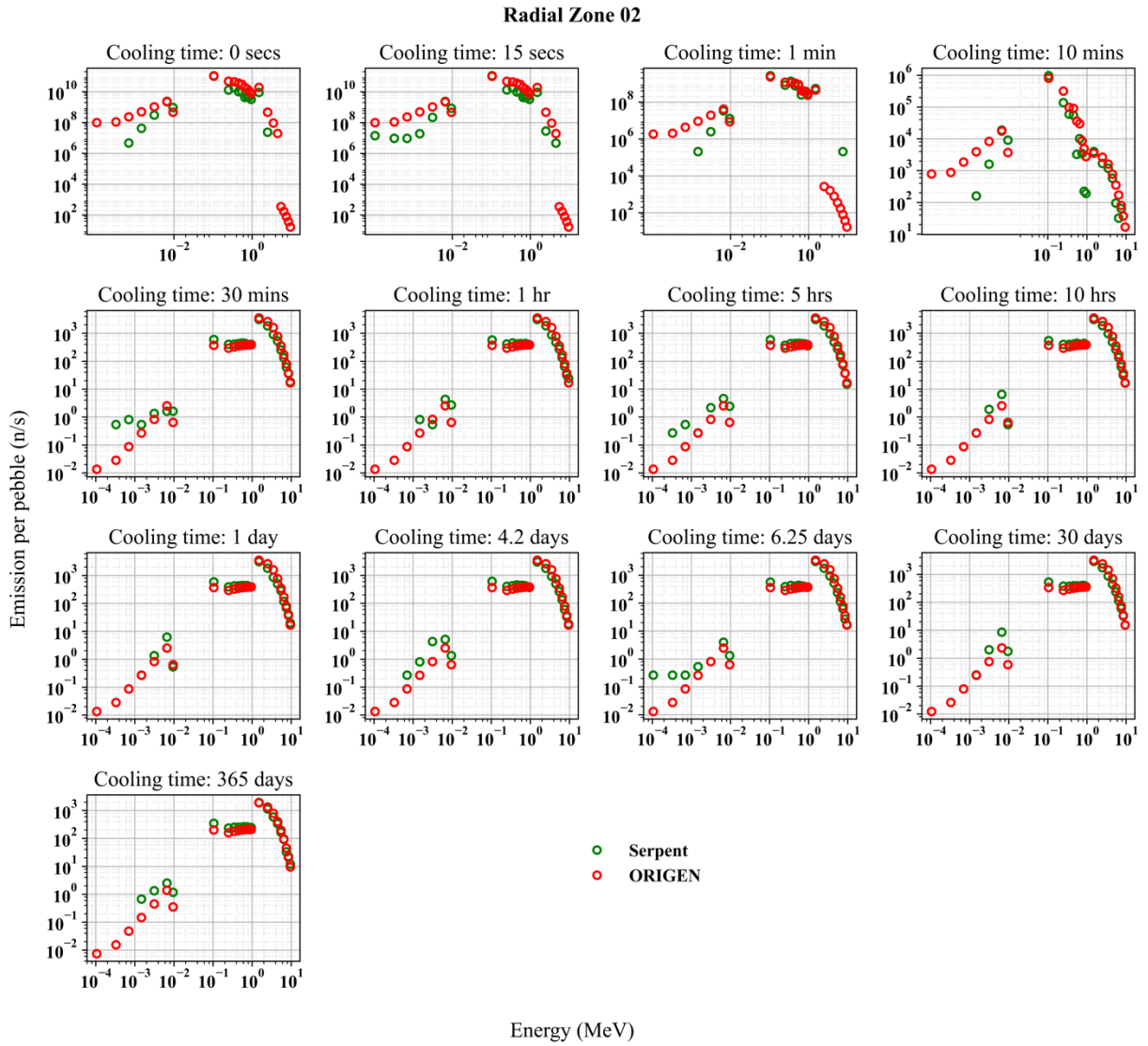


Figure 8: Neutron emission spectra for radial zone 2

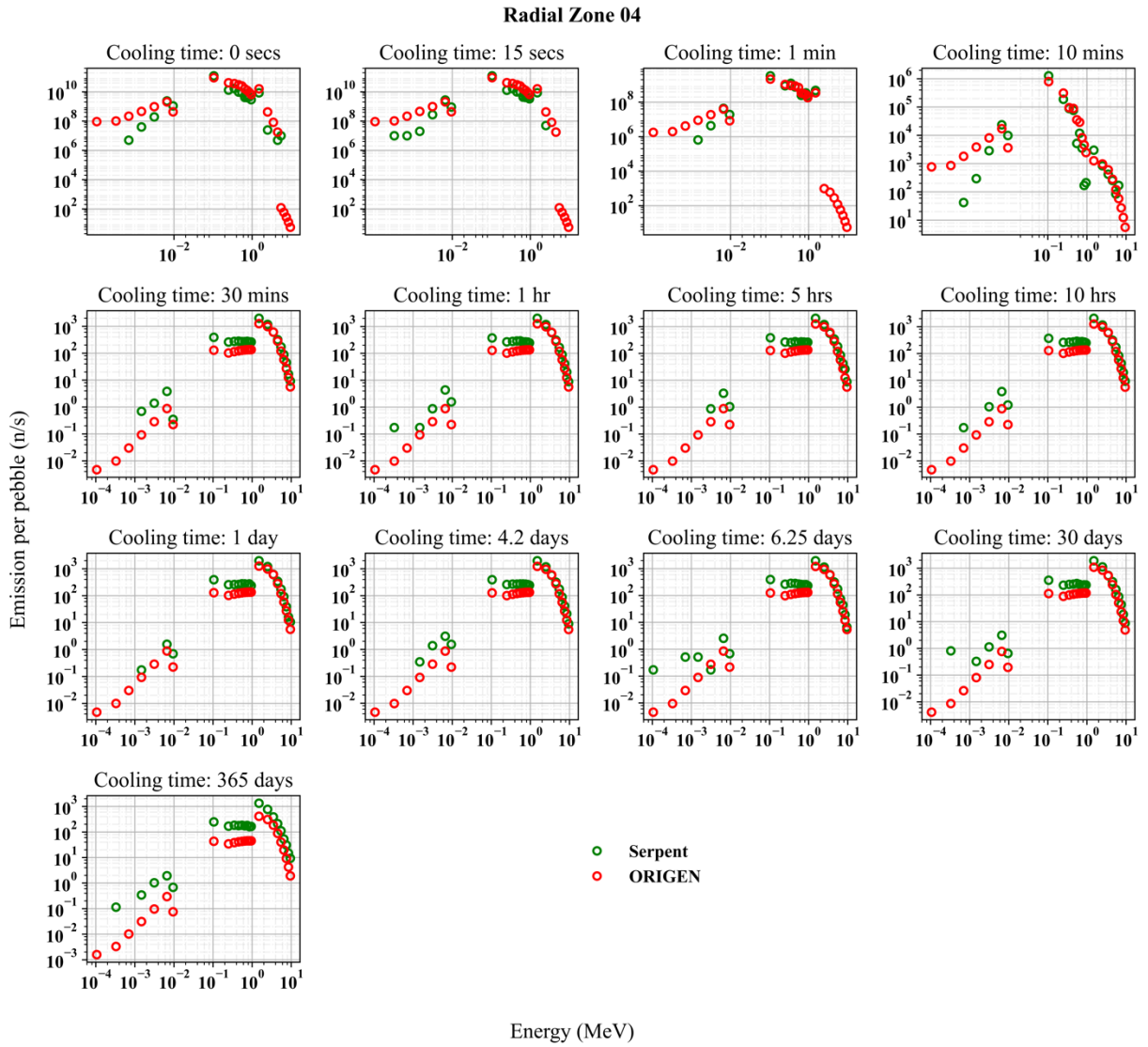


Figure 9: Neutron emission spectra for radial zone 4

Discussion

There is agreement in the results obtained with Serpent and ORIGEN; however, this is less so for the gamma emission spectra. The disagreements seen in Figures 2-9 can be attributed to two factors. Firstly, there may have been an insufficient number of particle histories run to populate the bins in Serpent. This is somewhat apparent from the uncertainties of 10 - 20 % recorded. Secondly, in Serpent, during the burnup stage, the fission and transmutation trajectory cut might have been set too high. This may specifically impact the short-lived isotopes and more obviously isotopes which have a relatively small composition compared to the overall mass in the TRISO.

Effects such as the decay of ^{135}I to ^{135}Xe on shutdown or zero power burnup can be observed to be simulated similarly in both Serpent and ORIGEN. Generally, isotopes which have a shorter half-life on the order of days or less respond drastically to power changes (i.e., both spatial and power shutdown). Isotopes which have a shorter half-life are seen to vary with the radial power of the reactor in comparison to longer-lived isotopes. For example, the concentration of ^{137}Cs is generally consistent across the radial zones of the core; however, for ^{134}Cs significant variation is observed in various radial zones due to power levels.

Some isotopes showed varying transient concentration between ORIGEN and Serpent. An example of this is seen in the concentration of ^{233}U and ^{60}Co . This behavior may be attributed to the isotope thresholds implemented in the Serpent models.

For Fissile isotopes we get mixed results in the transient concentration of ^{235}U and ^{239}Pu . For ^{235}U , there is a good agreement in the concentration estimates in Serpent and ORIGEN. This observation holds true irrespective of the radial location of the pebble. The maximum percent difference over the duration was about 25 % and occurs mostly midway full burn duration, i.e., about 400-600 days. The concentration estimates by Serpent and ORIGEN for ^{239}Pu agree up to about 100 days after which Serpent consistently predicts less than ORIGEN. Estimates of the concentration of fissionable material ^{238}U agree very well between Serpent and ORIGEN.

There are two main types of discrepancies which were observed regarding the fission products estimate that are of concern to us. The first kind of discrepancy is related to isotopes such as ^{239}Pu , ^{240}Pu where these isotopes build up as expected but at a point seem to experience a decrease in concentration that appears like a sudden increase in absorption. Another type of discrepancy is one observed with ^{154}Eu , ^{244}Cm and ^{238}Pu (shown in Figures 2 - 5). In this case there is agreement between ORIGEN and Serpent at the initial duration of burnup, however, in the later stages and at higher burnup, there a steadily increasing difference observed.

The neutron emission spectra as shown above in Figures 2 – 9 compare well between ORIGEN and Serpent. However, the gamma emission spectra seem to suffer from some level of disagreement at energies below 100 keV. This discrepancy in the gamma emission spectra is consistent irrespective of the cooling time or the radial zone. There are a few reasons which we suspect could be responsible for the observations (such as the differences in cross-section data used between ORIGEN and Serpent) however, more studies need to be performed to verify these.

Overall, we believe that the models in Serpent are good enough to generate data representative of burnup in a pebble bed reactor. We would, however, need to resolve the observed discrepancies and consider making a few improvements that will reduce the uncertainties without drastically reducing the efficiency of the simulation process.

References

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- [2] O. U. Dim, C. Soto, Y. Cui and e. al, "Verification of TRISO fuel burnup using machine learning algorithms," in *INMM and ESARDA Joint Virtual Meeting*, New York, 2021.
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- [4] S. Skutnik and W. Wieselquist, "Assesment of ORIGEN reactor library development for pebble bed reactors based on the PBMR-400 benchmark," Oak Ridge, Tennessee, 2021.