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Statistical error propagation in HTR burnup model

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ABSTRACT

In this study we use independent replica calculations in order to assess statistical error propagation in whole-core actinide-burner High Temperature Reactor model. We use the MCB5 code for modeling a single irradiation cycle with reactivity control. We made 100 simulations of representative neutron precision, each having different initial random number generator seed. We analyze the real-to-apparent tally variation for neutron multiplication factor and nuclear reaction rates. While k_{eff} uncertainty is well-predicted, local reaction uncertainties have exhibited under-prediction of several times since the very beginning of irradiation. Additionally, we correlate the increasing dominance ratio with the emergence of numerical instability and source convergence problems at a high burnup. Our conclusions indicate that the neutron cycle-to-cycle correlation must be considered by code users dealing with computationally expensive HTR models.

1. Introduction

The following types of uncertainty sources can be distinguished in Monte Carlo (MC) burnup calculations:

– Statistical – result from the statistical approach to solution of the neutron transport problem. Random fluctuation of scored physical quantities comes from the limited number of tracked particle histories. Various seeds for random number generator provide different results of simulation. This uncertainty component in burnup calculation has been studied in articles (Tohjoh et al., 2006a; Garcia-Herranz et al., 2008) for various models.
– Nuclear data – cross section libraries, thermal collision tables, decay constants, branching ratios and fission yields of isotopes are burdened with uncertainties. These errors are systematic, as nuclear data remain constant in simulation steps. The problem has been presented in article (Frosio et al., 2016) and studied by Rochman et al. (2010) and Rochman and Sciolla, 2014.
– Input data/modeling – specifications of nuclear system model are provided with a limited precision. In addition, the way the system is modeled (spatial and temporal discretization, various simplifications, etc.) systematically influences the results of neutron transport and burn-up calculations (investigated in the article by Kępisty et al. (2016)).
– Numerical truncation – various discrimination levels are applied in MC neutron transport and fuel depletion procedures. These settings are described in code user manuals such as those by X-5 MONTE CARLO TEAM (2003), Leppänen et al. (2015). Eventually, even floating-point variables in codes have a limited numerical precision.
– Nuclide densities error – isotopic densities at each time step contain cumulated errors from previous steps. This directly influences current MC neutron transport run and its results. It has been investigated analytically in the works by Park et al. (2012), Takeda et al. (1999).
– Renormalization – models assume that constant power during burnup steps and transmutations coefficients must be renormalized to represent this period. Different techniques used to reduce this error have been discussed by Isotalo et al. (2016).

The majority of Monte Carlo burnup codes lack information about errors other than apparent variance of tallies. It turns out that the direct analytical approach to the propagation of uncertainties at each step is substantially difficult due to the structure and complexity of Bateman equations (as discussed in the articles by Tohjoh et al. (2006a), Rochman and Sciolla, 2014; Park et al., 2012).

Abbreviations: BPR, Burnable Poison Rod; BWR, Boiling Water Reactor; EFPD, Equivalent Full Power Days; HTR, High Temperature Reactor; k_{eff}, effective neutron multiplication factor; MC, Monte Carlo; MCB, continuous energy Monte Carlo burnup (code); MCNP, Monte Carlo N-Particle (code); MOX, Mixed Oxide (fuel); PWR, Pressurized Water Reactor; SD, standard deviation; TRISO, tristructural-isotropic (fuel); TTA, Transmutation Trajectory Analysis.

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The independent replica method for MC simulations is usually applied to criticality calculations as a solution to overcome the problem of cross-correlation between neutron cycles. A code user can compare the real variance of tallies to the apparent variance predicted by a single MC neutron transport run (as demonstrated in Ueki et al. (1997)). Analogical methodology has already been applied in the context of burnup calculations, which can be considered as a brute force approach in the lack of other methods. In the paper by Sternat et al. (2011) the authors studied 200 MCNPX/MONTEBURNS simulations of fuel assembly with varying number of neutron histories in order to prove that burnup results undergo normal distribution. In the master thesis by Wyant (2012) the author studied 2D models of fuel assemblies and core from Pressurized Water Reactor (PWR) using the SERPENT code and 19 independent replica samples of burnup simulation. The evolution of real/apparent tallies variation as well as nuclide densities spread has been studied in detail in this work. Another example is the study by Bennett et al. (2013) in which the burnup of 4 Boiling Water Reactor (BWR) assemblies has been studied using 23 independent replica simulations. As one can observe, this method is usually applied to simplified reactor models, which is certainly logical due to computational burden of the approach itself.

In this article we focus on the propagation and assessment of statistical error in whole-core simulation of High Temperature Reactor (HTR). We apply the independent replica method to full 3D reactor geometry model, which can be found as novelty. Core physics in HTR systems differ from PWRs due to double heterogeneity, strong interaction with neutron reflectors, strong axial streaming effects and annular geometry. These factors motivate us to compare statistical error propagation in HTR with results obtained by other researchers. We analyzed 100 simulations with changed random number generator seed in order to observe the dispersion of physical quantities, both global (total mass of isotopes in the system, neutron multiplication factor) and local, for each burnable cell (reaction rates, power density, nuclide concentrations) at each time step. We put special attention to the ratio between real and apparent variation of tallies. The dominance ratio and source convergence are also studied due to reaching instability regime at a high burnup.

In Section 2 we present the methodology applied in burnup simulations. Specification of the numerical model is presented in Section 3, while the computational results are described in Section 4. Section 5 contains the summary and conclusions.

2. Methodology

The computational tool chosen for the purpose of this research is continuous energy Monte Carlo burnup code MCB (Cetnar et al., 1999) version 5 (Oettingen et al., 2011).

Below we present prominent elements of the MCB code methodology:

- Neutron transport calculations are based on MCNP5 (described in X-5 MONTE CARLO TEAM (2003));
- Reaction rates are scored for each cell and nuclide in continuous energy mode;
- Heating in cells is calculated either using heating cross section libraries with gamma heating or using Q-values (Zerovnik et al., 2014);
- Neutron source efficiency is normalized to the total generated power based on heating in cells and decay heat (Oettingen et al., 2011);
- Bateman equations are formulated and solved with TTA method (Cetnar, 2006),
- Available coupling schemes are Euler predictor and Stochastic Implicit Euler (explained and discussed in the articles by Kępisty and Cetnar (2014), Kotlyar and Shwageraus (2012));
- Numerical values of thresholds in depletion part and discrimination levels of neutron transport can be adjusted to required numerical precision, as described in the works by Cetnar et al. (1999), X-5 MONTE CARLO TEAM (2003);

Other depletion codes based on Monte Carlo neutron transport should be successfully applicable for the independent replica method, as long as it is possible to change input seed for random number generator. In case of MCB, output data have been post-processed using the C++ code in order to compute considered averages and standard deviation (SD) values.

Calculations have been performed on the Prometheus cluster computer (Cyfronet AGH, Krakow) with Intel Xeon E5-2680v3 processors. The independent replica simulations have been run in parallel using the MPI standard. We have adopted each replica simulation on 2 nodes and estimated the total computational cost at 274,000 core-hours. The main origin of computational burden comes from particle transport, which is particularly slow in HTR geometry.

3. Numerical model

The model chosen for numerical demonstration originates from the *PUMA* project of the European Union's 6th framework program, EURATOM (Jonnet and Kloosterman, 2008; Kuijper et al., 2010). It is an annular prismatic HTR with fuel comprising plutonium in the form of TRISO particles. Sufficient specification is provided in the report by Cetnar et al. (2013). Potential application of TRISO particles for actinides burning has already been investigated numerically by Jonnet and Kloosterman (2008), Dufek et al. (2007), Urbatsch (1995), thus we assume that the model chosen is sufficiently reliable. The model represents full reactor core with fresh fuel loading. The isotopic composition of fresh heavy metal vector is presented below (Table 1).

The key aspects of the core model are the following:

- Annular core design;
- 240 fuel zones (24 axial and 10 radial);
- Compensation rods inserted during operation;
- Burnable Poison Rods (BPR) with Eu_2O_3 in the corners of graphite prisms;
- Active core surrounded by radial and axial reflectors;
- Fixed fuel and graphite temperature (1200 K);
- Nominal thermal power of 600 MW_{th};
- Irradiation period of 1200 Equivalent Full Power Days (EFPD);
- Average output fissions per initial metal atom of 46.0%;
- JEFF.3.1 library applied for cross section neutron data.

The scheme of geometry in radial section is shown in Fig. 1.

Table 2 shows details of MC neutron transport calculations. The number of inactive neutron cycles can be considered as sufficient to avoid source convergence problems in the context of former studies concerning HTR geometry (Kępisty and Cetnar, 2015b, 2015c).

The densities of BPRs have been adjusted to provide the neutron multiplication factor between 0.99 and 1.04 during irradiation without compensation rods withdrawal. The initial volumetric neutron source is comprised between two coaxial cylinders covering the active area of the core. Short step of 2 days at the beginning-of-cycle ensures reaching xenon equilibrium. All replica samples have been computed independently, having the same