Implementation of Quadratic-Order Predictor-Corrector Method in KARMA

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1. Introduction

KEPCO Nuclear Fuel Company (KNF) has developed the KARMA/ASTRA code system for commercial core design [1]. KARMA (Kernel Analyzer by Ray-tracing Method for Fuel Assembly) is a lattice code based on the method of characteristics. It employs the subgroup method to account for self-shielding effects and applies the B_1 method to determine the criticality spectrum [2]. ASTRA (Advanced Static and Transient Reactor Analyzer) is a multigroup nodal code designed to analyze steady-state characteristics and transient core behavior based on multigroup diffusion theory.

KARMA conducts transport calculation and generates homogenized few-group cross sections for fuel assemblies. KARMA uses a predictor-corrector method, which iteratively performs prediction and correction steps to track the time evolution of the depletion system. In the current implementation of KARMA, the depletion matrix is assumed to remain constant within each burnup time step. To accurately capture the time-dependent behavior of the burnup system affected by gadolinium depletion, this approach employs short burnup steps of 0.5 MWd/kgU or less during the gadolinium depletion period. However, in reactors using enriched gadolinium, such as innovative Small Modular Reactor (i-SMR), the gadolinium depletion phase lasts longer, requiring more computational steps.

In this study, we introduce high-order predictor-corrector methods that effectively account for the time-varying behavior of the burnup system. By employing these methods, we aim to enhance the efficiency of burnup calculations in KARMA, particularly for i-SMR utilizing enriched gadolinium.

2. Predictor-Corrector Methods for Burnup Calculation

2.1 Bateman equation

The time-dependent change in nuclide densities can be described by the Bateman equation in Eq. (1) which considers neutron-induced reactions and radioactive decay.

$$\frac{dn_i(t)}{dt} = \left(\sum_{j=1}^{N} \langle \gamma_{j\to i}(E)\sigma_j(E,t)\phi(E,t)\rangle + \lambda_{j\to i}\right) n_j(t) - \left(\langle \sigma_i(E,t)\phi(E,t)\rangle + \sum_{j\neq i}^{N} \lambda_{i\to j}\right) n_i(t), \quad i = 1,2,\dots,N \tag{1}$$

where $n_i(t)$ is nuclide number density of i-th nuclide at time t, $\sigma_i(E,t)$ is transmutation cross section for i-th nuclide at energy E and time t, $\phi(E,t)$ is neutron flux at energy E and time t, and $\gamma_{j\to i}(E)$ is fraction of transmutation reactions in j-th nuclide that produce i-th nuclide.

The depletion system described by Eq. (1) can be expressed in a matrix form, as shown in Eq. (2). Here, the depletion matrix **A** is influenced by the decay constants of nuclides and neutron flux. As indicated in Eq. (2) the depletion matrix **A** varies over time.

$$\frac{dn(t)}{dt} = \mathbf{A}(n,t)n(t), \qquad n(0) = n_0 \tag{2}$$

If the depletion matrix **A** is a time-independent constant matrix, the solution to Eq. (2) can be expressed using the matrix exponential as follows:

$$n(t) = \exp(t\mathbf{A})\, n_0 \tag{3}$$

2.2 Predictor-Corrector Methods

The Predictor-Corrector method is widely used to obtain numerical solutions for time-dependent systems. Currently, the KARMA code uses the Heun method, which is defined by Eq. (4). In the Heun method, it is assumed that the depletion matrix remains constant throughout the depletion interval.

$$\begin{aligned} n_{k+1}^{(p)} &= \exp\left(h \times \mathbf{A}(n_k, t_k)\right) n_k \\ n_{k+1} &= \left(n_{k+1}^{(p)} + \exp\left(h \times \mathbf{A}\left(n_{k+1}^{(p)}, t_{k+1}\right)\right) n_k\right) / 2 \end{aligned} \tag{4}$$

where h is depletion interval, n_k is nuclide number density at the current time step, $n_{k+1}^{(p)}$ is predicted nuclide number density at the next time step, n_{k+1} is the nuclide number density at the next time step, t_k is the current time step, t_{k+1} is next time step, $\mathbf{A}(n_k, t_k)$ is depletion matrix at time t_k based on nuclide density n_k, $\mathbf{A}(n_{k+1}^{(p)}, t_{k+1})$ is deletion matrix at time t_{k+1} based on the predicted nuclide density $n_{k+1}^{(p)}$.

The higher-order predictor-corrector methods can be expressed as follows.

Prediction:

$$\frac{d\tilde{n}(t)}{dt} \approx \tilde{\mathbf{A}}_{approx}\left(t, \mathbf{A}_{ext}^{(l)}(t_{k+1}), \mathbf{A}(n_k, t_k), \dots\right) n_k$$
$$n_{k+1}^{(p)} = \tilde{n}(t_k + h_k) \quad (5)$$

Correction:

$$\frac{d\tilde{n}(t)}{dt} \approx \tilde{\mathbf{A}}_{approx}\left(t, \mathbf{A}(n_{k+1}^{(p)}, t_{k+1}), \mathbf{A}(n_k, t_k), \dots\right) n_k$$
$$n_{k+1} = \tilde{n}(t_k + h_k) \quad (6)$$

where $\tilde{\mathbf{A}}_{approx}$ represents the approximated depletion matrix, and $\mathbf{A}_{ext}^{(l)}(t_{k+1})$ denotes the depletion matrix at time t_{k+1} obtained through l th order extrapolation. Linear and quadratic approximations for the depletion matrix ($\tilde{\mathbf{A}}_{lin}$ and $\tilde{\mathbf{A}}_{quad}$) are usually considered.

- Constant Extrapolation, Constant Midpoint (CECM)

CECM is a method that, like Heun method, uses a constant depletion matrix. The key difference from Heun method is that the correction step uses the depletion matrix evaluated at the midpoint of the depletion interval, $\mathbf{A}(n_{k+1/2}^{(p)}, t_{k+1/2})$.

- Constant Extrapolation, Linear Interpolation (CELI)

CELI predicts the nuclide number density $n_{k+1}^{(p)}$ at time t_{k+1} using a constant depletion matrix and calculates $\mathbf{A}(n_{k+1}^{(p)}, t_{k+1})$. In the correction step, the depletion system is approximated using linear interpolation between the depletion matrices $\mathbf{A}(n_k, t_k)$ and $\mathbf{A}(n_{k+1}^{(p)}, t_{k+1})$.

- Linear Extrapolation, Linear Interpolation (LELI)

LELI approximates the depletion system using linear methods for both prediction and correction steps. During the prediction step, the depletion system is approximated by a linear extrapolation of the depletion matrices $\mathbf{A}(n_{k-1}, t_{k-1})$ and $\mathbf{A}(n_k, t_k)$.

- Linear Extrapolation, Quadratic Interpolation (LEQI)

LEQI [3] uses a linear approximation to the burnup system in the same way as LELI. In the correction step, the depletion system is approximated using a quadratic polynomial based on the depletion matrices at the previous time step, the current time step, and the predicted depletion matrix $\mathbf{A}(n_{k+1}^{(p)}, t_{k+1})$.

- Quadratic Extrapolation, Quadratic Interpolation (QEQI)

QEQI [4] is a method that approximates the depletion system using a quadratic polynomial approximation in both the prediction and correction steps. In the prediction step, quadratic extrapolation is used to approximate the depletion matrix and compute $n_{k+1}^{(p)}$. In the correction step, quadratic interpolation is performed in the same way as in LEQI.

2.3 Magnus Integrator

Solution of the time-dependent depletion matrix can be obtained by performing the sub-steps in Eq. (7). The depletion interval is subdivided so that the depletion matrix is treated as constant within each subinterval. Since a system with constant matrices can be numerically solved using the matrix exponential, the solution for the time-dependent depletion matrix can be obtained by successively computing the matrix exponentials for each subinterval, as shown in the equation below.

$$\mathbf{A}_s = \int_{t_k + \frac{s-1}{m}h}^{t_k + \frac{s}{m}h} \mathbf{A}(s)ds \ ,$$
$$n(t_k + h) = \exp(\mathbf{A}_m)\exp(\mathbf{A}_{m-1}) \dots \exp(\mathbf{A}_1)\, n(t_k) \quad (7)$$

However, solving the system using Eq. (7) requires multiple matrix exponential computations, which leads to high computational costs. To improve efficiency, KARMA applies the Magnus integrator. As shown in Eq. (8), the solution can be obtained using the Magnus integrator $\exp(\mathbf{\Omega}(t))$. In the case of linear and quadratic matrices, the Magnus integrator can be derived analytically. We used the Magnus integrator as derived by Josey, C [5, 6].

$$\frac{dn(t)}{dt} = \mathbf{A}(t)n(t), n(0) = n_0 \ ,$$
$$n(t) = \exp\left(\mathbf{\Omega}(t)\right) n_0 \quad (8)$$

The LELI method, a linearly approximated depletion system, can be calculated using the Magnus integrator as follows

Prediction:

$$n_{k+1}^{(p)} = \exp\left(\mathbf{\Omega}\left(t, \mathbf{A}(n_k, t_k), \mathbf{A}_{ext}^{(1)}(t_{k+1})\right)\right) n_k \quad (9)$$

Correction:

$$n_{k+1} = \exp\left(\mathbf{\Omega}\left(t, \mathbf{A}(n_k, t_k), \mathbf{A}^{(p)}(n_{k+1}^{(p)}, t_{k+1})\right)\right) n_k \quad (10)$$

where $\mathbf{A}_{ext}^{(1)}(t_{k+1})$ is the linearly extrapolated burnup matrix, and the Magnus integrator for a linear system is given by

$$\exp\left(\mathbf{\Omega}(t, \mathbf{A}_0, \mathbf{A}_1)\right) =$$
$$\exp\left(\frac{h_k}{12}\mathbf{A}_0 + \frac{5h_k}{12}\mathbf{A}_1\right)\exp\left(\frac{5h_k}{12}\mathbf{A}_0 + \frac{h_k}{12}\mathbf{A}_1\right) \quad (11)$$

The QEQI method, a quadratically approximated depletion system, can be calculated as follows

Prediction:

$$n_{k+1}^{(p)} = \exp\left(\mathbf{\Omega}\left(t, \mathbf{A}(n_{k-1}, t_{k-1}), \mathbf{A}(n_k, t_k), \mathbf{A}_{ext}^{(2)}(t_{k+1})\right)\right) n_k \quad (12)$$

Correction:

$$n_{k+1} = \exp\left(\mathbf{\Omega}\left(t, \mathbf{A}(n_{k-1}, t_{k-1}), \mathbf{A}(n_k, t_k), \mathbf{A}^{(p)}(n_{k+1}^{(p)}, t_{k+1})\right)\right) n_k \quad (13)$$

where $\mathbf{A}_{ext}^{(2)}(t_{k+1})$ is the quadratically extrapolated burnup matrix, and the Magnus integrator for a quadratic system is given by

$$\exp\left(\mathbf{\Omega}(t, \mathbf{A}_{-1}, \mathbf{A}_0, \mathbf{A}_1)\right) = \quad (14)$$

$$\exp\left(-\frac{h_k^3}{12h_{k-1}(h_{k-1}+h_k)}\mathbf{A}_{-1} + \frac{(h_{k-1}^2+2h_{k-1}h_k+h_k^2)h_k}{12h_{k-1}(h_{k-1}+h_k)}\mathbf{A}_0 + \frac{(5h_{k-1}^2+4h_{k-1}h_k)h_k}{12h_{k-1}(h_{k-1}+h_k)}\mathbf{A}_1\right)$$

$$\exp\left(-\frac{h_k^3}{12h_{k-1}(h_{k-1}+h_k)}\mathbf{A}_{-1} + \frac{(5h_{k-1}^2+6h_{k-1}h_k+h_k^2)h_k}{12h_{k-1}(h_{k-1}+h_k)}\mathbf{A}_0 + \frac{h_{k-1}h_k}{12h_{k-1}(h_{k-1}+h_k)}\mathbf{A}_1\right)$$

As can be seen from Eqs. (11) and (14), the Magnus integrator requires two matrix exponential operations for both linear and quadratic cases.

3. Results and Discussion

Burnup calculations were performed with various assemblies to evaluate the predictor-corrector (PC) method implemented in KARMA. The U-235 enrichment of the UO_2 fuel rods was set to 4.95 wt%, and enriched gadolinium (Gd-155 and Gd-157) was used. Gd_2O_3 was blended at enrichment levels of 8 wt% and 2 wt%. The layout of the evaluation fuel assemblies, used to evaluate the PC methods, is shown in Figure 1 and its specifications are listed in Table I. The KARMA calculations were performed using a cross section library based on ENDF/B-VI.8 with a 47-group structure. A quadrature set with three polar angles and eight azimuthal angles was used. The UO_2 fuel rods were divided into three sections, while the Gd_2O_3 rods were subdivided into seven sections to construct the cell.

The PC algorithms in the KARMA burnup module were evaluated, with a focus on how well it reproduced the results of the CECM method, which was calculated over very short intervals. The CECM reference calculation was performed with high precision, applying a burnup interval of 0.1 MWd/kgU, excluding the initial burnup period. The HEUN, CELI, LELI, LEQI, and QEQI methods were applied using relatively wider burnup intervals, and each algorithm was compared to the reference calculation. Burnup intervals of 0.5, 1.0, 1.5, and 2.0 MWd/kgU were used until the point at which Gd was depleted.

Table I. Assemblies Specification for Bunrup Calculation

Type	U_{235} enrichment	Gd enrichment	Number of Gd_2O_3 rods
A01	4.95 wt%	enriched	8 wt% Gd_2O_3 (x20) 2 wt% Gd_2O_3 (x4)
A02	4.95 wt%	enriched	8 wt% Gd_2O_3 (x28) 2 wt% Gd_2O_3 (x4)
A03	4.95 wt%	enriched	8 wt% Gd_2O_3 (x20) 2 wt% Gd_2O_3 (x8)
A04	4.95 wt%	enriched	8 wt% Gd_2O_3 (x24) 2 wt% Gd_2O_3 (x8)
A05	4.95 wt%	enriched	8 wt% Gd_2O_3 (x28) 2 wt% Gd_2O_3 (x8)
C01	4.95 wt%	nat.	8 wt% Gd_2O_3 (x20) 2 wt% Gd_2O_3 (x4)
C02	4.95 wt%	nat.	8 wt% Gd_2O_3 (x28) 2 wt% Gd_2O_3 (x4)
C03	4.95 wt%	nat.	8 wt% Gd_2O_3 (x20) 2 wt% Gd_2O_3 (x8)
C04	4.95 wt%	nat.	8 wt% Gd_2O_3 (x24) 2 wt% Gd_2O_3 (x8)
C05	4.95 wt%	nat.	8 wt% Gd_2O_3 (x28) 2 wt% Gd_2O_3 (x8)

The effective multiplication factor and peaking factor for each assembly, derived from the burnup calculations, are shown in Figure 2. The assemblies A01-05, which used enriched gadolinium, underwent gadolinium depletion by the 35 MWd/kgU point, while the assemblies C01-05, which used natural gadolinium, underwent gadolinium depletion by the 15 MWd/kgU point.

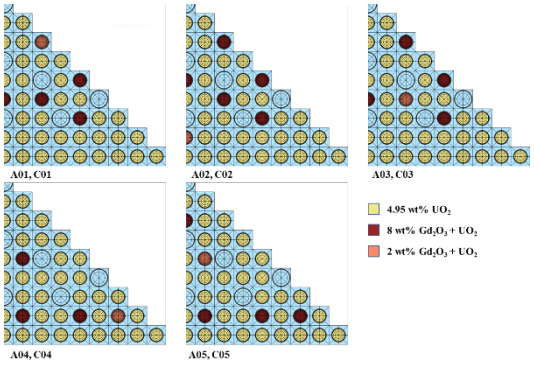

Fig. 1. Fuel Assembly Layout for KARMA Burnup Calculation

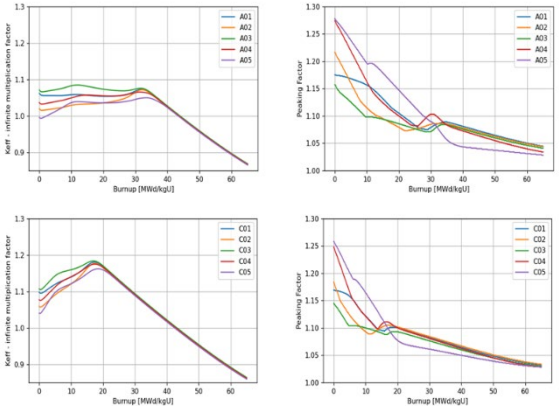

Fig. 2. k_{eff} and Peaking Factor from KARMA Burnup Calculation

Figures 3 and 4 show the k_{eff} deviation from the reference calculation for assemblies A01 and A05 for different PC algorithms. In the A01 assembly, the CECM algorithm showed a maximum k_{eff} deviation of -93 pcm with a burnup interval of 0.5 MWd/kgU, while a burnup interval of 1.0 MWd/kgU produced a deviation of -326 pcm. The CELI method showed the same trend as the CECM method in all assemblies and burnup intervals. In contrast, the LELI, LEQI, and QEQI, methods demonstrated improved accuracy compared to HEUN and CECM.

The results show that gadolinium has a significant impact on burnup calculations, a trend consistently observed in other assemblies, including A02–A04 and C01–C05. The QEQI, which approximates the burnup matrix using a quadratic polynomial, demonstrated high accuracy. For example, in the C01 assembly, when using

QEQI with a burnup interval of 1.5 MWd/kgU, the maximum deviation in criticality from the reference calculation was found to be -39 pcm.

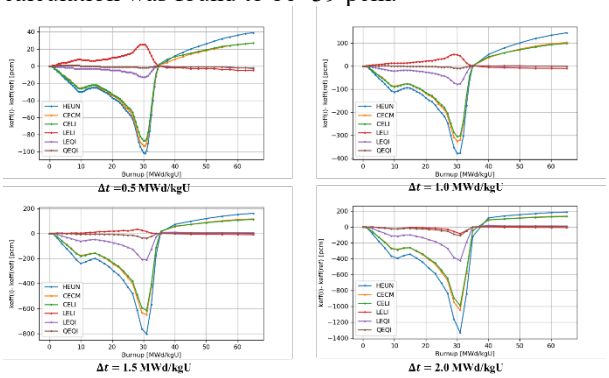

Fig. 3. The Δk_{eff} from the reference for the A01 assembly corresponding to the burnup interval

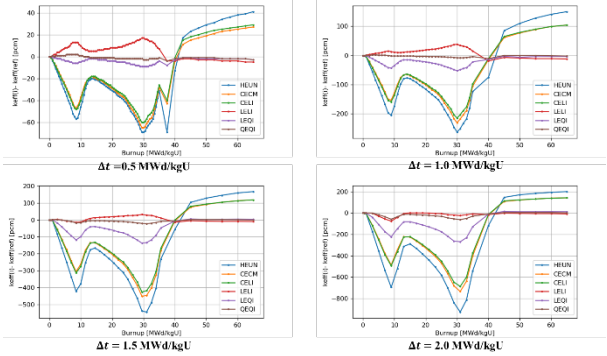

Fig. 4. The Δk_{eff} from the reference for the A05 assembly corresponding to the burnup interval

The maximum criticality deviation (Δk_{eff}) between the PC methods and the reference calculation for different fuel assemblies is presented in Table II. The QEQI, which approximates the burnup matrix quadratically, exhibited the highest accuracy among all the methods. The LEQI method demonstrated computational accuracy similar to that of QEQI at a time interval of 0.5 MWd/kgU. However, its error increased with larger time intervals. Unlike the other algorithms, LELI showed a positive deviation and remained relatively insensitive to the time interval.

Table II. Maximum Δk_{eff} of the Assemblies for Each the Predictor-corrector Method

Assembly	Burnup Interval [MWd/kgU]	HEUN [pcm]	CECM [pcm]	CELI [pcm]	LELI [pcm]	LEQI [pcm]	QEQI [pcm]
A01	0.5	-102	-93	-87	25	-13	-2
	1.0	-379	-326	-306	50	-79	-10
	1.5	-803	-650	-615	34	-212	-38
A02	0.5	-116	-107	-100	28	-15	-2
	1.0	-436	-375	-352	56	-91	-12
	1.5	-897	-732	-687	37	-242	-43
A03	0.5	-82	-76	-71	21	-11	2
	1.0	-311	-268	-251	42	-64	-8
	1.5	-646	-522	-493	28	-170	-30
A04	0.5	-78	-73	-68	19	-10	-2
	1.0	-293	-252	-237	39	-58	-8
	1.5	-619	-510	-484	25	-162	-25
A05	0.5	-69	-65	-60	17	-9	-3
	1.0	-263	-231	-215	38	-52	-8
	1.5	-545	-452	-426	32	-138	-23
C01	0.5	-123	-106	-104	32	-13	3
	1.0	-463	-638	-363	48	-97	-3
	1.5	-928	-706	-696	-21	-254	-39
C02	0.5	-141	-121	-119	37	-15	4
	1.0	-531	-420	-416	55	-107	-3
	1.5	-1047	-822	-809	-25	-296	-44
C03	0.5	-100	-86	-85	26	-10	3
	1.0	-375	-299	-295	40	-75	2
	1.5	-755	-575	-568	-23	-205	-31
C04	0.5	-102	-87	-86	26	-10	2
	1.0	-382	-303	-302	40	-75	2
	1.5	-787	-597	-594	-11	-210	-27
C05	0.5	-94	-82	-80	25	-9	4
	1.0	-353	-282	-280	42	-66	-2
	1.5	-750	-571	-566	-33	-188	-22

4. Conclusions

This study introduced high-order predictor-corrector methods into KARMA to enhance the accuracy of burnup calculations. The higher-order PC methods demonstrated significant improvements over the methods previously implemented in KARMA, particularly for Gd-containing rods. The results indicated that gadolinium has a substantial impact on burnup calculations, and accurate modeling of its depletion is critical for precise reactor simulations. The QEQI, which employ quadratic polynomial approximations, was found to offer the highest computational accuracy, with minimal deviation from the reference calculations.

This work provides a foundation for enhancing the accuracy and efficiency of burnup calculations in nuclear reactor core design, providing improved insights into fuel behaviour and reactor performance over the entire burnup cycle.

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REFERENCES

[1] Han, T. Y., Yoon, J. I., Kim, J. H., Lee, C. K., and Cho, B. J. Benchmark verification of the karma/astra code with oecd/nea and us nrc pwr mox/uo2 transient problem.
[2] Kim, K. S., Hong, S. G., Cho, J. Y., and Song, J. S. Transport lattice code karma 1.1. In Transactions of KNS Autumn Meeting, Gyeongju, Korea (2009).
[3] A. Isotalo, P.A. Aarnio, Higher order methods for burnup calculations with bateman solutions, Ann. Nucl. Eng. 38 (2011) 1987.
[4] H. J. Park et al, Monte Carlo burnup and its uncertainty propagation analyses for VERA depletion benchmarks by McCARD, Nucl. Eng. Technol. 50 (2018) 1043-1050
[5] Josey, C. Development and analysis of high order neutron transport depletion coupling algorithms. PhD thesis, Massachusetts Institute of Technology, 2017.
[6] Romano, P. K., Josey, C. J., Johnson, A. E., and Liang, J. Depletion capabilities in the openmc monte carlo particle transport code. Annals of Nuclear Energy 152 (2021), 107989.
[7] Saad, Y. Analysis of some krylov subspace approximations to the matrix exponential operator. SIAM Journal on Numerical Analysis 29, 1 (1992), 209–228.