Uncertainty Analysis of Fission Product Yields in Pebble Bed High Temperature Gas-Cooled Reactors Based on Detailed Burnup Chains

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Date: 2025-06-20T14:58:28+00:00

Abstract

Pebble bed high-temperature gas-cooled reactors (HTGRs) are cores with online refueling, and their fuel is in the shape of spheres. In an equilibrium core, each fuel pebble undergoes 15 cycles of being loaded into the core from the top and discharged from the bottom under gravity, resulting in a complex burnup history. During the burnup process in the equilibrium core of a pebble bed HTGR, fission product yields and their uncertainties primarily affect the composition of the nuclide inventory, nuclide concentrations, and the distribution of nuclides at different positions within the equilibrium core; these factors related to the core nuclide inventory remain constant in the equilibrium core. After reactor shutdown, fission product yield uncertainties will propagate to decay heat uncertainties through nuclide concentration uncertainties. The decay heat uncertainty in pebble bed HTGRs determines the maximum fuel pebble temperature under accident conditions, which is related to the inherent safety of the reactor. Therefore, it is necessary to conduct in-depth research on the contribution of fission product yield uncertainties to nuclide concentration uncertainties during the burnup process in the equilibrium core of pebble bed HTGRs.

[Methods] Currently, although the VSOP-UAM core physics design and uncertainty analysis code for pebble bed HTGRs can quantify the contribution of fission product yield uncertainties to the uncertainties in keff and nuclide concentrations in the equilibrium core, VSOP-UAM simplifies the burnup calculation process for pebble bed HTGRs by omitting many burnup chains and can only output information for approximately one hundred nuclides, making it incapable of performing detailed quantitative analysis of fission product yield uncertainties. Therefore, it is necessary to develop a detailed burnup uncertainty analysis capability for pebble bed HTGRs based on detailed burnup chains and a complete nuclide inventory. The core source term calculation code NUIT can perform constant-power burnup calculations and decay heat calculations for pebble bed HTGRs, provides complete burnup and nuclide inventory information, and already possesses the NUIT-EMBAD fission product yield uncertainty analysis code for 235U.

[Results] Based on the NUIT-EMBAD burnup calculation uncertainty analysis code, this paper developed fission product yield uncertainty analysis capabilities for 233U, 239Pu, and 241Pu based on detailed burnup chains to quantitatively analyze the contribution of each fission product yield uncertainty to burnup calculation uncertainties. Through comparison, it was found that the contribution of fission product yield uncertainties from 239Pu and 235U to the burnup process is comparable, and NUIT-EMBAD's contribution to nuclide concentration uncertainties for actinides is mostly smaller than that of VSOP-UAM. For fission product nuclide concentration uncertainties, the results from the two codes show little difference.

[Conclusion] This conclusion demonstrates the accuracy of the NUIT-EMBAD uncertainty analysis code. Moreover, NUIT-EMBAD can output complete nuclide concentration uncertainty information, enabling detailed decay heat uncertainty studies for pebble bed HTGRs based on these results.

Full Text

Fission Yield Uncertainty Analysis for Pebble-Bed High-Temperature Gas-Cooled Reactors Based on Detailed Burnup Chains

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Abstract

[Objective] The pebble-bed high-temperature gas-cooled reactor (HTGR) is a continuously refueled reactor with spherical fuel elements. In the equilibrium core, each fuel pebble undergoes approximately 15 passes through the core—loaded from the top and discharged from the bottom under gravity—resulting in a complex burnup history. During equilibrium core burnup, fission yields and their uncertainties primarily affect the composition, concentration levels, and spatial distribution of nuclides in the core's nuclide inventory. In the equilibrium state, these nuclide-related factors remain constant. After reactor shutdown, fission yield uncertainty propagates to decay heat uncertainty through nuclide concentration uncertainty. Since decay heat uncertainty determines the maximum fuel temperature under accident conditions and thus impacts inherent safety, investigating the contribution of fission yield uncertainty to nuclide concentration uncertainty during equilibrium core burnup is essential.

[**Methods**] Currently, the VSOP-UAM code for pebble-bed HTGR core physics design and uncertainty analysis can quantify contributions from fission yield uncertainty to keff and nuclide concentration uncertainties in the equilibrium core. However, VSOP-UAM simplifies the burnup calculation process, omits many burnup chains, and outputs information for only about one hundred nuclides, preventing detailed quantitative analysis of fission yield uncertainties. Therefore, developing a refined burnup uncertainty analysis capability based on detailed burnup chains and a comprehensive nuclide library is necessary. The core source term calculation code NUIT can perform constant-power burnup and decay heat calculations for pebble-bed HTGRs while providing complete burnup and nuclide library information. NUIT-EMBAD, an existing module for 235U fission yield uncertainty analysis, serves as the foundation for this work.

[**Results**] This study developed fission yield uncertainty analysis capabilities for 233U, 239Pu, and 241Pu based on the NUIT-EMBAD burnup uncertainty analysis code, quantifying each fission yield's contribution to burnup calculation uncertainty. Comparison reveals that 239Pu and 235U fission yield uncertainties contribute comparably to the burnup process. For actinide nuclides, NUIT-EMBAD's concentration uncertainty contributions are generally smaller than VSOP-UAM's, while results for fission products show minimal differences between the two codes.

[**Conclusion**] These findings demonstrate the accuracy of the NUIT-EMBAD uncertainty analysis code. Furthermore, NUIT-EMBAD can output complete nuclide concentration uncertainty information, enabling refined decay heat uncertainty studies for pebble-bed HTGRs.

[**Keywords**] pebble-bed HTGR; fine burnup uncertainty analysis; fission yield uncertainty; nuclide concentration uncertainty; NUIT-EMBAD

[**DOI**] 10.16516/j.ceec.2025-083

Funding: National Natural Science Foundation of China "Research on Uncertainty Propagation Methodology for Multi-Pass Fuel Through Core Mode" (11505102)

Compared to fixed-fuel-layout pressurized water reactors, the pebble-bed

HTGR's unique refueling mode and flowing core make precise simulation of each fuel pebble's irradiation history from loading to discharge extremely challenging [1]. The equilibrium core theoretical refueling model is illustrated in [Figure 1: see original paper], where the core is axially divided into 20 layers. Fuel pebbles move downward one layer every 3 days under gravity, with each pebble undergoing a complete refueling cycle of 1056 days. This complexity introduces significant uncertainty inputs into pebble-bed HTGR burnup calculations [2-3]. Burnup uncertainty analysis is crucial for operational design and inherent safety evaluation, representing an important component of pebble-bed HTGR uncertainty analysis [4-5].

Fission yield uncertainty, as one source of nuclear data uncertainty, affects burnup process uncertainty and contributes substantially to uncertainties in key operational parameters such as keff and equilibrium core nuclide concentrations [4]. Due to the high burnup characteristics of pebble-bed HTGRs, 239Pu fission fraction exceeds that of 235U in later burnup stages, as shown in [Figure 2: see original paper]. Therefore, accurately quantifying the contribution of fissionable nuclides like 239Pu to burnup uncertainty is essential [6].

Current burnup uncertainty analysis tools for pebble-bed HTGRs include VSOP-UAM [7], SCALE/SAMPLER [2, 8], and NUIT-EMBAD [9]. VSOP-UAM can analyze uncertainties in multi-group cross-sections and fission yields of fissionable nuclides, but simplifies the burnup calculation process and chains, outputting only about one hundred nuclides [6, 10] without providing complete burnup information. While other tools offer refined burnup calculation and uncertainty analysis capabilities, they lack the detailed power history simulation of pebble flow movement [11]. NUIT-EMBAD, developed from the pebble-bed HTGR source term analysis code NUIT [12], performs constant-power burnup calculations with a complete nuclide library, including intermediate and short-lived nuclides from all burnup and decay processes. The existing 235U fission yield uncertainty analysis module outputs complete nuclide concentration information for the equilibrium core, providing the foundation for refined decay heat calculations. This study extends NUIT-EMBAD with fission yield uncertainty analysis capabilities for 233U, 239Pu, and 241Pu, producing detailed nuclide concentration uncertainty information for comparison with VSOP-UAM results to validate the developed functionality.

1 NUIT-EMBAD Uncertainty Analysis Process

The NUIT-EMBAD uncertainty analysis workflow is shown in [Figure 3: see original paper]. Based on sampling statistics, the code is treated as a "black box." Fission yields are randomly perturbed according to uncertainties provided in the ENDF/B-VII.1 library, and output parameter uncertainties are quantified through physical calculation simulations of the pebble-bed HTGR [13-14]. The analysis comprises four main steps:

1. **Covariance Calculation:** Using Bayesian updating with fission yield

and decay data from ENDF/B-VII.1 to compute covariances for independent fission yield data from thermal neutron-induced fission [15-16].

2. **Sample Generation:** Assuming a multivariate log-normal probability density distribution for independent fission yields (based on physical non-negativity constraints), with distribution parameters derived from mean values and covariance data. Latin hypercube sampling generates multiple sets of perturbed independent fission yield samples [17-19].
3. **Database Matching:** Matching independent fission yield perturbation samples with the NUIT-EMBAD fission yield library (as shown in [Figure 4: see original paper]) to generate perturbed sample libraries for numerical simulation in NUIT-EMBAD.
4. **Statistical Analysis:** Analyzing the standard deviation of nuclide concentrations from NUIT-EMBAD outputs as the quantification result [4].

1.1 Refined Burnup Uncertainty Calculation Process

The NUIT-EMBAD burnup calculation process is illustrated in [Figure 4: see original paper] [2]. Based on the pebble-bed HTGR equilibrium core, this method uses NUIT's constant-power burnup capability and complete nuclide library information to simulate the detailed power history experienced by each fresh fuel batch from initial loading through multiple burnup cycles until final discharge, obtaining complete nuclide composition and concentration information for the core.

During uncertainty analysis, each fission yield perturbation sample library produces a corresponding set of nuclide concentration results. Statistical analysis of these complete nuclide library results yields comprehensive uncertainty information. For validation purposes, fission yield uncertainties were also obtained using VSOP-UAM for comparison. This study performs fission yield covariance matrix evaluation and uncertainty analysis based on the NUIT-EMBAD program.

1.2 Evaluation of Fission Yield Covariance Matrices

The fission yield covariance matrix evaluation process uses ENDF/B-VII.1 independent fission yield data for 239Pu thermal fission and decay data as the foundation. Bayesian updating incorporates four constraints on independent fission yields: cumulative fission yield constraint, total independent fission yield constraint, mass number conservation, and charge number conservation [4]. The constraints are listed in , and the procedure is shown in [Figure 5: see original paper]. After four levels of Bayesian updating, the resulting correlation coefficient matrices for each fission yield are presented in [Figure 6: see original paper] [20]. Perturbation samples are then generated through log-normal sampling based on the updated matrices.

1.3 NUIT-EMBAD Perturbation Database Matching Process

Following covariance matrix updates, consistency evaluation between the fission yield sample libraries and the NUIT-EMBAD database is performed, as shown in [Figure 7: see original paper]. Analysis reveals that since NUIT-EMBAD's fission yield database is constructed from ENDF/B-VII.1 independent fission yield data for fissionable nuclides, perturbation sample libraries generated from ENDF/B-VII.1 can be directly mapped to NUIT-EMBAD's independent fission yield library, satisfying consistency requirements. Thus, ENDF/B-VII.1-based independent fission yield sample libraries can be directly used in NUIT-EMBAD burnup calculations for uncertainty analysis.

2 Calculation Results and Validation

Decay heat calculation for HTGRs is critical for inherent safety evaluation, making quantification of nuclide library parameter contributions to burnup uncertainty essential [1]. This analysis examines fission yield uncertainties for thermal fission of 233U, 235U, 239Pu, and 241Pu. First, contributions from 239Pu and 235U fission yield uncertainties to nuclide concentration uncertainties in NUIT-EMBAD are compared. Second, contributions from all four nuclides' fission yield uncertainties to burnup calculation uncertainties are compared between VSOP and NUIT-EMBAD to validate NUIT-EMBAD's accuracy. Results for actinides and fission products are presented separately in – and [Figure 8: see original paper].

**** Comparison of relative uncertainty contributions (%) of U fission yield uncertainties to actinide nuclide concentration uncertainties.
**** Comparison of relative uncertainty contributions (%) of Pu fission yield uncertainties to actinide nuclide concentration uncertainties.
**** Comparison of relative uncertainty contributions (%) of U isotope fission yield uncertainties to fission product nuclide concentration uncertainties.
**** Comparison of relative uncertainty contributions (%) of Pu isotope fission yield uncertainties to fission product nuclide concentration uncertainties.
[Figure 8: see original paper] Comparison of nuclide concentration uncertainties.

The results in – and [Figure 8: see original paper] demonstrate that fission yield uncertainties contribute far less to actinide concentration uncertainties than to fission product uncertainties. For actinides, NUIT-EMBAD results are generally smaller than VSOP-UAM's because VSOP, as a core design code, handles strong reactor coupling. During burnup calculations, perturbed fission yields affect batch power values, influencing the neutron physics calculation integrated with pebble flow movement and ultimately impacting actinide concentrations. NUIT-EMBAD performs constant-power calculations without neutron physics coupling, yielding smaller statistical results where fission yield uncertainty contributes negligibly to actinide concentration uncertainty.

For fission products, VSOP-UAM and NUIT-EMBAD show nearly identical nuclide concentration uncertainties. This agreement arises because both codes use the ENDF/B-VII.1 fission yield library, and fission yield uncertainty directly propagates to fission product concentrations. These results validate the reliability of NUIT-EMBAD's fission yield uncertainty analysis for subsequent studies.

Specifically, 239Pu contributes to actinide concentration uncertainties in the range of 4.6$\times10^{-7}$ to 9.6$\times10^{-5}$, while its contribution to fission product concentration uncertainties ranges from 0.095% to 12.73%. The 109Ag nuclide shows particularly high uncertainty at 12.73%, with 235U contributing only 0.93%. This occurs because 109Pd produced from 239Pu thermal fission decays to 109Ag with a very short half-life of 13.7 hours, and the fission yield and its uncertainty for 109Pd from 239Pu are larger than from 235U. Thus, 239Pu fission yield uncertainty must be considered. The 109Ag decay scheme is shown in [Figure 9: see original paper].

This study extends NUIT-EMBAD with fission yield uncertainty analysis capabilities for 233U, 239Pu, and 241Pu thermal fission, refining the program's functionality and enabling detailed quantitative analysis of fission yield uncertainty contributions to equilibrium core nuclide concentration uncertainties. Comparison with VSOP-UAM validates NUIT-EMBAD's accuracy. During shutdown or accident conditions, fission yield uncertainty propagates to decay heat uncertainty through nuclide concentration uncertainty, representing one source of decay heat uncertainty. Therefore, this program enables refined decay heat uncertainty studies for pebble-bed HTGRs.

Key findings include:
1) For equilibrium core fission yield uncertainties in pebble-bed HTGRs, fission product uncertainties far exceed actinide uncertainties.
2) Comparing both codes, fission product concentration uncertainties show close agreement, while VSOP-UAM yields larger actinide uncertainties due to its integrated neutron physics calculations versus NUIT-EMBAD's constant-power approach.
3) The close agreement between VSOP-UAM and NUIT-EMBAD validates NUIT-EMBAD's burnup uncertainty analysis.
4) 239Pu fission yield uncertainty contributes comparably to 235U and cannot be neglected, with up to 12.73% contribution to 109Ag concentration uncertainty.

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