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Calculation of reactor kinetics parameters with Monte Carlo differential operator sampling

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ABSTRACT

The methods to calculate the reactor kinetics parameters of β_{eff} and Λ with the differential operator sampling have been reviewed. The comparison of the results obtained with the differential operator sampling and iterated fission probability approaches has been performed. It is shown that the differential operator sampling approach gives the same results as the iterated fission probability approach within the statistical uncertainty. In addition, the prediction accuracy of the evaluated nuclear data library JENDL-4.0 for the measured $\beta_{\text{eff}}/\Lambda$ and β_{eff} values is also examined. It is shown that JENDL-4.0 gives a good prediction except for the uranium-233 systems. The present results imply the need for revisiting the uranium-233 nuclear data evaluation and performing the detailed sensitivity analysis.

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1. Introduction

The effective delayed neutron fraction β_{eff} and the neutron generation time Λ are the very important reactor kinetics parameters in nuclear reactor applications. Thus, extensive work has been done to calculate the kinetics parameters with Monte Carlo. Approximate methods have been proposed by Meulekamp and van der Marck (2006) and Nauchi and Kameyama (2005). Both the methods for the $\beta_{\rm eff}$ calculation are similar; they are based on the interpretation of the $\beta_{\rm eff}$ value as the ratio of the average number of fissions/fission neutrons induced by delayed and all neutrons. These methods include an approximation of the socalled next fission probability (Meulekamp and van der Marck, 2006); namely a single generation approximation of the iterated fission probability (Hurwitz, 1964) is introduced. Nauchi and Kameyama also proposed a method to calculate the Λ value with the next fission probability approximation. However, the approximation yields a significant discrepancy in the $\beta_{\rm eff}$ value for some cases as pointed out by Nagaya et al. (2010).

Recently, some work has been done to calculate the kinetics parameters with the exact implementation of the iterated fission probability. Feghhi et al. (2008) calculated the neutron generation time with the MCNIC method; the adjoint flux is calculated with the iterated fission probability approach but the neutron generation time is calculated in the deterministic way. Nauchi and Kameyama (2010) and Kiedrowski et al. (2011) proposed the

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http://dx.doi.org/10.1016/j.anucene.2014.08.064 0306-4549/© 2014 Elsevier Ltd. All rights reserved. method to calculate the adjoint-weighted kinetics parameters directly in the continuous-energy Monte Carlo method. The other approach based on the perturbation method has been developed. Verboomen et al. (2006) calculated the neutron generation time from the change in the effective multiplication factor due to the introduction of uniform 1/v poisoning into a system. Nagaya and Mori (2011) calculated the effective delayed neutron fraction with the Monte Carlo perturbation techniques: correlated sampling and differential operator sampling.

In the present work, we calculated the kinetics parameters of both $\beta_{\rm eff}$ and Λ with the differential operator sampling, and compare the results obtained with the iterated fission probability and perturbation approaches. In addition, we examine the prediction accuracy of the recently released evaluated nuclear date library JENDL-4.0 (Shibata et al., 2011) for the measured $\beta_{\rm eff}/\Lambda$ values.

2. Methods

2.1. Effective delayed neutron fraction

The method to calculate β_{eff} with the differential operator sampling has been already proposed by Nagaya and Mori (2011). It is briefly reviewed in what follows.

The time-independent transport equation for a system without external source can be written as follows:

$$L\Phi(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) = \frac{1}{k} S_{\rm f}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}), \tag{1}$$

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where $\Phi(\mathbf{r}, E, \Omega)$ is the angular neutron flux at position \mathbf{r} with energy E and direction Ω ; L is the net-loss operator, k the effective multiplication factor and $S_{\rm f}(\mathbf{r}, E, \Omega)$ is the fission source. The operator L is defined as follows:

$$L\Phi(\mathbf{r}, E, \mathbf{\Omega}) \equiv \mathbf{\Omega} \cdot \nabla \Phi(\mathbf{r}, E, \mathbf{\Omega}) + \Sigma_{t}(\mathbf{r}, E)\Phi(\mathbf{r}, E, \mathbf{\Omega}) - \int d\mathbf{\Omega}' \int dE' \Sigma_{s}(\mathbf{r}, E, \mathbf{\Omega} \leftarrow E', \mathbf{\Omega}')\Phi(\mathbf{r}, E', \mathbf{\Omega}'),$$
(2)

where Σ_t and Σ_s the total and scattering cross sections, respectively. The fission source can be split into the prompt and delayed fission sources:

$$S_{\rm f}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) = S_{\rm f}^{\rm p}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) + \sum_{i} S_{{\rm f},i}^{\rm d}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}), \tag{3}$$

where S_{f}^{p} and $S_{f,i}^{d}$ are the prompt and delayed fission sources, respectively; *i* is the *i*-th delayed neutron family.

Let us consider a perturbed system where the number of delayed neutrons is changed. The transport equation for the perturbed system is then expressed as

$$L\Phi(\mathbf{r}, E, \mathbf{\Omega}; a) = \frac{1}{k(a)} S_{\mathbf{f}}(\mathbf{r}, E, \mathbf{\Omega}; a),$$
(4)

$$S_{\rm f}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}) = S_{\rm f}^{\rm p}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}) + (1+\boldsymbol{a}) \sum_{i} S_{{\rm f}, i}^{\rm d}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}), \tag{5}$$

where a is the fractional change of the number of delayed neutrons. Considering the change in the effective multiplication factor k with the perturbation theory and taking the limit as the parameter a approaches zero, then we obtain

$$\beta_{\rm eff} = \frac{1}{k(0)} \left[\frac{\partial k}{\partial a} \right]_{a=0}.$$
 (6)

The differential coefficient in the right hand side of Eq. (6) can be estimated with the differential operator sampling.

2.2. Neutron generation time

The neutron generation time is conventionally defined as follows:

$$\Lambda = \frac{\left\langle \Phi^{\dagger}(\mathbf{r}, E, \mathbf{\Omega}) \frac{1}{v} \Phi(\mathbf{r}, E, \mathbf{\Omega}) \right\rangle}{\left\langle \Phi^{\dagger}(\mathbf{r}, E, \mathbf{\Omega}) S_{\mathbf{f}}(\mathbf{r}, E, \mathbf{\Omega}) \right\rangle},\tag{7}$$

where the angle brackets denote $\int d\mathbf{r} \int d\Omega \int dE$; v is the neutron speed; $\Phi^{\dagger}(\mathbf{r}, E, \Omega)$ is the adjoint angular flux. The adjoint angular flux is obtained from the following equation:

$$L^{\dagger}\Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) = \frac{1}{k} S_{\mathrm{f}}^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}), \tag{8}$$

$$L^{\dagger}\Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) \equiv -\boldsymbol{\Omega} \cdot \nabla \Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) + \Sigma_{\mathrm{t}}(\boldsymbol{r}, \boldsymbol{E})\Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega})$$

$$-\int d\mathbf{\Omega}' \int dE' \Sigma_{\rm s}(\mathbf{r}, E', \mathbf{\Omega}' \leftarrow E, \mathbf{\Omega}) \Phi^{\dagger}(\mathbf{r}, E', \mathbf{\Omega}'), \qquad (9)$$

$$S_{\rm f}^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}) \equiv \int d\boldsymbol{\Omega}' \int d\boldsymbol{E}' \chi(\boldsymbol{E}' \leftarrow \boldsymbol{E}, \boldsymbol{\Omega}') \nu(\boldsymbol{E}) \Sigma_{\rm f}(\boldsymbol{r}, \boldsymbol{E}) \Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}', \boldsymbol{\Omega}').$$
(10)

To calculate the neutron generation time with the differential operator sampling, we consider a perturbed system where a fictitious 1/v absorber is uniformly introduced in the system. The transport equation is then expressed as

$$L(a)\Phi(\mathbf{r}, E, \mathbf{\Omega}; a) = \frac{1}{k(a)}S_{\mathbf{f}}(\mathbf{r}, E, \mathbf{\Omega}; a),$$
(11)

and the perturbed net-loss operator is defined as

$$\begin{split} L(a)\Phi(\boldsymbol{r},\boldsymbol{E},\boldsymbol{\Omega}) &\equiv \boldsymbol{\Omega}\cdot\nabla\Phi(\boldsymbol{r},\boldsymbol{E},\boldsymbol{\Omega}) + [\Sigma_{\mathrm{t}}(\boldsymbol{r},\boldsymbol{E}) + a\Sigma_{\mathrm{v}}]\Phi(\boldsymbol{r},\boldsymbol{E},\boldsymbol{\Omega}) \\ &- \int d\boldsymbol{\Omega}' \int d\boldsymbol{E}'\Sigma_{\mathrm{s}}(\boldsymbol{r},\boldsymbol{E},\boldsymbol{\Omega}\leftarrow\boldsymbol{E}',\boldsymbol{\Omega}')\Phi(\boldsymbol{r},\boldsymbol{E}',\boldsymbol{\Omega}'), \end{split}$$
(12)

where Σ_v is the 1/v absorber defined as

$$\Sigma_{\rm v} = \frac{1}{\nu}.\tag{13}$$

Since Eq. (8) is the adjoint equation of Eq. (11) for a = 0, Eq. (8) can be expressed as

$$L^{\dagger}(0)\Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; 0) = \frac{1}{k(0)} S_{\mathrm{f}}^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; 0).$$
(14)

Using Eqs. (11) and (14), we can derive the following equality:

$$\frac{\left\langle \Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{0}) \Sigma_{\mathbf{v}} \Phi(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}) \right\rangle}{\left\langle \Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{0}) S_{\mathbf{f}}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}) \right\rangle} = -\frac{1}{k(a)k(0)} \frac{k(a) - k(0)}{a}.$$
(15)

Note that the following equality is used to derive Eq. (15):

$$\left\langle \Phi(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}) S_{\mathrm{f}}^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{0}) \right\rangle = \left\langle \Phi^{\dagger}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{0}) S_{\mathrm{f}}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\Omega}; \boldsymbol{a}) \right\rangle.$$
(16)

Taking the limit of Eq. (15) as the parameter *a* approaches zero, then we obtain

$$\Lambda = -\frac{1}{k^2(0)} \left[\frac{\partial k}{\partial a} \right]_{a=0}.$$
(17)

This method is essentially the same as Verboomen et al. (2006) proposed. The difference lies in the direct estimation of the differential coefficient in the right hand side of Eq. (17) with the differential operator sampling in the present work.

3. Verification and validation

3.1. Code implementation and benchmark cores

In order to perform verification and validation, we have implemented the above-mentioned methods into the MVP2 code (Nagaya et al., 2005). The details of the algorithm can be consulted in Nagaya and Mori (2005) and Nagaya and Mori (2011). Benchmark cores examined in Kahler et al. (2011) and van der Marck (2006) are selected for the β_{eff}/Λ and β_{eff} values, respectively. The following are the brief explanation for the benchmark cores. The benchmark models in the ICSBEP (NEA Nuclear Science Committee, 2008) and IRPhEP (OECD Nuclear Energy Agency, 2012) handbooks are employed for the MVP calculations. The ICS-BEP/IRPhEP identifiers are given in the parentheses.

Bare spheres: Jezebel (PU-MET-FAST-001), Godiva (HEU-MET-FAST-001) and Jezebel-23 (U233-MET-FAST-001) are metal spherical cores for plutonium, uranium-235 and uranium-233, respectively.

Spherical cores with a fertile reflector: Flattop-Pu (PU-MET-FAST-006), Flattop-25 (HEU-MET-FAST-028) and Flattop-23 (U233-MET-FAST-006) are metal spherical cores surrounded by a normal uranium reflector for plutonium, uranium-235 and uranium-233, respectively.

Heterogeneous fast cores:

- **ZEUS:** Zeus-1 (HEU-MET-INTER-006) is a graphite-HEU (highly enriched uranium) core surrounded by a copper reflector. Zeus-5 (HEU-MET-FAST-073) is a HEU cylindrical core surrounded by a copper reflector.
- **Big Ten:** Big Ten (IEU-MET-FAST-007) is a large mixed-uranium-metal cylindrical core with a depleted uranium reflector. The detailed model was employed for MVP calculations.
- **ZPR:** ZPR-9/34 (HEU-MET-INTER-001) is a HEU-iron cylindrical core reflected by stainless steel (SST). ZPR-6/9 (IEU-MET-FAST-010) is a uranium metal (9% enriched) cylindrical core with a depleted uranium reflector. ZPR-6/10 (PU-MET-INTER-002) is a plutonium-carbon-SST

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