Variable Fidelity Estimations of Radiation Source Term for HTR-PM Equilibrium Core

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1. Introduction

High-temperature reactors (HTRs) are thrilling technologies for the new generation of nuclear energy production, providing inherent safety features. HTR-PM is a Chinese pebble-bed HTR design that ensures inherent safety and higher thermal efficiency for the priority of the design, which was developed by Tsinghua University, Institute of Nuclear and New Energy Technology (INET) [1]. Pebble-type fuels are to retrain the fission products inside the power and provide additional defense depth. Pebble-bed HTRs are also capable of online refueling and discharging depleted fuel pebbles. Therefore, it also opens a new concept, the "equilibrium core." The equilibrium core concept refers to the number of pebbles discharged equal to the number of fresh fuel pebbles loaded into the core. It takes almost three years to reach the equilibrium core for a pebble-bed HTR [2]. After reaching the equilibrium core, the core's power, flux, and radiation source inventory are stabilized. That way, source terms during normal operation and accident conditions can be minimized. In the licensing and design processes of nuclear power plants, the source term estimation is a vital process that holds up to calculating the radiation source term inventory inside the core during normal operation and under accident conditions. Each reactor state requires a new model to estimate the source term regarding radioactivity units and concentration levels. It is essential for emergency preparedness and response and the nuclear safety of the design. Because of the importance of the source term estimation, the process requires the highest fidelity of the calculation possible.

In the field of nuclide inventory calculations, there are computer codes commonly used such as SCALE/ORIGEN [3,4], KORIGEN [5], CINDER [6], FISPACT [7], DEPTH [8], and NUIT [9]. HTR technology is relatively new, and the lack of extended cross-section libraries causes simplifications in the source term calculation. On the other hand, in recent years, Monte Carlo codes have been developed to couple the transport and depletion, providing additional details on the geometry of the fuel elements and reactor structures. In that way, the cross-sections are calculated separately due to temperature, energy, and materials, providing detailed simulations. The stochastic algorithm of the Monte Carlo method provides randomness and better simulation of the depletion process. Since Monte Carlo methods are probabilistic and geometry-dependent, computation time is a significant concern for highly detailed simulations. The primary aim of this study is to provide source term estimation approaches to the HTR-PM reactor using a Monte Carlo code and a deterministic

point depletion tool to compare the efficiency and accuracy of the methodology. This study provides four different approaches to source term estimation of HTR-PM reactor with increasing the fidelity of the simulations step by step by the Monte Carlo tool OpenMC. OpenMC is an open-source Monte Carlo particle transport code developed by the Massachusetts Institute of Technology (MIT) [10]. It has coupling and parallel computing features for depletion and transport simulations with the capability of radioactive decay, decay heat calculations, and radioactive isotope inventory estimation. ENDF/B-VIII.0 libraries were used in this study, and a detailed depletion chain file was used for depletion calculations [11]. For the final approach, a deterministic depletion tool, Nuclide Inventory Tool (NUIT), which INET developed, is utilized for point depletion of the fuel of the HTR-PM. The NUIT code uses extensive nuclear data libraries, cutting-edge burnup solvers, and a userfriendly I/O interface compared to the code KORIGEN. Both OpenMC and NUIT can be utilized for depletion calculations. However, OpenMC will cost too much computation time for the last approach; therefore, for the last approach, NUIT was used for burnup calculations with the newly developed "Randomized Flux Distribution Algorithm" (RFDA). For the last approach, a new library for NUIT was utilized, which is also a burnup-dependent library that makes the cross-section calculation more specific to the depletion. Therefore, the fidelity of the NUIT itself is also improved.

This study shows the importance of improving fidelity if the computation cost is acceptable by applying four approaches with different fidelities to the HTR-PM source term estimation. For source term estimation, there are some essential radioisotopes must be analyzed such as ^{85m}Kr, ⁹⁰Sr, ⁹¹Y, ⁹⁵Nb, ^{99m}Tc, ¹⁰⁵Ru, ¹⁰⁹Pd, ²³¹Th, ²³²Pa, ^{234m}Pa, ²³⁶U, ²³⁸U, ²³⁷Np, ²³⁸Pu, ²⁴¹Am, ²⁴²Cm, ¹¹⁰Ag, ¹²⁸Sn, ¹²⁷Te, ¹³¹I, ¹³⁴Cs, ¹³⁷Cs, ¹⁴¹La, ¹⁴⁷Pm, ¹⁵⁶Sm, ²³⁴Th, ²³³Pa, ²³⁵U, ²³⁷U, ²³⁶Np, ²³⁸Np, ²³⁹Pu, ²⁴²Am, ²⁴⁵Cm. This study estimates concentrations of these isotopes using four different approaches. For analysis of the results and execution of the codes, generic Python codes were developed to increase the efficiency of the methods.

2. Methods for Source Term Estimation

The study's primary aim is to investigate the efficiencies and accuracies of the different approaches and how the fidelity of the study affects the results of source term estimation. To do so, the OpenMC Monte Carlo tool and NUIT were utilized to increase the fidelity of the estimation of source term HTR-PM, regular operation, and equilibrium core. The first step is to develop a comparative study to see the accuracy of the tools of the study.

2.1 HTR-PM Equilibrium Core

OpenMC is an open-source Monte Carlo code that couples transport and depletion in the same simulation. OpenMC can utilize the detailed power and flux distributions and specified timesteps of the demand for depletion. For this study, HTR-PM fuels are considered to circulate in a reactor with a multi-pass fuel scheme with 15 passes in 1050 days of depletion. The total depletion time is considered as 1050 days for each of the simulations. For the first three approaches with OpenMC, a detailed power distribution was calculated using VSOP [12] calculations of the HTR-PM core. The data was provided by INET (Fig. 1.). For the last approach, the flux distribution that was calculated by INET and NUIT code was used, which was calculated by PANGU code [13] (Fig. 2.). The study aims to increase the fidelity of the source term estimation step by step from 1 pebble state to 420,000 pebble states. Depletion of nuclear fuel depends on several parameters, such as thermal power, fuel temperature, initial enrichment level of the fuel, and fuel geometry. The HTR-PM core is designed to have 250 MW thermal power for the equilibrium core state, and at the equilibrium core, there are 420,000 fuel pebbles in the core. The radiation source term will be stabilized in this state. As it is known, the pebbles are randomly distributed in HTR cores. Therefore, the depletion levels of each pebble have different characteristics. Table 1 represents the constant simulation parameters of OpenMC and NUIT. These parameters are kept constant for four different approaches. For the fourth approach, a newly developed burnup-dependent cross-section library was used.

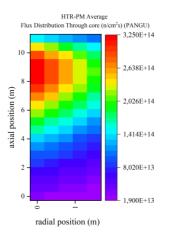


Fig. 1. HTR-PM average equilibrium core flux distribution over the core (PANGU).

Table 1. HTR-PM fuel parameters.

Parameter	Value
Type of Fuel	UO_2
Fuel Enrichment, w/o	8.5
Fuel geometry	Pebble
Moderator Material	Graphite
Coolant Material	Helium, gas
Fuel density, g/cm ³	10.4
Number of TRISO-coated particles	11667
Fuel region diameter, cm	5
Pebble diameter, cm	6
Fuel Temperature, K	900

2.2 Core Averaged Power Approach

For the first assumption, it is assumed that each fuel pebble has the same thermal power, and it is averaged to the number of pebbles in the core. The lifetime of each pebble in the core is assumed to reach its design burnup value (90,000 MWd/tHM) is approximately 1050 days, and with the multi-pass cycle, each pebble is designed to circulate in the reactor core 15 times. So, each pass will take 70 days for a pebble. Therefore, each pebble will reach its design burnup.

$$\frac{(250 MW_{th} \times 10^6 W/1 MW)}{420,000 \ pebbles} \cong 595 \frac{W_{th}}{pebble}, \frac{1050 \ days}{15 \ passes} = 70 \frac{days}{pass}$$

2.3 Layer-Wise Pass-Averaged Power Approach

For this study, the power distribution of the HTR-PM, which Tsinghua University INET generated, was used to estimate the fuel inventory for 15 passes of fuel circulation. The core is divided into 20 layers with 1400 pebbles for each region. Absolute power distributions were calculated concerning 15 passes. The average lifetime of one pebble in the core is estimated at around 1050 days to reach its design burnup, so each total circulation of pebble is 70 days. The pass-average technique was used to simplify the problem, and the power and timesteps were defined as follows.

$$\begin{bmatrix} W_1 \\ \vdots \\ W_{20} \end{bmatrix}_1, \begin{bmatrix} W_1 \\ \vdots \\ W_{20} \end{bmatrix}_2, \dots, \begin{bmatrix} W_1 \\ \vdots \\ W_{20} \end{bmatrix}_{15}, Timesteps = [70 \ days] * 15$$

$$Power = Average \begin{bmatrix} W_1 \\ \vdots \\ W_{20} \end{bmatrix}_1 * 1 + Average \begin{bmatrix} W_1 \\ \vdots \\ W_{20} \end{bmatrix}_2 + \dots + Average \begin{bmatrix} W_1 \\ \vdots \\ W_{20} \end{bmatrix}_{15} * 1$$

In this way, it is possible to simulate each pass with a specified power level and calculated fuel composition as the batches of the simulation change. In the Single-Pebble Average Power investigation, the power level is assumed to be constant for each pebble of the core. However, now the core is divided into regions, so the fidelity of the problem improved. For the depletion results, to get the source term, since all the pebbles have different radiation levels and isotopic concentrations, the activity levels are averaged at the time of equilibrium core, and final radiation levels are obtained.

2.4 Layer-Wise Pass-Wise Power Distribution Approach

For that simulation, the power values of each cell were used, and the timesteps of the problem were set to 3.5 days. This will help to improve the fidelity and give more details about the previous assumptions. To do so, each power level was used as input to the power, and 300 power values were simulated. In that way, the calculation steps of the problem are increased from 15 to 300.

$$\begin{bmatrix} W_{1} \\ \vdots \\ W_{20} \end{bmatrix}_{1}, \begin{bmatrix} W_{1} \\ \vdots \\ W_{20} \end{bmatrix}_{2}, \dots, \begin{bmatrix} W_{1} \\ \vdots \\ W_{20} \end{bmatrix}_{15}, Timesteps = [3.5 days] * 300$$

Power = $[W_{1,1}] * 1 + [W_{1,2}] * 1 + [W_{1,3}] * 1 + \dots [W_{19,15}] * 1 + [W_{20,15}] * 1$

This approach covers 300 different pebble states at one simulation; therefore, to get the equilibrium core average operation source term, results were multiplied by 1400 and summed to get the source term from the depletion results.

2.5 Pebble-wise Randomized Flux Distribution Approach (RFDA)

The new algorithm will randomly decide the first pass region, and the pebble will be depleted in that radial ring for the first pass. Then, for the second pass, it will randomly decide on the radial ring again, and according to the second pass flux distribution on that radial ring, the pebble will be depleted, and so on. Each pebble will have 15 passes and a total of 300 flux histories randomly. This flux distribution will be input for the NUIT point depletion code. Therefore, the randomness of the pebble circulation can be simulated as well. The calculation will take place for 1400 pebbles, which means the depletion of one region is distributed randomly. Each depletion result will be stored and added at the end of the 1400 pebbles. Finally, $300 \times 1400 = 420,000$ pebble states, which can be assumed as a pebble-wise source term estimation. This algorithm will add randomness to the pebble flow in the core and generate high-fidelity data. Fig. 2. describes the workflow of the designed algorithm.

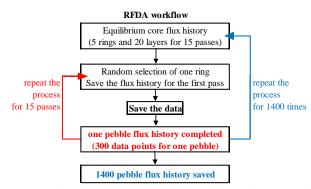


Fig. 2. RFDA workflow

The algorithm is not limited to NUIT. It can be easily implemented in OpenMC media by changing the input file creation steps and execution settings of the algorithm. However, as explained, the current methodology will have a high computational cost.

After the RFDA determined the flux histories for the depletion, the NUIT was implemented into the code. RFDA can also easily be implemented into the OpenMC code to execute an MC simulation. However, the calculation time, as mentioned, is too high. That makes the OpenMC not efficient for extensive data utilization. A newly developed generic Python script has been developed to generate and execute NUIT input files continuously; then, the same code also fetches the desired isotope data from the output files. After executing the 1400 input files, the desired isotopic radioactivity data was fetched and averaged from the output files to compare with the OpenMC data. A newly developed burnup-dependent sub-library specially developed for HTRs was utilized for NUIT. This new sub-library provides burnup data for fuel depletion, developed with the OpenMC single pebble model. Therefore, the accuracy and fidelity of the source term estimation are expected to be increased.

2.6 Total Core Radioactivity Analysis

For HTRs, the equilibrium core concept is already explained, which means each pebble will have different isotopic concentrations and depletion levels in the core. For the accuracy of the approaches, it was assumed that there are different pebble states in the nuclear reactor core. For the most straightforward and pass-averaged methods, there are 30 burnup histories, meaning there are 30 different types of pebbles with increasing depletion levels. However, the layer-wise approach increases this number to 300 pebble states. Moreover, finally, for the NUIT-RFDA, there will be 420,000 pebble states, which can be summed up to pebble-wise equilibrium core radioactive isotope inventory. The equation below was utilized for total core radioactivity analysis to obtain radioactivity levels in Curies (Ci) units.

$$Open[Source Term]_{i,Ci} = \left(\frac{\# of \ pebbles}{\# of \ PS}\right) \times \frac{\sum_{i=0}^{n} (PS)_i \times \lambda_i}{3.7 \times 10^{10} \ Bq \ / \ Ci}$$

Where n is the number of pebbles states and starts with initial condition because at equilibrium core, it is assumed that there are also fresh fuel pebbles loaded to the core as well, PS_i is the concentration of i_{th} pebble state for isotope i, λ_i is the decay constant in a unit of s⁻¹ for isotope i and several pebbles are assumed as 420,000 in equilibrium core state.

3. Results

According to the results of the different runs, the results were compared concerning the approach. In this section, there are two significant subtitles. The first one investigates the performance of the OpenMC with NUIT and newly developed burnup-dependent sub-library accuracy on the source term estimation, a Code-to-Code Comparative Study. In this section, the same simulation parameters results were represented as the last concentrations of the desired isotopes of the source term.

After proving that the OpenMC and NUIT are consistent, for the next step, four different approaches on the source term and their results were investigated according to the source term estimation methods while increasing the fidelity of the simulations.

3.1 Verification of NUIT for Pebble-wise Depletion

The same simulation parameters were used for both OpenMC and NUIT for the code-to-code comparative study. The same power levels and the same concentration for fuel material were defined. One thousand fifty days of depletion were selected for the study. Also, for the code-to-code study, the performance of the source term of the newly developed burnup-dependent sub-library was investigated (Table 2). For some critical isotopes, the OpenMC model and newly developed burnup sublibrary, including NUIT simulation, became closer. The primary expectation of this study is to show that the new burnup-dependent sub-library would result in the highest accuracy with the single-pebble OpenMC model.

Table 2. Comparison of essential fission products and actinides concentration levels for HTR-PM single pebble model between OpenMC and NUIT after 1050 days of depletion ($n \times 1.0E+24$)

Nuclide	OpenMC (ref)	NUIT old lib (Err %)	NUIT new lib (Err %)	
Th234	2.27E-13	2.27E-13(-0.05)	2.27E-13(-0.01)	
Pa232	3.31E-15	3.17E-15(-4.33)	3.27E-15(-1.25)	
Pa233	4.49E-13	4.85E-13(8.13)	4.46E-13(-0.61)	
Pa234m1	7.75E-18	7.78E-18(0.39)	7.76E-18(0.11)	
Np236	2.04E-12	2.08E-12(1.99)	2.01E-12(-1.21)	
Np237	1.32E-05	1.46E-05(10.58)	1.32E-05(0.38)	
Np238	5.14E-08	5.91E-08(14.87)	5.22E-08(1.60)	
U234	3.03E-08	3.15E-08(3.87)	3.09E-08(1.86)	
U235	2.40E-04	2.37E-04(-1.47)	2.33E-04(-2.87)	
U236	2.04E-04	2.02E-04(-1.00)	2.05E-04(0.28)	
U237	3.45E-07	4.15E-07(20.53)	3.47E-07(0.83)	
U238	1.54E-02	1.54E-02(-0.07)	1.54E-02(-0.01)	
Pu238	5.11E-06	5.71E-06(11.75)	5.21E-06(2.10)	
Pu239	8.94E-05	9.75E-05(9.01)	8.75E-05(-2.18)	
Pu240	7.46E-05	6.17E-05(-17.35)	7.48E-05(0.27)	

Pu241	4.01E-05	4.53E-05(12.92)	3.97E-05(-0.99)
Pu242	3.71E-05	3.94E-05(6.06)	3.79E-05(2.08)
Kr85m1	3.17E-09	3.06E-09(-3.66)	3.11E-09(-1.92)
Kr85	3.51E-06	3.42E-06(-2.49)	3.43E-06(-2.33)
Kr87	1.75E-09	1.68E-09(-3.90)	1.72E-09(-1.87)
Kr88	5.15E-09	5.05E-09(-1.98)	5.16E-09(0.19)
Rb86	2.29E-09	2.62E-09(14.25)	2.39E-09(4.44)
Sr89	3.17E-06	3.06E-06(-3.42)	3.14E-06(-0.89)
Sr90	7.01E-05	6.85E-05(-2.22)	6.86E-05(-2.07)
Sr91	3.09E-08	2.99E-08(-3.24)	3.05E-08(-1.35)
Sr92	9.52E-09	9.53E-09(0.07)	9.64E-09(1.29)
Y90	1.89E-08	1.85E-08(-2.38)	1.86E-08(-1.75)
Y91	4.82E-06	4.67E-06(-2.94)	4.78E-06(-0.81)
Zr95	7.53E-06	7.50E-06(-0.42)	7.54E-06(0.13)
Nb95	4.16E-06	4.15E-06(-0.31)	4.17E-06(0.24)
Mo99	3.64E-07	3.62E-07(-0.35)	3.58E-07(-1.45)
Tc99m1	2.91E-08	2.90E-08(-0.37)	2.87E-08(-1.44)
Rh103m1	4.54E-09	4.67E-09(2.69)	4.56E-09(0.31)
Ru105	1.59E-08	1.65E-08(3.91)	1.57E-08(-1.07)
Ru106	1.63E-05	1.68E-05(2.85)	1.65E-05(0.79)
Rh106	1.88E-11	1.95E-11(3.91)	1.93E-11(2.52)
Pd109	1.59E-08	1.52E-08(-4.58)	1.42E-08(-11.00)
Ag110m1	6.88E-08	6.26E-08(-9.03)	5.92E-08(-13.93)
Te131	1.06E-09	1.06E-09(0.41)	1.05E-09(-1.28)
Te132	3.24E-07	3.24E-07(0.02)	3.20E-07(-1.42)
Te134	3.68E-09	3.74E-09(1.65)	3.72E-09(1.15)
I130	1.09E-09	1.36E-09(24.90)	1.46E-09(33.60)
I131	5.80E-07	5.84E-07(0.70)	5.75E-07(-0.72)
I132	9.96E-09	9.87E-09(-0.95)	9.72E-09(-2.40)
I133	1.27E-07	1.27E-07(0.33)	1.25E-07(-0.98)
I134	5.95E-09	5.71E-09(-4.00)	5.66E-09(-4.93)
I135	3.81E-08	3.78E-08(-0.77)	3.73E-08(-2.24)
Xe133m1	1.00E-08	9.77E-09(-2.67)	9.64E-09(-4.03)
Xe133	7.74E-07	7.74E-07(0.04)	7.66E-07(-1.03)
Xe135	8.31E-09	9.00E-09(8.25)	7.88E-09(-5.15)
Xe138	1.21E-09	1.18E-09(-2.55)	1.17E-09(-3.19)
Cs134	8.98E-06	1.03E-05(14.85)	9.77E-06(8.76)
Cs136	3.91E-08	3.56E-08(-8.79)	3.44E-08(-12.04)
Cs137	9.95E-05	9.92E-05(-0.32)	9.91E-05(-0.42)
Cs138	3.15E-09	3.09E-09(-1.82)	3.06E-09(-2.72)
Ba140	1.59E-06	1.60E-06(0.39)	1.59E-06(0.17)
La140	2.20E-07	2.20E-07(0.09)	2.21E-07(0.20)
Ce141	3.82E-06	3.79E-06(-0.99)	3.78E-06(-1.01)
Ce143	1.49E-07	1.47E-07(-1.03)	1.47E-07(-1.22)
Pr143	1.48E-06	1.45E-06(-1.97)	1.45E-06(-1.64)
Ce144	2.76E-05	2.75E-05(-0.38)	2.76E-05(-0.20)
Pr144	1.17E-09	1.18E-09(0.18)	1.18E-09(0.37)

In Table 2, the burnup difference between the codes is represented. As it is clear, OpenMC and NUIT will result in almost the same burnup histories for the same simulation parameters. For this study, the percentage difference is 0.125% between OpenMC and NUIT. Therefore, it can be assumed that the simulations are accurate for different simulations in case of fuel material depletion. Figures 3, 4, and 5 are burnup-dependent comparisons of isotopic mass change of important isotopes concerning burnup represented.

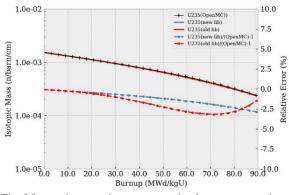


Fig. 3 Isotropic mass change concerning burnup comparison with different methods for ²³⁵U.

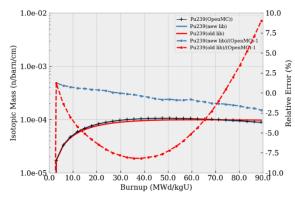


Fig. 4 Isotropic mass change concerning burnup comparison with different methods for ²³⁹Pu.

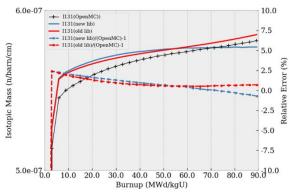


Fig. 5 Isotropic mass change concerning burnup comparison with different methods for ¹³¹I.

3.2 HTR-PM Core Source Term Estimations

For an approach-wise comparative study, the total core radioactivity was estimated according to the results of the fission products. For observation of the results, the total radioactivity of the isotopes of concern was analyzed, and the results were listed as the total radioactivity of the core in Table 3 and the total radioactivity of the important nuclides individually in Table 4. From the radioactive source term results of 4 approaches, it was observed that 4 methods can be accepted as source term estimation methods due to minor discrepancies considering the application conservatively. The NUIT- RFDA method is considered the reference source term estimation approach due to its randomness of the pebble flow and pebble-wise estimation algorithm. The OpenMC results show that these approaches are also acceptable in engineering design, nuclear safety, and applications.

Table 3. Radioactivity of important nuclides of HTR-PM equilibrium core

Total Equilibrium Core Source Term of important nuclides (Ci)				
Nuclide Category	OpenMC (1) [*]	OpenMC (2)**	OpenMC (3)***	NUIT RFDA
Total	1.31E+09	1.32E+09	1.38E+09	1.30E+09
Fission	1.11E+09	1.12E+09	1.17E+09	1.08E+09
Products				
Actinides	2.03E+08	2.03E+08	2.12E+08	2.17E+08
**OpenMC (2):	Core averaged Power Pass-averaged Power	r approach		

***OpenMC (3): Layer-wise Power approach

Table	4.	Source	term	comparison	for	HTR-PM
equilibrium core under normal operation.						

equilion	Total concentrations (Ci)				
Nuclide	OpenMC	MC OpenMC OpenMC		NUIT	
	$(1)^{*}$	(2)**	(3)***	RFDA	
^{85m} Kr	1.96E+06	1.96E+06	2.08E+06	2.03E+06	
⁹⁰ Sr	3.35E+05	3.79E+05	3.87E+05	3.59E+05	
⁹¹ Y	8.61E+06	8.79E+06	9.09E+06	8.97E+06	
⁹⁵ Nb	1.03E+07	1.07E+07	1.10E+07	1.07E+07	
^{99m} Tc	1.06E+07	1.06E+07	1.11E+07	1.08E+07	
¹⁰⁵ Ru	5.27E+06	5.27E+06	5.47E+06	5.22E+06	
¹⁰⁹ Pd	1.33E+06	1.33E+06	1.37E+06	1.11E+06	
²³¹ Th	2.61E-01	2.28E-01	2.38E-01	2.51E-01	
²³² Pa	1.88E-01	1.58E-01	1.59E-01	1.68E-01	
^{234m} Pa	8.43E-01	8.40E-01	8.54E-01	8.59E-01	
²³⁶ U	1.28E+00	1.46E+00	1.49E+00	1.43E+00	
²³⁷ Np	5.75E-01	7.11E-01	7.23E-01	6.59E-01	
²³⁸ Pu	3.60E+03	4.82E+03	4.87E+03	4.27E+03	
²⁴¹ Am	2.08E+02	2.79E+02	2.79E+02	2.46E+02	
²⁴² Cm	1.16E+05	1.42E+05	1.44E+05	1.37E+05	
¹¹⁰ Ag	3.43E+05	3.41E+05	3.51E+05	2.80E+05	
¹²⁸ Sn	8.10E+05	8.09E+05	8.49E+05	8.62E+05	
¹²⁷ Te	4.61E+05	4.62E+05	4.81E+05	4.71E+05	
131 I	6.22E+06	6.22E+06	6.49E+06	6.35E+06	
¹³⁴ Cs	3.72E+05	4.43E+05	4.52E+05	4.43E+05	
¹³⁷ Cs	4.18E+05	4.78E+05	4.87E+05	4.56E+05	
¹⁴¹ La	1.09E+07	1.10E+07	1.15E+07	1.13E+07	
¹⁴⁷ Pm	9.25E+05	1.01E+06	1.03E+06	8.76E+05	
¹⁵⁶ Sm	1.12E+05	1.12E+05	1.16E+05	1.13E+05	
²³⁴ Th	8.38E-01	8.35E-01	8.49E-01	8.54E-01	
²³³ Pa	5.42E-01	6.75E-01	6.86E-01	6.20E-01	
²³⁷ U	2.30E+06	2.36E+06	2.42E+06	2.30E+06	
²³⁶ Np	1.17E-06	1.46E-06	1.47E-06	1.33E-06	
²³⁸ Np	6.64E+05	6.92E+05	7.08E+05	6.47E+05	
²³⁹ Pu	9.02E+02	9.25E+02	9.43E+02	9.38E+02	
²⁴² Am	2.47E+05	2.80E+05	2.83E+05	2.71E+05	
²⁴⁵ Cm	1.68E-01	2.33E-01	2.39E-01	3.41E-01	

*OpenMC (1): Core averaged Power approach **OpenMC (2): Pass-averaged Power approach

***OpenMC (3): Layer-wise Power approach

4. Conclusions

In conclusion, it was proven that both OpenMC and NUIT could be utilized for normal operation source term estimation of HTR-PM at the equilibrium core. Also, this paper showed the importance of the highest fidelity on the source term estimation. This paper provided four approaches to increasing the fidelity of the source term estimation from 30 burnup histories to 420,000 burnup histories, which may be considered pebble-wise source term estimation for HTR-PM.

For the proof of the concept at first, the same depletion simulation was adapted by OpenMC and NUIT to see the accuracies of the codes under the same simulation parameters and depletion conditions. This study showed that the NUIT and OpenMC are consistent under the same simulation parameters. The first three approaches were utilized for OpenMC, and the last was for NUIT. The last approach used for NUIT is the high computational cost of Monte Carlo studies, which makes the OpenMC inefficient for highly detailed simulations. However, a newly developed random flux distribution algorithm can also be applied to OpenMC, considering the high computational cost of operation. The VSOP power distribution was used for the OpenMC simulations for the first three approaches; for the NUIT-RFDA simulation, the PANGU HTR-PM equilibrium core flux distribution was utilized. The idea of the RFDA is to simulate the randomness of the pebble flow inside the reactor core. It selects random flux histories for each pass and depletes the pebbles.

For NUIT and NUIT-RFDA simulations, a newly developed burnup-dependent cross-section sub-library was introduced. The effects of the new sub-library are estimated by carrying out NUIT simulations with and without the sub-library. The results showed that the new burnup-dependent sub-library improved the simulation.

Finally, with four different approaches, the total source term for the equilibrium core is estimated with four different approaches in units of Curies for the isotopes included for OpenMC and NUIT libraries. In conclusion, the fidelity of the source term estimation is vital due to the randomness of the pebble flow and the randomness of the depletion of the pebbles. For the final approach, a new pebble-wise source term estimation concept introduced the highest fidelity possible for source term estimation. Regarding the computation time and memory consumption, the RFDA can be improved and used for 420,000 individual pebbles to achieve the source term's highest detailed performance.

Results showed that OpenMC and NUIT are acceptable in source term estimation methods with variable-feasible fidelity. This paper proved the importance of the fidelity of the source term estimation process with four different approaches to increasing the fidelity of the calculations. The first three approaches with OpenMC are considered conservative to the source term estimation, which can also be accepted in engineering design, nuclear safety, and applications. Since this study aims to prove the fidelity difference between different approaches of source term estimation, the NUIT-RFDA method has the highest accuracy due to its random flux history selection and calculation of 420,000 pebble states, which makes it pebble-wise, and it is also accepted as a reference for the source term calculations.

In the code-to-code comparative study, the aim was focused on the consistency between the methods before applying four different approaches. Table 2 shows that the results on the nuclide inventory are consistent for OpenMC and NUIT simulations with the same simulation parameters. Also, Table 2 shows that the newly developed burnup-dependent cross-section library improved the results. For the source term estimation with four different approaches, the results are listed in Tables 3 and 4. As it is clear, four of the results were consistent with minor discrepancies, in which the last method was considered the reference due to its high fidelity and pebble-wise characteristics. The potential reasons for the discrepancies between the isotropic concentration and source term differences between the codes are differences in the algorithms of OpenMC and NUIT, the simulation technique difference, and model differences. OpenMC is a transport and depletion coupled code that calculates the cross-sections by the particles' transport and re-calculates the cross-section and then depletion. Since NUIT is a deterministic point depletion code, the algorithm depletes the number of materials according to the solution of the Bateman equation only with a constant cross-section. However, the newly developed burnupdependent sub-library is increasing the fidelity of the burnup calculation of the fuel by adding a burnupdependent cross-section to the nuclides. Therefore, the results are improved regarding the OpenMC.

This study concludes that a direct correlation exists between the enhancement of source term estimation fidelity and the computational load associated with processing larger datasets, considering the computation cost and efficiency of the algorithms.

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