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Nuclear data uncertainty propagation analysis for depletion calculation in PWR and FR pin-cells

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ABSTRACT

In order to assess the nuclear data uncertainty propagation in the depletion calculation, a computational code named SUNDEW has been developed based on the home-developed lattice code NECP-CACTI. In the SUNDEW, Generalized Perturbation Theory (GPT) is applied to calculate sensitivity coefficients of response function with respect to the nuclear cross sections. Method of Characteristics (MOC) is employed to solve the transport equation, adjoint and generalized adjoint transport equations. Chebyshev Rational Approximation Method (CRAM) is implemented to solve the depletion equation and adjoint depletion equation. The sensitivity coefficients of K_{eff} and nuclide density with respect to the nuclear cross sections are verified by comparing with the results of direct perturbation calculation. The uncertainties on K_{eff} and the nuclide density at different depletions, which are induced by the nuclear cross sections uncertainties, are analyzed based on ENDF/B-VII.1 covariance data for LWR and fast reactor pin-cells. The numerical results show that there are significant differences between LWR and fast reactor pin-cells. The differences are mainly caused by the differences of the sensitivity coefficients between the LWR and fast reactor pin-cells. In addition, to identify the cross section improvement priority for nuclides, reactions and energy ranges, the dominant contributors to K_{eff} and nuclide density uncertainties are analyzed at different depletions.

1. Introduction

The accurate prediction of nuclear parameters in depletion calculation is of great significance for the management of spent nuclear fuel, core design, and even economy and safety of nuclear reactor. However, the reliability of neutron transport and depletion calculations is subject to some degree of uncertainties due to a lot of approximations made in the computational model and inaccuracy of input parameters. Traditionally, conservative safety margins are used in safety analysis of reactor because the uncertainties are not quantified. Reasonable safety margins, which are conducive to improve the economy of reactor, can be given if the uncertainties are quantified.

The nuclear cross sections are used as basic input data for the neutron transport and depletion calculations, whose uncertainties are likely one of the most significant sources of uncertainties of response functions (Pusa, 2012a,b). Therefore, the interest towards sensitivity and uncertainty analysis with respect to the nuclear cross sections has increased markedly in recent years. With the larger availability of covariance files, as in the ENDF/B-VII.1 library (Chadwick et al., 2011), the JENDL4.0 (Shibata et al., 2011) and TENDL-2009 libraries (Koning and Rochman, 2009), the uncertainty quantification of the response function using covariance data prepared in these nuclear data libraries has been carried out by two different approaches: stochastic sampling method and first order generalized perturbation method. The stochastic sampling method can get a probability distribution of output with different input data samples. The probability distribution characterizes the uncertainty related to output. This method is easy to be implemented by running existing transport and depletion codes with different input data samples, but at the expense of high computational costs. It has been carried out in XSUSA/SCALE (Zwermann et al., 2012), TMC/SERPENT (Rochman et al., 2012) and NUDUNA (Diez et al., 2015). In the first order perturbation method, the uncertainty of the response function is quantified with the sensitivity coefficient regarding to input parameters by error propagation formulation. The formulation to calculate the sensitivity coefficient was proposed by Takeda based on a differential approach in 1985 (Takeda and Umano, 1985). This approach employs first order approximation but can provide the sensitivity coefficient, which only requires one time forward depletion calculation and one time adjoint depletion calculation. It is very efficient when the number of considered response functions is not too large.

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So it is applicable for the sensitivity and uncertainty analysis in the pin-cell micro-depletion calculation. Up to now, however, most uncertainty studies based on the first order perturbation method have different levels of approximations, such as neglecting the nuclide density uncertainties induced by the nuclear cross sections uncertainties in the depletion calculation (Oak Ridge National Laboratory, 2009) or neglecting the flux uncertainties (Aliberti et al., 2002), or based on diffusion theory (Yokoyama, 2014).

In order to make a comprehensive assessment, the sensitivity and uncertainty analysis is carried out based on the first order perturbation method in this paper. Both the nuclide density uncertainties and flux uncertainties induced by the uncertainties of the nuclear cross sections in the depletion calculation are considered. The transport code is used to obtain the flux, which can make the result more reliable. A new code named SUNDEW is developed. The SUNDEW code is verified by comparing with the result of direct perturbation (DP) calculation.

In 2006, the NEA/OECD Uncertainty Analysis in Modeling (UAM) workshop established a depletion benchmark for propagating cross section uncertainties in LWR design and safety calculations, and the objective was to address the uncertainty induced by the basic nuclear data in the depletion calculation (Ivanov et al., 2012). In 2008, the NEA/OECD Working Party on Evaluation Cooperation (WPEC) Subgroup 26 published a report, which pointed out that a comprehensive sensitivity and uncertainty analysis should be performed to evaluate the impact of nuclear cross sections uncertainties on the significant integral parameters of innovative systems, even beyond the Gen-IV range of systems (Salvatores and Jacqmin, 2008). Nowadays, the neutronics experience with UO_2 fuel and thermal reactors such as Light Water Reactors (LWR) is extremely extensive, but nuclear data uncertainties are still one of the most significant sources of uncertainties of neutronics calculations. For fast reactor, most nuclear data are available in modern data files, but their accuracy and validation are still a major concern. It is widely accepted that the uncertainties of nuclear data for fast reactor design should still be significantly reduced (Palmiotti et al., 2009). In this paper, the SUNDEW code is used to perform the nuclear data uncertainty propagation analysis for a LWR burn-up pin-cell benchmark proposed by the NEA/OECD (Ivanov et al., 2012) and a fast reactor (FR) burn-up pin-cell to assess the effect of nuclear data uncertainties on a different system with a fast spectrum. The uncertainties of K_{eff} and the nuclide densities at different depletions are analyzed based on the ENDF/B-VII.1 covariance data. In addition, to identify the cross section improvement priority for nuclide, reaction and energy range, the dominant contributors of K_{eff} and nuclide density uncertainties are analyzed.

The organization of this paper is as follows: Section 2 describes the theoretical models of this work. The calculation results of sensitivity coefficient and uncertainty analysis associated with the LWR and FR pin-cells are given in Section 3. Finally, conclusions are provided in Section 4.

2. Uncertainty propagation methodology

The depletion analysis consists of two components: transport calculation and depletion calculation. The transport calculation is used to calculate fluxes and prepare weighted cross sections with updated nuclide densities. Microscopic reaction rates estimated at the beginning of a depletion step are used to solve depletion equation to update the nuclide density at the end of the depletion step. So the transport calculation and depletion calculation have a strong relationship. Any data perturbations which affect one will also affect the other. The first order perturbation method taking account of the nuclide density uncertainties and flux uncertainties induced by the nuclear cross sections in the depletion calculation is introduced in this section.

2.1. Depletion sensitivity coefficient theory

The sensitivity coefficient of R with respect to the nuclear cross section is expressed by

$$S^k_{x,g,z} = \frac{dR}{R} \Big/ \frac{d\sigma^k_{x,g,z}}{\sigma^k_{x,g,z}} \tag{1}$$

where k, x, g, and z are the indices of nuclide, reaction type, neutron energy group and region, respectively.

In the depletion analysis, the calculated nuclear response functions R, such as K_{eff} or nuclide density ($\mathbf{N}$), are a function of the nuclear cross sections (σ), nuclide density, neutron flux ($\mathbf{\Phi}$), and adjoint neutron flux ($\mathbf{\Phi}^*$). Namely, the R can be written as

$$R = f(\sigma, \mathbf{N}, \mathbf{\Phi}, \mathbf{\Phi}^*) \tag{2}$$

Expanding the left-hand side of Eq. (1) with a function Taylor series and neglecting the higher-order terms:

$$S^k_{x,g,z} = \frac{\sigma^k_{x,g,z}}{R}\left(\frac{\partial R}{\partial \sigma^k_{x,g,z}} + \frac{\partial R}{\partial \mathbf{N}}\frac{d\mathbf{N}}{d\sigma^k_{x,g,z}} + \frac{\partial R}{\partial \mathbf{\Phi}}\frac{d\mathbf{\Phi}}{d\sigma^k_{x,g,z}} + \frac{\partial R}{\partial \mathbf{\Phi}^*}\frac{d\mathbf{\Phi}^*}{d\sigma^k_{x,g,z}}\right) \tag{3}$$

In reactor design studies, it is frequently desired to determine the response functions that are time-dependent. So the R is represented as integration over all depletion period from t_0 (the beginning of depletion period) to t_f (the end of depletion period). Assuming that $\mathbf{\Phi}$ and $\mathbf{\Phi}^*$ are constant in each depletion step, Eq. (3) can be written as

$$\begin{aligned} S^k_{x,g,z} = \frac{\sigma^k_{x,g,z}}{R}\Bigg(& \int_{t_0}^{t_f} \frac{\partial R}{\partial \sigma^k_{x,g,z}} dt + \int_{t_0}^{t_f} \frac{\partial R}{\partial \mathbf{N}}\frac{d\mathbf{N}}{d\sigma^k_{x,g,z}} dt \\ & + \sum_{i=0}^{I-1} \frac{d\mathbf{\Phi}_i}{d\sigma^k_{x,g,z}} \int_{t_i}^{t_{i+1}} \frac{\partial R}{\partial \mathbf{\Phi}_i} dt + \sum_{i=0}^{I-1} \frac{d\mathbf{\Phi}^*_i}{d\sigma^k_{x,g,z}} \int_{t_i}^{t_{i+1}} \frac{\partial R}{\partial \mathbf{\Phi}^*_i} dt + \frac{\partial R}{\partial \mathbf{N}_I}\frac{d\mathbf{N}_I}{d\sigma^k_{x,g,z}} \\ & + \frac{\partial R}{\partial \mathbf{\Phi}_I}\frac{d\mathbf{\Phi}_I}{d\sigma^k_{x,g,z}} + \frac{\partial R}{\partial \mathbf{\Phi}^*_I}\frac{d\mathbf{\Phi}^*_I}{d\sigma^k_{x,g,z}} \Bigg) \end{aligned} \tag{4}$$

where i is the index of the depletion step; I is the total number of steps; t_i and t_{i+1} are the beginning and end of the ith depletion step, respectively.

Depletion analysis is to solve three coupled equations which are given by Eqs. (5)–(7)

$$\frac{d\mathbf{N}_i(\mathrm{t})}{dt} = \mathbf{M}_i \mathbf{N}_i(t) \tag{5}$$

$$\mathbf{B}_i \mathbf{\Phi}_i = 0 \tag{6}$$

$$P_i = \int_V \sum_k \kappa^k \boldsymbol{\sigma}^k_f N^k_i \mathbf{\Phi}_i dV \tag{7}$$

$$\mathbf{B}^*_i \mathbf{\Phi}^*_i = 0 \tag{8}$$

where Eq. (5) is the depletion equation; Eq. (6) is the neutron transport equation; Eq. (7) is the equation of power calculation; $\mathbf{M}_i$ is the transmutation matrix containing the rate coefficients for neutron absorption and radioactive decay; $\mathbf{B}_i$ is the multi-group transport operator; P_i is the total power over core volume; κ^k is the energy released per fission for nuclide k; $\boldsymbol{\sigma}^k_f$ is the microscopic fission cross section for nuclide k; Eq. (8) is the adjoint transport equation; $\mathbf{B}^*_i$ is the adjoint operator of $\mathbf{B}_i$.

In this paper, a formulation for calculating depletion sensitivity coefficients is derived according to the variation method described