FISSION YIELD UNCERTAINTY PROPAGATION IN MULTI-PASS REFUELING PEBBLE-BED HTGR

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ABSTRACT

Multi-pass refueling scheme is a highlighted feature of pebble bed HTGR which spatially mixes the burnup calculation inside core. Such refueling scheme relate burnup calculation in one region of the core to others and thus affects the uncertainty propagation of nuclear data, e.g. fission product yield. In this work, thermal neutron induced U-235 fission product yield uncertainties are propagated in HTR-PM models with various refueling schemes in V.S.O.P. code. And the effect of multi-pass refueling scheme is studied. Bayesian method is applied to estimate the covariance of fission product yield based on ENDF/B-VII.1 fission yield sub-library. Uncertainty quantification is performed with stochastic sampling method and log-normal based correlated sampling method is used to generate reasonable and self-consistent fission product yield samples. The analyzed results indicate that multi-pass refueling scheme could affect the uncertainty propagation of reactor local responses.

KEYWORDS: Multi-pass refueling scheme, fission yield uncertainty, pebble-bed HTGR

1. INTRODUCTION

The continued research and design of pebble-bed High Temperature Gas-cooled Reactor (HTGR) require not only high-fidelity codes to provide accurate reactor system predictions, but also systematic uncertainty analysis to assign confidence bounds to those predictions. Specifically, uncertainty analysis of fuel pebble maximum temperature under accidental scenario serves as primary aspect for assessing reactor safety margin and design. Such analysis needs propagate nuclear data’s uncertainty throughout reactor burnup process to released decay heat after accident occurrence. Although previous research has investigated nuclear data’s uncertainty contribution to neutronics calculation [1, 2], few research has extended it to reactor burnup calculation and even little has involved fission yields’ uncertainty propagation, whose contribution is presumably important to decay heat release [3, 4]. This study aims to establish fission yields uncertainty analysis method throughout pebble-bed HTGR burnup calculation based on V.S.O.P. computer code system [5]. It serves as a preliminary study for further conducting reactor accidental safety analysis.

Most notably, this study places additional attention on investigating what effect does multi-pass refueling fuel management scheme have on uncertainty propagation inside the core. Multi-pass refueling fuel management scheme or multi-pass refueling scheme is a highlighted feature of pebble-bed HTGR. What is distinct from Light Water Reactor (LWR) burnup calculation is that isotopes’ compositions evolve not merely within each

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individual spectrum region, but are mixed and related among all regions via fuel refueling. It is therefore quantified uncertainty in every corner of the core stems from both temporal accumulation and spatial mixing of fuel burnup during reactor operation. This novel investigation addressing uncertainty analysis related to non-fixed flowing pebble bed core would provide knowledge about uncertainty propagation characteristics of pebble-bed HTGR.

This paper is organized as follows: Chapter 2 recaps the description about HTR-PM with emphasis on its refueling process modeling. Chapter 3 presents the methodology applied in this work, including established framework for fission yields uncertainty propagation based on stochastic sampling method as well as independent yields covariance estimation based on ENDF/B-VII.1 by Bayesian method. Analyzed reactor responses are categorized into two types, namely global response and local response. Their uncertainties quantified under different adopted multi-pass refueling schemes are compared and discussed in result chapter.

2. CORE MODEL DESCRIPTION

HTR-PM (High Temperature gas-cooled Reactor Pebble-bed Module) consists of two pebble-bed reactor modules and each of them includes a reactor core and a steam generator, shown as in Figure 1 (left). Large amount of spherical fuel elements or fuel pebbles stacks inside reactor core forming the cylindrical-like pebble bed, whose diameter and height are 3 m and 11 m, respectively. These fuel pebbles are of 60 mm diameter with thousands of small UO\textsubscript{2} coated particles embedded inside. Detailed description and main design parameters of the HTR-PM could be referred to these review articles [6, 7].

![Figure 1. Cross-section view of HTR-PM reactor building [6] (left); V.S.O.P. burnup 2D model with adoption of eight times refueling scheme (right). The core is divided into five channels radially from the center to the outside, labelled from I to V. Each channel is subdivided axially into 20 regions from top of the core to bottom, with each representing individual spectrum region (orange shading). Each region contains eight fuel batches numbered by the times of fuel pebbles passing through the core.](image-url)

One of the noteworthy feature of HTR-PM is the adoption of “multi-pass” refueling fuel management scheme. Fresh fuel pebbles of 8.5\%wt enrichment are loaded into the top of the core, while spent fuel pebbles are
discharged at the bottom. During the irradiation of fresh fuels to spent fuels, fuel pebbles would be consistently reloaded into the core several times before their average burn-up reaching to design burnup depth 90 GWd/tU. To be specific, fuel pebbles whose burnup does not reach to design burn-up depth would be loaded into the core to pass through it once again, while others reaching design burn-up depth would be discharged from the core[6]. After long term operation, an equilibrium core state is expected in the reactor whose materials’ composition remains constant over time. This continuous loading fuel management is beneficial for achieving a fairly uniform fissile material distribution and a flatter power distribution throughout the core.

In this study, the multi-pass refueling burnup process is modelled and simulated in V.S.O.P. computer code system [5]. A 2D R-Z geometry spectrum region discretization of reactor core is depicted in Figure 1 (right). It is noteworthy to mention that 100 spectrum regions are volume-equally partitioned throughout the core. Fuel batches characterize different fuel pebbles corresponding to different passing times and the number of them within each region is identical to the adopted refueling times. Therefore, fuel shuffling operation is introduced to simulate pebbles’ flow inside core. In proceeding a shuffling, materials of all fuel batches within each region will be transferred to the corresponding batches labeled with identical number in the subsequent region. The first batches appear at the top of the core will be loaded fresh fuel, and the last batches reside in the bottom region will be discharged. All other batches running out of the core will be collected into corresponding storage box and re-allocated equally into the corresponding subsequent batches in the top regions. This process follows the grey dash line depicted in Figure 1 (right).

| Table I. Main Equilibrium Core Parameters in 8x, 10x and 15x |
|-----------------------------------------------------------|
| Parameters                                               | Eight times pass (8x) | Ten times pass (10x) | Fifteen times pass (15x) |
|----------------------------------------------------------|
| Total thermal power [MW]                                 | 250                  | 250                   | 250                     |
| Average burnup [MWd/tU]                                  | 90000.0              | 90000.0               | 90000.0                 |
| Heavy metal mass per fuel pebble [g]                     | 7                    | 7                     | 7                       |
| Number of loaded fresh fuel pebbles per day [-]          | 397.0                | 397.0                 | 397.0                   |
| Number of refueling times [-]                            | 8                    | 10                    | 15                      |
| Refueling cycle length [d]                               | 6.60                 | 5.28                  | 3.52                    |
| Time for pebbles going through the core per times [d]    | 132.0                | 105.6                 | 70.4                    |
| Total residence time of pebbles in the core [d]          | 1056.0               | 1056.0                | 1056.0                  |
| Calculated average discharge burnup depth [-]            | 89912.0              | 89997.0               | 90212.0                 |

Thereafter, Reactor burnup evolution process is discretized into many fuel cycles with identical cycle length. Cycle length represents the time interval between two successive fuel shuffling. Smaller cycle length indicates a faster refueling and it allows fuel pebbles run through the core more times at given total residence time. In this study, three multi-pass refueling schemes are simulated, namely eight times pass (8x), ten times pass (10x) and fifteen times pass (15x), and their equilibrium core main parameters are listed in table I. Reactor responses of multiplication factor and region relative power are calculated and compared. Further, with the established fission yield uncertainty analysis framework described in the following chapter, yields’ uncertainty contributions to those responses are quantified and compared to address the multi-pass refueling effect on yields uncertainty propagation.
3. METHODOLOGY

3.1. Fission Yield Covariance Estimation

Fission product yields characterize the fraction of fission products produced per fission. Depending on different fissile isotope and incident neutron energy, different fission system are categorized and recorded in ENDF/B-VII.1 library. This study focuses thermal neutron-induced U-235 fission system in this evaluated nuclear data library. However, yields data in this system originate from England and Rider’s work [8] in 1994. Although they provided a recommended independent and cumulative yield data set along with corresponding uncertainties, covariance information is lacked from their work. In this study, independent yields’ covariance information is estimated by Bayesian method [9-11]. Because yield library adopted in V.S.O.P. uses a combined set of cumulative and independent yields for sake of shortening fission product decay chain, and also cumulative yields are dependent with independent yields by Q-matrix proposed by M. F. James [12], sampling directly on independent yields is critical to generate self-consistent combined V.S.O.P. yields library samples. Furthermore, because of the existence of consistency between independent and cumulative yields as well as inherent physical constrains imposed on independent yields, properly estimated covariance information is indispensable for generating self-consistent independent yield samples to permit an unbiased uncertainty analysis results.

Bayesian method is feasible for updating and combining prior information of independent yields with upcoming new knowledge about them. By assigning initial Gaussian prior of independent yields and following M.T. Pigni’s derivation [11], the updating process is listed in Table II. It is noteworthy to mention that updating formulation of posterior independent yields mean value is not listed here.

| Index | Procedure Name | Independent yield distribution | Covariance updating formulation | Prior | Likelihood |
|-------|----------------|-------------------------------|--------------------------------|-------|------------|
| 0     | Prior distribution | $I - N(I_0, Z_0)$ | $Z_i = Z_{i0} - Z_i Q (V + QZ_i Q^T)^{-1} Q Z_{i0}$ | $I - N(I, Z)$ | $Z_{i0}$ |
| 1     | Cumulative yields consistency | $I - N(I_0, Z_0)$ | $C = Q I$ | $Z_i = Z_{i0} - Z_i Q (V + QZ_i Q^T)^{-1} Q Z_{i0}$ | $I - N(I, Z)$ | $Z_{i0}$ |
| 2     | Total yields conservation | $I - N(I_0, Z_0)$ | $y = Z_i^T U (x^2 + U^T Z_i U) U^T Z_i$ | $I - N(I, Z)$ | $U^T = \sum_{i=1}^{n} j_i = 2.0$ |
| 3     | Mass number conservation | $I - N(I_0, Z_0)$ | $m = Z_i^T U (x^2 + U^T Z_i U) U^T Z_i$ | $I - N(I, Z)$ | $N^T = \sum_{i=1}^{n} j_i = 233.57915$ |
| 4     | Charge number conservation | $I - N(I_0, Z_0)$ | $z = W^T I (x^2 + W^T Z_i W)^{-1} W^T Z_i$ | $I - N(I, Z)$ | $W^T = \sum_{i=1}^{n} j_i = 92.05318$ |

Here, $I_0 \in \mathbb{R}^{nx1}$ and $Z_0 \in \mathbb{R}^{nxn}$ are prior independent yields value and diagonal covariance matrix with each element directly taken from ENDF/B-VII.1 neutron induced fission yield sub-library (MF=8, MT=454), while $C_0 \in \mathbb{R}^{nx1}$ and $V \in \mathbb{R}^{nxn}$ are those for cumulative yields taken from fission yield sub-library (MF=8, MT=459). $Q \in \mathbb{R}^{nxn}$ is the Q-matrix constructed according to radioactive decay information provided in ENDF/B-VII.1 radioactive decay sub-library (MF=8, MT=457). $\sigma^2$ is summation precision and is taken as $10^{-10}$. The updating process is implemented sequentially from index 1 to index 4 and the final resulting posterior distribution of independent yields is $I - N(I_4, Z_4)$.

Independent yields distribution of 0.0253 eV neutron induced U-235 fission follows a two-humped pattern, with light hump having mass number range of 90 to 100 and heavy hump having mass number range of 132 to
Corresponding to this pattern, two features could be noticed in Figure 2. First, there are many correlations appear within each hump and between humps (shown as hump-hump correlation), while few correlations are overserved between hump and valley part. These correlations are derived from the physical constrains imposed on independent yields, which are fission system conservation of total yields, mass number and charge number. Another feature is that many strong negative correlations appear alongside the diagonal part, which suggests fission product yields within each mass chain correlated with each other negatively. This is induced by the imposing consistency with cumulative yields on independent yields, because most radioactive decay fission products within each mass chain will contribute to its corresponding final stable or long-lived products by $\beta^-$ decay. Uncertainty and measured yields of these stable or long-lived products suggest negative correlations among its precursor products.

Figure 2. Estimated independent yield correlation matrix. Upper diagonal is omitted in the figure. The axis is the mass number of these fission products. These fission products are ordered firstly by decreasing mass number, and then increasing charge number within each mass chain.

3.2. Stochastic Sampling of Fission Product Yields

Stochastic sampling based uncertainty analysis method is applied to propagate fission yield uncertainty in pebble-bed HTGR burnup simulations. Figure 3 (left) illustrates fission yield uncertainty analysis flowchart. As is described in section 3.1, stochastic sampling of posterior independent yields is conducted in this study. However, direct sampling independent yield under normal distribution would generate inconsistent negative value yield samples. This is because most independent yields have larger posterior relative uncertainty (larger than 30%) as is shown in Figure 3 (right), and the PDF of these yields would expand a lot to their negative range [13]. As is suggested by the principle of maximum entropy [14], instead of sampling yields under normal distribution, lognormal distribution is assigned to posterior independent yields. Although lognormal distribution would approximate normal distribution when the relative uncertainty of yield is small, the uncertainty of posterior independent yield is large enough that assigning normal distribution would be insufficient to describe its randomness and result in involving incorrect samples into the following burnup uncertainty analysis.
Figure 3. Fission product yield uncertainty propagation flowchart (Left) and relative uncertainty of prior and posterior independent yields (Right). Several larger posterior relative uncertainty (larger than 60%) result from large discrepancy between calculated prior cumulative yields and those provided in ENDF/B-VII.1.

Figure 4. Histogram of 2,000 independent yield samples of Cs-134 (Left) and Nd-143 (Right). Dark brown parts are the overlaps between these two bar graphs.

Figure 4 presents histograms of 2,000 yield samples sampled under normal and lognormal distribution. Nd-143 has larger relative uncertainty 64.0%, while Cs-133 has smaller relative uncertainty 32.0%. Their sampling results are compared in this figure to highlight the negative sample value issue discussed above. Histograms of Cs-133 obtained from normal and lognormal distribution are fairly similar (Figure 4 left), while those for Nd-143 are completely different (Figure 4 right) and many negative value yield samples are observed. Log-normal distribution could capture the skewness of inherently positive yields’ distribution and provide more reasonable and self-consistent perturbation samples sets.
4. RESULTS

4.1. Multiplication Factor Uncertainty

Table III shows uncertainty analysis results of multiplication factor in equilibrium core and comparison among three multi-pass refueling schemes. 1,000 samples are analyzed to obtain the following results.

| Refueling Scheme | Nominal Prediction | Fission Yield Uncertainty Analysis Results |
|------------------|--------------------|--------------------------------------------|
|                  | V.S.O.P. | Samples Mean | Relative Uncertainty | 95% CI | Normality Test |
| 8x               | 0.99881 | 0.99879 | 2.5755E-04 | [2.4346E-04, 2.7465E-04] | Failed: p=1.057E-04 |
| 10x              | 0.99990 | 0.99989 | 2.5759E-04 | [2.4360E-04, 2.7461E-04] | Failed: p=9.035E-05 |
| 15x              | 1.00106 | 1.00105 | 2.5867E-04 | [2.4438E-04, 2.7548E-04] | Failed: p=1.103E-04 |

* 95% confidence interval is estimated by bootstrapping method with 100,000 bootstrap samples;
* Normality test is conducted on the z-score of multiplication factor samples with K-S test;

From the above table, it could be noted that yields uncertainty contribute a little to multiplication factor’s uncertainty in equilibrium core. This is fairly consistent with only considering yields contribution, as yields have little impact on neutron multiplication and absorption compared with other dominant parameters, like cross section. These relative uncertainty results are agree with the results in magnitude (around $10^{-4}$) obtained in LWR [4], and this indicates the feasibility of proposed yields uncertainty propagation framework in this study. In future work, this will be applied to study yields uncertainty contribution to reactor decay heat release under accidental scenario, where yields are expected to be important.

Another observation is that multi-pass refueling scheme has little impact on yields uncertainty contribution to reactor global responses, like multiplication factor. From table II, multiplication factors predicted under 8x, 10x and 15x are slightly different from each other, while their corresponding relative uncertainty are fairly similar. Multiplication factor is a global response which is affected by the overall burnup of the core. Considering all these three refueling schemes have reached similar average discharge burnup depth, it is therefore their overall nuclide compositions in the core are similar. Because of that, yields have similar contributions among different refueling schemes. Although equilibrium cores reached via different refueling schemes could have overall similar average fuel burnup, the distribution of those burnup throughout the core could vary a lot with different adopted refueling schemes. Subject to similar average discharge burnup depth, more fueling times indicates faster reloading speed of the fuels. It allows more fuel batches mixed within each spectrum region, and smaller burnup difference among those fuel batches. Hence, more fueling times foresees a more “homogeneous” equilibrium core. Except for global responses, it is therefore expected that yields uncertainty contribution to local responses, like region relative power, are likely to be affected by fuel refueling times, as is going to be discussed in the following section.

4.2. Region Relative Power Uncertainty

Channel I is the inner most channel of HTR-PM and it is partitioned into 20 spectrum regions axially, namely layer 1 to layer 20. The relative power of each region in channel I is presented in Figure 5, and it could be seen that multi-pass refueling scheme could flatten the power distribution inside the core. The more refueling fuel pebbles undergo, the more fuel batches are within each region. Therefore, burnup difference among different regions is smaller when more refueling procedures are adopted. Therefore region relative power is flattened.
Figure 5. Regional relative power distribution alongside Channel I. Each spectrum region is mixed with different fuel batches corresponding to the adopted refueling times. Number of fuel batch is identical to refueling times.

Figure 8. U-235 fission fraction alongside Channel I (left) and standard deviation of regional relative power in Channel I (right). This fraction accounts for U-235 fission among all fissile fission, including U-233, U-235, Pu-239 and Pu-241. Upper section stands for region 1 to region 8 and lower section stands for region 9 to region 20. 

Figure 8 (right) presents the quantified standard deviation of relative power in each region of Channel I and results from 8x, 10x and 15x are compared in this figure. Yields have small contributions on relative power (standard deviation is smaller than 0.12%) and it coincides with our belief that yields are small.
effect in relative power prediction. Though yields are small effect, their uncertainty contributions to relative power are still affected by the adopted refueling scheme. As shown in Figure 8(right), more refueling times provide a more “flattened” uncertainty distribution and the uncertainty of peak relative power is reduced. As only thermal neutron induced U-235 fission yields uncertainty are considered in this study, this power uncertainty distribution is related to fission fraction of U-235 within each region. Fission fraction of U-235 is shown in Figure 8 (left). It is observed that, in the upper section, fission fraction distribution resembles standard deviation distribution of relative power. This is because the more fission from U-235, the more its yields uncertainty would contribute to the release power. Additionally, in the lower section of all these three refueling scheme, U-235 fission fractions become smaller and thus yields’ contribution to relative power is smaller than upper section in general.

5. CONCLUSIONS

Based on ENDF/B-VII.1, thermal neutron induced U-235 fission product yield uncertainty propagation in HTR-PM burnup process is studied. As one feature of HTR-PM, the effect of multi-pass refueling fuel management scheme on yields uncertainty propagation is addressed and the following conclusions are drawn from this study:

(1) A V.S.O.P. computer code system based fission yields uncertainty analysis framework is proposed in this work to investigate yields uncertainty contribution to reactor responses during burnup simulation.
(2) Compared with cross section, yields uncertainty contribution to reactor responses is small for both global response, like multiplication factor, and local response, like region relative power. This is coincide with common belief.
(3) Multi-pass refueling scheme in HTR-PM could affect the propagation of yields uncertainty contribution to reactor local responses. Specifically, more refueling times could allow a more “flattened” region relative power uncertainty distribution and smaller uncertainty for peak relative power, whereas global response uncertainty is not affected by refueling scheme.

Based on the proposed yields uncertainty framework in this study, yields uncertainty contribution to released decay heat under accidental scenario will be investigated in further work and the multi-pass refueling effect on it will be further addressed.

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