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# Development of a fuel depletion sensitivity calculation module for multi-cell problems in a deterministic reactor physics code system CBZ

Go Chiba *, Yosuke Kawamoto, Tadashi Narabayashi

*Hokkaido University, Kita-ku, Sapporo, Hokkaido 060-8628, Japan*

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ABSTRACT

A new functionality of fuel depletion sensitivity calculations is developed as one module in a deterministic reactor physics code system CBZ. This is based on the generalized perturbation theory for fuel depletion problems. The theory for fuel depletion problems with a multi-layer depletion step division scheme is described in detail. Numerical techniques employed in actual implementation are also provided. Verification calculations are carried out for a $3 \times 3$ multi-cell problem consisting of two different types of fuel pins. It is shown that the sensitivities of nuclide number densities after fuel depletion with respect to the nuclear data calculated by the new module agree well with reference sensitivities calculated by direct numerical differentiation. To demonstrate the usefulness of the new module, fuel depletion sensitivities in different multi-cell arrangements are compared and non-negligible differences are observed. Nuclear data-induced uncertainties of nuclide number densities obtained with the calculated sensitivities are also compared.



## 1. Introduction

Accurate and reliable prediction of nuclide number densities after fuel depletion is quite important in various applications in the field of nuclear engineering, including safety analyses of nuclear power plants and nuclear waste fuel management. Since safety margins, which should be considered for various functionalities of nuclear systems, significantly affect construction and operation costs, an important issue is the quantitative evaluation of accuracy and reliability. Uncertainty quantification (UQ) is one of promising ways to fulfill this requirement; much research and development of UQ has been conducted to date in the field of reactor physics.

One of numerical procedures for UQ is the adjoint-based method, in which sensitivities of observed (target) parameters with respect to input parameters that include uncertainties are calculated and input parameter-induced uncertainties are evaluated by manipulation of the sensitivities and uncertainty information on the input parameters. In the field of reactor physics, the perturbation theory and the generalized perturbation theory (GPT) are well established and implemented to application codes to calculate the sensitivities of reactor physics parameters with respect to nuclear data, which is a principal source of uncertainty. Fuel depletion problems for heterogeneous systems are complicated because they are coupled problems between fuel depletion and neutron transport problems. A theory for these problems, GPT for fuel depletion problems, however, has been established (Williams, 1979; Takeda and Umano, 1985). While this theory exists, actual implementation to lattice physics codes is quite rare.

A deterministic reactor physics code system CBZ, which has been under development at Hokkaido University in Japan, has various functionalities for UQ, including fuel depletion problems for a single fuel pin cell. In order to enhance this capability, a new fuel depletion sensitivity calculation module has been developed and implemented. The purpose of the present paper is to describe this new CBZ functionality.

The present paper is organized as follows: Section 2 describes the generalized perturbation theory for fuel depletion problems and actual implementation. Sections 3 and 4 are devoted, respectively, to the description of numerical procedures and results. Finally, Section 5 provides the conclusions of the present study and future perspectives.

## 2. Theory and implementation

### 2.1. General description of fuel depletion calculations

Generally in fuel depletion calculations, the fuel depletion period is divided into *steps* and each of the steps is further divided into *sub-steps*. In the frame of the deterministic numerical procedure, resonance self-shielding and neutron flux calculations are carried

* Corresponding author.
*E-mail address:* go_chiba@eng.hokudai.ac.jp (G. Chiba).

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out at the beginning of each step; and the calculated multi-group cross sections and neutron flux distributions are commonly used during each step. At the beginning of each sub-step, neutron flux distribution is normalized and fuel depletion during the sub-step is calculated with the normalized neutron flux.

Let us consider a step which is divided into $I$ sub-steps. The beginning and end of sub-step $i$ are denoted as $t_i$ and $t_{i+1}$, while the beginning and end of this step are denoted as $t_0$ and $t_I$. Note that sub-steps are denoted as $0, 1, \ldots, I-1$.

Neutron flux distribution $\Phi$ at a particular step is defined as the solution to the following neutron transport equation:

$$\mathbf{B}_0\Phi = \left(\mathbf{A}_0 - \frac{1}{k_{\text{eff},0}}\mathbf{F}_0\right)\Phi = 0, \tag{1}$$

where $k_{\text{eff}}$ is the effective neutron multiplication factor, and $\mathbf{A}$ and $\mathbf{F}$ are operators for neutron loss and production, respectively. The subscript for $k_{\text{eff}}$ and the operators describes the time at which these are defined. The neutron flux distribution $\Phi$ is normalized by the following equation:

$$\left\langle \nu\Sigma_{f,0}\Phi \right\rangle = \text{Const.} \tag{2}$$

Neutron flux distribution at sub-step $i$, $\phi_i$, is assumed to be proportional to $\Phi$ and is defined as

$$\phi_i = f_i\Phi. \tag{3}$$

The normalization factor $f_i$ is defined so as to satisfy the following equation:

$$\mathbf{G}_i\phi_i = f_i\mathbf{G}_i\Phi = P, \tag{4}$$

where $\mathbf{G}_i$ is an operator for the normalization at sub-step $i$ and $P$ denotes values of the normalization. We denote average of energy-integrated value for $\Phi$ (average total neutron flux) in a fuel region $j$ as $\tilde{\Phi}^j$, which is defined as

$$\tilde{\Phi}^j = \frac{\int dE \int_{\mathbf{r}\in j}\Phi(\mathbf{r},E)d\mathbf{r}}{\int_{\mathbf{r}\in j} d\mathbf{r}}. \tag{5}$$

Total neutron flux in a region $j$ at sub-step $i$, $\tilde{\phi}_i^j$, can be written as

$$\tilde{\phi}_i^j = f_i\tilde{\Phi}^j. \tag{6}$$

Let us assume that we consider a system in which there are $J$ fuel regions.

A number density vector in a region $j$ at time $t$ is denoted as $\mathbf{N}^j(t)$. The number density vectors at $t_0$, $\mathbf{N}^j(t_0)$, are given as an initial condition. The fuel depletion equation in this region at sub-step $i$ is written as

$$\frac{d\mathbf{N}^j(t)}{dt} = \mathbf{M}_i^j\mathbf{N}^j(t), \quad (t_i \leqslant t < t_{i+1}). \tag{7}$$

The fuel depletion matrix in a region $j$ at sub-step $i$, $\mathbf{M}_i^j$, can be decomposed as follows:

$$\mathbf{M}_i^j = \mathbf{M}_\lambda + \mathbf{M}_\phi^j\tilde{\phi}_i^j = \mathbf{M}_\lambda + \mathbf{M}_\phi^j f_i\tilde{\Phi}^j, \tag{8}$$

where $\mathbf{M}_\lambda$ and $\mathbf{M}_\phi$ are fuel depletion matrix components for radioactive decay and neutron-nuclide reaction. Note that entries of $\mathbf{M}_\phi$ are composed of the one-group cross sections.

A fuel depletion equation for the whole system at sub-step $i$ is written as

$$\frac{d\mathbf{N}(t)}{dt} = \frac{d}{dt}\begin{pmatrix}\mathbf{N}^1(t)\\ \mathbf{N}^2(t)\\ \vdots\\ \mathbf{N}^J(t)\end{pmatrix} = \begin{pmatrix}\mathbf{M}_i^1 & \mathbf{0} & \cdots & \mathbf{0}\\ \mathbf{0} & \mathbf{M}_i^2 & \cdots & \mathbf{0}\\ \vdots & \vdots & \ddots & \cdots\\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{M}_i^J\end{pmatrix}\begin{pmatrix}\mathbf{N}^1(t)\\ \mathbf{N}^2(t)\\ \vdots\\ \mathbf{N}^J(t)\end{pmatrix} = \mathbf{M}_i\mathbf{N}(t), \quad (t_i \leqslant t < t_{i+1}). \tag{9}$$

### 2.2. Generalized perturbation theory for fuel depletion problems

Although several papers on GPT for fuel depletion problems have been published and the theoretical detail of GPT has well been documented (Williams, 1979; Takeda and Umano, 1985), there are none that explicitly describe GPT for fuel depletion problems with a multi-layer depletion step division scheme consisting of depletion steps and sub-steps.

Let us focus on the number density of nuclide $k$ in region $j$ after fuel depletion, $N_k^j(t_I)$. The sensitivity of this quantity with respect to arbitrary nuclear data $\sigma$ is defined as

$$S = \frac{\sigma}{N_k^j(t_I)}\frac{dN_k^j(t_I)}{d\sigma} = \frac{\sigma}{N_k^j(t_I)}\mathbf{e}_{(j-1)\times K+k}^T\frac{d\mathbf{N}(t_I)}{d\sigma}, \tag{10}$$

where $\mathbf{e}_j$ is a vector in which the $j$th entry is unity and others are zero, and $K$ denotes the number of nuclides in each fuel region. The superscript $T$ for vectors and matrices is for the transposition.

In order to calculate $\frac{dN_k^j(t_I)}{d\sigma}$ in Eq. (10), vector $\mathbf{w}(t)$, whose size is the same as that of $\mathbf{N}$, is multiplied to both sides of Eq. (9), both the sides are integrated over the entire period $[t_0, t_I]$, and then the following equation is derived.

$$\begin{aligned}
&\int_{t_0}^{t_I}\mathbf{w}^T\frac{d\mathbf{N}}{dt}dt = \sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\mathbf{M}_i\mathbf{N}dt,\\
&\left[\mathbf{w}^T\mathbf{N}\right]_{t_0}^{t_I} = \int_{t_0}^{t_I}\frac{d\mathbf{w}^T}{dt}\mathbf{N}dt + \sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\mathbf{M}_i\mathbf{N}dt,\\
&\mathbf{w}^T(t_I)\mathbf{N}(t_I) = \mathbf{w}^T(t_0)\mathbf{N}(t_0) + \int_{t_0}^{t_I}\frac{d\mathbf{w}^T}{dt}\mathbf{N}dt + \sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\mathbf{M}_i\mathbf{N}dt.
\end{aligned} \tag{11}$$

For simplicity, dependence of $\mathbf{N}$ and $\mathbf{w}$ on time in integrations is omitted. Setting

$$\mathbf{w}(t_I) = \mathbf{e}_{(j-1)\times K+k}, \tag{12}$$

as the final condition of $\mathbf{w}(t)$, $N_k^j(t_I)$ can be written as

$$N_k^j(t_I) = \mathbf{w}^T(t_0)\mathbf{N}(t_0) + \int_{t_0}^{t_I}\frac{d\mathbf{w}^T}{dt}\mathbf{N}dt + \sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\mathbf{M}_i\mathbf{N}dt. \tag{13}$$

By differentiating both sides of Eq. (13) by $\sigma$, the following equation is derived:

$$\begin{aligned}
\frac{dN_k^j(t_I)}{d\sigma} = &\int_{t_0}^{t_I}\frac{d\mathbf{w}^T}{dt}\frac{d\mathbf{N}}{d\sigma}dt + \sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\frac{d\mathbf{M}_i}{d\sigma}\mathbf{N}dt\\
&+\sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\mathbf{M}_i\frac{d\mathbf{N}}{d\sigma}dt.
\end{aligned} \tag{14}$$

The first and third terms in the right hand side (RHS) of Eq. (14) disappear if the vector $\mathbf{w}$ is properly defined as described later.

Let us consider the second term in the RHS of Eq. (14). This can be rewritten as

$$\begin{aligned}
\sum_{i=0}^{I-1}\int_{t_i}^{t_{i+1}}\mathbf{w}^T\frac{d\mathbf{M}_i}{d\sigma}\mathbf{N}dt &= \sum_{i=0}^{I-1}\sum_{j=1}^{J}\int_{t_i}^{t_{i+1}}\mathbf{w}^{jT}\frac{d\mathbf{M}_i^j}{d\sigma}\mathbf{N}^j dt = \sum_{i=0}^{I-1}\sum_{j=1}^{J}\int_{t_i}^{t_{i+1}}\mathbf{w}^{jT}\frac{\partial\mathbf{M}_i^j}{\partial\sigma}\mathbf{N}^j dt\\
&+\sum_{i=0}^{I-1}\sum_{j=1}^{J}\sum_{g}\frac{d\tilde{\Phi}_g^j}{d\sigma}\int_{t_i}^{t_{i+1}}\mathbf{w}^{jT}\frac{\partial\mathbf{M}_i^j}{\partial\tilde{\Phi}_g^j}\mathbf{N}^j dt\\
&+\sum_{i=0}^{I-1}\sum_{j=1}^{J}\int_{t_i}^{t_{i+1}}\mathbf{w}^{jT}\frac{df_i}{d\sigma}\frac{\partial\mathbf{M}_i^j}{\partial f_i}\mathbf{N}^j dt,
\end{aligned} \tag{15}$$

where $\tilde{\Phi}_g^j$ denotes average neutron flux of group $g$ in region $j$. The first term in the RHS of Eq. (15) corresponds to direct effect of nuclear data to fuel depletion matrix, and partial differentiation $\frac{\partial\mathbf{M}_i^j}{\partial\sigma}$ can be easily calculated. The second and third terms correspond