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Effect of error propagation of nuclide number densities on Monte Carlo burn-up calculations

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Abstract

As a result of improvements in computer technology, the continuous energy Monte Carlo burn-up calculation has received attention as a good candidate for an assembly calculation method. However, the results of Monte Carlo calculations contain the statistical errors. The results of Monte Carlo burn-up calculations, in particular, include propagated statistical errors through the variance of the nuclide number densities. Therefore, if statistical error alone is evaluated, the errors in Monte Carlo burn-up calculations may be underestimated. To make clear this effect of error propagation on Monte Carlo burn-up calculations, we here proposed an equation that can predict the variance of nuclide number densities after burn-up calculations, and we verified this equation using enormous numbers of the Monte Carlo burn-up calculations by changing only the initial random numbers. We also verified the effect of the number of burn-up calculation points on Monte Carlo burn-up calculations. From these verifications, we estimated the errors in Monte Carlo burn-up calculations including both statistical and propagated errors. Finally, we made clear the effects of error propagation on Monte Carlo burn-up calculations by comparing statistical errors alone versus both statistical and propagated errors. The results revealed that the effects of error propagation on the Monte Carlo burn-up calculations of 8×8 BWR fuel assembly are low up to 60 GWd/t.

1. Introduction

The current methods commonly used in commercial BWR core analysis consist of two separate stages: the assembly calculation by a lattice physics code at a first stage, and the core analyses by a three-dimensional neutronic-thermal hydraulic core calculation code using the assembly constants from the first stage. Recently, deterministic theories such as the current coupling collision probability method (e.g., LANCER (Ikehara et al., 2001)) or characteristics method (e.g., CASMO (Edenius et al., 1991)) have been used to perform assembly calculations. These deterministic lattice codes have enabled high accurate assembly calculation. However, they involve approximations such as space and energy discretizations, and their calculation geometries are limited to two dimensions. On the other hand, a continuous energy Monte Carlo calculation method involves less approximation of energy and geometries. It can treat three-dimensional heterogeneous regions directly. However, the continuous energy Monte Carlo calculation requires an enormous calculation time to obtain highly accurate assembly calculations. Therefore, Monte Carlo calculation methods have been used as reference codes of assembly calculation in the BWR production calculation field.

High burn-up fuel assemblies have been developed to reduce the fuel cycle cost. Therefore, recent fuel assembly designs have been further complicated by high ^{235}U enrichment, high Gd content, and complex shapes in geometry. In these circumstances, coupled with recent advancement in computer performance, the continuous energy Monte Carlo calculation method has garnered attention (Tohjoh et al., 2005) because of its less reliance on approximation.

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However, Monte Carlo calculation results contain statistical errors. In the case of single-step Monte Carlo calculation, these statistical errors can be estimated from the number of neutron histories. However, the results of Monte Carlo burn-up calculations include propagated statistical errors may arise from the variance of nuclide number densities. Therefore, the errors in Monte Carlo burn-up calculations evaluated solely on the basis of statistical errors may be underestimated. Such propagation errors on the nuclide number densities have been reported (Takeda et al., 1999). In that study, these errors were evaluated by using a burn-up matrix. And in the case of fast reactors, Takeda et al. proposed that these errors are relatively smaller than errors of the cross-section libraries. However, quantitative analysis of propagations of statistical errors on the nuclide number densities has not been carried out in their study. Furthermore, the effects of these propagation errors on the Monte Carlo burn-up calculations have not been studied.

To make clear this effect of error propagation on the Monte Carlo burn-up calculations, we here proposed an equation that can predict the variance of the nuclide number densities after burn-up calculations, and we verified this equation from the results of enormous times in Monte Carlo burn-up calculations. To do this, we executed Monte Carlo burn-up calculations 400 times by changing only initial random numbers. We also verified the effect of the number of burn-up calculation points on variance of nuclide number densities.

From these verifications, we estimated the errors of the Monte Carlo burn-up calculations, including both statistical and propagated errors, under several different neutron history numbers. Finally, we made clear the effects of error propagation on Monte Carlo burn-up calculations by comparing statistical errors alone versus both statistical and propagated errors. The results showed that the effects of error propagation on Monte Carlo burn-up calculations of an 8×8 BWR fuel assembly are low up to 60 GWd/t.

Section 2 describes three case studies on the propagation of errors examined in this paper. Each case has a different object. Section 3 proposes the equations that predict these propagated errors, and we verify these equations by using the results of large numbers of Monte Carlo burn-up calculations with different initial random numbers. Section 4 discusses the effects of the number of burn-up calculations points on the nuclide number densities of the Monte Carlo burn-up calculations. This section also verifies this effect through a comparison of the results of large numbers of burn up calculations between 20 and 40 burn-up calculation points. Section 5 examines the propagated errors of nuclide number densities in the Monte Carlo burn-up calculations of a BWR fuel assembly. It also quantitatively shows the effects of these propagated errors on the results of the Monte Carlo burn-up calculations, which are including the k-infinity, the corner-rod peaking (CRP), and the neutron flux. The concluding remarks are given in Section 6.

2. Calculation cases and conditions

This section describes our approach to this study and the calculation conditions used. We have executed three cases of calculations:

Case 1: Burn-up calculations were performed 400 times under the same calculation conditions except for changes in the initial random numbers. There were 20 burn-up calculation points and 20,000 neutron histories per burn-up calculation point.
Case 2: Burn-up calculations were performed 400 times under the same calculation conditions except for changes in the initial random numbers. There were 40 burn-up calculation points and 20,000 neutron histories per burn-up calculation point. The only difference between Cases 1 and 2 is the number of burn-up calculation points.
Case 3: Burn-up calculations were performed 10 times under the same calculation conditions except for changes in the initial random numbers. There were 20 burn-up calculation points, and the numbers of neutron histories per burn-up calculation point were 20,000, 200,000, and 2,000,000. (The burn-up calculations were totally carried out 30 times in Case 3.)

From Case 1, we discuss the mechanism underlying the propagations of errors of nuclides number densities in Section 3. The reaction rate of Monte Carlo calculation has a normal distribution. These deviations of in reaction rate reflect the number densities through the burn-up calculation with exponential functions. Therefore, the number densities of Monte Carlo burn-up calculations have a "log-normal" distribution after burn-up calculation.

From the comparison of the deviation of the nuclide number density between Cases 1 and 2, we will describe the effect of the number of burn-up calculation points on the variance of the nuclide number densities. We will predict that the deviation of nuclide number density with relation to the number of burn-up calculation points.

From Case 3, we will discuss the effects of the deviation in nuclide number densities on the results of Monte Carlo burn-up calculations. We will extend the calculation conditions in order to generalize on the effect of deviation in nuclide number densities on the results of the Monte Carlo burn-up calculations verified above from Cases 1 and 2. In Cases 1 and 2, the numbers of neutron histories are very low, only 20,000. In Case 3, we executed three conditions of neutron histories per burn-up calculation point: 20,000, 200,000 and 2,000,000 histories. We verify that the quantitative effects of the propagated error of the nuclide number densities depend on the neutron histories.

We used the continuous energy Monte Carlo burn-up calculation code MVP-BURN (Nakagawa et al., 1990; Mori et al., 1999; Okumura et al., 2000; Nagaya et al., 2005). This Monte Carlo burn-up calculation code can execute branch calculations from a base case. Therefore, we have already

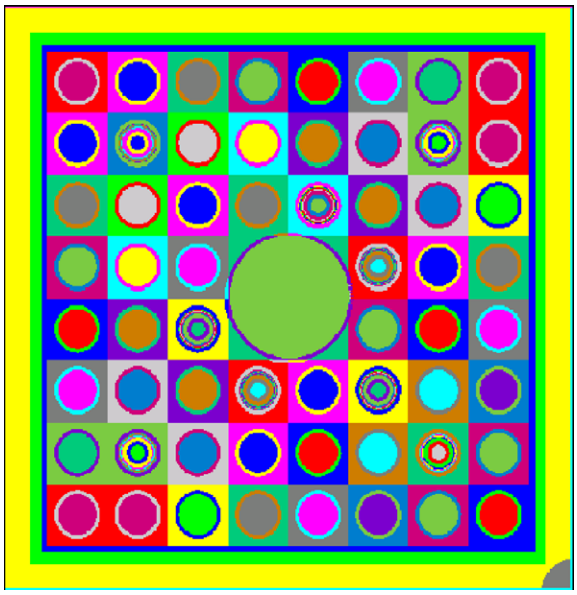

Fig. 1. Calculation regions.

reported the application of this Monte Carlo burn-up calculation code as a cross-section generator of BWR (Tohjoh et al., 2005). We used JENDL-3.3 (Shibata et al., 2002) as the evaluated nuclear data file. The calculation target is the hot condition of the 8×8 with a wide-water-rod fuel assembly for BWR5. The volume-averaged temperature of the fuel is 610 °C and the structure of fuel assembly is 286 °C. The in-channel void fraction is 40%, and a uniform water density distribution was assumed. The burn-up spatial discretized regions of Gd_2O_3 rods are annularly divided into 8, and the UO_2 rods are not annularly divided. The spatial discretization of burn-up calculation regions is shown in Fig. 1. The calculation conditions of this study are summarized in Table 1.

The next section describes the mechanism underlying error propagation of the nuclide number densities.

3. Error propagation in the number densities of Monte Carlo burn-up calculation (from Case 1)

The number density of nuclides after the burn-up calculation is described as follows when variation of these nuclides were dominated by absorption reactions:

$$N_i = N_{i-1} \exp(\mathrm{RR}_i \Delta t_i) \tag{1}$$

where N_i is the number density of nuclides at step i of the burn-up calculation, N_{i-1} is that at the previous step, RR_i is the absorption reaction rate of the nuclide, and Δt_i is the burn-up period of step i.

The number density of the previous step can be described as follows:

$$N_i = N_0 \exp(\mathrm{RR}_1 \Delta t_1) \exp(\mathrm{RR}_2 \Delta t_2) \cdots \exp(\mathrm{RR}_{i-1} \Delta t_{i-1}) \exp(\mathrm{RR}_i \Delta t_i) \tag{2}$$

$$N_i = N_0 \exp(\mathrm{RR}_1 \Delta t_1 + \mathrm{RR}_2 \Delta t_2 + \cdots + \mathrm{RR}_{i-1} \Delta t_{i-1} + \mathrm{RR}_i \Delta t_i) \tag{3}$$

$$\ln\left(\frac{N_i}{N_0}\right) = \sum_i (\mathrm{RR}_i \Delta t_i) \tag{4}$$

where N_0 is the initial number density of the nuclide.

We assume that there is a standard deviation s_i at the reaction rate of the burn-up calculation step i. Eqs. (1)–(4) can be written as follows:

$$N'_i = N'_{i-1} \exp\{(\mathrm{RR}_i \pm s_i)\Delta t_i\} \tag{5}$$

$$N'_i = N_0 \exp\{(\mathrm{RR}_1 \pm s_1)\Delta t_1 + (\mathrm{RR}_2 \pm s_2)\Delta t_2 + \cdots + (\mathrm{RR}_{i-1} \pm s_{i-1})\Delta t_{i-1} + (\mathrm{RR}_i \pm s_i)\Delta t_i\} \tag{6}$$

$$N'_i = N_0 \exp\left\{\sum_i (\mathrm{RR}_i \Delta t_i) \pm \sqrt{\sum_i (s_i^2 \Delta t_i^2)}\right\} \tag{7}$$

$$\ln\left(\frac{N'_i}{N_0}\right) = \sum_i (\mathrm{RR}_i \Delta t_i) \pm \sqrt{\sum_i (s_i^2 \Delta t_i^2)}. \tag{8}$$

Table 1
Assembly calculation conditions

Calculation code	The continuous-energy Monte Carlo burn-up code MVP-BURN
Cross section library	JENDL-3.3
Energy groups	1st group (fast): $1.0000e+7 \sim 5.5300e+3$ eV 2nd group (resonance): $5.5300e+3 \sim 6.8250e-1$ eV 3rd group (thermal): $6.8250e-1 \sim 1.0000e-5$ eV
History	1 batch: 200, 2000, and 20,000 neutron histories (3 case) Calculation batch: 120 batches Skip batch: 20 batches (total effective neutron histories are 20,000, 200,000, and 2,000,000)
Temperature	Hot condition: 286 °C for structures and water, 610 °C for fuel pellets
Void	40% void
Burn-up point	0, 0.2, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16, 20, 30, 40, 50, 60 (GWd/t) (Total 20 points for Case 1, Case 3) 0, 0.1, 0.2, 0.6, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8, 8.5, 9, 9.5, 10, 11, 12, 13, 14, 15, 16, 18, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65 (GWd/t) (Total 40 points for Case 2)
Burn-up calculation	"Predictor corrector" was adopted for all burn-up calculation points

Substituting Eq. (4) into Eq. (8), the logarithm of the ratio of the final number density to initial number density, $\ln\left(\frac{N_i'}{N_0}\right)$, can be obtained as follows:

$$\ln\left(\frac{N_i'}{N_0}\right) = \ln\left(\frac{N_i}{N_0}\right) \pm \sqrt{\sum_i (s_i^2 \Delta t_i^2)}. \tag{9}$$

Namely, when there is a standard deviation s_i at the reaction rate RR_i, the logarithm of the ratio of the number density to initial number density, $\ln\left(\frac{N_i'}{N_0}\right)$, has a standard deviation $\sqrt{\sum_i (s_i^2 \Delta t_i^2)}$. In general, a distribution like that shown above, whose logarithm has a standard distribution is called a log-normal distribution. The log-normal distribution has been used in the field of finance. It lacks a symmetrical shape. In the case of decreasing nuclide number densities, the rate of the increase $\sum_i (RR_i \Delta t_i)$ is negative; the mode of this log-normal distribution is on the right side. As we mentioned in Section 2, in Case 1 the distribution of ^{238}U's number density at 20 GWd/t is shown in Fig. 2.

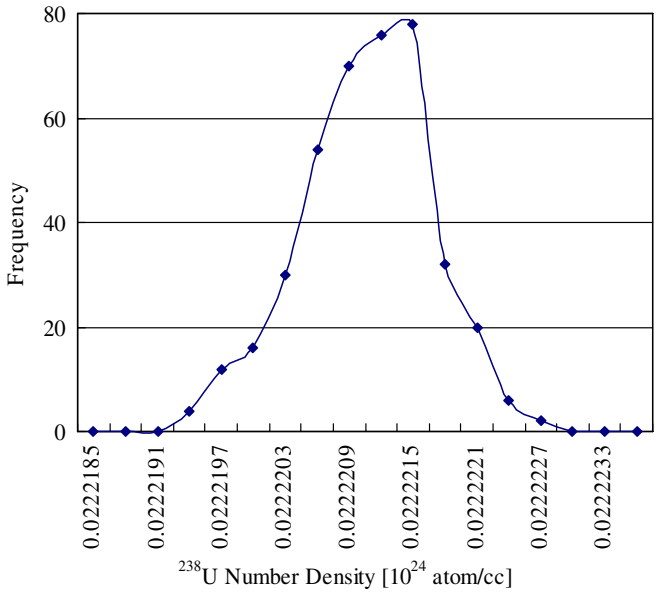

Fig. 2. Histogram of the ^{238}U number density.

Generally, the variance of the log–normal distribution, $VAR(X)$, can be written as follows:

$$\begin{aligned} VAR(X) &= E(X^2) - \{E(X)\}^2 \\ &= \exp(2\mu + 2S^2) - \exp(2\mu + S^2) \\ &= \exp(2\mu + S^2)\{\exp(S^2) - 1\} \end{aligned} \tag{10}$$

where μ is the mean value of the normal distribution after the logarithm transformation of this log–normal distribution and S is the standard deviation of the normal distribution after the transformation.

In the case of the normal distribution, we can use a notational system such as $A \pm a$, where A is the mean value and a is the standard deviation. In this paper, we use the same notations for the log-normal distribution. From Eqs. (9) and (10), the standard deviation of the rate of the increase (or decrease) of the nuclide number density, $\frac{N_i'}{N_0}$, after i times of burn-up calculation can be written as

$$\frac{N_i'}{N_0} = \frac{N_i}{N_0} \pm \sqrt{VAR} = \frac{N_i}{N_0} \pm \sqrt{\exp\left[2\sum_i (RR_i \Delta t_i) + \left\{\sqrt{\sum_i (s_i^2 \Delta t_i^2)}\right\}^2\right]\left[\exp\left\{\left(\sqrt{\sum_i (s_i^2 \Delta t_i^2)}\right)^2\right\} - 1\right]} \tag{11}$$

$$\frac{N_i'}{N_0} = \frac{N_i}{N_0} \pm \sqrt{\exp\left[2\sum_i (RR_i \Delta t_i) + \sum_i (s_i^2 \Delta t_i^2)\right]\left[\exp\left\{\sum_i (s_i^2 \Delta t_i^2)\right\} - 1\right]} \tag{12}$$

$$N_i' = N_i \pm N_0 \sqrt{\exp\left[2\sum_i (RR_i \Delta t_i) + \sum_i (s_i^2 \Delta t_i^2)\right]\left[\exp\left\{\sum_i (s_i^2 \Delta t_i^2)\right\} - 1\right]} \tag{13}$$

Consequently, after i times burn-up calculations, the nuclide number density has the standard deviation $N_0\sqrt{\exp\left[2\sum_i (RR_i \Delta t_i) + \sum_i (s_i^2 \Delta t_i^2)\right]\left[\exp\left\{\sum_i (s_i^2 \Delta t_i^2)\right\} - 1\right]}$.

This equation can be applied only to the nuclides those decreasing can be written as the absorption reaction of a single nuclide. This would place one log–normal distribution on the other log-normal distributions, if there were several contributions to the generation of the nuclide concerned. However, if there are several components to the reactions of generating concerned nuclide, we cannot grasp the practical errors of these reaction rates separately, especially under the case of the fixed value of burn-up exposures.

In the case of fixed value of burn-up exposure, the deviations in the number densities of the fissile nuclides are not in good agreement with Eq. (13), when analyst input the value of burn-up exposure. This is because the number of fission reactions is controlled by the value of burn-up exposure. For example, when fission rate obtained in Monte Carlo calculation is smaller than mean value due to statistical deviation, exposure time is increased to adjust thermal output (i.e. number of fissions) of current burn-up step; power normalization is carried out in burn-up calculation.

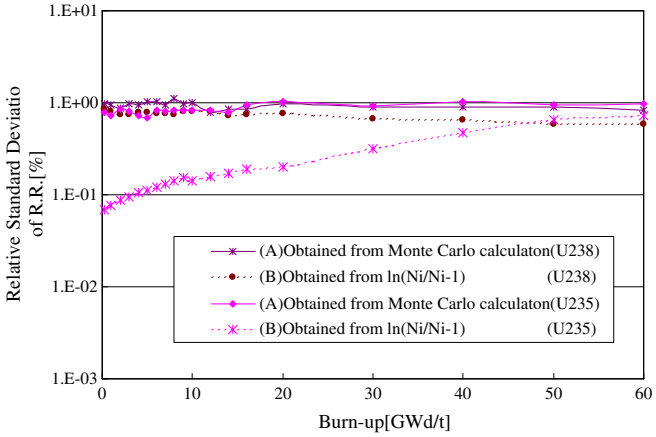

Fig. 3. Error of the reaction rate (RR) of ^{235}U and ^{238}U, (A) obtained from Monte Carlo calculation, (B) obtained from $\ln(N_i/N_{i-1})$.

The errors in the reaction rates of ^{235}U and ^{238}U with 400 burn-up calculations, Case 1, are shown in Fig. 3. The errors in reaction rate (A), which is statistically evaluated in Monte Carlo calculations, and those in reaction rate (B), calculated from the logarithm of the ratio of number densities, $\ln\left(\frac{N_i'}{N_{i-1}'}\right)$, are plotted in Fig. 3. From this figure, we can observe that the errors of fissile nuclide ^{235}U, (A) and (B), are not in good agreement. The error of the reaction rate (B) is controlled because the number of the fission reactions is normalized as described above. Therefore, the actual error (B) is lower than the statistical error (A). On the other hand, the errors of ^{238}U's (A) and (B) are in good agreement with each other.

The results of the relative standard deviations of number density ^{235}U and ^{238}U are shown in Fig. 4. In this figure there are the observed relative standard deviations and the predicted relative standard deviations, which are calculated by the errors of reaction rates (A) and (B). In the case of ^{238}U of Fig. 4, the prediction of the relative standard deviation of the number density is in good agreement with the observed for both (A) and (B). On the other hand, in the case of ^{235}U in Fig. 4, the predicted relative standard deviation using error (A) is overestimated compared with the observed relative standard deviation because of the normalized number of the fission reactions. This overestimation is large at BOL because of the large contribution of ^{235}U to the number of fission reactions. The overestimation at BOL is about 10-fold. This is in good agreement with the error in reaction rate shown in Fig. 3. The predicted relative standard deviation using error (B) is in good agreement with observed relative standard deviations. From Figs. 3 and 4, we can verify that Eq. (13) is appropriate for the prediction of the relative standard deviation of nuclide number densities, which follow simple burn-up chain like Eq. (1).

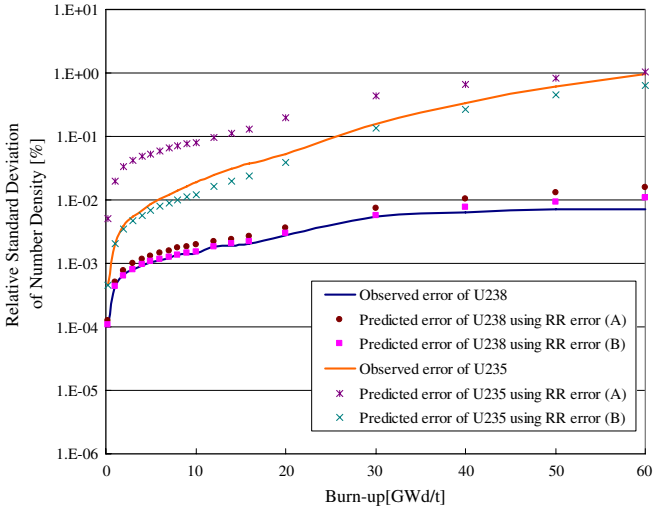

Fig. 4. Observed and predicted relative standard deviations of ^{235}U, ^{238}U number densities.

4. Effect of the number of burn-up calculation points on the number densities of Monte Carlo burn-up calculations (from Case 2)

In the Monte Carlo burn-up calculations, the errors of reaction rate are transformed into the nuclide number densities through the exponential functions, and these errors are propagated through the burn-up calculations, as we mentioned in Section 3. In these circumstances, there is a possibility that the errors of the number densities are affected by changes in the number of burn-up calculation points.

Generally speaking, the spectrum of neutron energy changes continuously during burn-up calculations. However, we have to execute the burn-up calculation by the discretized calculation point. Therefore, the results of the burn-up calculation would be affected by the choice of burn-up calculation points this is true both for Monte Carlo and deterministic calculations. However, this change in results, i.e. discretization effect of neutron spectrum, is not within the scope of this paper. The question we have to ask here concerns the statistical error of the number densities of the Monte Carlo burn-up calculation.

To consider these circumstances, we describe the following problem, called the symmetric random walk model. For example, consider starting the n times random walking from "0" in one dimension. In one random walking, the point can walk $+\delta$ distance with 50% likelihood and it can walk $-\delta$ distance with 50% likelihood. This problem is called the random walk model; and, because $+\delta$ and $-\delta$ are equal, the problem is especially called the symmetric random walk model. The range of existence of the point is from $-n\delta$ to $+n\delta$ after n times random walking. The mean value $\mu(n)$ and the variance $\sigma^2(n)$ can be written as follows:

$$\mu(n) = 0 \tag{14}$$

$$\sigma^2(n) = n\delta^2. \tag{15}$$

We will consider that the number of random walkings was changed from n to kn and that the distance was changed

from δ to $\frac{\delta}{k}$. After kn times random walking, the range of existence of the point is unchanged, from $-n\delta$ to $+n\delta$, and the mean value is also unchanged, $\mu(kn) = 0$. The variance can be written as follows:

$$\sigma^2(kn) = kn\left(\frac{\delta}{k}\right)^2 = \frac{1}{k}n\delta^2. \quad (16)$$

From Eq. (16), if the number of burn-up calculation points was multiplied by k, the deviation in nuclide number density would be divided by $\sqrt{k}$. This symmetric random walking model can be applied to the number density of Monte Carlo burn-up calculations. We will verify this effect using results of Case 2.

As mentioned in Section 3, the nuclide number density distribution is, strictly speaking, a log–normal distribution. However, in this section we will demonstrate about the relation of the number of burn-up calculation points and deviation in nuclide number density, using the approximation that the deviation of nuclide number density is in agreement to a normal distribution. The symmetric random walking model can be applied to the distribution of the number density. To verify this point, we execute 400 Monte Carlo burn-up calculations using different initial random numbers; this is called Case 2, as mentioned in Section 2. In Case 2, the number of burn-up calculation points is 40, twice that in Case 1. The distributions of the ^{238}U and ^{244}Cm number densities in Cases 1 and 2 are shown in Figs. 5 and 6, respectively. From these figures, we can verify that increasing the number of burn-up calculation points broadens the span of the number density distributions. From Fig. 5, we can also confirm that the mode of the ^{238}U number density is shifted. It is caused by the fact that the discretized calculation method of burn-up calculation under the spectrum is continuously changing, as we mentioned before. However, this shift is not our target in this paper as described above. The targets of this paper are the deviations of the nuclide number densities. The standard deviations of the ^{238}U and ^{244}Cm number densities in Cases 1 and 2 are shown in Figs. 7 and 8, respectively. The predicted standard deviations from Eq. (16) are shown in these figures. From these figures, we can confirm that the symmetric random-walk model is applicable. The deviation in the number density would be divided by $\sqrt{2}$ when the number of burn-up calculation points was doubled.

In actual Monte Carlo burn-up calculations, the total number of neutron histories dominates the calculation cost. Therefore, we cannot increase the number of burn-up calculation points endlessly; we have to limit the calculation time reasonably. Then, the increase in the number of burn-up calculation points causes a reduction in the neutron number histories of each step in the Monte Carlo calculations. When the neutron histories were multiplied by k,

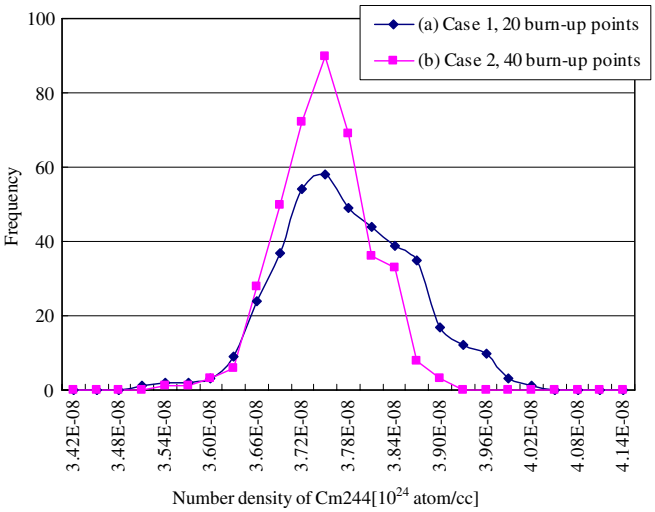

Fig. 6. Histogram of the ^{244}Cm number density, (a) Case 1, 20 burn-up points and (b) Case 2, 40 burn-up points.

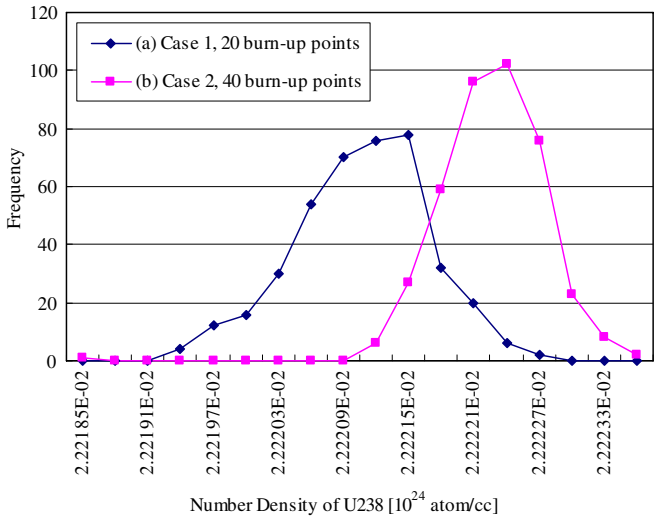

Fig. 5. Histogram of the ^{238}U number density, (a) Case 1, 20 burn-up points and (b) Case 2, 40 burn-up points.

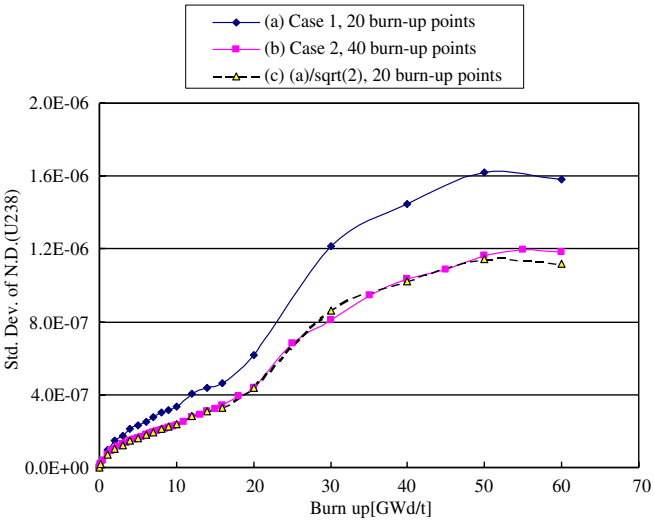

Fig. 7. Standard deviation of the ^{238}U number density, (a) Case 1, (b) Case 2, and (c) Case 2 divided by $\sqrt{2}$.

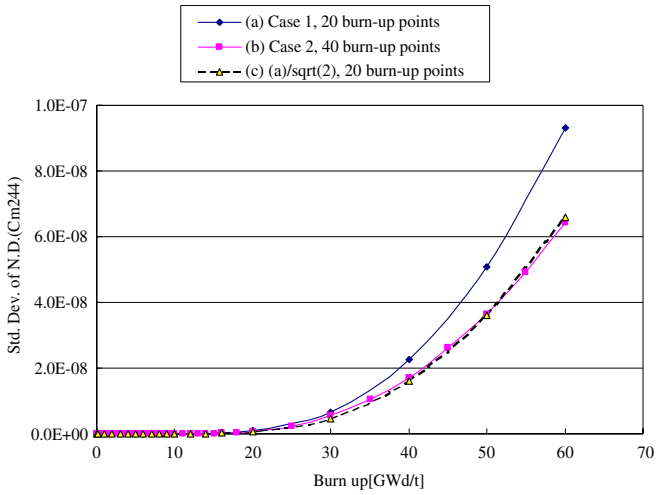

Fig. 8. Standard deviation of the ^{244}Cm number density, (a) Case 1, (b) Case 2, and (c) Case 2 divided by $\sqrt{2}$.

the deviation in k-infinity would be divided by $\sqrt{k}$. On the other hand, when the neutron histories were multiplied by $1/k$, the deviation in the number density would also be multiplied by $\sqrt{k}$. However, the sensitivity of the number densities to k-infinity is lower than that of the number of neutron histories, as described in Section 5. Therefore, a larger number of neutron histories (a smaller number of burn-up calculation points) is desirable for the analyses, which demand highly accurate results of k-infinity. On the other hand, a smaller number of neutron histories (a larger number of burn-up calculation points) is desirable for the PIE analyses, which demand highly accurate results of the nuclide number densities.

5. Accuracy of the Monte Carlo burn-up calculations including propagated errors of the nuclide number densities (from Case 3)

5.1. Verification of the equations for propagation errors

In Section 3 we verified the mechanism underlying the error propagation of nuclide number densities, and in Section 4 we verified the effect of the number of burn-up calculation points on the nuclide number densities. However, the neutron histories of those verifications were very low – only 20,000 – because of the large number (400) of executions of burn-up calculations using different initial random numbers. This section verifies that mechanisms and those effects described in previous sections are generally applicable to Monte Carlo burn-up calculations with various number of neutron histories. Furthermore, we will obtain the accuracy of Monte Carlo burn-up calculations on a BWR fuel assembly, including the propagated errors of the nuclide number densities.

We executed three sets of calculations, each including 10 burn-up calculations using different initial random numbers. The only different point among three sets is the num-

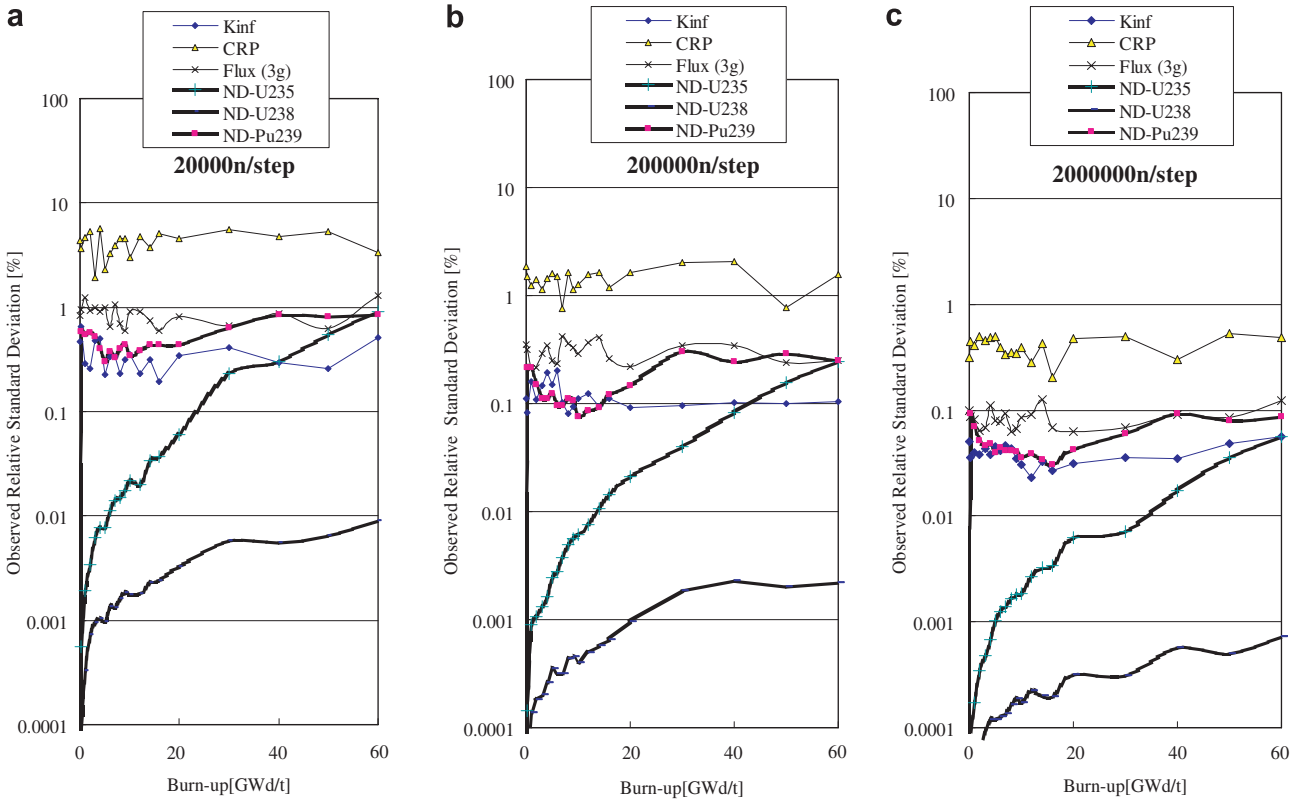

Fig. 9. Observed relative standard deviations of the k-infinity, CRP, flux, and number densities, (a) 20,000 histories/batch, (b) 200,000 histories/batch, (c) 2,000,000 histories/batch.

ber of neutron histories: 20,000, 200,000 and 2,000,000. This was Case 3 in Section 2.

In this section, we call the errors of *k*-infinity, the corner-rod peaking (CRP), and neutron flux, "Observed (Statistical + Propagated)", which obtained from the statistical analysis of these 10 burn-up calculations. The Observed (Statistical + Propagated) errors include not only statistical errors at particular burn-up point but also those of propagated errors during burn-up calculations. To the contrary, the errors of *k*-infinity, CRP, and neutron flux evaluated from statistical analysis of Monte Carlo calculations are defined as "Calculated (Statistical)". The Calculated (Statistical) errors include statistical errors only at particular burn-up point, and they are listed in the output of MVP-BURN.

We call the error of nuclides number densities "Observed (Propagated)", which obtained from the statistical analysis of these 10 burn-up calculations. To the contrary, we call the error of nuclides number densities

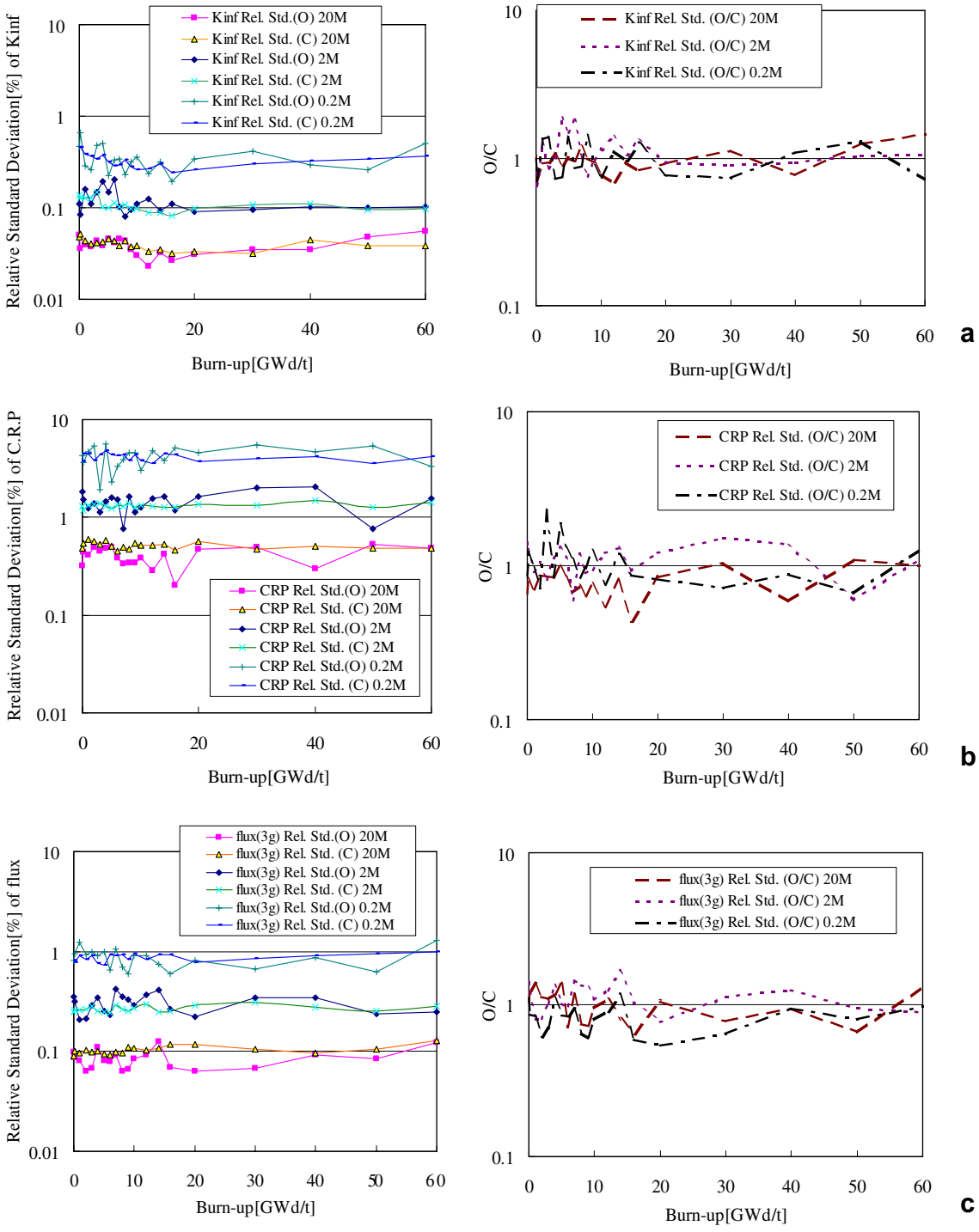

Fig. 10. Relative standard deviations and O/C (Observed (S + P)/Calculated (S)), (a) *k*-infinity, (b) CRP, and (c) flux.

"Predicted (Propagated)", which is obtained from Eq. (13). It is inferred from Sections 3 and 4 that the Observed (Propagated) errors and the Predicted (Propagated) errors of number density are in good agreement.

The Observed (Statistical + Propagated) relative standard deviations of *k*-infinity, corner-rod peaking (CRP), and neutron flux and are shown in Fig. 9. This figure also shows that the Observed (Propagated) relative standard deviations of the nuclide number densities. The Observed (Propagated) errors of the nuclide number densities depend not only on neutron histories but also on burn-up exposure. On the other hand, the Observed (Statistical + Propagated) errors of *k*-infinity, CRP, and flux became larger depending only on the neutron histories. Strictly speaking, these Observed (Statistical + Propagated) errors would be large with relation to the burn-up exposure due to the propagation error of number density. However, they do not depend clearly on the burn-up exposures due to the lower effect of the propagation errors than statistical errors. The relative standard deviations of those parameters at the EOL are roughly in agreement with the BOL. This indicates that the errors in those parameters (*k*-infinity, peaking factors, and flux) can be predicted in the rough from statistical errors alone due to the low effect of the propagations on these parameters. The errors in the Observed (Statistical + Propagated), Calculated (Statistical) and O/C (Observed (Statistical + Propagated)/Calculated (Statistical)) for *k*-infinity, flux, and CRP are shown in Fig. 10. From this figure, we can understand that O/C (Observed (Statistical + Propagated)/Calculated (Statistical)) is roughly 1.0 from BOL to EOL. Nevertheless the propagated errors of nuclide number densities increase as the burn-up exposure increases. The reason why these Observed (Statistical + Propagated) errors do not dependent on burn-up exposure, is that the effect of the propagated errors of nuclides number densities to *k*-infinity is much lower than the effects of the neutron histories as we mentioned below.

Next, we again verify Eq. (13) described in Section 3. The Observed (Propagated) and the Predicted (Propagated) errors from Eq. (13) of the ^{235}U and ^{238}U are shown in Figs. 11 and 12, respectively. In these figures, the reaction rates were calculated from the logarithm of the ratio of number densities, $\ln\left(\frac{N'_i}{N'_{i-1}}\right)$, which were called (B) in Section 3. From these figures, the errors of the Predicted (Propagated) and Observed (Propagated) are in good agreement. We can consider Eq. (13) reasonable for these nuclides.

5.2. Verification of the effects of propagation errors on Monte Carlo burn-up calculations through sensitivity analyses

In this section, we verify the sensitivity of the statistical and propagated errors of the nuclide number density to the

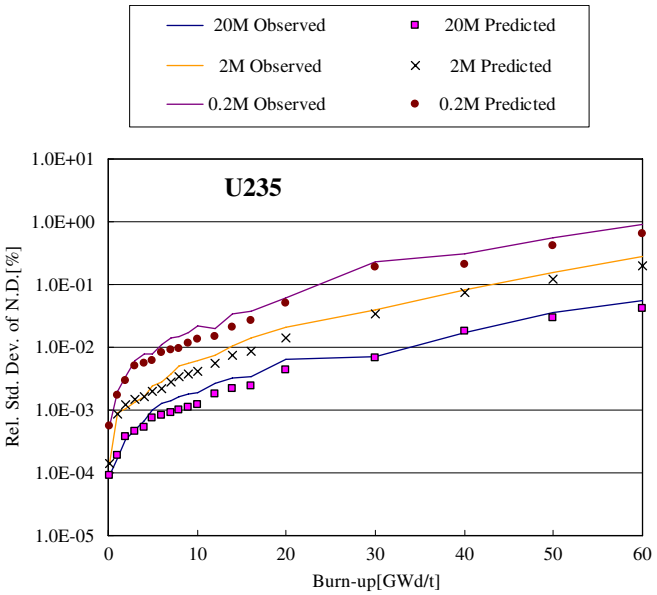

Fig. 11. Observed (Propagated) and Predicted (Propagated) errors of the ^{235}U dependence on the neutron histories.

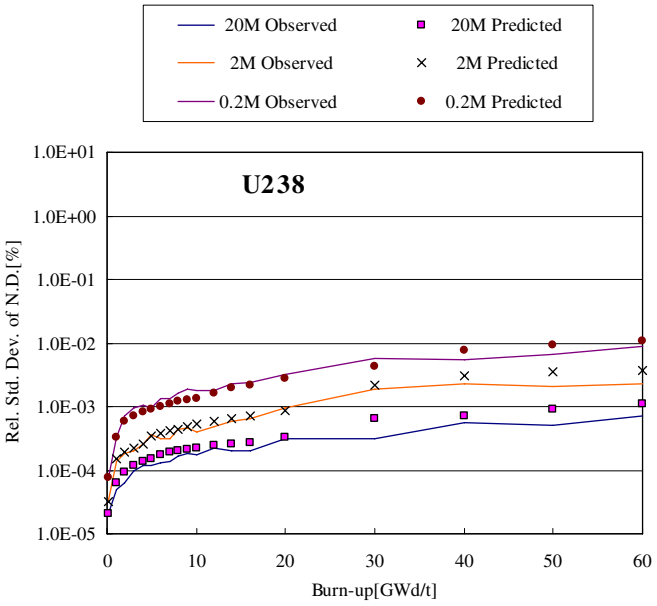

Fig. 12. Observed (Propagated) and Predicted (Propagated) errors of the ^{238}U dependence on the neutron histories.

results of the Monte Carlo burn-up calculations. As mentioned above, Eq. (13) can predict the errors in the nuclide number densities after burn-up calculations. However, this equation is applicable to the nuclide number densities whose reactions consist of single absorption reactions. In case of the multiple reactions are included in the absorption reactions, and under the fixed burn-up exposure calculations, these errors in number densities are overestimated as in Fig. 4. Therefore, we use the fitting equations to predict the statistical and propagated errors of the fissile nuclide number densities.

The dominant nuclides in the results of k-infinity are major absorption nuclide ^{238}U and major fissile nuclides ^{235}U, ^{239}Pu, and ^{241}Pu. However, as shown in Fig. 12, the errors of the number density of ^{238}U are very low because of its large initial number density. Therefore, we use equations that fit from the total number densities of ^{235}U, ^{239}Pu, and ^{241}Pu. The (Propagated) errors are shown in Fig. 13. In this figure, we show the equations of the fissile number density fit depend to the burn-up exposures, and several neutron histories.

We also show the sensitivity of these fissile nuclides in Fig. 14. This figures compares the results of the sensitivity analyses of the total number densities of ^{235}U, ^{239}Pu, and ^{241}Pu to the results of k-infinity in the deterministic assembly calculation. The calculation code of this sensitivity analysis is NEUPHYS-C. NEUPHYS-C calculates the effective macroscopic cross sections depending on the collision probability method, and execute the lattice calculation depend on the diffusion theory. The accuracy of this assembly calculation code is verified through the in-core management of the HAMAOKA-2 and 3. From Fig. 14, we can observe that the sensitivity of the fissile number density to k-infinity is small. The effect of a 0.1% change in fissile number density (e.g., for the 3 wt% UO_2 fuels, this means not 3.3 wt% but 3.003 wt%.) on k-infinity is only about 0.05% Δk.

Section 4 showed the effects of the number of burn-up calculation points on nuclide number densities. The deviation in the nuclide number densities would be divided by $\sqrt{k}$ if the number of burn-up calculation points was multiplied by k. On the other hand, the number of neutron histories also affects the results for k-infinity. The deviation in k-infinity would be divided by $\sqrt{k}$ if the number of neutron histories was multiplied by k. There is a trade-off between the number of the calculation points and the number of neutron histories per burn-up step. However, the sensitivity of the fissile number densities is half that of the neutron histories, as we shown in Fig. 14. From this figure, we can understand that a larger number of neutron histories (a smaller number of burn-up calculation points) is desirable for the analyses, which demand highly accurate results of k-infinity, as we mentioned in Section 4.

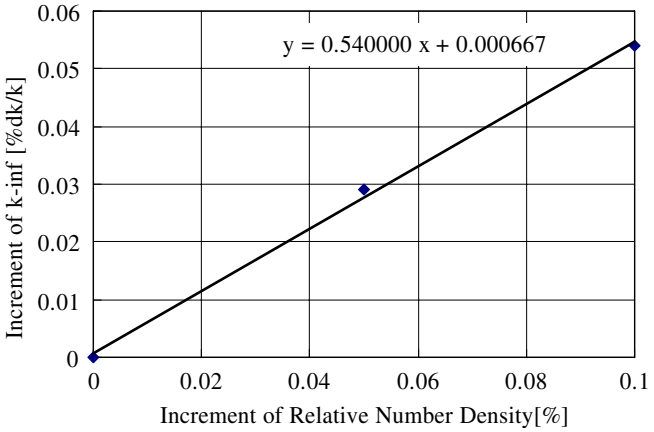

Fig. 14. Sensitivity of the fissile nuclide number densities to k-infinity.

From the errors of the fissile number densities shown in Fig. 13 and the sensitivity of these fissile number densities shown in Fig. 14, we can predict the dependence of the total statistical and propagated errors on the burn-up exposures. The dependencies of the Statistical + Propagated, Statistical, and (Statistical + Propagated)/(Statistical) errors on the neutron histories are shown in Table 2 and Fig. 15. From Fig. 10, we could not observe clearly the effects of the propagations due to the lower effect of the propagations than statistical errors. Actually, Fig. 15

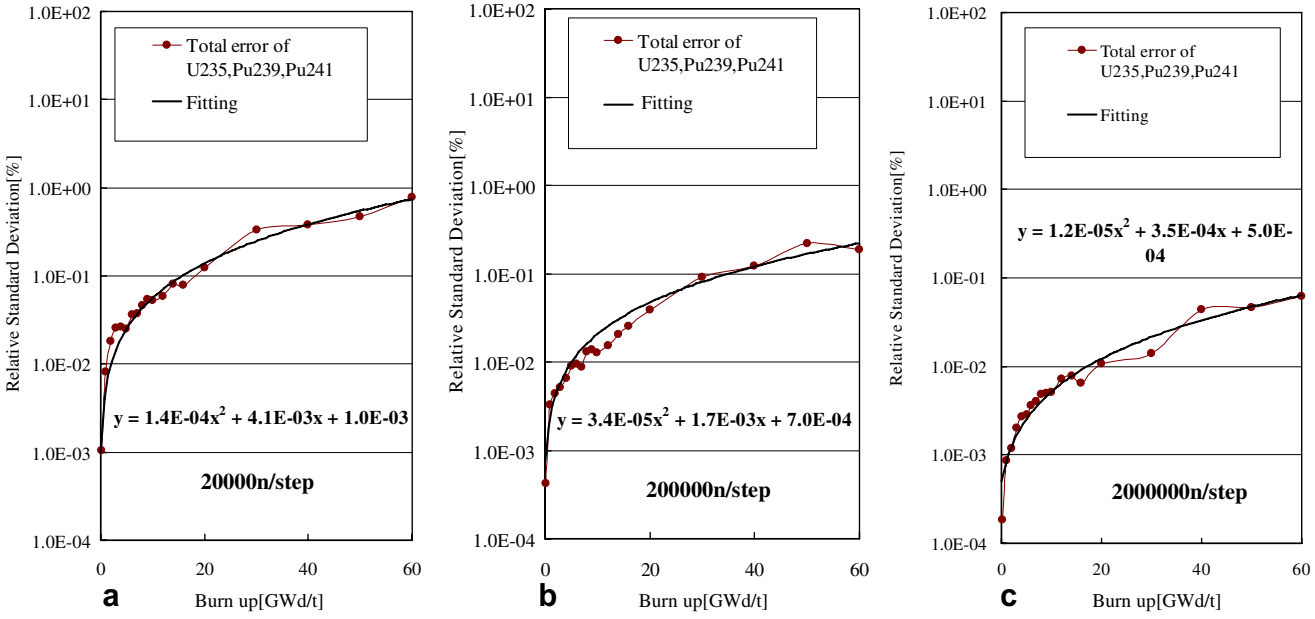

Fig. 13. Total (Propagated) errors of fissile number density, (a) 20,000 histories, (b) 200,000 histories, and (c) 2,000,000 histories.

Table 2
"Statistical + Propagated", Statistical, and (Statistical + Propagated)/(Statistical) errors of *k*-infinity

Burn up (GWd/t)	2,000,000					200,000					20,000				
	ND (%)	Prop. error (%dk/k)	Static error (%)	S + P error (%)	(S + P)/(S)	ND (%)	Prop. error (%dk/k)	Static error (%)	S + P error (%)	(S + P)/(S)	ND (%)	Prop. error (%dk/k)	Static error (%)	S + P error (%)	(S + P)/(S)
0	0.0005	0.0009	0.048	0.048	1.00	0.0007	0.0010	0.138	0.138	1.00	0.0010	0.0012	0.461	0.461	1.00
0.2	0.0006	0.0010	0.052	0.052	1.00	0.0010	0.0012	0.129	0.129	1.00	0.0018	0.0017	0.457	0.457	1.00
1	0.0009	0.0012	0.043	0.043	1.00	0.0024	0.0020	0.126	0.126	1.00	0.0052	0.0035	0.388	0.388	1.00
2	0.0013	0.0014	0.040	0.040	1.00	0.0042	0.0029	0.129	0.129	1.00	0.0096	0.0059	0.363	0.363	1.00
3	0.0018	0.0016	0.041	0.042	1.00	0.0061	0.0039	0.148	0.148	1.00	0.0142	0.0083	0.343	0.343	1.00
4	0.0023	0.0019	0.043	0.043	1.00	0.0080	0.0050	0.103	0.103	1.00	0.0190	0.0109	0.374	0.374	1.00
5	0.0028	0.0022	0.046	0.046	1.00	0.0100	0.0060	0.100	0.100	1.00	0.0240	0.0136	0.316	0.317	1.00
6	0.0033	0.0024	0.044	0.044	1.00	0.0120	0.0071	0.112	0.112	1.00	0.0292	0.0164	0.286	0.287	1.00
7	0.0038	0.0027	0.038	0.038	1.00	0.0141	0.0083	0.103	0.103	1.00	0.0346	0.0194	0.297	0.298	1.00
8	0.0043	0.0030	0.044	0.044	1.00	0.0162	0.0094	0.108	0.108	1.00	0.0402	0.0224	0.332	0.332	1.00
9	0.0049	0.0033	0.037	0.037	1.00	0.0184	0.0106	0.097	0.097	1.01	0.0460	0.0255	0.277	0.278	1.00
10	0.0055	0.0036	0.039	0.039	1.00	0.0207	0.0118	0.098	0.099	1.01	0.0520	0.0287	0.259	0.260	1.01
12	0.0067	0.0043	0.033	0.033	1.01	0.0254	0.0144	0.089	0.091	1.01	0.0646	0.0356	0.263	0.266	1.01
14	0.0081	0.0050	0.035	0.035	1.01	0.0304	0.0171	0.089	0.091	1.02	0.0780	0.0428	0.303	0.306	1.01
16	0.0095	0.0058	0.032	0.032	1.02	0.0356	0.0199	0.083	0.085	1.03	0.0922	0.0505	0.240	0.246	1.02
20	0.0125	0.0074	0.033	0.034	1.02	0.0467	0.0259	0.097	0.101	1.03	0.1230	0.0671	0.263	0.271	1.03
30	0.0215	0.0123	0.031	0.034	1.07	0.0787	0.0432	0.108	0.117	1.08	0.2140	0.1162	0.302	0.324	1.07
40	0.0325	0.0182	0.045	0.049	1.08	0.1167	0.0637	0.109	0.127	1.16	0.3250	0.1762	0.321	0.366	1.14
50	0.0455	0.0252	0.039	0.046	1.19	0.1607	0.0874	0.097	0.131	1.35	0.4560	0.2469	0.337	0.418	1.24
60	0.0605	0.0333	0.039	0.051	1.32	0.2107	0.1144	0.097	0.150	1.55	0.6070	0.3284	0.369	0.494	1.34
70	0.0775	0.0425	0.039	0.058	1.48	0.2667	0.1447	0.097	0.174	1.80	0.7780	0.4208	0.369	0.560	1.52
80	0.0965	0.0528	0.039	0.066	1.68	0.3287	0.1782	0.097	0.203	2.09	0.9690	0.5239	0.369	0.641	1.74
90	0.1175	0.0641	0.039	0.075	1.92	0.3967	0.2149	0.097	0.236	2.43	1.1800	0.6379	0.369	0.737	2.00
100	0.1405	0.0765	0.039	0.086	2.20	0.4707	0.2548	0.097	0.273	2.81	1.4110	0.7626	0.369	0.847	2.30

ND (%), relative standard deviation of total fissile number densities; Prop. error (%dk/k), propagated errors; S + P error (%), Statistical + Propagated errors; (S + P)/S, (Statistical + Propagated)/(Statistical) errors.

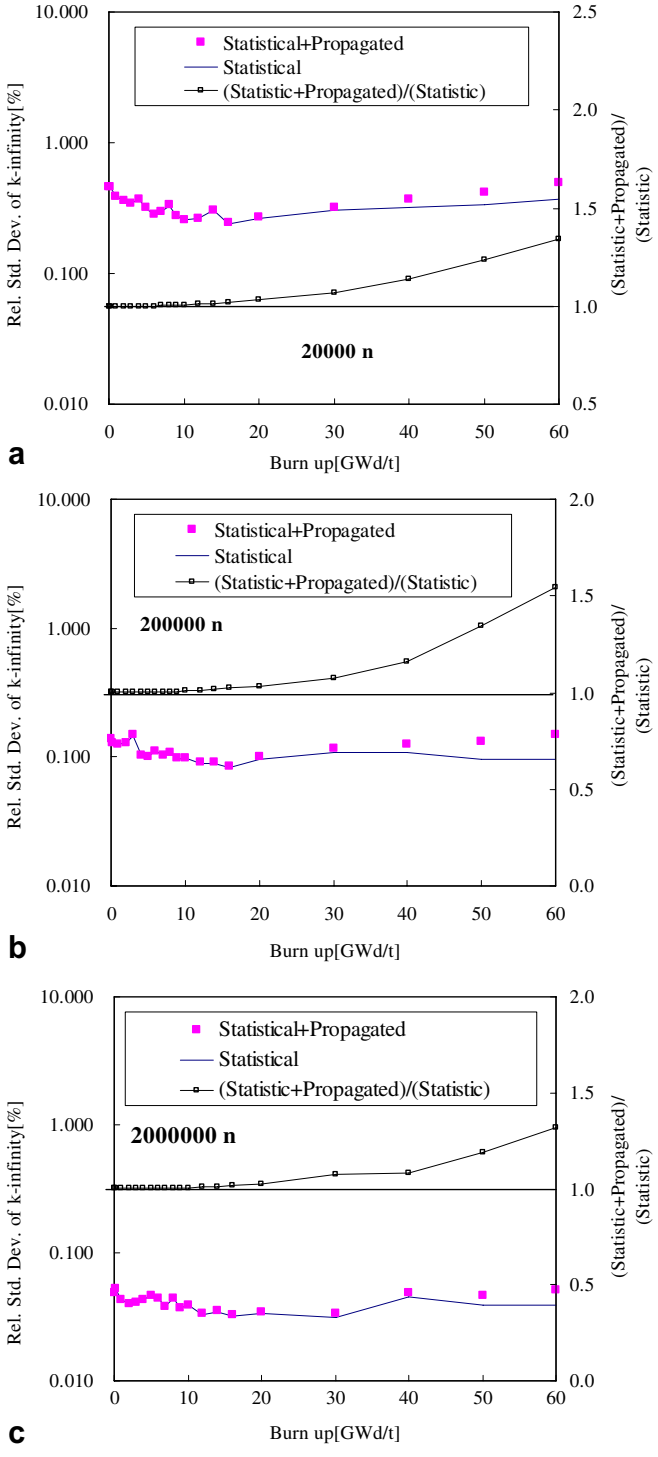

Fig. 15. Statistical + Propagated, Statistical and (Statistical + Propagated)/(Statistical) errors of k-infinity, (a) 20,000 histories, (b) 200,000 histories, and (c) 2,000,000 histories.

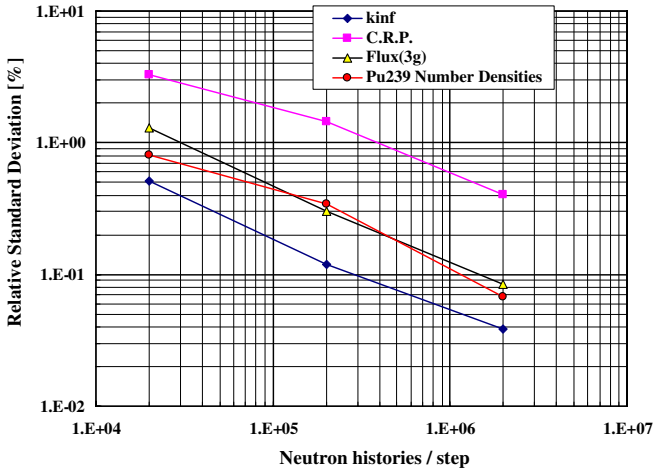

Fig. 16. Accuracy of the Monte Carlo burn-up calculation for the BWR fuel assembly at 20 GWd/t.

demonstrates that the effect of the Statistical + Propagated errors on the 8×8 BWR assembly is only about 7% that of the MOL (30 GWd/t), due to the quantitative analysis of propagations and statistical errors. This means that the effect of the statistical error propagation of Monte Carlo burn-up calculations is not important to the present BWR fuel assemblies, because the reactivity of the core is dominated by the young fuel bundles like fresh or once-burned fuels. However, for the future high burn-up fuels, such as those exceeding 100 GWd/t, the Monte Carlo burn-up calculation needs to take into consideration the propagated errors through the nuclide number densities.

From Figs. 9–15, we can see that the results of k-infinity, CRP, and flux do not depend on the propagation errors. We have also found that the errors of the nuclide number densities depend on the burn-up exposure. To define these errors, the dependence of the accuracy of these parameters on the neutron histories is shown in Fig. 16. In this figure, the accuracy of each parameter is at 20 GWd/t. The figure shows that we can find the reasonable neutron histories depending on the necessary calculation accuracy without over cost of the Monte Carlo burn-up calculations.

6. Conclusions and recommendations

To make clear the effects of error propagations on Monte Carlo burn-up calculations, we studied the mechanism underlying such propagations and we verified this effect quantitatively.

First, we proposed an equation that can predict the variance in the nuclide number densities after burn-up calculations, and we verified this equation by performing huge numbers of Monte Carlo burn-up calculations using different initial random numbers. The nuclide number densities of the Monte Carlo burn-up calculations have a log-normal distribution, which is widely used in the field of finance. The proposed equations are applicable to general Monte Carlo burn-up calculations.

We also verified the effect of the number of burn-up calculation points on the nuclide number densities. The deviation in the nuclide number densities would be divided by $\sqrt{k}$ if the number of calculation points is multiplied by k. This sensitivity is equal to the effect of the neutron histories on k-infinity. However, the sensitivity of the nuclide number

density to the results of k-infinity is only half as great as the sensitivity of the neutron histories. Therefore, it is desirable to reduce the number of burn-up calculation points for analyses that require highly accurate estimation of k-infinity. On the other hand, it is desirable to reduce the number of neutron histories for the analyses that require highly accurate of nuclide number densities, like PIE analyses. This effect of the number of calculation points is applicable to the general Monte Carlo burn-up calculations.

Finally, based on these verifications, we have estimated the Monte Carlo burn-up calculation errors, including both statistical and propagated errors, by comparing statistical errors alone versus both statistical and propagated errors. These comparisons revealed that the effects of error propagation on the Monte Carlo burn-up calculations of the 8×8 BWR fuel assembly are low up to 60 GWd/t. However, for future high burn-up fuels, such as those exceeding 100 GWd/t, Monte Carlo burn-up calculations must take propagated errors into consideration.

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