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Validation of Kinetics Parameter Calculation Capability of McCARD

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1. Introduction

Reactor kinetics parameters like the effective delayed neutron fraction, β_{eff}, and the prompt neutron generation time, Λ, in the point kinetics equation [1, 2] are weighted quantities. The adjoint angular flux from the solution to a relevant adjoint eigenvalue equation is preferred as the weighting function in order to improve the accuracy of the eigenvalue perturbation calculations [2]. There have been several studies [3-5] on how to calculate the adjoint-weighted kinetics parameters by the continuous-energy Monte Carlo (MC) forward eigenvalue calculations. They can be grouped into two categories according to the adopted adjoint solution: the constant source adjoint function and the self-consistent adjoint function. The constant source adjoint function, ϕ_S^*, is the solution of

$$\mathbf{M}^*\phi_S^* = \Sigma_d\,, \tag{1}$$

while the self-consistent adjoint function, ϕ_0^* is the fundamental-mode solution of the following adjoint eigenvalue equation.

$$\mathbf{M}^*\phi_0^* = \frac{1}{k_0}\mathbf{F}^*\phi_0^* \tag{2}$$

Σ_d is the cross-section characterizing a fictitious detector placed in the reactor core and k_0 is the fundamental-mode eigenvalue. $\mathbf{M}^*$ and $\mathbf{F}^*$ are the adjoint operators corresponding to the direct operators for the destruction **M** and the fission **F**, respectively.

The kinetics parameter calculation capability has been implemented into McCARD [6] with both the constant source adjoint function and the self-consistent adjoint function. The purpose of this paper is to present a comparison of McCARD results of both methods with measurements for several critical facility problems.

2. Adjoint-Weighted Kinetics Parameters

β_{eff} and Λ in the point kinetics equation are defined with the adjoint flux by

$$\beta_{eff} = \frac{1}{F}\int d\mathbf{r}\int dE\int d\mathbf{\Omega}\int dE'\int d\mathbf{\Omega}'\phi^*(\mathbf{r},E,\mathbf{\Omega}) \times (1/4\pi)\,\chi_d(E,E')\nu_d(E')\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',\mathbf{\Omega}'), \tag{3}$$

$$\Lambda = \frac{1}{F}\int d\mathbf{r}\int dE\int d\mathbf{\Omega}\phi^*(\mathbf{r},E,\mathbf{\Omega})\frac{1}{v(E)}\phi(\mathbf{r},E,\mathbf{\Omega}); \tag{4}$$

$$F = \int d\mathbf{r}\int dE\int d\mathbf{\Omega}\int dE'\int d\mathbf{\Omega}'\phi^*(\mathbf{r},E,\mathbf{\Omega}) \times (1/4\pi)\,\chi(E,E')\nu(E')\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',\mathbf{\Omega}'), \tag{5}$$

where χ and χ_d are the fission spectrum of a neutron and a delayed neutron, respectively. ν and ν_d are the mean number of neutrons and delayed neutrons, respectively, produced in a fission. Σ_f is the fission cross section. v is the neutron velocity.

2.1 Constant Source Adjoint Function

In terms of the Green's function G, ϕ_S^* in Eq. (1) can be expressed as [7]

$$\phi_S^*(\mathbf{r},E,\mathbf{\Omega}) = \int d\mathbf{r}'\int dE'\int d\mathbf{\Omega}'\,G(\mathbf{r},E,\mathbf{\Omega}\rightarrow\mathbf{r}',E',\mathbf{\Omega}')\Sigma_d(\mathbf{r}',E',\mathbf{\Omega}'), \tag{6}$$

where $G(\mathbf{r}',E',\mathbf{\Omega}'\rightarrow\mathbf{r},E,\mathbf{\Omega})$ is defined by

$$\mathbf{M}G(\mathbf{r}',E',\mathbf{\Omega}'\rightarrow\mathbf{r},E,\mathbf{\Omega}) = \delta(\mathbf{r}-\mathbf{r}')\delta(E-E')\delta(\mathbf{\Omega}-\mathbf{\Omega}'), \tag{7}$$

and means the angular flux at $\mathbf{r}$, E, $\mathbf{\Omega}$ produced from a unit point source located at $\mathbf{r}',E',\mathbf{\Omega}'$.

Let us choose $\nu\Sigma_f$ as Σ_d. Because of the physical meaning of G in Eq. (6), $\phi_S^*(\mathbf{r},E,\mathbf{\Omega})$ then is interpreted as the number of fission neutrons produced at the next generation due to the source at $\mathbf{r}$, E, $\mathbf{\Omega}$.

From this meaning of $\phi_S^*(\mathbf{r},E,\mathbf{\Omega})$, kinetics parameters at cycle i, $\beta_{eff,i}$ and Λ_i can be calculated by the collision estimator as

$$\beta_{eff,i} = \frac{1}{M_i}\sum_{j\in D_i}\sum_{k=1}^{K_{ij}} w_{ijk}\frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}} \Bigg/ \frac{1}{M_i}\sum_{j=1}^{M_i}\sum_{k=1}^{K_{ij}} w_{ijk}\frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}}, \tag{8}$$

$$\Lambda_i = \frac{\dfrac{1}{M_i}\displaystyle\sum_{j=1}^{M_i}\sum_{k=1}^{K_{ij}} w_{ijk}\frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}}\sum_{k'=1}^{k}\Delta t_{ijk}}{\dfrac{1}{M_i}\displaystyle\sum_{j=1}^{M_i}\sum_{k=1}^{K_{ij}} w_{ijk}\frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}}\sum_{k'=1}^{k}\nu\Sigma_{f,ijk}\Delta l_{ijk}}. \tag{9}$$

i, j, and k are cycle, history, and collision indices, respectively. M_i is the number of histories of i-th cycle and K_{ij} is the total number of collisions experienced by j-th history of cycle i. D_i is the domain of delayed fission neutron sources among all the sources of cycle i. w_{ijk} is the neutron weight for k-th collision of history j at cycle i. Δl_{ijk} is the track length between (k-1)-th and k-th collision of history j at cycle i. v_{ijk} is the velocity of incident neutron for collision k of history j at cycle i. The flight time, Δt_{ijk} is defined by $\Delta l_{ijk}/v_{ijk}$.

In another way, the denominator of the right hand side (RHS) of Eq. (9) can be calculated using the cycle-wise eigenvalues as

$$F_i = k_i k_{i-1}\,, \tag{10}$$

where k_i denotes the eigenvalue estimated at cycle i.

From the cycle-wise results, β_{eff}, Λ and their statistical uncertainties can be readily calculated.

2.2 Self-Consistent Adjoint Function

The adjoint eigenvalue equation of Eq. (2) can be expressed as

$$\phi_0^* = \frac{1}{k_0}\left(\mathbf{M}^*\right)^{-1}\mathbf{F}^*\phi_0^* = \frac{1}{k_0}\left(\mathbf{F}\mathbf{M}^{-1}\right)^*\phi_0^* = \frac{1}{k_0}\mathbf{H}^*\phi_0^*\,, \tag{11}$$

where the fission operator **H** is defined by [8]

$$\mathbf{H} = \mathbf{F}\mathbf{M}^{-1}. \tag{12}$$

By the power method for Eq. (11), an unnormalized fundamental-mode eigenfunction can be calculated as

$$\phi_0^* = \lim_{n\to\infty} \phi_{0,n}^* ; \phi_{0,n}^* = \frac{1}{k_0{}^n} \left(\mathbf{H}^n\right)^* \phi_{0,init.}^* , \quad (13)$$

n is the iteration or generation index. $\phi_{0,n}^*$ denotes the n-th iterated solution and $\phi_{0,init.}^*$ can be an arbitrary non-zero function as a starting distribution.

Then when $\phi_{0,init.}^*(\mathbf{r}, E, \mathbf{\Omega}) = 1$, $\phi_0^*(\mathbf{r}, E, \mathbf{\Omega})$ of Eq. (13) can be interpreted as the number of fission neutrons produced in the n-th generation due to a unit source neutron located at $(\mathbf{r}, E, \mathbf{\Omega})$ as n approaches infinity. This physical interpretation is well-known as the iterated fission probability [9]. When n is large enough to converge the iterative solution, ϕ_0^* can be approximated by $\phi_{0,n}^*$. In the conventional MC forward calculations, $\phi_{0,n}^*$ required at cycle i can be estimated by tallying the number of fission neutrons generated at (i+n-1)-th cycle, which means that the kinetics parameters calculated at cycle i requires the flux or fission source data of (i-n+1)-th cycle. Then from the physical meaning of $\phi_{0,n}^*$, $\beta_{eff,i}$ and Λ_i can be calculated by the collision estimator as

$$\beta_{eff,i} = \frac{1}{M_i} \sum_{j\in D_{i-n+1}} \sum_{k=1}^{K_{ij}} w_{ijk} \frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}} \Bigg/ \frac{1}{M_i} \sum_{j=1}^{M_i} \sum_{k=1}^{K_{ij}} w_{ijk} \frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}} , \quad (14)$$

$$\Lambda_i = \frac{\frac{1}{M_i} \sum_{j=1}^{M_i} \left(\sum_{k=1}^{K_{ij}} w_{ijk} \frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}} \right) \left(w_{(i-n+1)j'1} \frac{\Delta l_{(i-n+1)j'k'}}{v_{i(i-n+1)j'k'}} \right)}{\frac{1}{M_i} \sum_{j=1}^{M_i} \left(\sum_{k=1}^{K_{ij}} w_{ijk} \frac{\nu\Sigma_{f,ijk}}{\Sigma_{t,ijk}} \right) \left(w_{(i-n+1)j'1} \nu\Sigma_{f,(i-n+1)j'k'} \Delta l_{(i-n+1)j'k'} \right)} , \quad (15)$$

where j' and k' is the history and collision indices of (i-n+1)-th cycle from which the progenitor of j-th fission source of cycle i is generated.

The denominator of the RHS of Eq. (15) can be also calculated by

$$F_i = k_i k_{i-n} . \quad (16)$$

3. Numerical Results

The MC forward eigenvalue calculations with continuous-energy cross-section libraries produced from ENDF/B-VII were conducted for two kinds of critical facilities: Godiva [10], the Tank-type Critical Assembly (TCA) [11]. In the MC calculations, the self-consistent adjoint functions are assumed to be converged after 10 power iterations. Table III shows a comparison of β_{eff} estimated from McCARD with measurements. From the table, it is noted that β_{eff}'s from the use of either ϕ_S^* or ϕ_0^* agree well with the measurements within 2% error. Table IV shows the comparisons of β_{eff}/Λ estimated from McCARD with experimental outputs. From the table, it is noted that the β_{eff}/Λ values from the use of ϕ_0^* agree well with the measurements within 3% error, while the maximum error of β_{eff}/Λ from the use of ϕ_S^* is 13%.

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Table III: Comparison of β_{eff} for Critical Facilities

Facility	Core Name	$(\beta_{eff})_{exp}$	$(\beta_{eff})_{MC}$ weighted by ϕ_S^*			$(\beta_{eff})_{MC}$ weighted by ϕ_0^*		
			Mean	RSD (%)	Ratio to Exp.	Mean	RSD (%)	Ratio to Exp.
Godiva	-	0.00640	0.00646	0.17	1.01	0.00649	0.42	1.01
TCA	1.50U	0.00771	0.00767	0.49	0.99	0.00774	1.32	1.00
	1.83U	0.00760	0.00758	0.53	1.00	0.00762	1.38	1.00
	2.48U	0.00765	0.00750	0.47	0.98	0.00748	1.31	0.98

Table IV: Comparison of β_{eff}/Λ for Critical Facilities

Facility	Core Name	$(\beta_{eff}/\Lambda)_{exp}$	$(\beta_{eff}/\Lambda)_{MC}$ weighted by ϕ_S^*			$(\beta_{eff}/\Lambda)_{MC}$ weighted by ϕ_0^*		
			Mean	RSD (%)	Ratio to Exp.	Mean	RSD (%)	Ratio to Exp.
Godiva	-	1.11×10^6	1.13×10^6	0.17	1.02	1.14×10^6	0.42	1.03
TCA	1.50U	219	191	0.49	0.87	220	1.34	1.01
	1.83U	201	175	0.53	0.87	197	1.39	0.98
	2.48U	175	154	0.47	0.88	170	1.32	0.97