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Computation time reduction of nuclear fuel burnup calculations with the predictor-corrector method using low-order model

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Abstract

Special attentions should be paid on the time discretization in nuclear fuel burnup calculations for systems including gadolinia, and several efficient methods based on the predictor-corrector method have been proposed so far. There are still requirements of the further reduction of the computation time, and we propose to use a low-order model (LOM) whose computation time is much shorter than that of a full-order model (FOM) in the corrector calculations. To mitigate the error caused by the LOM adoption, correction factors for one-group quantities are devised and introduced. The proposed method is tested on the lattice physics problems under the condition that FOM is a deterministic method based on MOC and LOM is also a deterministic method based on MOC with the coarse ray-tracing condition with fewer-group cross sections. The proposed method gives results whose accuracy is almost equivalent with that of FOM, and computation time is reduced to 60-65%.

Key words: fuel burnup calculation, predictor-corrector method, gadolinia, low-order model, method of characteristics

1. Introduction

It is common to use burnable poisons in light water reactors (LWRs) in order to suppress the large excess reactivity around at the beginning of operation cycle, and gadolinia is often used as burnable poisons in presently operating LWRs. In fuel assemblies including gadolinia, the microscopic neutron capture reaction rates of Gd-155 and -157 change rapidly with time. In nuclear fuel burnup calculations for such systems, it is necessary to adopt a small burnup step size to accurately simulate the rapid time variation of these reaction rates. The use of the small burnup step size leads to an increase in computation time since the required number of time-consuming neutron transport calculations becomes large. Various burnup calculation methods that can provide highly accurate solutions even with large burnup step size have been developed so far (Yamamoto, 1985; Carpenter, 2010; Isotalo, 2011; Fiorito, 2013). Among them, the predictor-corrector

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(PC) method(Stamm'ler, 1983) has widely been employed in many computer codes. While the PC method is computationally much more efficient than the simple Euler-type method, typical burnup step size used for systems with gadolinia is still on the order of 0.2 GWd/t(Knott, 2007), and the further reduction in computational burden was desired.

Under this circumstance, Yamamoto et al. have proposed the projected PC (PPC) method(Yamamoto, 2008, 2009) in 2008. They have specified the cause of the errors in the conventional PC method: the error in the number densities obtained by the predictor calculations. This error is caused by the assumption of the constant reaction rates during a burnup step in the predictor calculations, and is inevitable in the PC method with one neutron transport calculation per one corrector step. The PPC method uses the linear correlation between the microscopic reaction rate and the number density of Gd-155 and -157, and better microscopic reaction rates are estimated through the extrapolation for the final number densities in the PC method. Significant improvement in the computational accuracy has been achieved even with the simple numerical procedure in the PPC method.

In 2009, Lee et al. have proposed the quadratic depletion (QD) method(Lee, 2009, 2013). The QD method constructs a quadratic function of the microscopic reaction rates of the Gd isotopes dependent on the number density of Gd-155 after the predictor calculation. Coefficients in this function are determined from the results of the concerned and last burnup steps and the predictor calculation result of the concerned step. The corrector calculations are performed with the time-dependent reaction rate represented by this quadratic function. Furthermore, to mitigate the error in the number densities obtained by the predictor calculations, the post-correction on these number densities is made using the calculation results on the last burnup step.

As another variation of the PC method, the weighted PC (WPC) method has been proposed by the research group of Hokkaido University and the Nuclear Fuel Industries, Ltd.(Okumura, 2017). In the conventional PC method, number densities (or microscopic reaction rates) obtained through the predictor and corrector steps are averaged with the same weight, but in the WPC method the different weights are adopted. The main motivation of this work is to develop a method which can easily be adopted to the depletion perturbation theory combined with the PC method(Chiba, 2018). The key issue in the WPC method is how to determine the optimum weight, and the optimally-weighted PC (OWPC) method and the advanced optimally-weighted PC (AOWPC) method have been proposed(Okumura, 2017; Sasuga, 2021). It has been demonstrated that the AOWPC method gives solutions of k_{∞} within approximately 150 pcm errors with large burnup step size of 2 GWD/t for several PWR and BWR assembly problems(Sasuga, 2021). In the AOWPC method, a quadratic function of the microscopic reaction rates of Gd-155 and -157 dependent on the Gd-155 number density is used, and the error in the number densities obtained by the predictor calculations is mitigated through correcting not the number densities themselves but the corresponding microscopic reaction rates (one-group cross sections) of these Gd isotopes using the results on the last

burnup step. Whereas the theoretical framework and the detailed implementation of the AOWPC method are different from those of the QD method, these two methods are very close to each other.

Recently, the nuclear fuel burnup calculations have often been carried out in the framework of the Monte Carlo neutron transport codes. Furthermore, burnup calculations with the computationally-expensive three-dimensional deterministic transport codes have also been attempted. Computational burden of these calculations is significant and its reduction is beneficial. In addition, in works requiring many calculation cases such as the stochastic-based uncertainty quantification, reduction of the computational burden is crucial. Using the advanced PC methods such as the PPC, QD, and AOWPC methods, relatively large burnup step size of approximately 2 GWD/t can be adopted without significant degradation of the computational accuracy, and further extension of the burnup step size would not be beneficial from the practical point of view. It is well known that the most time-consuming part in the nuclear fuel burnup calculations is the neutron transport calculation part, and the neutron transport calculation should be carried out twice per one burnup step at least when the PC-based methods are employed. In the present work, we propose to use a low-order model (LOM) for the PC method; a full-order model (FOM) is used only at the predictor step calculation and LOM is used at the corrector step. To mitigate the error caused by the LOM adoption, another calculation with LOM is also carried out at the predictor step, and this error is quantified as the difference between the FOM and LOM results. Using this information, the LOM results at the corrector step can be corrected. If the computation time of the LOM calculations is much shorter than that of the FOM calculations, total computation time can possibly be reduced to around half.

The combination of FOM and LOM is arbitrary: the continuous-energy Monte Carlo method as FOM and the deterministic method as LOM, for example. In the present work, we focus on the two-dimensional lattice physics computations; the 172-group neutron transport calculations with the method of characteristics (MOC) is considered as FOM and the coarse-group neutron transport calculations with MOC with the coarse ray-tracing conditions as LOM. This combination is realistic and practical since many modern lattice physics codes employ MOC for the spatial discretization and the same numerical method, MOC in this work, is used commonly in FOM and LOM. This proposed procedure to reduce the computation time using LOM can be adopted to any PC-based methods, and is adopted to the AOWPC method in the present work.

Section 2 describes the theory of the AOWPC method briefly and the procedure of how to correct the errors caused by the LOM adoption. Section 3 provides the detailed information on LOM used in the present work. Numerical methods and problem specification are explained in Section 4, and numerical results including the investigation on the proper choice of the numerical conditions in LOM and the comprehensive verification are described in Section 5. Finally, Section 6 is devoted to conclude the present work.

2. Theory

2.1. Brief review of advanced optimally-weighted predictor-corrector method

Let us assume that the number densities at the time step n are known and those at $n + 1$ are target of the calculation. First, the neutron transport equation at the step n is solved, and the microscopic reaction rates, R_n^p , are calculated. Using them, the Bateman equation is defined assuming the constant microscopic reaction rates from the step n to $n + 1$. Then, this equation is solved and the number densities at $n + 1$, N_{n+1}^p , are obtained. This is the predictor step. Next, the neutron transport equation at $n + 1$ defined from N_{n+1}^p is solved, and the corresponding microscopic reaction rates, R_{n+1}^c , are calculated. Using them, the Bateman equation is again defined and solved, and the number densities at $n + 1$, N_{n+1}^c , are obtained. This is the corrector step. The WPC method finally determines the number density at the step $n + 1$, N_{n+1} , using a weight parameter ω as

$$N_{n+1} = (1 - \omega)N_{n+1}^p + \omega N_{n+1}^c, \quad (1)$$

or

$$N_{n+1} = \exp \left((1 - \omega) \ln N_{n+1}^p + \omega \ln N_{n+1}^c \right). \quad (2)$$

The concept of the WPC method is briefly presented in **Fig. 1**. In the following, Eq. (2) is used because of the better accuracy than Eq. (1).

In the AOWPC method, ω is determined using a simple burnup problem that takes into account the properties of Gd-155 and -157 as follows. Since the change in the number densities of Gd-155 and -157 is dominated by neutron capture reactions of themselves, the burnup equation used in the simple burnup problem is defined as

$$\frac{d\hat{N}(t)}{dt} = -R(t)\hat{N}(t), \quad (3)$$

with the initial condition $\hat{N}(0) = N_n$. In Eq. (3), $R(t)$ is the microscopic neutron capture reaction rate of the concerned nuclide. The accurate solution to this simple burnup equation at the end of the concerned burnup step, $\hat{N}_{n+1}$, can easily be obtained if $R(t)$ is known. With the same manner as the QD method, $R(t)$ is represented in the AOWPC method as

$$R(t) = aN^2(t) + bN(t) + c, \quad (4)$$

where $N(t)$ is the Gd-155 number density at t . The coefficients a , b , and c are determined from the results at the steps $n - 1$ and n , (N_{n-1}, R_{n-1}^p) and (N_n, R_n^p) , and the predictor calculation result at the concerned step, (N_{n+1}^p, R_{n+1}^c) . The same simple problem is solved also by the conventional PC method, and $\hat{N}_{n+1}^p$ and $\hat{N}_{n+1}^c$ are obtained. Finally, the proper weight ω is obtained from

$$\hat{N}_{n+1} = \exp \left((1 - \omega) \ln \hat{N}_{n+1}^p + \omega \ln \hat{N}_{n+1}^c \right), \quad (5)$$

117 and ω is explicitly represented as

$$118 \quad \omega = \frac{\ln \hat{N}_{n+1} - \ln \hat{N}_{n+1}^p}{\ln \hat{N}_{n+1}^c - \ln \hat{N}_{n+1}^p}. \quad (6)$$

119 As mentioned in the introduction, the results of the predictor calculations N_{n+1}^p should include errors
 120 since the constant reaction rates are assumed when solving the Bateman equation, and thus the correspond-
 121 ing reaction rates calculated from N_{n+1}^p , R_{n+1}^c , should include errors. Since the pair (N_{n+1}^p, R_{n+1}^c) is used
 122 to determine the quadratic function represented in Eq. (4), this quadratic function should have the errors,
 123 and this finally causes the error on N_{n+1} . In the QD method, the post-correction is made on N_{n+1}^p , and
 124 it can successfully reduce this error. In the AOWPC method, corrections are adopted not to N_{n+1}^p but to
 125 R_{n+1}^c . There should exist “true” reaction rate corresponding to N_{n+1}^p . Using the result in the last burnup
 126 step calculation, the difference of R_n^c from the true value (the error of R_n^c) is quantified. To estimate the true
 127 value, the reaction rate is assumed a linear or quadratic function on the number density of the correspond-
 128 ing nuclide, and the coefficients in this function are determined from (N_n, R_n^p) , (N_{n-1}, R_{n-1}^p) , and $(N_{n-2},$
 129 $R_{n-2}^p)$ if exists. Unlike R^c , these reaction rates R^p are expected accurate. The concept of the correction to
 130 R^c is briefly presented in **Fig. 2**.

131 In burnup calculations with the constant power condition, one burnup step is further divided into sub-
 132 steps, and the neutron flux is normalized at each sub-step. Therefore, it is convenient to correct the one-group
 133 cross sections rather than the microscopic reaction rates. The AOWPC method adopts the correction factors
 134 for the one-group cross section σ : the absolute difference of σ_n^c from the true value based on the linear or
 135 quadratic function at the last burnup step. The correction on the microscopic reaction rate is made as

$$136 \quad R_{mod,n+1}^c = R_{n+1}^c - \Delta\sigma_n^c \cdot \phi \cdot \frac{\Delta B_n}{\Delta B_{n-1}}, \quad (7)$$

137 where $\Delta\sigma_n^c$ is the correction factor, ϕ is the total neutron flux at the concerned sub-step, and ΔB_n is the
 138 burnup size from the step n to $n+1$. This corrected $R_{mod,n+1}^c$ is used to define the quadratic function shown
 139 as Eq. (4). Note that the above procedure using the optimum weight is adopted only to Gd-155 and -157,
 140 and the conventional PC method with the equal weight is adopted to other nuclides.

141 2.2. Corrections to reduce errors caused by low-order model

142 In the present work, we assume that the common set of the burnup regions is used in both FOM and
 143 LOM, and there is a unique burnup region in the LOM calculation which corresponds to that in the FOM
 144 calculation. This means that we do not intend to use the fraction of the entire system of FOM as LOM.

145 The results obtained with LOM should include errors and are different from the results with FOM.
 146 These errors are expected considerable when the degree of the model simplification in LOM is large. If
 147 one wants to correct the LOM results to make them close to the FOM results, the preservation of the
 148 reaction rate between LOM and FOM would be attempted. While there are several methods to attain this

purpose, the superhomogenization (SPH) method(Kavenoky, 1980), which has originally been proposed to reduce the errors induced by spatial homogenization of the cross sections, would be the first candidate. For example, the SPH method has successfully been adopted to correct the MOC calculation results with the coarse numerical conditions: coarse ray-tracing conditions and coarse energy groups(Giho, 2014). In the present work, we tested the SPH method for the correction, and, however, it was found difficult to obtain the converged SPH factors due to the existences of the strong neutron absorbers in the concerned problems. Thus, the following simple method which corrects the one-group cross sections and the total neutron flux of each burnup region has been adopted. As described later, this simple method works satisfactorily.

In the predictor calculation at the step n , the one-group cross sections and the total neutron flux in each burnup region are calculated with FOM and LOM. Those obtained with FOM are denoted to as σ_n^p and ϕ_n^p , and those with LOM are as $\tilde{\sigma}_n^p$ and $\tilde{\phi}_n^p$. The correction factors to reduce the errors caused by LOM are defined as $f_{\sigma,n} = \sigma_n^p / \tilde{\sigma}_n^p$ and $f_{\phi,n} = \phi_n^p / \tilde{\phi}_n^p$. In the corrector calculation with LOM at this step, the one-group cross sections and the total neutron flux at $n+1$, $\tilde{\sigma}_{n+1}^c$ and $\tilde{\phi}_{n+1}^c$, are calculated. In the proposed method, these are corrected using $f_{\sigma,n}$ and $f_{\phi,n}$, and the microscopic reaction rates used in the corrector step are obtained as

$$R_{n+1}^c = (f_{\sigma,n} \tilde{\sigma}_{n+1}^c) \cdot (f_{\phi,n} \tilde{\phi}_{n+1}^c). \quad (8)$$

The above correction method assumes that the errors caused by LOM in the one-group cross sections and the total neutron flux are unchanged throughout a burnup step. It should be noted that these corrections should be made on the one-group cross sections not only of Gd-155 and -157 but also of the other nuclides.

The calculation algorithm of the proposed method combined with the AOWPC method is summarized as follows:

1. In the predictor calculation of the burnup step n , σ_n^p and ϕ_n^p are obtained through the neutron transport calculation with FOM, and the number density N_{n+1}^p is calculated using $R_n^p = \sigma_n^p \phi_n^p$.
2. The neutron transport calculation at the predictor step is also performed with LOM, and $\tilde{\sigma}_n^p$ and $\tilde{\phi}_n^p$ are calculated. Using them, the correction factors for the one-group cross sections and the total neutron flux, $f_{\sigma,n}$ and $f_{\phi,n}$, are obtained.
3. The neutron transport equation defined from N_{n+1}^p is solved with LOM, and $\tilde{\sigma}_{n+1}^c$ and $\tilde{\phi}_{n+1}^c$ are obtained. Then, the corrected microscopic reaction rates R_{n+1}^c are calculated with Eq. (8).
4. Using the pairs of (N_n, R_n^p) and (N_{n+1}^p, R_{n+1}^c) , the AOWPC method is adopted and the final estimation of the number densities of the next burnup step N_{n+1} is obtained.

The above procedure is briefly presented in **Fig. 3**.

3. Low-order model in the present work

The present work focuses on the burnup calculations of lattice physics problems with deterministic methods, and the neutron transport equation is solved by MOC with a fine-group energy discretization such as the XMAS 172-group structure(Sartori, 1990). Relative to FOM with the fine ray-tracing condition with fine-group treatment, the present work uses the model with the coarse ray-tracing condition with coarse-group treatment as LOM. The same spatial mesh discretization scheme, 72 flat-flux regions per one fuel pin-cell consisting of a normal fuel rod, is adopted to FOM and LOM.

3.1. Ray-tracing condition

In the ray-tracing of the MOC calculation, it is necessary to set the number of azimuthal angle divisions M (per 2π) and standard tracing width Δl . The total number of rays (or trajectories), on which the computation time significantly depends, is determined from these setting. The “standard” in the standard tracing width means that the tracing width cannot rigorously be set to the specified value when the cyclic trajectory scheme is adopted(Sanchez, 2002). The number of trajectories can be reduced by decreasing M and/or increasing Δl . There is a trade-off between the number of trajectories and calculation accuracy, and careful parameter setting is required for LOM.

3.2. Energy group collapsing for coarse-group condition

In the present LOM, the coarse-group cross sections are used. These are obtained through energy group collapsing of the fine-group cross sections using the neutron flux as a weight. The LOM calculations are carried out at both the predictor and corrector steps. At the predictor step, the energy group collapsing from the fine-group cross section can be done using the fine-group neutron flux obtained in the predictor calculations with FOM. On the other hand, at the corrector step, no neutron transport calculations with the fine-group cross section are performed. Thus, in the present work, fine-group neutron flux calculated at the predictor step is also used in the collapsing at the corrector step. This can be an error source in the proposed method. In the present work, the fine-group cross sections at the corrector step are calculated with the number densities at the corrector step; the resonance self-shielding calculations are carried out twice per one burnup step as well as the conventional PC method.

4. Numerical methods and problem specification

4.1. Brief description of numerical methods of CBZ

All calculations in the present work were performed with the MulticellBurner module(Chiba, 2023) of CBZ, a deterministic reactor physics code system under development at Hokkaido University. The 172-group library with the XMAS structure based on JENDL-4.0(Shibata, 2011) were used, and the 172-group effective

cross sections were calculated based on the advanced Bondarenko model(Chiba, 2016). Lattice effects were taken into account by the Dancoff factor method. In FOM, the 172-group neutron transport equation was solved with MOC, and the condition of the ray-tracing was set as $M=64$ and $\Delta l=0.02$ cm. The two-point Tabuchi-Yamamoto optimum quadrature set(Yamamoto, 2007) was used for polar angle treatment. Anisotropy of scattering was taken into account by the P0 transport approximation. A simplified burnup chain consisting of 138 fission products(Chiba, 2015) was used and the Bateman equation was solved by the matrix exponential method. The matrix exponential was calculated numerically by the minimax polynomial approximation method(Kawamoto, 2015; Chiba, 2019). The Gd-bearing fuel rod was divided into eight ring-type burnup regions of equal volume, and each of the normal fuel rods was treated as a single burnup region. No spatial dependence of multi-group cross sections inside fuel pellets was considered. The first and second burnup step sizes were set 0.1 and 0.4 GWD/t, and the size of the following burnup steps were set 2.0 GWD/t. The reference solutions were obtained with the AOWPC method with the burnup step size of 0.1 GWD/t.

4.2. Problem specification

4.2.1. 3×3 multicell

Nine cases of the 3×3 multicell are prepared. The center rod is a Gd-bearing fuel rod and the others are the normal UO_2 fuel rods as shown in **Fig. 4**. The compositions of these fuel rods are dependent on the cases as shown in **Table 1**. Values of the line power of the cases 8 and 9 are different from those in the other cases. The reference k_∞ with the fuel burnup is shown in **Fig. 5**.

4.2.2. PWR fuel assemblies

Four PWR fuel assemblies are concerned. The first two are taken from the VERA benchmark problem (2O and 2P)(Kim, 2015) and the other two are taken from the previous work(Sasuga, 2021). The fuel specifications of these PWR assembly problems are shown in **Table 2** and **Fig. 6**.

4.2.3. BWR fuel assemblies

As the BWR fuel assembly problem, the OECD/NEA burnup credit benchmark phase III-C(NEA, 2015) is used. Since the void fraction varies along the vertical direction in BWRs, calculations were performed for three different void fractions (0, 40, and 70%). Geometrical specification of the BWR assembly problem is shown in **Fig. 7**.

5. Numerical results

5.1. Impact of low-order model condition on accuracy

In this subsection, the impact of the LOM condition on the accuracy is quantified using the case 1 of the 3×3 multicell problem. We examine the computational accuracy with the reproduction error of k_∞

obtained by the proposed method. As the initial setting of LOM, the ray-tracing conditions were $M=8$ and $\Delta l=0.1$ cm, and the CASMO 9-group structure was used.

In order to quantify the effect of the correction to the one-group quantities in the proposed method, the errors in k_∞ with and without the correction are shown in **Figure 8**. If the errors caused by the LOM adoption are negligible, the curves of “w LOM” coincide with that of “FOM”. It is interesting to point out that the correction to the one-group quantities shows rather small impact on the accuracy improvement by 25 GWD/t, and after 25 GWD/t the correction begins to work. The reason of this unexpected small error by 25 GWD/t is due to the correction to R^c in the AOWPC method represented in Eq. (7), which is a different correction from that for the one-group quantities newly proposed in the present work. Since the uncorrected R^c should include the error due to the LOM adoption in addition to the error inherent to the PC method, Eq. (7) in the AOWPC method also includes the correction to the error by the LOM adoption. In other words, the errors brought by LOM is corrected by the inherent procedure in the AOWPC method, and thus the correction to the one-group quantities in the proposed method has small impact on the results by 25 GWD/t. To confirm this, the reproduction error of k_∞ with and without the AOWPC-inherent correction to R^c is shown in **Figure 9**. Note that the corrections to the one-group quantities for the LOM adoption are not considered. If the correction to R^c is not considered, the proposed method using LOM gives worse results than that with the R^c correction. The above result, however, does not mean that the correction to the one-group quantities is unnecessary. As shown in Fig. 8, significant overestimation in k_∞ is observed after the Gd burnout when this correction is not adopted. This is because the correction to R^c in the AOWPC method is adopted only to Gd-155 and -157, and thus errors due to the LOM adoption in microscopic reaction rates of the other nuclides including important actinoids should still remain.

Even if the corrections to the one-group quantities in the proposed method and the correction to R^c in AOWPC are considered, there is a non-negligible error of over 100 pcm in the results with LOM. This suggests that the present LOM condition, $M=8$, $\Delta l=0.1$ cm, and the CASMO 9-group structure as the coarse group, is too coarse. In order to quantify sensitivities of these setting to the results, additional calculations changing each of M and Δl were carried out, and the results are shown in **Figures 10 and 11**. These suggest that the initial setting of $M=8$ and $\Delta l=0.1$ cm is coarse, and it is better to use a finer setting of $M=16$ and $\Delta l=0.05$ cm. This new setting for M and Δl is adopted in the following. This, however, does not contribute to the accuracy improvement, and the coarse-group structure was addressed next. Through numerical surveys on the coarse-group structure, we reached the conclusion that a new 20-group structure shown in **Table 3** is effective. This 20-group structure is characterized by the fact that the group structure in the thermal neutron region is almost kept while the other energy regions are grouped together. This seems reasonable since neutron capture reactions of Gd isotopes are dominant in the thermal region. In order to demonstrate the effectiveness of this 20-group structure, the errors in k_∞ are shown in **Figure 12** with the results obtained by the CASMO 9- and 25-group structures as the coarse-group structure. Even though the

number of energy groups is smaller than that in the CASMO 25-group structure, results with high accuracy, which are almost equivalent to those with FOM, are obtained when the new 20-group structure is employed.

5.2. Comprehensive performance test

The proposed method with the coarse calculation condition, $M=16$, $\Delta l=0.05$ cm, and the 20-group structure for the coarse-group, has been tested against the nine cases of the 3×3 multicell problem, four PWR assembly problems, and the BWR assembly problem with three different void fractions. Reproduction errors of k_∞ are concerned, and the results with and without the proposed method are compared. **Figure 13** shows the results of the 3×3 multicell problems. As shown in Figure (a), the AOWPC method predicts k_∞ within 150 pcm errors in all the cases. The results with the proposed method (Figure (b)) show quite similar trend to those with AOWPC, and the good agreement to the references within 150 pcm difference is observed also. The maximum difference to the AOWPC results only with FOM is 20 pcm. **Figure 14** shows the results of the PWR and BWR assembly problems. Although slight accuracy degradation of about 20 pcm is observed in some problems, the reproduction errors of k_∞ of the proposed method are less than 150 pcm for all these assembly problems except PWR-2 (VERA-2P). In PWR-2, the error of the AOWPC method is over 200 pcm. In the previous work(Sasuga, 2021), the maximum error of the AOWPC method in this PWR assembly problem was reported 150 pcm. This difference is due to the burnup step division around the initial burnup; finer burnup steps were adopted in the previous work. Compared with the other PWR assembly problems, the Gd content of PWR-2 is small and the number of Gd-bearing rods is large. The former causes the rapid Gd burnout and the latter enlarges the impact of the time discretization on k_∞ . This is the reason why the reproduction errors are relatively large in PWR-2 compared with the other problems. It should be noted that the smaller burnup step size of 1.5 GWD/t gives much better results in PWR-2 as shown in **Figure 15**; the reproduction error was reduced to less than 60 pcm. The computation time with FOM and that with the proposed method with the recommended LOM condition are summarized in **Table 4**. The computation time values reported in this table were obtained on a PC featuring AMD Ryzen 9 5950X 3.4 GHz processor. In all the problems, the reduction of 35-40% in the computation time is attained.

6. Conclusion

Special attentions should be paid on the time discretization in nuclear fuel burnup calculations for systems including gadolinia due to the rapid change of the reaction rates with time. To tackle with this issue, several efficient methods based on the PC method, such as the PPC, QD, and AOWPC methods, have been proposed and successfully been adopted to many computer codes. There, however, are still requirements of the further reduction of the computation time for the burnup calculations coupled with the

Monte Carlo method or the three-dimensional deterministic transport methods. In the PC-based method, at least two neutron transport calculations are required. In the present work, we have used the low-order model whose computation time is shorter than that of the full-order model for the corrector calculations in order to reduce the computation time of the corrector calculation. To mitigate the error caused by the low-order model adoption, we have proposed to do the calculation with the same low-order model and to quantify the error at the predictor calculation step. The correction factors obtained from this quantified error are adopted to the results with low-order model calculation at the corrector step to mitigate the error. If the computation time of the low-order model is negligible compared with that of the full-order model, the computation time is expected to be reduced to around half.

In the present work, this proposed method has been combined with the AOWPC method, and has been tested for the lattice physics problems including the 3×3 multicell problems and the PWR and BWR assembly problems. The full-order model is the deterministic method based on MOC with the 172-group cross sections, and the low-order model is also the deterministic method based on MOC with the coarse ray-tracing condition with fewer-group cross sections. We have also proposed the coarse calculation condition which restricts the increase of the errors due to the model simplification. It has been demonstrated that the proposed method gives the results whose accuracy is almost equivalent with that of the original model; the differences are less than 20 pcm. Computation time has been reduced to 60-65% for all the concerned problems.

The proposed method can be adopted to arbitrary combinations: the Monte Carlo method as the full-order model and the deterministic method as the low-order model, for example. If the computation time of the low-order model, whose accuracy degradation is acceptable, is much shorter than that of the full-order model, the computation time can be reduced to around half by using the proposed method.

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Appendix

The favorable coarse-group structure for the SHEM 361-group structure(Hebert, 2008) was also investigated, and the 21-group structure shown in **Table 5** is recommended.

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Table 1: 3×3 multicell problem specification

Case	Line power [W/cm]	U-235 enrichment [wt%]		Gd content [wt%]
		UO ₂ rod	Gd-bearing rod	
1	179.0	4.8	3.2	10
2	179.0	4.8	3.2	8
3	179.0	4.8	3.2	6
4	179.0	4.8	3.2	4
5	179.0	4.8	3.2	2
6	179.0	4.1	2.6	10
7	179.0	3.4	2.0	10
8	268.5	4.8	3.2	10
9	89.5	4.8	3.2	10

Table 2: PWR fuel assemblies specification

ID	Gd content [wt%]	Number of Gd rods	U-235 enrichment [wt%]	
			UO ₂ rod	Gd-bearing rod
PWR-1 (VERA-2O)	5.0	12	3.1	1.8
PWR-2 (VERA-2P)	5.0	24	3.1	1.8
PWR-3	9.6	12	4.1	2.6
PWR-4	10.0	24	4.8	3.2

Table 3: 20-group structure as the coarse condition with the XMAS 172-group library

Group	Upper energy [eV]
1	1.9640×10^7
2	1.1500×10^0
3	1.0970×10^0
4	9.9600×10^{-1}
5	9.7200×10^{-1}
6	3.9100×10^{-1}
7	3.5000×10^{-1}
8	2.4800×10^{-1}
9	2.2000×10^{-1}
10	1.8900×10^{-1}
11	1.6000×10^{-1}
12	1.3400×10^{-1}
13	1.1500×10^{-1}
14	1.0000×10^{-1}
15	9.5000×10^{-2}
16	8.0000×10^{-2}
17	6.7000×10^{-2}
18	5.8000×10^{-2}
19	5.0000×10^{-2}
20	3.5000×10^{-2}
	1.0000×10^{-5}

Table 4: Computational time with FOM and LOM

Problem	Computation time (Min.)	
	FOM	LOM (Ratio to FOM)
PWR-1 (VERA-2O)	259	166 (0.64)
PWR-2 (VERA-2P)	267	174 (0.65)
PWR-3	323	206 (0.64)
PWR-4	256	167 (0.65)
BWR (0% void)	189	121 (0.64)
BWR (40% void)	158	95 (0.60)
BWR (70% void)	142	86 (0.61)

Table 5: 21-group structure based on the SHER 361-group structure

Group	Upper energy [eV]
1	1.96403×10^7
2	1.11605×10^0
3	1.07799×10^0
4	9.96500×10^{-1}
5	9.63960×10^{-1}
6	3.90001×10^{-1}
7	3.52993×10^{-1}
8	2.54997×10^{-1}
9	2.31192×10^{-1}
10	2.09610×10^{-1}
11	1.90005×10^{-1}
12	1.61895×10^{-1}
13	1.37999×10^{-1}
14	1.19995×10^{-1}
15	1.04298×10^{-1}
16	8.97968×10^{-2}
17	7.64969×10^{-2}
18	6.51994×10^{-2}
19	5.54981×10^{-2}
20	4.73019×10^{-2}
21	3.43998×10^{-2}
	1.10003×10^{-4}

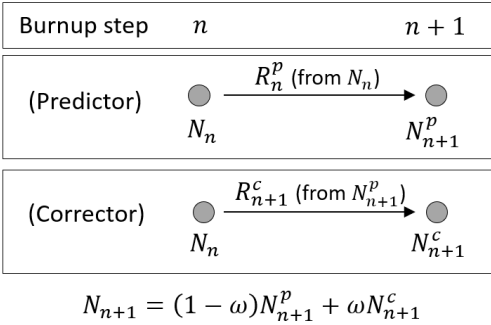


Figure 1: Brief descrption of the weighted predictor-corrector method

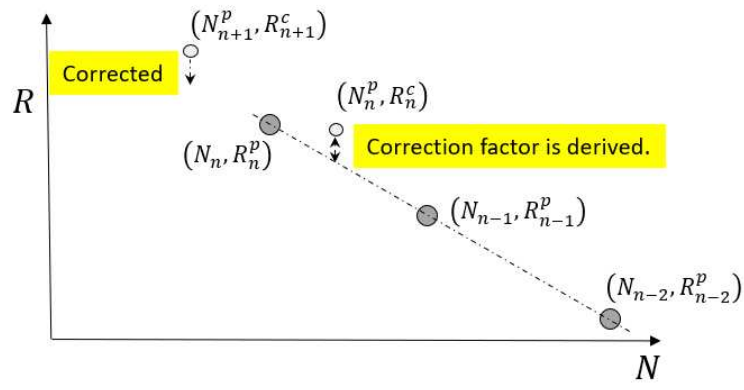


Figure 2: Correction scheme for R^c in the advanced optimally-weighted predictor-corrector method

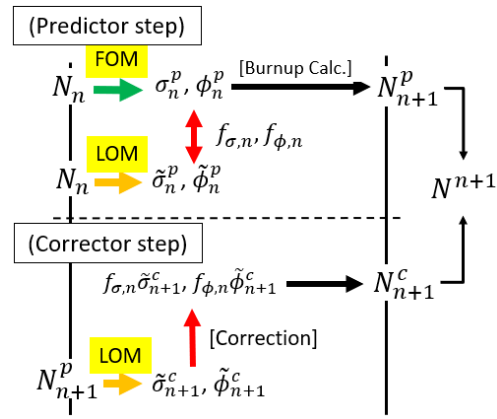


Figure 3: Proposed burnup calculation scheme using FOM and LOM

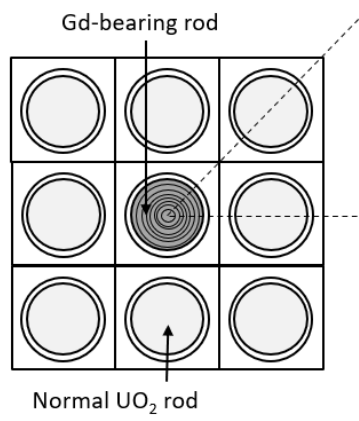


Figure 4: Geometrical specification of 3×3 multicell problems

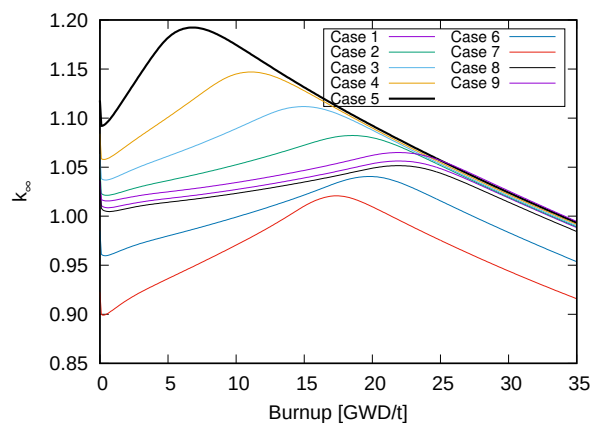


Figure 5: k_{∞} with fuel burnup of the 3×3 multicell problem

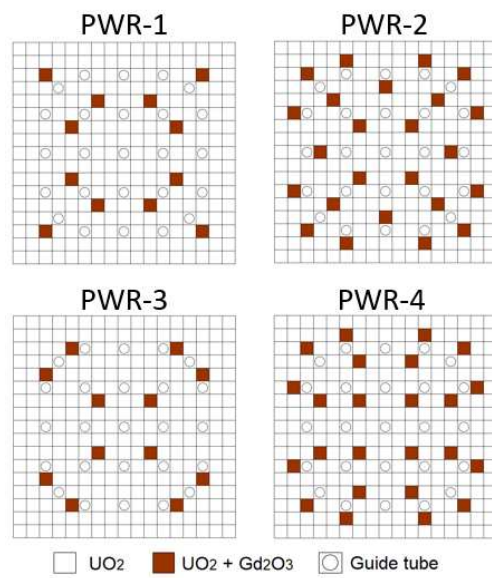


Figure 6: Geometrical specification of the PWR assembly problems

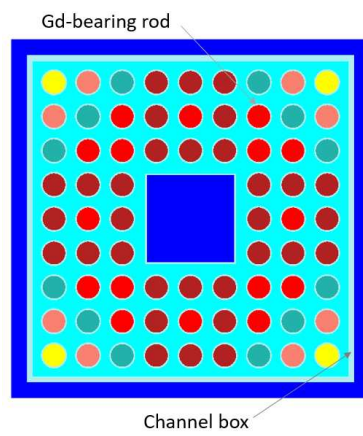


Figure 7: Geometrical specification of the BWR assembly problem

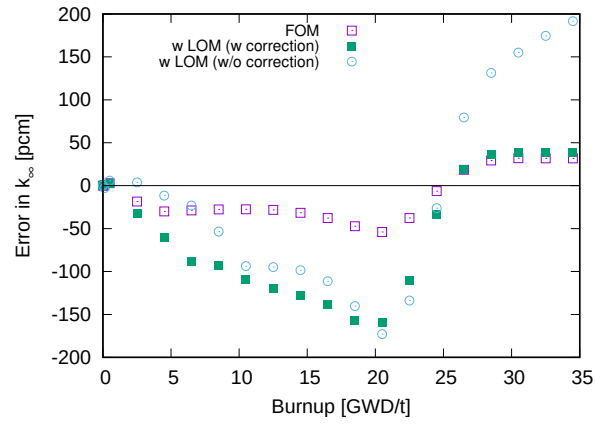


Figure 8: Errors in k_∞ in the case 1 of the 3×3 multicell problem with the correction to R^c

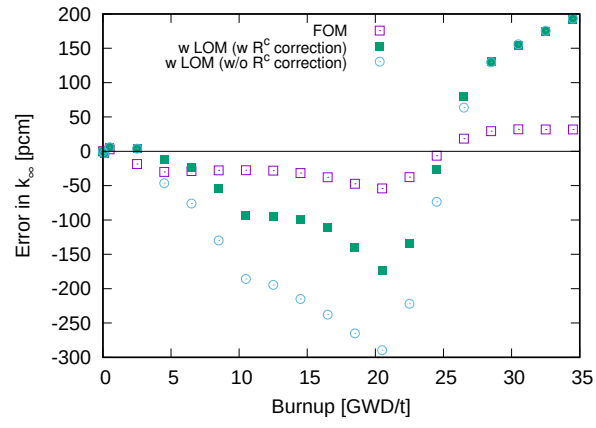


Figure 9: Errors in k_{∞} in the case 1 of the 3×3 multicell problem without the correction to the one-group quantities

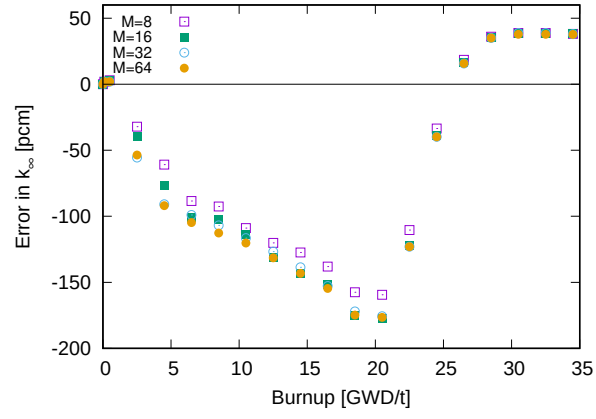


Figure 10: Errors in k_∞ in the case 1 of the 3×3 multicell problem with different values of M and $\Delta t=0.1$

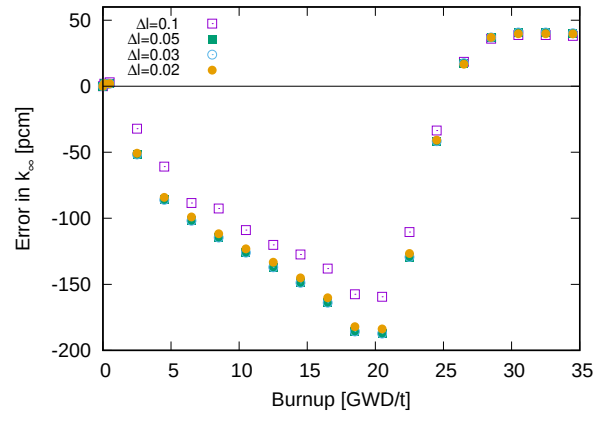


Figure 11: Errors in k_∞ in the case 1 of the 3×3 multicell problem with different values of Δl and $M=8$

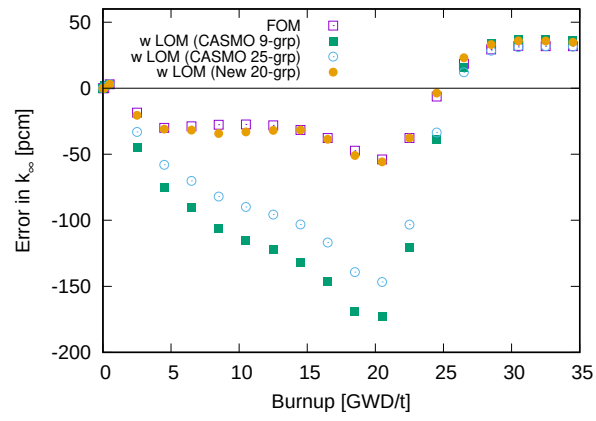


Figure 12: Errors in k_{∞} in the case 1 of the 3×3 multicell problem with several different coarse-group structures

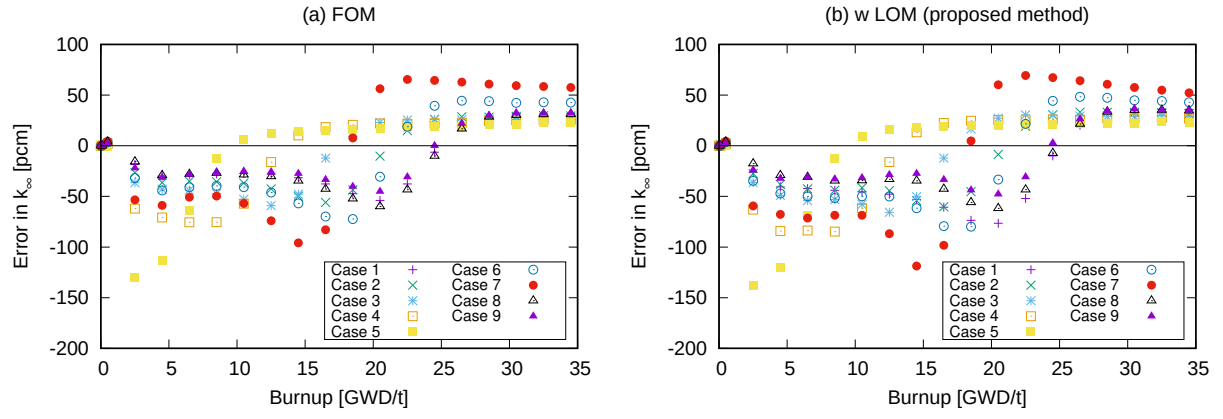


Figure 13: Reproduction errors in k_{∞} of the 3x3 multicell problem

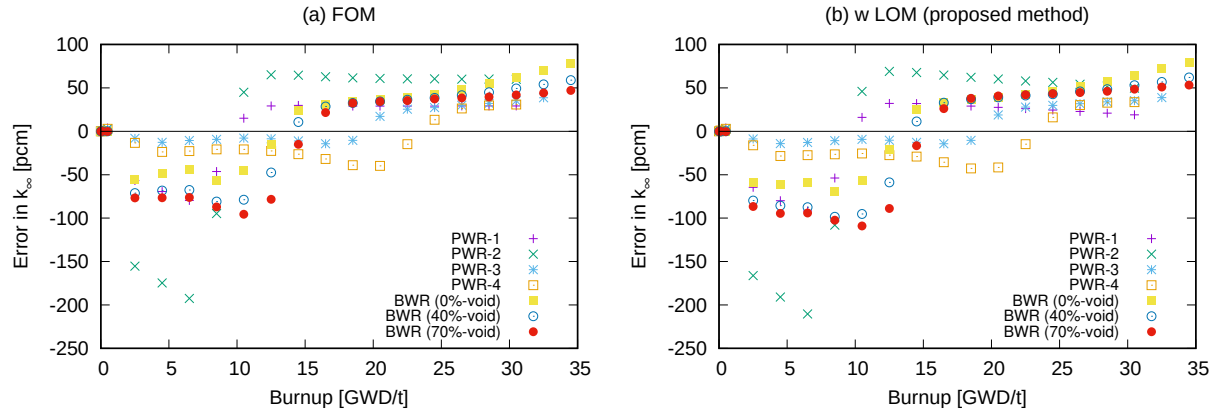


Figure 14: Reproduction errors in k_{∞} of the PWR and BWR assembly problems

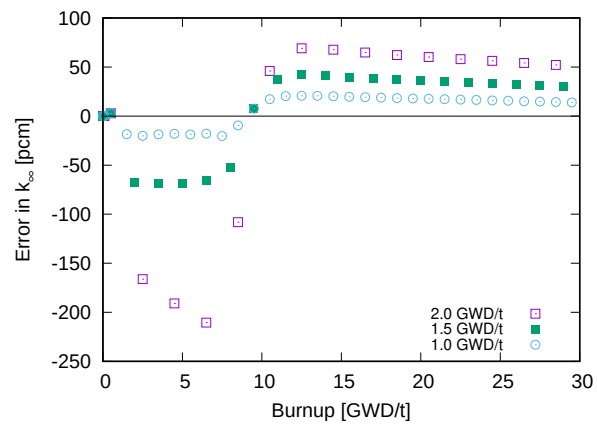


Figure 15: Reproduction errors in k_{∞} of the PWR-2 problem with different burnup step size

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