Implementation of Burnup Interval Optimization Module Based on Monte Carlo Perturbation Technique

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Keywords : burnup analysis, depletion time steps, burnup interval, optimization, perturbation,

1. Introduction

In nuclear core design analyses, general neutron transport equation is typically expressed as a function of position, energy, direction, and time. For computational efficiency, time discretization is broadly divided into three categories: steady-state analysis, transient analysis, and depletion analysis for long-term periods. In nuclear engineering field, depletion analysis means the computational process of calculating how the number densities of isotopes in a nuclear system change over time as it is burned.

Generally, the number densities can be calculated by the depletion equation, which represents a balance equation for nuclear reactions and decays. The depletion equation can calculate the number density at a specific time point. Accordingly, the depletion time discretization is essential to solve the depletion equation. Finer discretization of depletion time intervals reduces errors but increases the computational burden.

There are a few studies on the topics to optimize depletion time steps or to enhance burnup analysis capabilities. W. Yang developed a linear time-dependent flux approximation for nuclide depletion based on a perturbation method. [1] In this method, a perturbation method is employed to derive the first-order expansion of the time-dependent flux. Moreover, Jan Dufek proposed the stochastic implicit Euler method [2] for burnup calculations. The implicit solution is obtained through stochastic approximation at each time step.

In this paper, we introduced a new concept of burnup interval optimization based on perturbation method.

2. New Concept of Burnup Interval Optimization

2.1 Source of Errors in Reactivity Over Burnup

In the depletion analysis, the depletion period of the nuclear system is split into non-overlapping depletion time step (DTS); $[t_n, t_{n+1}]$ $(n=1,2,\cdots)$ with n denoting depletion time index. The change in the number density of nuclide i in cell m of the operating nuclear system during DTS n can be determined by solving the depletion equations;

$$\frac{dN_{m,i}(t)}{dt} = \sum_j l_{ij}\lambda_j N_{m,j}(t) + \sum_j \gamma^n_{m,ij} N_{m,j}(t) - \left(\lambda_i + \gamma^n_{m,i}\right) N_{m,i}(t),$$
$$t \in [t_n, t_{n+1}],\ N^n_{m,i} = N_{m,i}(t_n), \quad \cdots (1)$$

where $\gamma^n_{m,i}$ is the microscopic absorption rate of nuclide i in cell m and $\gamma^n_{m,ij}$ is the fraction of the microscopic reaction rate of nuclide j in cell m which leads to the creation of nuclide i. The other notations follow the convention. To determine the number density at the $(n+1)^{th}$ DTS, the number density at the $(n)^{th}$ DTS and 1-group reaction rates are required. In the depletion equation, it is assumed that the 1 group reaction rates remain constant between the $(n)^{th}$ and $(n+1)^{th}$ DTS. This assumption is based on the premise that there are not significant changes in reaction rates or reaction cross sections between burnup intervals.

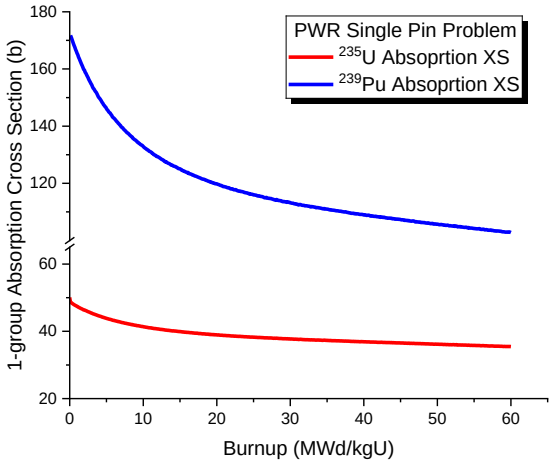

Fig. 1. Comparison of one-group cross sections of a PWR single pin problem over burnup.

Figure 1 compares one-group absorption cross sections of a PWR single pin problem over burnup. It is observed that the changes in one-group cross sections over burnup can cause significant errors depending on the burnup interval. The errors in one-group cross sections can propagate to the inaccuracies in number density. Finally, it leads to the error in reactivity over burnup [3].

2.2 Algorithm for Burnup Interval Optimization

In this study, a new concept of optimized burnup interval is introduced by considering the source of error in reactivity over burnup. Let's assume that one-group reaction rates at the previous and current DTS are RR(t_0) and RR(t_1) and the next DTS can be arbitrarily set as $t_1+\Delta t$. The reaction rate at the next DTS, RR($t_1+\Delta t$), can be predicted by linear extrapolation method. The goal of this algorithm is to ensure that the reactivity change caused by changes in the reaction rates remains within a tolerance of ε.

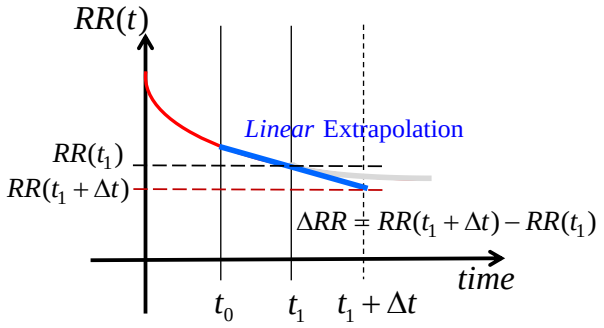

Fig. 2. Reaction rates estimations by linear extrapolation for a next depletion time step(t_2).

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1: Input: RR(tn-1), RR(tn), Δtmax, Δtitv
2: Δt= Δtmax
3: Estimate RR(tn+Δt) from RR(tn-1) and RR(tn)
4: Calculate ∂N/∂R(tn) and ∂k/∂N(tn)
5: while (Δk<ε)
6:    ΔRR=RR(tn+Δt)-RR(tn)
7:    ΔN= ∂N/∂R(tn)x ΔRR
8:    Δk= ∂k/∂N(tn)x ΔN
9:    Δt= Δt- Δtitv
10: end while
11: tn+1=tn+Δt
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Fig. 3. Algorithm of new burnup interval optimization method for next depletion time step(t_{n+1}).

To quantify the change in reactivity due to change of reaction rates, the MC perturbation technique and direct subtraction were used in this approach. The direct subtraction can provide the changes in number densities caused by variations in reaction rates, ∂N/∂RR, while the MC perturbation technique reveals changes in reactivity or k_{eff} resulting from variations in the number densities, ∂k/∂N. The change in reactivity due to the change of reaction rate can be expressed as:

$$\Delta k(t_n) = \sum_{i,\alpha} \left\{ \frac{\partial k}{\partial N_i} \times \frac{\partial N_i}{\partial RR_{\alpha,i}} \times \left(RR_{\alpha,i}(t_n + \Delta t) - RR_{\alpha,i}(t_n) \right) \right\} \quad \ldots (2)$$

where $RR_{\alpha,i}$ is an one-group α-type microscopic reaction rate for *i*-isotope. When Δ*k* falls within the convergence criterion ε, the current Δ*t* is confirmed as the next DTS, t_{n+1}. If it has not yet converged, Δ*t* is reduced by Δt_{itv}, and Δ*k* is recalculated by Eq. (2). Figure 3 shows the algorithm of MC perturbation technique-based burnup interval optimization method. In this burnup interval optimization, the incorporation of perturbation technique computations may result in a considerable increase in computation time.

3. Numerical Results for Burnup Interval Optimization Method

3.1 VERA depletion benchmark problem

To examine the new concept of the burnup interval optimization, VERA 1C pin depletion problem [4] was performed by the McCARD MC code [5]. Table I provides the geometrical and material data for VERA 1C pin depletion problem. In this study, all burnup analyses were conducted from a constant extrapolation at the predictor stage and a backward extrapolation at the corrector stage (CEBE) by matrix exponential method (MEM) depletion equation solver.

Table I: Geometrical and material data for problem 1C

Material	Parameter	Value
Fuel	Pellet radius (cm)	0.4096
	^{235}U w/o	3.1
	Density (g/cm3)	10.2570
	Temperature (K)	900
Clad	Inner radius (cm)	0.4180
	Outer radius (cm)	0.4750
	Density (g/cm3)	6.5600
	Temperature (K)	600
Core	Pressure (bar)	155.13
	Power density (w/gU)	40.00
	Pin pitch (cm)	1.2600

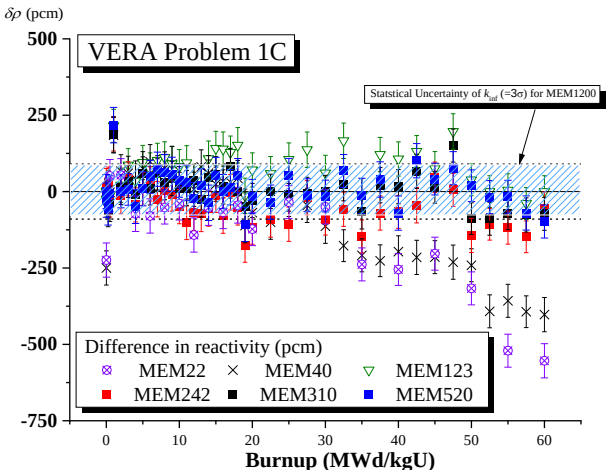

Fig. 4. k_{inf} convergence plots for problem 1C with varying the number of depletion time steps.

To obtain the reference solution for the VERA 1C pin problem, the McCARD depeltion calculations were

performed by the CEBE/MEM varying the number of DTSs as 22, 40, 123, 242, 310, and 520, 1200. Figure 4 shows differences of the infinite multiplication factors from the 1200 DTS results with MEM solver (hereafter MEM1200). The difference in reactivity between MEM1200 and other cases decreases as the number of depletion time steps increases. The interval of burnup in MEM22, MEM40, MEM520, MEM1200 are roughly 4, 1, 0.1, 0.05 MWd/kgU, respectively. Table II compares the root mean square (RMS) errors and k_{inf} at 60 MWd/kgU burnup for each case. It can be observed that MEM310 was fully converged with considering the statistical uncertainties (< 30pcm).

Table II: RMS errors and k_{inf} at EOC (60MWd/kgU) for problem 1C with varying the number of depletion time steps.

Case	RMS errors (pcm)	k_{inf} (EOC)
MEM22	157	0.79210
MEM40	129	0.79305
MEM123	84	0.79559
MEM242	64	0.79524
MEM310	43	0.79513
MEM520	45	0.79497
MEM1200 (Reference)		0.79559

* statistical uncertainties are less than 30 pcm.

3.2 Application of the Burnup Interval Optimization Algorithm for VERA Depletion Problem 1C

In this study, the optimized DTSs are calculated by the MC perturbation technique-based burnup interval optimization algorithm. Table III shows the results of the DTS for the convergence parameters (i.e., Δt_{itv}, ε) for problem 1C. As mentioned in the previous section, Δt_{itv} indicates the time interval reduction applied to the previous time step when the calculated Δk under the current conditions does not fall within the convergence criterion ε. Δt_{max} represents the initial time interval for the next burnup calculation, and a value of 100 EFPD was used for all cases.

Table III: Optimized DTSs by the burnup interval optimization algorithm for problem 1C.

Case	Nuclides	ε (pcm)	Δt_{itv} (EFPD)	DTS
I	^{235}U, ^{238}U	10	3	46
II	^{235}U, ^{238}U	5	3	82
III	^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu	10	3	151
IV	^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu	5	3	385

For Cases I and II, the effects by ^{235}U and ^{238}U were considered whereas in Cases 3 and 4 the effect of four nuclides – ^{235}U, ^{238}U, ^{239}Pu, and ^{240} Pu were considered.

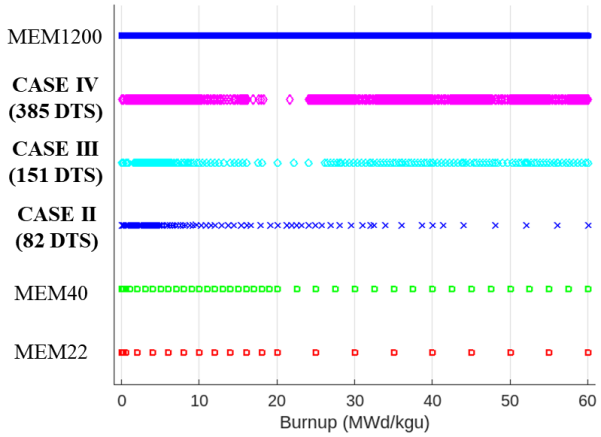

Fig. 5. Distributions of depletion time steps for problem 1C.

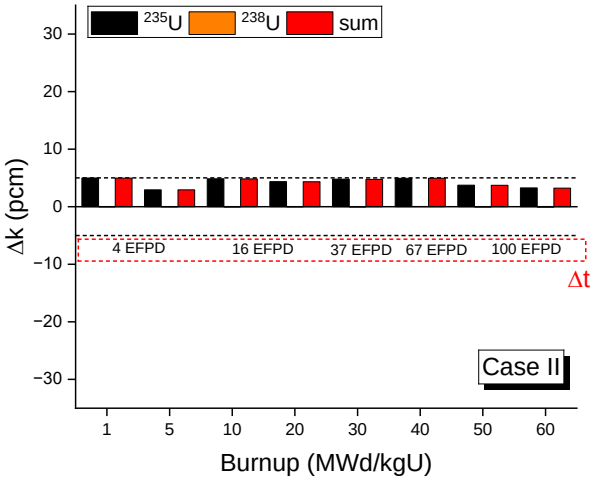

Fig. 6. Change of k with varying the time interval (Δt) by the optimization algorithm for Case II.

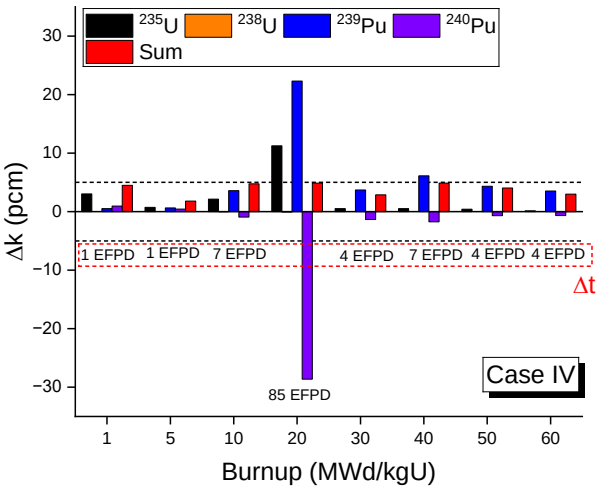

Fig. 7. Change of k with varying the time interval (Δt) by the optimization algorithm for Case IV.

Figure 5 shows the distributions of depletion time steps for Case II, Case III, Case IV, MEM22, MEM40, and MEM1200 (Reference). Figures 6 and 7 show the Δk with varying the time interval by the optimization algorithm for Case II and IV, respectively.

Table IV: RMS errors and k_{inf} at EOC (60MWd/kgU) for each optimized DTS case.

Case	DTS	RMS errors (pcm)	k_{inf} (EOC)
I	46	141	0.79301
II	82	125	0.79319
III	151	55	0.79555
IV	385	47	0.79583
MEM1200 (Reference)			0.79559

* statistical uncertainties are less than 30 pcm.

Table IV compares the RMS errors and k_{inf} at 60 MWd/kgU burnup for four optimized DTS cases. Cases I and II give RMS errors in reactivity exceeding 100 pcm. In both cases, the reactivity error was more than 380 pcm. In Cases III and IV, where plutonium was considered, the RMS errors were at a similar level to the converged error (e.g., 40~50 pcm) as shown in Table II. From the results, it was confirmed that it is necessary to consider both Uranium and Plutonium isotopes for the optimization of the burnup intervals in a UO_2 pin problem. Additionally, the proposed burnup interval optimization algorithm demonstrated a burnup accuracy similar to Case III, which used 151 burnup steps, compared to MEM242, which employed 242 equally divided burnup intervals. It was noted that this algorithm has been verified to be efficient and capable of automatically optimizing the burnup intervals.

3. Conclusions

In this study, a new concept of burnup interval optimization was proposed. This algorithm uses the MC perturbation technique and direct subtraction method to quantify the error in reactivity due to the changes in one-group cross sections over burnup. Through a simple UO_2 fuel pin problem (i.e., VERA 1C problem), it was confirmed that the proposed algorithm effectively provides optimized burnup intervals.

In the near future, a sensitivity analysis of the convergence parameters and an additional analysis of Gd_2O_3-UO_2 burnable absorber pin problem (i.e., VERA 1I problem) will be conducted.

Acknowledgment

This work was supported by the Innovative Small Modular Reactor Development Agency grant funded by the Korea Government (MSIT) (No.RS-2023-00258205) and the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. RS-2024-00422848).

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