Comparison among MCNP-based depletion codes applied to burnup calculations of pebble-bed HTR lattices

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ABSTRACT

The double-heterogeneity characterising pebble-bed high temperature reactors (HTRs) makes Monte Carlo based calculation tools the most suitable for detailed core analyses. These codes can be successfully used to predict the isotopic evolution during irradiation of the fuel of this kind of cores. At the moment, there are many computational systems based on MCNP that are available for performing depletion calculation. All these systems use MCNP to supply problem dependent fluxes and/or microscopic cross sections to the depletion module. This latter then calculates the isotopic evolution of the fuel resolving Bateman’s equations.

In this paper, a comparative analysis of three different MCNP-based depletion codes is performed: Monteburns2.0, MCNPX2.6.0 and BGCore. Monteburns code can be considered as the reference code for HTR calculations, since it has been already verified during HTR-N and HTR-N1 EU project. All calculations have been performed on a reference model representing an infinite lattice of thorium–plutonium fuelled pebbles. The evolution of k-inf as a function of burnup has been compared, as well as the inventory of the important actinides.

The k-inf comparison among the codes shows a good agreement during the entire burnup history with the maximum difference lower than 1%. The actinide inventory prediction agrees well. However significant discrepancy in Am and Cm concentrations calculated by MCNPX as compared to those of Monteburns and BGCore has been observed. This is mainly due to different Am-241 (n,γ) branching ratio utilized by the codes.

The important advantage of BGCore is its significantly lower execution time required to perform considered depletion calculations. While providing reasonably accurate results BGCore runs depletion problem about two times faster than Monteburns and two to five times faster than MCNPX.

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1. Introduction

With increasing computer performances there is a growing interest in Monte Carlo (MC) based depletion codes due to their capability of handling complex geometries of advanced reactor systems. An example for such system is pebble-bed high temperature reactor (HTR). The so-called “double-heterogeneity” characterizing HTR fuel elements, while challenges existing deterministic lattice codes, can be directly treated by the MC methods.

Currently a number of MC depletion codes are available. These codes usually couple MC neutronic solver with a depletion code in a way that MC code provides one group problem dependent fluxes and microscopic cross sections to depletion module, which performs burnup calculation and provides end-of-timestep material compositions.

MC depletion codes can be divided into two groups according to the cross-section generation methodology. The first group of the codes uses the “standard” approach according to which one-group reaction rates for all cross sections of interest are directly tallied by the MC code. The second group of the MC depletion codes uses multi-group approach for cross-section generation which is different from the standard one. According to this methodology, only multi-group flux is calculated by MC code while reaction
rates for particular nuclides are not tallied. Then, reaction rates are calculated separately using pre-generated multi-group cross-section set and the fine group neutron spectrum obtained from the MCNP code. Multi-group coupling approach significantly reduces the code execution time without compromising the accuracy of the results due to reduced number of tracked tallies. This approach was implemented in several computational systems including OCTOPUS (Kloosterman et al., 1996; Kuiper et al., 2004), ALEPH (Haecck and Verboomen, 2007), and BGCore (Fridman et al., 2008b) codes. In this work, we performed intercomparison among three MC depletion codes as applied to burnup analysis of HTR fuel element. Initially, we present a brief description of the codes while highlighting the difference in coupling methodology and depletion modules in use. The model of HTR fuel element will be described. Then, the results of depletion calculations will be compared including evaluation of nuclide inventories, neutron multiplication factor, and execution time required by codes.

2. Computer codes description

In this work, depletion calculations were performed with Monteburns, MCNPX, and BGCore MC-depletion code. In this section, a brief description of the codes is presented.

2.1. Monteburns2.0

Monteburns (Poston and Trellue, 1999) couples MCNP a general-purpose Monte Carlo radiation transport code (Briefmeister, 2005) with either ORIGEN2.2 (Cropp, 1980) or CINDER90 (Wilson et al., 1994) depletion codes. The Monteburns uses the standard coupling approach where MCNP provides one-group microscopic cross-sections and fluxes to the chosen depletion code. Monteburns uses Perl (http://www.perl.com) script interacting with a FORTRAN77 program (monteb.f) for linking between MCNP and depletion code. The current version 2.0 is able to use MCNP4C, MCNP5 or MCNPX2.5. Monteburns uses predictor–corrector methodology to increase the accuracy of the burnup calculation. Initially a “predictor” step is used, in which ORIGEN (or CINDER) is run halfway through the designated step to obtain half-timestep isotopic composition. Then, this composition is used by MCNP to recalculate half-timestep one-group cross-sections and neutron fluxes. The assumption is that half-timestep cross-sections and neutron fluxes represent a reasonable approximation of the cross-sections and neutron fluxes averaged over the timestep. Finally, half-timestep values are used to perform depletion calculation for entire timestep. Monteburns provides a user with various time dependent data such as neutron multiplication factor, neutron fluxes, microscopic cross-section per material, nuclide inventories, activity, and radiotoxicity. In this work ORIGEN2.2 was used as a depletion code.

2.2. MCNPX2.6.0

The MCNPX (Pelowitz, 2008) is a general-purpose Monte Carlo N-Particle code that has been developed as an extension of the MCNP code. CINDER90 depletion code was integrated into the latest 2.6.0 version of MCNPX to provide it with built-in burnup capabilities. CINDER90 has inherent decay and 63-group cross-section data library for 3400 isotopes. In general, CINDER90 utilizes one group cross sections tallied by MCNPX. However, for isotopes without continuous energy cross sections data, one group cross sections are obtained by collapsing 63-group CINDER90 cross-section set and 63-group neutron spectrum calculated by MCNPX. MCNPX utilizes predictor–corrector procedure which is similar to that of MONTEBURNS (Fensin et al., 2006).

2.3. BGCore

BGCore (Fridman et al., 2008b) reactor analysis system, recently developed at Ben-Gurion University, couples MCNP4C with an independently developed burnup and decay module SARAF. The BGCore utilizes a multi-group approach for generation of one group cross-sections (Fridman et al., 2008a). The BGCore approach for generation of one group cross-sections takes advantage of the fact that dividing the neutron flux tally into multiple energy bins has practically no effect on the MCNP execution time. The following calculation procedure is therefore adopted. A fine group spectrum (currently 50,000 lethargy points) is tallied at each burnable region by MCNP and passed on to the SARAF module. The one-group cross-sections are not tallied, but calculated in a separate subroutine using pre-generated multi-group cross-section set and the fine group neutron spectrum obtained from MCNP. The SARAF data library required for its execution is based on JEFF3.1 evaluated data files (Koning et al., 2006). Careful choice of about 1700 isotopes allows covering all potentially significant aspects of fuel irradiation and decay including calculations of post-irradiation fuel characteristics such as, activity, radiotoxicity, and decay heat with high degree of accuracy.

Considerable effort was made to ensure that the multi-group approach gives one group cross-section values identical to those obtained with the conventional direct reaction rate tally approach. It was found that for the nuclides with complex resonance structure, which present in the fuel at high concentrations, increasing the number of energy groups does not reduce the error in one group cross-section below ~1% especially at low fuel temperatures. The error originates almost exclusively from the unresolved resonances energy region. This is due to the probabilistic treatment of unresolved resonances in MCNP, which correctly predicts the average value of reaction rates but in principle cannot provide the fine structure of the neutron flux. As a result, the self-shielding effect in the unresolved resonances energy region is not accounted for correctly. The error introduced is not statistical in nature but systematic since shielded cross-section is always smaller than the infinite dilution one.

In order to overcome that inaccuracy, the multi-group approach was extended by introducing the background cross-section ($\sigma_0$) tabulation into the calculation scheme. A series of multi-group cross-section sets is generated for selected isotopes with significant resonance cross-sections for several values of $\sigma_0$. The approximate value of the $\sigma_0$ is then used to extract the appropriate set of multi-group cross-section set for a specific resonance isotope, which is further used to obtain the “shielding corrected” 1-$\sigma$ cross-section value. The simplified model for estimation of $\sigma_0$ is described in (Fridman et al., 2008a). Introduction of such extension reduces the difference between directly tallied and collapsed from multi-group cross-sections to well below 1% while still taking advantage of the fast MCNP execution (Fridman et al., 2008a).

The BGCore predictor–corrector approach is somewhat different from that of Monteburns and MCNPX. BGCore performs only one MCNP run per timestep for calculating the spectrum and one-group cross sections. The flux value calculated by MCNP is used for predictor depletion calculations to obtain predictor end-of-timestep isotopic composition of burnable materials. Then, the corrector flux value is recalculated using end of time isotopic composition and beginning-of-timestep one-group cross sections. After that, the depletion calculation is repeated using the corrector flux value. The final end of time isotopic composition is an average of predictor and corrector isotopic compositions. This approach accounts for changing magnitude of the neutron flux during the timestep, while it neglects changes in the flux spectrum and thus, cross-section values. In some cases, such as Gadolinium depletion, this limitation needs to be circumvented by careful choice of timestep size.
Substantial reduction in the BGCore code execution time allows consideration of problems with much higher degree of complexity, such as an introduction of thermal hydraulic feedback into the Monte Carlo calculations. Currently, a new T-H feedback module for BGCore system is under development. The results of the preliminary verification analysis (Kotlyar et al., 2009) show a good agreement with deterministic code and indicate the importance of introduction of T-H feedback into the calculation scheme.

3. Methodology

The reference model used in this framework is the following:

1. A single HTR pebble with white boundary conditions in order to simulate a stochastic arrangement like that we find in a typical HTR pebble-bed core.
2. The considered pebble is a standard one (6 cm diameter), with an average power density that is around 5 kW/l (Reitsma et al., 2006).
3. The TRISO particle arrangement was modelled as a regular cubic lattice (Bomboni et al., 2009), whose pitch was chosen on the basis of the kernel dimension and of the total HM mass per pebble (Cerullo et al., 2005).

The main assumed calculation parameters are the following:

- 3 g of HM per pebble (Cerullo et al., 2005)
- HM elemental composition: 33% Pu-RG, 67% thorium (Cerullo et al., 2005)
- Fuel temperature: 900 K. Please note that it is the same for each kernel inside the pebble. It has been kept constant during the whole irradiation. It has been chosen on the basis of the cross-section set available, i.e. ZZ-MCJEFF3.1NEA
- Non-burnable material temperature: 700 K
- Number of initial particles for MC calculation: 1000
- Number of cycles in each MC calculation: 250
- Number of cycles skipped: 50
- Number of irradiation steps: 30
- Length of each irradiation step: 25.

Please note that 3 g of HM per pebble as well as their elemental composition given above have been chosen since they are the reference configuration used in the framework of an international benchmark on burnup calculation for HTR fuel elements.

The total number of initial particles and of cycles has been chosen in order to obtain a standard deviation on k-inf that is lower than 200 pcm. This standard deviation is generally considered acceptable for pebble-bed burnup calculations, and it allows the possibility to obtain a reasonably short calculation time. The total irradiation length has been set to reach around 250 GWd/tHM burnup. This value is based on previous investigation on Th–Pu fuelled pebbles (Rodriguez et al., 2002). Indeed, irradiation experiments on Th/Pu fuelled TRISO particles were successfully performed in the past up to this burnup value (Rodriguez et al., 2002).

4. Results

This section presents the results of depletion calculations performed by the three codes. Since Monteburns has been verified for burnup calculation of HTR fuel during HTR-N and HTR-N1 European projects, we consider its results as a reference (Bufalino et al., 2004). Of course, this does not imply that Monteburns results are necessarily the most accurate, and a future code-to-experiment validation should be undoubtedly performed. Fig. 1 shows k-inf as function of burnup calculated by the three codes. Figs. 2 and 3 show the relative difference in k-inf including 2σ error bars and 2σ uncertainty band of Monteburns. MCNPX and Monteburns k-inf values are in good agreement while the majority of the values agree within statistical uncertainty (Fig. 2). The maximum relative difference in k-inf between Monteburns and MCNPX is lower than 0.8%. The BGCore k-inf results show slightly higher discrepancy with those of the Monteburns attributed to the different predictor corrector approaches implemented in Monteburns and BGCore. Smaller timesteps might improve the results.

Fig. 1. Comparison of k-inf calculated by MCNPX, BGCore, and Monteburns.

Fig. 2. Relative difference in k-inf: MCNPX vs. Monteburns.

Fig. 3. Relative difference in k-inf: BGCore vs. Monteburns.
Fig. 4. Th$^{232}$ inventory vs. burnup.

Fig. 5. Pa$^{233}$ inventory vs. burnup.

Fig. 6. U$^{233}$ inventory vs. burnup.

Fig. 7. Pu$^{238}$ inventory vs. burnup.

Fig. 8. Pu$^{239}$ inventory vs. burnup.

Fig. 9. Pu$^{240}$ inventory vs. burnup.

Fig. 10. Pu$^{241}$ inventory vs. burnup.

Fig. 11. Pu$^{242}$ inventory vs. burnup.
Fig. 12. Am\textsuperscript{241} inventory vs. burnup.

The concentrations of important actinides as function of burnup are presented in Figs. 4–18. Table 1 shows the maximum relative difference in actinide concentrations. A very good agreement in concentration of nuclides in Th chain can be observed (Figs. 4–6). The maximum relative difference between Monteburns results and those of MCNPX and BGCore is lower than 2.5% and 2.0%, respectively (see Table 1). The predicted Pu inventories (from Pu-239 to Pu-242) agree within 1.0% between Monteburns and MCNPX and within 3.0% between Monteburns and BGCore (Figs. 8–11). Significantly higher discrepancies in concentration of Am and Cm isotopes can be observed (Figs. 13–18). MCNPX systematically underestimates concentrations of Am isotopes (Figs. 12 and 13) and overestimates concentrations of Cm isotopes (Figs. 14–18) in comparison with Monteburns and BGCore. The relative difference

Fig. 13. Am\textsuperscript{243} inventory vs. burnup.

Fig. 14. Cm\textsuperscript{242} inventory vs. burnup.

Fig. 15. Cm\textsuperscript{243} inventory vs. burnup.

Fig. 16. Cm\textsuperscript{244} inventory vs. burnup.

Fig. 17. Cm\textsuperscript{245} inventory vs. burnup.

Fig. 18. Cm\textsuperscript{246} inventory vs. burnup.
is as high as 15% and 20% for Am and Cm isotopes, respectively (see Table 1) while Am and Cm inventories calculated by Monteburns and BGCore are in better agreement (about 2% and 9%, respectively). Relatively high discrepancy in MCNPX results can be explained using Pu-241 transmutation path presented in Fig. 19. Pu-241 decays into Am-241 with a $T_{1/2} = 14.7$ years. Am-241 which is relatively stable captures neutron and generates either Am-242m or Am-242 with branching ratios $\overline{b}$ and $1 - \overline{b}$, respectively. Short lived Am-242 ($T_{1/2} = 16$ h) decays into Cm-242 and starts Cm transmutation chain. Relatively long lived Am-242m ($T_{1/2} = 141$ years) continues Am transmutation chain. It is obvious that amounts of Am-242 and Am-242m obtained from the neutron capture reaction in Am-241 are strongly dependent on the capture branching ratio. The branching ratio utilized by MCNPX ($b \approx 0.1$) is lower than that of BGCore and Monteburns ($b = 0.2$). As a result MCNPX overestimates the production of Am-242 and underestimates the production of Am-242m as compared to BGCore and Monteburns. Moreover concentration of Pu-238 which is generated by $\alpha$ decay of Cm-242 is also overestimated. Currently there is a substantial degree of uncertainty in the branching ratio among the different databases (Fig. 20). Therefore further investigation is required to determine the most suitable database. In addition, new experimental measurement of the Am-241 ($n,\gamma$) reaction branching ratio might be necessary in order to reduce its uncertainty in evaluated data files. The use of problem dependent branching ratio would be necessary to improve the accuracy of Am, Cm, and Pu-238 inventory prediction.

Fig. 21 compares the calculation time as function of burnup required by the three codes. Please note that the execution time is normalized to that of the beginning of life (BOL) MCNP run (no tallies, BOL fuel composition). Fig. 21 shows that BGCore has a clear advantage over Monteburns and MCNPX. BGCore is two times faster than Monteburns and two to five times faster than MCNPX. The BGCore execution time exhibits only moderate increase with burnup mainly due to constantly increasing number of neutronically important nuclides to be considered in the MCNP material card. The Monteburns execution time has a higher slope because of both increasing number of considered nuclides and increasing number of reaction rates tallies. MCNPX execution time is essentially constant with burnup. This is due to the fact that during every time step MCNPX tallies reaction rates for a constant number of nuclides regardless to their neutronic importance. MCNPX tracks all nuclides “listed on the MCNPX material cards, produced by the isotope generator algorithm, or selected by the specified fission-product tier” (Pelowitz, 2008). This approach significantly increases the running time as compared to other MCNP-based depletion codes.

<table>
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<th>Table 1</th>
<th>Maximum relative difference in nuclide concentration.</th>
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5. Summary

A burnup calculation on a Pu–Th fuelled pebble up to 250 GWd/THM burnup has been performed with three different MCNP-based depletion codes namely Monteburns 2.0, MCNPX 2.6.0, and BGCore. Monteburns has been previously validated for Pu-based HTR pebbles (Bowman et al., 2005) and it has been considered as a reference code.

The results of depletion calculation show a good agreement in k-inf prediction. The predicted nuclide inventory of important actinides agrees well. However there is a significant discrepancy in Am and Cm concentrations calculated by MCNPX as compared to those supplied by Monteburns and BGCore (differences up to 20%). This difference can be explained by different capture branching ratio for the production of Am–242 and Am–242m used by the codes. The higher prediction accuracy in Am and Cm inventory can be achieved if “correct” problem dependent branching ratio would be used.

Among the three codes, BGCore exhibits superior computational performance. The computational time required by BGCore to run considered depletion problem is lower by factor of 2 and 2–5 as compared to that of Monteburns and MCNPX, respectively.

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