Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 17-18, 2018

Inline Critical Boron Concentration Search Iteration with p-CMFD Feedback in Continuous-Energy Monte Carlo Simulation

YuGwon Jo and Nam Zin Cho*
Korea Advanced Institute of Science and Technology (KAIST)
291 Daehak-ro, Yuseong-gu, Daejeon, Korea 34141
**nzcho@kaist.ac.kr*

1. Introduction

For the fuel depletion analysis in the pressurized water reactors (PWRs), it is necessary to search the critical boron concentration (CBC). In the deterministic reactor analysis [1], the CBC search is usually based on a Newton-like method as:

$$p^{(l)} = \left(\frac{p^{(l-1)} - p^{(l-2)}}{k^{(l-1)} - k^{(l-2)}} \right) \left(1 - k^{(l-2)}\right) + p^{(l-2)} , \quad (1)$$

where l is the CBC search iteration index. The boron concentration $p^{(l)}$ is updated by using the last two pairs of boron concentrations ($p^{(l-1)}$ and $p^{(l-2)}$) and the multiplication factors ($k^{(l-1)}$ and $k^{(l-2)}$). However, the application of this method in the Monte Carlo (MC) simulation is problematic due to the uncertainty. As $k^{(l)}$ goes to the unity, the difference between the two recent multiplication factors (Δk) can be buried in the uncertainty in k's, which may lead to the inaccurate gradient $\Delta p / \Delta k$ for the CBC update.

In Ref. [2], a neutron balance approach for the determination of the critical parameters such as the CBC and the critical control rod position was proposed. The eigenvalue of the neutron balance equation is set as the critical parameter, instead of the multiplication factor (k_{eff}). In the deterministic diffusion and transport calculations [2], the neutron balance approach showed faster and more stable convergence, compared to a Newton-like algorithm. Furthermore, it does not require the evaluation of the gradient $\Delta p / \Delta k$, which is a good feature for the MC simulation. This approach was applied to the continuous-energy MC calculation [3].

In this paper, the inline CBC search iteration method based on the neutron balance approach is applied to the continuous-energy MC simulation with acceleration. To accelerate the convergence of both the CBC and the fission source distribution (FSD), the p-CMFD feedback is applied [4-8], where the p-CMFD equation is constructed correspondingly. On a typical PWR problem, the performance of the inline CBC search algorithm is tested. Furthermore, it is also shown that the p-CMFD feedback effectively accelerates the convergence of both the CBC and the FSDs.

2. Methodology

In a typical PWRs, the boric acid (H_3BO_3) is dissolved in the coolant (H_2O). It is assumed that the boron concentration p is uniform over the entire coolant. Then, p in unit of [ppm] can be expressed as:

$$p = \frac{\rho_{z,H_3BO_3} w_{B/H_3BO_3}}{\rho_{z,H_3BO_3} + \rho_{z,H_2O}} \times 10^6 \text{ , for } z = 1 \text{ to } Z, \quad (2)$$

where z is the index of local coolant cell to consider the thermal-hydraulics feedback and Z is the total number of local coolant cells. In Eq. (2), ρ_{z,H_2O} is the water density [g/cc] of the borated water in the local coolant cell z, ρ_{z,H_3BO_3} is the boric acid density [g/cc] of the borated water in the local coolant cell z, and w_{B/H_3BO_3} is the weight fraction of boron in the boric acid.

Then, ρ_{z,H_3BO_3} can be expressed in terms of p and ρ_{z,H_2O} , as follows:

$$\rho_{z,H_3BO_3} = \frac{p}{w_{B/H_3BO_3} \times 10^6 - p} \rho_{z,H_2O} \text{ , for } z = 1 \text{ to } Z, \quad (3)$$

where p will be iteratively updated to be the CBC (see Section 2.1) and ρ_{z,H_2O} will be determined by the thermal-hydraulics calculations.

2.1. Inline CBC Search Iteration Method

The neutron transport equation can be written in the kernel form with the CBC search iteration index l as:

$$L\psi^{(l)} + T^{(l-1)}\psi^{(l)} - S^{(l-1)}\psi^{(l)} = F\psi^{(l-1)} , \quad (4)$$

where the kernels are defined as:

$$L\psi^{(l)} \equiv \vec{\Omega} \cdot \nabla \psi^{(l)}(\vec{r}, E, \vec{\Omega}) , \quad (5)$$

$$T^{(l-1)}\psi^{(l)} \equiv \Sigma_t^{(l-1)}(\vec{r}, E)\psi^{(l)}(\vec{r}, E, \vec{\Omega}) , \quad (6)$$

$$S^{(l-1)}\psi^{(l)} \equiv \int d\vec{\Omega}' \int dE' \times m\Sigma_s^{(l-1)}(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega})\psi^{(l)}(\vec{r}, E', \vec{\Omega}') , \quad (7)$$

with scattering multiplicity m,

$$F\psi^{(l-1)} \equiv \frac{\chi(E)}{4\pi} \int d\vec{\Omega}' \int dE' \nu\Sigma_f(\vec{r}, E')\psi^{(l-1)}(\vec{r}, E', \vec{\Omega}') , \quad (8)$$

and the multiplication factor can be evaluated as:

$$k^{(l)} = \frac{\left\langle F\psi^{(l)} \right\rangle}{\left\langle T^{(l-1)}\psi^{(l)} - S^{(l-1)}\psi^{(l)} \right\rangle + J_{leak}^{(l)}} , \quad (9)$$

where $\langle\ \rangle \equiv \int d\vec{r} \int dE \int d\vec{\Omega}$ for the convenient notation of multiple integrations and $J_{leak}^{(l)}$ is the total leakage of neutrons at the space domain boundary.

By iteratively solving Eq. (4), the multiplication factor converges to unity, while the boron concentration converges to the CBC. In this framework, the role of the eigenvalue is taken by the CBC, $p^{(l-1)}$, which is hidden in the macroscopic cross sections $\Sigma_t^{(l-1)}(\vec{r}, E)$ and $\Sigma_s^{(l-1)}(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega})$.

To derive an equation to update the CBC, the neutron balance equation can be obtained by integrating Eq. (4) over the space, energy, and angle, as:

$$J_{leak}^{(l)} + \left\langle R_{B-10}^{(l-1)}\psi^{(l)} \right\rangle + \left\langle R_{others}^{(l-1)}\psi^{(l)} \right\rangle = \left\langle F\psi^{(l)} \right\rangle , \quad (10)$$

where $\left\langle R_{B-10}^{(l-1)}\psi^{(l)} \right\rangle$ is the total removal reaction rate by B-10 and $\left\langle R_{others}^{(l-1)}\psi^{(l)} \right\rangle$ is the total removal reaction rate by other nuclides, which are defined, respectively, as:

$$\left\langle R_{B-10}^{(l-1)}\psi^{(l)} \right\rangle \equiv \sum_{z=1}^{Z} \left\langle N_{z,B-10}^{(l-1)} \sigma_{a,B-10}(\vec{r}, E)\psi^{(l)}(\vec{r}, E, \vec{\Omega}) \right\rangle_{\vec{r} \in V_z} , \quad (11)$$

with $\langle\ \rangle_{\vec{r} \in V_z} \equiv \int_{\vec{r} \in V_z} d\vec{r} \int dE \int d\vec{\Omega}$,

$$\left\langle R_{others}^{(l-1)}\psi^{(l)} \right\rangle \equiv \sum_{nuclide \neq B-10} \left\langle N_{nuclide}^{(l-1)}(\vec{r}) \sigma_{t,nuclide}(\vec{r}, E)\psi^{(l)}(\vec{r}, E, \vec{\Omega}) - \int dE' \int d\vec{\Omega}'\, N_{nuclide}^{(l-1)}(\vec{r}) \times m\sigma_{s,nuclide}(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega})\psi^{(l)}(\vec{r}, E', \vec{\Omega}') \right\rangle . \quad (12)$$

The followings are notations used in Eqs. (11) and (12). V_z is the volume of the local coolant cell z, N_A is the Avogadro constant, $f_{B-10/B}$ is the atomic fraction of B-10 in boron, $M_{H_3BO_3}$ is the molecular mass of the boric acid [g/mole], and $N_{z,B-10}^{(l-1)}$ is the atomic number density of B-10 in the local coolant cell z, which can be expressed as:

$$N_{z,B-10}^{(l-1)} = r^{(l-1)} \frac{\rho_{z,H_2O} N_A f_{B-10/B}}{M_{H_3BO_3}}, \quad (13)$$

with $r^{(l-1)} \equiv \frac{p^{(l-1)}}{w_{B/H_3BO_3} \times 10^6 - p^{(l-1)}}$.

In Eq. (13), $p^{(l-1)}$ is initially guessed and iteratively updated as:

$$p^{(l)} = \frac{r^{(l)} w_{B/H_3BO_3}}{1 + r^{(l)}} \times 10^6 , \quad (14)$$

where $r^{(l)}$ is updated based on Eq. (10), as:

$$r^{(l)} = \frac{\left\langle F\psi^{(l)} \right\rangle - \left\langle R_{others}^{(l-1)}\psi^{(l)} \right\rangle - J_{leak}^{(l)}}{\left\langle \tilde{R}_{B-10}\psi^{(l)} \right\rangle} , \quad (15)$$

with $\left\langle \tilde{R}_{B-10}\psi^{(l)} \right\rangle$ being defined as:

$$\left\langle \tilde{R}_{B-10}\psi^{(l)} \right\rangle \equiv \sum_{z=1}^{Z} \left\langle \frac{\rho_{z,H_2O} N_A f_{B-10/B}}{M_{H_3BO_3}} \sigma_{a,B-10}(\vec{r}, E)\psi^{(l)}(\vec{r}, E, \vec{\Omega}) \right\rangle_{\vec{r} \in V_z} . \quad (16)$$

Then, the nuclide number densities of H, B-10, B-11, and O in the local coolant cell z can be updated, respectively, as:

$$N_{z,H}^{(l)} = 3N_{z,H_3BO_3}^{(l)} + 2N_{z,H_2O} , \quad (17)$$

$$N_{z,B-10}^{(l)} = f_{B-10/B} N_{z,H_3BO_3}^{(l)} , \quad (18)$$

$$N_{z,B-11}^{(l)} = \left(1 - f_{B-10/B}\right) N_{z,H_3BO_3}^{(l)} , \quad (19)$$

$$N_{z,O}^{(l)} = 3N_{z,H_3BO_3}^{(l)} + N_{z,H_2O} , \quad (20)$$

where $N_{z,H_3BO_3}^{(l)}$ and N_{z,H_2O} can be obtained, respectively, as:

$$N_{z,H_3BO_3}^{(l)} = \frac{\rho_{z,H_3BO_3}^{(l)} N_A}{M_{H_3BO}} , \quad (21)$$

with $\rho_{z,H_3BO_3}^{(l)} = \frac{p^{(l)}}{w_{B/H_3BO_3} \times 10^6 - p^{(l)}} \rho_{z,H_2O}$,

$$N_{z,H_2O} = \frac{\rho_{z,H_2O} N_A}{M_{H_2O}} . \quad (22)$$

For both inactive and active cycles, the CBC and the nuclide number densities are updated at each MC cycle as Eqs. (14) to (22). At the end of active cycles, the average CBC and its standard deviation can be estimated. Of course, the multiplication factor is still available to check the criticality.

For a near critical system with zero boron concentration, Eq. (15) can occasionally give a negative CBC due to the uncertainty. In this case, the boron concentration is forced to be zero to prevent the negative probability problem,

which may introduce a bias in the CBC search iteration. To avoid such a bias, we may need to consider an extended particle-tracking algorithm to treat the negative number density problem.

2.2. p-CMFD Feedback in Inline CBC Search Iteration

In this section, the p-CMFD feedback for the acceleration of the convergence in the inline CBC search iteration will be presented. The detailed description of the p-CMFD feedback for the MC simulation (MC/p-CMFD) itself is given in Refs. [7] and [8]. The space domain is divided into I coarse-mesh cells. After the MC simulation for iteration l, the p-CMFD equation is constructed as:

$$\begin{aligned}&\frac{1}{V_i}\sum_j A_{ij}\left(\left(\tilde{D}^{(l)}_{MC,ij}+\hat{D}^{+,(l)}_{MC,ij}\right)\phi^{(l)}_{pCMFD,i}\right.\\&\left.-\left(\tilde{D}^{(l)}_{MC,ij}+\hat{D}^{-,(l)}_{MC,ij}\right)\phi^{(l)}_{pCMFD,j}\right)\\&+r^{(l)}_{pCMFD}\tilde{\Sigma}^{B-10,(l)}_{MC,removal,i}\phi^{(l)}_{pCMFD,i}+\Sigma^{others,(l)}_{MC,removal,i}\phi^{(l)}_{pCMFD,i}=\\&\Sigma^{(l)}_{MC,production,i}\phi^{(l)}_{pCMFD,i}\ ,\ \text{for } i=1\ to\ I,\end{aligned}\tag{23}$$

where the same notations are used as in Ref. [8], except for $\tilde{\Sigma}^{B-10,(l)}_{MC,removal,i}$ and $\Sigma^{others,(l)}_{MC,removal,i}$, which are defined, respectively, as:

$$\tilde{\Sigma}^{B-10,(l)}_{MC,removal,i}\equiv\frac{\left\langle\tilde{R}_{B-10}\psi^{(l)}\right\rangle_{\vec{r}\in V_i}}{\left\langle\psi^{(l)}(\vec{r},E,\vec{\Omega})\right\rangle_{\vec{r}\in V_i}}\ ,\tag{24}$$

$$\Sigma^{others,(l)}_{MC,removal,i}\equiv\frac{\left\langle R^{(l-1)}_{others}\psi^{(l)}\right\rangle_{\vec{r}\in V_i}}{\left\langle\psi^{(l)}(\vec{r},E,\vec{\Omega})\right\rangle_{\vec{r}\in V_i}}\ ,\tag{25}$$

with $\langle\ \rangle_{\vec{r}\in V_i}\equiv\int_{\vec{r}\in V_i}d\vec{r}\int dE\int d\vec{\Omega}$, and $r^{(l)}_{pCMFD}$ is defined as:

$$\begin{aligned}r^{(l)}_{pCMFD}\equiv&\left(\sum_{i=1}^{I}\Sigma^{(l)}_{MC,production,i}\phi^{(l)}_{pCMFD,i}-\sum_{i=1}^{I}\Sigma^{(l),others}_{MC,removal,i}\phi^{(l)}_{pCMFD,i}\right.\\&\left.-J^{(l)}_{leak,pCMFD}\right)\Big/\sum_{i=1}^{I}\tilde{\Sigma}^{(l),B-10}_{MC,removal,i}\phi^{(l)}_{pCMFD,i}\ .\end{aligned}\tag{26}$$

Equation (23) can be solved by the power method. The resulting p-CMFD scalar flux distributions are used to adjust the FSDs, while $r^{(l)}_{pCMFD}$ can be used to update the CBC as in Eq. (14).

3. Numerical Results

The inline CBC search iteration method was implemented in the in-house 3-D continuous-energy MC code, McBOX [9]. The proposed method was tested on a typical pressurized water reactor (PWR) problem.

Figure 1 shows the configurations of the test problem. The material densities and compositions are taken from BEAVRS [10]. The ENDF/B-VII.0 continuous-energy nuclear data library at 293 K is used in this study.

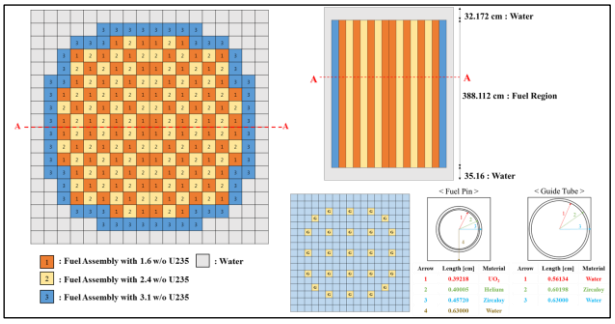

Fig. 1. Configurations of 3-D continuous-energy whole-core test problem.

For the inline CBC search iteration, 4,000,000 histories per cycle, 300 inactive cycles, and 500 active cycles are used, where the initial CBC is set as 0 ppm. To verify the inline CBC search iteration, another MC simulation is performed with a fixed boron concentration to the average CBC obtained from the inline CBC search iteration, which means the usual power iteration.

The inline CBC search iteration with the p-CMFD feedback is also tested, where the p-CMFD calculation is performed with the coarse-mesh cell being set as a single assembly in x-y plane, with 20 divisions in z-axis. The accumulation of the coarse-mesh MC tallies for the p-CMFD parameters is skipped for the initial 30 cycles. The first-in-first-out queue is set as 10 cycles to stabilize the fluctuations in the FSDs and reduce the bias from the p-CMFD feedback. For the source convergence and stabilization, 40 inactive cycles are used in the MC/p-CMFD.

Figures 2, 3, and 4 graphically examine the convergence of the k_{eff}, the CBC, and the Shannon entropy, respectively. The quantities from both inline CBC search iterations with and without p-CMFD feedback converge to the quantities from the fixed CBC calculation, while the p-CMFD feedback accelerates the convergence speed significantly, especially for the Shannon entropy.

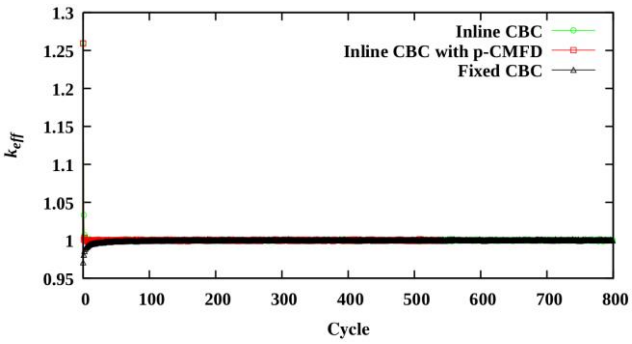

Fig. 2. Comparison of k_{eff} as cycle proceeds.

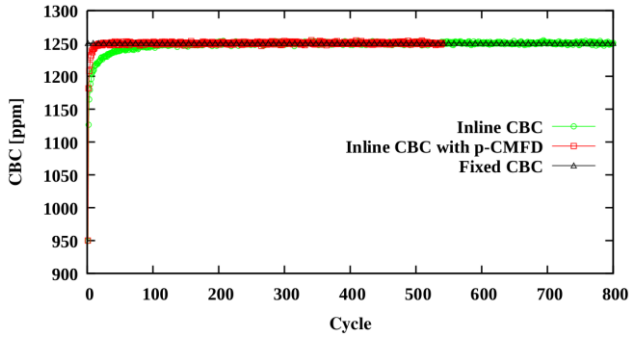

Fig. 3. Comparison of CBC as cycle proceeds.

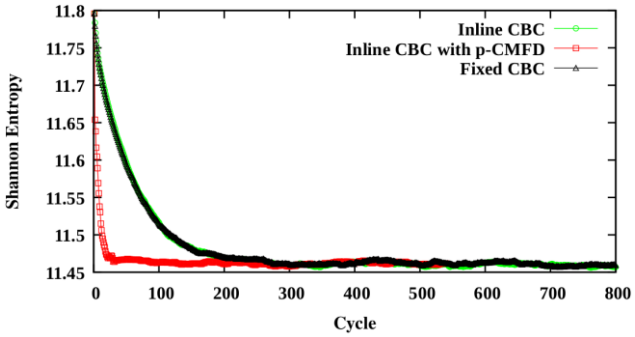

Fig. 4. Comparison of Shannon entropy as cycle proceeds.

Table 1 shows the mean and the standard deviation of the k_{eff} and the p-value in the Jarque-Bera normality test [11]. The p-value means the risk to reject the null hypothesis that the extracted sample (k_{eff}) follows normal distribution, while it is true. Table 2 shows the corresponding quantities for the CBC.

Table 1. Mean and standard deviation of k_{eff} and p-value in Jarque-Bera normality test

	Inline CBC	Inline CBC with p-CMFD	Fixed CBC
Mean	0.999997	1.000008	0.999987
Standard Deviation	0.000016	0.000015	0.000013
p-value	0.762	0.392	0.881

Table 2. Mean and standard deviation of CBC and p-value in Jarque-Bera normality test

	Inline CBC	Inline CBC with p-CMFD
Mean	1250.347	1250.308
Standard Deviation	0.063	0.065
p-value	0.618	0.321

For all the test cases, the k_{eff}'s agree well with unity within the 1σ and the p-value is higher than the significance level of 0.05 for the Jarque-Bera normality test.

4. Summary and Conclusions

The inline CBC search iteration with the p-CMFD feedback was tested on a typical PWR problem. The p-CMFD feedback accelerated the convergence of the CBC and the Shannon entropy. Since the inline CBC search iteration can yield a negative number density for a near critical system, an extended particle-tracking algorithm to treat the negative number density problem is being studied and its results will be presented at the meeting.

Acknowledgement

This work was supported by a National Research Foundation grant funded by the Korean government (NRF-2015M2B2A9029928).

References

[1] T. Downar, Y. Xu and V. Seker, "PARCS v3.0 U.S. NRC Core Neutronics Simulator Theory Manual", University of Michigan, USA (2012).

[2] A. Dall'Osso, "A neutron balance approach in critical parameter determination," *Annals of Nuclear Energy*, **35**, 1686-1694 (2008).

[3] L. Rui, et al., "Criticality search of soluble boron iteration in MC code JMCT," *Energy Procedia*, **127**, 329-334 (2017).

[4] N.Z. Cho et al., "On a New Acceleration Method for 3D Whole-Core Transport Calculations," *Annual Meeting of the Atomic Energy Society of Japan*, Sasebo, Japan, March 27-29, 2003.

[5] N.Z. Cho et al., "Partial Current-Based CMFD Acceleration of the 2D/1D Fusion method for 3D Whole-Core Transport Calculations," *Trans. Am. Nucl. Soc.*, **88**, 594 (2003).

[6] N.Z. Cho, "The Partial Current-Based CMFD (p-CMFD) Method Revisited," *Trans. Kor. Nucl. Soc.*, Gyeongju, Korea, October 25-26, 2012.

[7] S. Yun and N.Z. Cho, "Acceleration of Source Convergence in Monte Carlo k-Eigenvalue Problem via Anchoring with a p-CMFD Deterministic Method," *Ann. Nucl. Energy*, **37**, 1649-1658 (2010).

[8] Y.G. Jo and N. Z. Cho, "Acceleration and Real Variance Reduction in Continuous-Energy Monte Carlo Whole-Core Calculation via p-CMFD Feedback," *Nucl. Sci. Eng.*, **189**, 26-40 (2018).

[9] Y.G. Jo, "Study of New Features and Their Implementations in the Nuclear Reactor Analysis Monte Carlo Code – McBOX," PhD Thesis, Korea Advanced Institute of Science and Technology (2017).

[10] N. Horelik et al., "Benchmark for Evaluation and Validation of Reactor Simulation (BEAVRS)," *Proc. M&C 2013*, Sun Valley, Idaho, May 5–9, 2013.

[11] A. Bera and C. Jarque, "Efficient Tests for Normality, Homoscedasticity and Serial Independence of Regression Residuals: Monte Carlo Evidence," *Econ. Lett.*, **7**, 313 (1981).