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Parametric studies of the PWR fuel assembly modeling with Monte-Carlo method

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ABSTRACT

In this paper we present results of studies concerning modeling of critical nuclear systems performed by continuous energy Monte Carlo burnup code. We consider a geometry model of fuel assembly for Pressurized Water Reactor neutronic simulations with depletion calculated in the infinite medium. A variety of modeling parameters and common simplifications concerning geometry complexity have been investigated in order to observe their impact on key reactor parameters like: neutron multiplication factor, nuclide concentrations, conversion ratio and distribution of generated power. Comparison of different factors helps to draw conclusions about their significance and to choose the reliable modeling approach. The presented results should be valuable for a beginning reactor researcher, but the specialists will also find a part of results interesting due to their seldom direct consideration in literature. The conclusions are general and valid not only in case of Monte Carlo simulations.

We found that the lack of reactivity control in the model biases the concentration of ^{235}U by more than 10% at end of irradiation. Next, calculation time steps longer than 50 days lead to average discrepancy of neutron multiplication factor of 100 pcm or more. Axial discretization of fuel requires more than 20 burnable zones to provide asymptotic behavior of burnup calculation. Lack of thermal collision tables results in underestimation of minor actinides concentrations of the order of 10% at low burnup and several percent at the end-of-life. The discrepancies caused by: the radial discretization of fuel pins, the presence of the clad–pellet gap, the applied precision of Monte Carlo calculations and the separate treatment of fuel rods, have been observed at the end-of-life to lead to a maximum relative difference in concentrations of ^{235}U and ^{239}Pu below 1%. Nevertheless, some studies should take also these effects into account.

1. Introduction

Continuous energy Monte Carlo (MC) burnup methodology, described in detail by Isotalo (2013), can provide a reliable tool for depletion and neutron calculations for critical and sub-critical nuclear systems. Due to the lack of serious physical model limitation, this methodology is frequently chosen as reference prediction tool for research and development of fuel cycle. Statistical solution of Boltzmann transport equation with acceptable uncertainties requires relatively high computational cost, but increasing efficiency of parallel calculation with cluster computers helps to overcome this problem. Depending on complexity of considered model, required memory may also be a challenge. Martin (2012) discussed the above-mentioned problems in his paper. New methodology is still being invented and code developers work currently on the new problems like dynamic Monte Carlo, better variance reduction procedures (Brun et al., 2015), quicker memory access and new parallelization techniques. It seems that Monte Carlo simulations have well-established share in the future of nuclear reactor science.

Complexity of system definition is usually a matter of choice and reliability of the result depends on its specification. Currently used Monte Carlo codes allow for any arbitrary geometry design using quadrics, where each cell can be filled with different mixture of isotopes, presented by X-5 Monte Carlo team (2003). Point-wise cross-section (XS) tables and thermal collision tables for various

Abbreviations: BOL, beginning-of-life; BWR, Boiling Water Reactor; CFD, Computational Fluid Dynamics; CRAM, Chebyshew Rational Approximation Method; ENDF, Evaluated Nuclear Data File; EOL, end-of-life; FA, fuel assembly; FIMA, Fissions per Initial Metal Atom; HTR, High Temperature Reactor; JEFF, Joint Evaluated Fission and Fusion File; JENDL, Japanese Evaluated Nuclear Data Library; LWR, Light Water Reactor; MC, Monte Carlo; PWR, Pressurized Water Reactor; RKG, Runge–Kutta method of Gauss type; TTA, Transmutation Trajectory Analysis; UOX, uranium oxide; XS, cross section.

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nuclides can be found in the large set of nuclear libraries such as ENDF (Evaluated Nuclear Data File), JEFF (Joint Evaluated Fission and Fusion File) and JENDL (Japanese Evaluated Nuclear Data Library). Nuclear data is an essential input of each neutron simulation and its choice may significantly impact computational results. Beside nuclear data, many other parameters should be prepared and tested that can influence our results. If we consider application of burnup calculation, temporal mesh with depletion conditions for system must be prepared. A code user can increase statistical neutron precision, declare thicker mesh of time, space or energy in simulated model, however the question is when this leads to better quality of results. Each increase of complexity induces longer time of tracking particle history. Total real time of MC calculation is always a serious drawback due to limited number of available processors and finite achievable speedup. Thus, code users must find a compromise between expected precision of result and speed of simulation. What is more, there is not much common recommendation about good practice in reactor simulations, however part of code developers give some advices in user manuals, such as Leppänen (2015).

For given computational resources, quality of obtained results depends on assumptions and simplifications applied to constructed model. In the majority science fields at least a part of the problem is modeled in a simplified way. The goal of such an approach is to decrease computational expense, while keeping obtained result without a significant bias. Many assumptions are commonly used also in case of nuclear reactor systems, however explanation and estimation of their impact on results is quite often omitted. This work presents the results of parametric studies of multiple modeling factors and key parameters essential for fuel cycle simulation. Large variety of factors related to geometry, depletion settings, Monte Carlo statistical precision, time mesh and nuclear data is tested to show the impact on k_{inf}, isotopic field, conversion ratio and power generation during irradiation period. The studies are performed on the example of PWR fuel assembly (FA) model, important for the market of current nuclear reactors. The results of parametric studies are presented one-by-one and compared with work of other authors dealing with modeling of nuclear reactors. We refer to studies performed either by statistical or by deterministic methods used in various codes. Finally, considered modeling factors are arranged together and discussion of qualitative findings and impact on core modeling is presented.

Section 2 presents the methodology of burnup calculation coupled with Monte Carlo neutron transport code. Section 3 describes and justifies specification of the fuel assembly model, chosen for our computational tests. The results of parametric studies are given in Section 4 and the review of modeling factors is presented in Section 5. Section 6 contains our conclusions and summary of the burnup procedure study with Monte Carlo code.

2. Monte Carlo burnup calculation

The goal of burnup calculation is to predict temporal evolution of the isotopic composition and to assess criticality of the nuclear system. Such a procedure is complicated but necessary task in the field of nuclear engineering. Present codes usually proceed in several steps:

- Specification of geometry, materials, parameters of system and simulation settings.
- Preparation of nuclear data and loading it into memory (cross-section libraries, decay and branching coefficients for nuclides, thermal collision tables, fission yields and energies).
- Neutron transport simulation to calculate the fundamental neutron flux distribution.
- Heating per source neutron computation.
- Source normalization and calculation of transmutation coefficients for each required reaction, nuclide and cell.
- Matrix exponent solution of Bateman equation for nuclide densities,
- Calculation of system characteristics.

Neutron interaction with nuclei is described by tabulated point-wise cross-sections that are defined for discrete temperatures of medium. It is worth stressing that piecewise-constant properties of cells are assumed, however a size of cell may be arbitrarily small.

When definition of a system is established, Monte Carlo neutronic simulation is called to calculate required physical quantities. The goal of this method is to obtain a statistical solution of the Boltzmann transport equation that has the following shortened form shown in Eq. (1).

$$\boldsymbol{B}(\boldsymbol{N},\boldsymbol{N_c})\phi(\vec{r}) = \left[\boldsymbol{L}(\boldsymbol{N},\boldsymbol{N_c}) - \frac{1}{K_{\text{eff}}}\boldsymbol{F}(\boldsymbol{N}\boldsymbol{N_c})\right]\phi(\vec{r}) = 0 \tag{1}$$

where $\boldsymbol{N}$ symbolizes the atomic densities of burnable materials, $\boldsymbol{N_c}$ represents the densities of control and structural materials, $\boldsymbol{B}$ stands for the shortened equation operator, $\boldsymbol{L}$ stays for the operator of neutron loss in $\boldsymbol{r}$, $\boldsymbol{F}$ represents fission neutrons production operator and k_{eff} stands for the effective neutron multiplication factor. In fact, the operators $\boldsymbol{L}$ and $\boldsymbol{F}$ are not computed explicitly and only a response to these operators is analyzed.

Methodology of the statistical solution is based on tracking histories of sufficiently high number of neutrons (in practice: 10^6–10^{10} particles) and tallying required quantities such as k_{eff} estimators, neutron flux, reaction rates, heating per nuclide etc. Converged neutron source distribution is required in order to collect results related to the fundamental-mode flux, the eigenfunction of the Boltzmann equation, which corresponds to reactor critical configuration. Very common approach – power iteration is used to solve problem, where fission neutrons of one generation become source particles for the next generation. For realistic nuclear systems source distribution always converges toward physical solution. In simulation initial cycles have to be discarded in order to achieve a correct distribution of neutron source bank. Tallying of chosen quantities begins in active cycles and a final result is given as an average over all active cycles. All tallies estimated with Monte-Carlo method contain statistical error, which is directly related to its statistical nature and some inherent bias coming from the cross-correlation between neutron cycles. It is worth underlining that statistical uncertainty decreases as $\sim N^{-1/2}$, where N is the number of neutron histories applied in simulation of active cycles. The apparent standard deviation of tally is an average of standard deviations output by the Monte Carlo code for a set of multiple cases. The real standard deviation is the sample standard deviation calculated from the tally results for a set of multiple code runs. The comparison between the apparent and the real variance of results is explained and exposed by Mervin et al. (2011).

It is possible to collect neutron flux ϕ in energy groups (often from 10^2 to 10^5 energy intervals). Next, it is used for averaging point-wise cross-sections, so as to calculate microscopic reaction rates R, required to compute transmutation coefficients of the Bateman equations. Another approach is applied in case of continuous energy burnup codes: reaction rates per nuclide and per reaction are tallied directly during neutron transport calculation. The self-shielding effects in energy are directly accounted, which is a big advantage of this method. In this work we used the tool *MCB – Continuous Energy Monte Carlo Burnup*, version 5 (Cetnar et al., 1999).