Estimation of the Number Density Uncertainty in McCARD Depletion Calculation on SALUS

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1. Introduction

In Monte Carlo (MC) burn-up calculations, the number densities of isotopes for the next step is determined by the burn-up matrix, which is composed by group-collapsed reaction rates obtained from MC simulation itself. Noting that the reaction rates already involve statistical error from finite random samples in MC, the burn-up matrix also includes statistical error, the error can be propagated over all the burn-up steps [1]. The propagated error of number density can be estimated by formulating the number density error terms in the depletion equations [2], or estimating the error terms in MC calculation by the sensitivity and uncertainty analysis method using the covariance data and related MC tallies in the error propagation formulation [3]. Both approaches have been applied to fuel assembly problems, and showed that the uncertainty tends to increase as the fuel burns, and it becomes major error component on criticality if the fuel burn-up is higher.

Meanwhile, depletion analysis for SALUS [4] was conducted to McCARD burn-up calculation capability [5]. SALUS aims extended cycle length up to 20 years, the impact of error propagation can be appeared greater than typical reactors. Also, the error propagation analysis has not been conducted to whole core problems, it is required to quantify the impact of number density uncertainty on the SALUS analysis. In this work, the uncertainty of number density is directly calculated by statistical treatment on the results of multiple MC runs and its impact on the uncertainty of criticality is investigated.

2. SALUS burn-up calculations procedure

SALUS is a Sodium-cooled Fast Reactor (SFR) with 100MWe power, which aims for 20 years of operation without refueling. The design features are similar to KAERI's Proto-type Gen-IV SFR (PGSFR), but the core configuration has been modified for extended fuel cycles with increased average discharge burn-up of 75GWd/MT. The reactor core takes advantage of breeding concept to reduce reactivity swing and to reach the target EFPD of 7300 days, so the enrichment of uranium is lower in the core center.

The uncertainty of number density can be estimated by multiple runs of MC simulations, and the uncertainty can be referred to the estimated error of number density. At each burn-up step, the number densities of major isotope are compared each other, and the variance of number density can be obtained by statistical treatment.

In this work, 26 independent MC burn-up calculations were conducted with ENDF/B-VII.1, and the number densities of major isotopes as well as criticality were investigated. The active core regions in the fuel assemblies are divided into 14 burn-up cells, so axial distribution of reaction rates can be reflected into the MC burn-up calculations. Burn-up cells from two different fuel assemblies are selected for the number density monitoring, that are the 7-th burn-up cells from the bottom, and their radial location can be found as Reg.1 and Reg.2 in Fig. 1. At each MC run, 100k neutron histories are tallied in a cycle, while 250 active cycles are assigned for estimating tallies. Note that the 29 burn-up steps are assigned over 20 years.

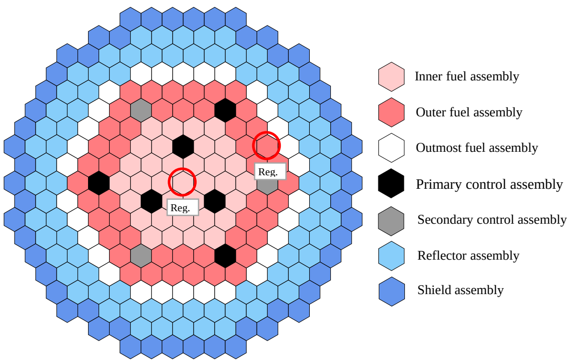

Fig. 1 Core layout of SALUS

The criticality of core for randomly selected 10 cases are plotted in Fig. 2, and they showed almost the same burn-up curve regardless of the different random seed. Some cases showed a large difference in criticality compared to others, but this tends to be recovered at the following burn-up steps.

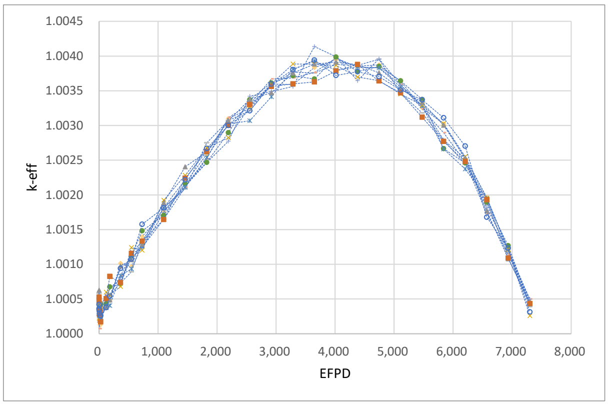

Fig. 2 Burn-up calculations w/ different random number seed

In order to confirm that 100k solutions are enough for avoiding the under sampling bias, the averaged criticality of 26 independent runs is compared to that of a single MC run with increased number of histories, 500k, in Fig. 3. Note that the error bar in this figure stands for 2-sigma, and the two results show a good agreement as the results are well overlapped within their error bars. Therefore, 100k histories per cycle can be considered accurate enough for the MC burn-up analysis of the SALUS core.

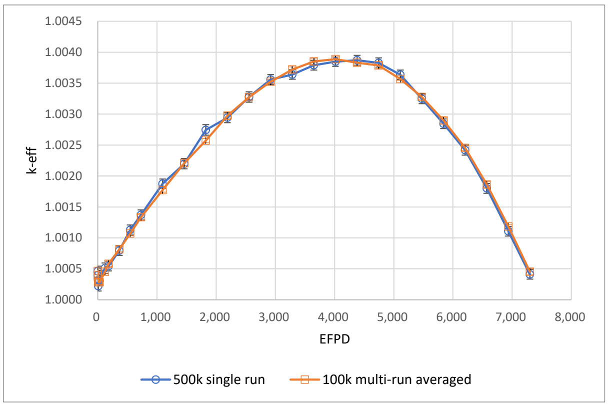

Fig. 3 Comparisons of MC Burn-up calculations between single run with 500k histories and average over 26 independent runs with 100k histories

3. Estimation of number density uncertainty

The number densities of isotopes in selected depletion cells are monitored along the burn-up steps of MC calculations. The number densities of major isotopes along the time are plotted in Fig. 4 for both Reg.1 and Reg. 2. Note that the number density is the averaged value over the 26 independent MC runs as:

$$\bar{N}_{\alpha,j} = \frac{1}{\mathrm{N_R}} \sum_{i=1}^{\mathrm{N_R}} N_{\alpha,i,j} \tag{1}$$

where $\mathrm{N_R}$ is the number of MC runs, and $N_{\alpha,i,j}$ stands for the number density of isotope α at burn-up step j in i-th MC run.

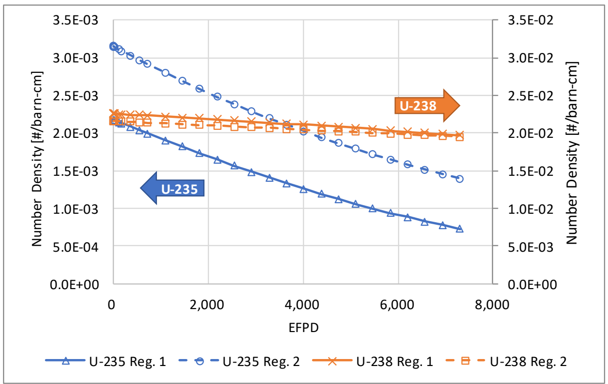

Fig. 4 Number density changes of U-235 and U-238 along the depletion calculation

The relative standard deviation of number densities in Reg. 1 are shown in Fig. 5, which are obtained from statistical treatment of 26 independent MC runs as:

$$s_r[N_{\alpha,j}] = \frac{1}{\bar{N}_{\alpha,j}} \sqrt{\frac{1}{\mathrm{N_R}-1} \sum_{i=1}^{\mathrm{N_R}} \left(N_{\alpha,i,j} - \bar{N}_{\alpha,j}\right)^2}. \tag{2}$$

According to the figure, the relative uncertainty of Pu-239 is decreasing as the fuel burns while those of U-235 and U-238 are increasing. The relative uncertainty of Pu-239 is the highest among three different isotopes, but it becomes smaller than that of U-235 after a certain burn-up step. One interesting observation is that the uncertainty of combined isotopes, U-235 and Pu-239, is significantly smaller than that of each isotope as shown in Fig. 5. This implies that the loss in U-235 fission reaction in a cell is compensated by the fission of Pu-239, so the total fission reaction rate can have relatively small uncertainty in the MC burn-up calculations. Since the major isotopes' uncertainties are increasing according to fuel burn-up, greater uncertainty of criticality is expected at the end of cycle.

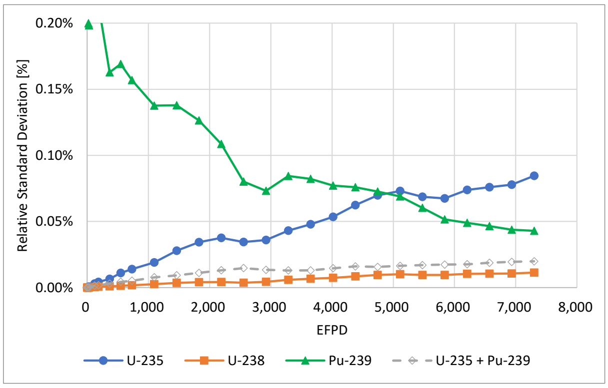

Fig. 5 Relative Std. Dev. of number density of major isotopes in Reg. 1

Fig. 6 shows the uncertainty of number densities in Reg. 2, and the observed behaviors are similar to the observations in Fig. 5. Because of higher enrichment in this cell, smaller amount of Pu-239 is generated in the core, and this leads to even higher uncertainty of Pu-239. This implies that the fission reaction compensation by Pu-239 is less effective, but the uncertainty of combined number density of U-235 and Pu-239 is smaller than that of each, as it is appeared in Fig. 5.

Since Reg.2 is in the outer core and the neutron flux is lower compared to the core center especially after the middle of cycle, the uncertainty is observed slightly greater than Reg. 1. However, the uncertainty of U-238 was estimated as less as only about 0.01% even for the EOC.

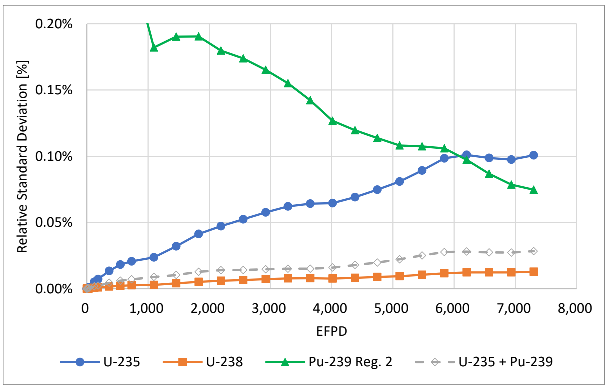

Fig. 6 Relative Std. Dev. of number density of major isotopes in Reg. 2

The uncertainty of U-235 and combined number density, U-235 and Pu-239 are compared to that of U-238, and the ratio is plotted Fig. 7. As shown in the figure, the ratio remains around 8 for U-235, and around 2 for the combined one. This implies that the uncertainty is less correlated to the initial composition of the fuel or the composition changes according to burn-up.

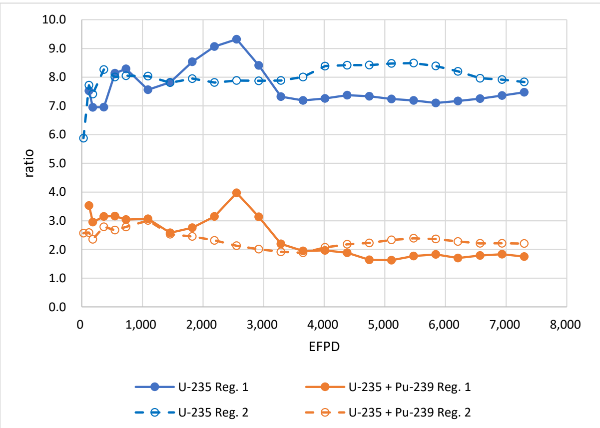

Fig. 7 Ratio of number density uncertainties: fissile isotopes to U-238

4. Impact of error propagation on criticality

As mentioned above, the uncertainty in number density tends to be increased as the fuel burns, so it can be expected that the uncertainty of criticality is also increased in the later burn-up steps. In order to compare the criticality at each step, a pseudo error is introduced and plotted for each MC run. The pseudo error at burn-up step *j* in the *i*-th MC run, $e_{i,j}$, can be defined as:

$$e_{i,j} = k_{i,j} - \bar{k}_j, \tag{3}$$

where $k_{i,j}$ is the criticality of MC calculation at burn-up step *j* in *i*-th run, and $\bar{k}_j$ is averaged criticality over the 26 independent runs at burn-up step *j*.

The pseudo errors of randomly selected 10 MC runs are plotted in Fig. 8. The solid red and blue line in the figure indicates the confidential intervals showing the uncertainty of criticality ($\hat{s}_j$), which is obtained from the variance of criticality defined as:

$$\hat{s}_j^{\,2} = \frac{1}{\mathrm{N_R} - 1} \sum_{i=1}^{\mathrm{N_R}} \left(k_{i,j} - \bar{k}_j\right)^2. \tag{4}$$

where $\bar{k}_j = \frac{1}{\mathrm{N_R}} \sum_{i=1}^{\mathrm{N_R}} k_{i,j}$.

According to Fig. 8, it is difficult to see the effect of the error propagation on the criticality. The distribution of error is not skewed, and all results are well distributed around the mean value, which is zero. Additionally, the variance of criticality seems similar over the all burn-up steps.

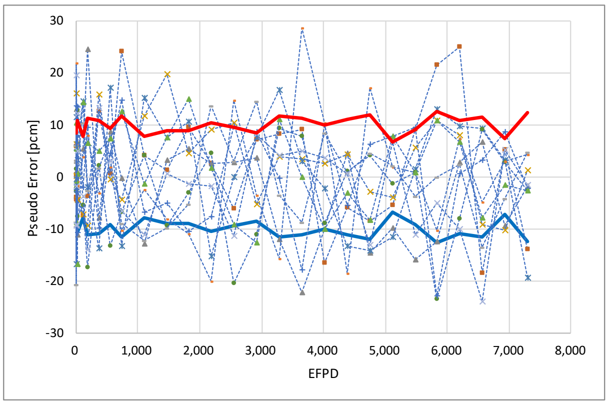

Fig. 8 Pseudo error of MC depletion calculations

The standard deviation in equation (4) is an estimation of uncertainty of MC burn-up calculations which includes the error propagation by number density uncertainty. On the other hand, the sample standard deviation of criticality from a single MC run ignores the error propagation since the sample standard deviation is obtained from fixed number densities that are calculated in the previous burn-up step. The expectation value of sample variance, can be obtained as:

$$\bar{s}_j^{\,2} = E\left[s^2\left[k_{i,j}\right]\right] = \frac{1}{\mathrm{N_R}} \sum_{i=1}^{\mathrm{N_R}} s^2\left[k_{i,j}\right], \tag{5}$$

where $s^2\left[k_{i,j}\right]$ is the sample standard deviation of criticality at burn-up step *j* in the *i*-th MC run.

The difference between $\hat{s}_j^{\,2}$ and $\bar{s}_j^{\,2}$ indicates that how much the sample standard deviation is biased in MC burn-up simulations. Fig. 9 shows two different standard deviations over the whole depletion steps: $\hat{s}_j$is appeared as 'Statistical + Propagated', while $\bar{s}_j$ is appeared as 'Statistical'. As shown in the figure, $\hat{s}_j$ is estimated greater than $\bar{s}_j$ for most depletion steps. Large fluctuation was observed for $\hat{s}_j$ estimation because limited number of MC runs were used for statistical treatment. The result showed that a typical MC burn-up calculation for SALUS would underestimate the uncertainty of criticality by up to 30%. One important observation is that $\widehat{s_j}$ seems slightly increasing at the later burn-up steps, which was expected from the increasing uncertainty of number densities as plotted in Fig. 5 and Fig. 6.

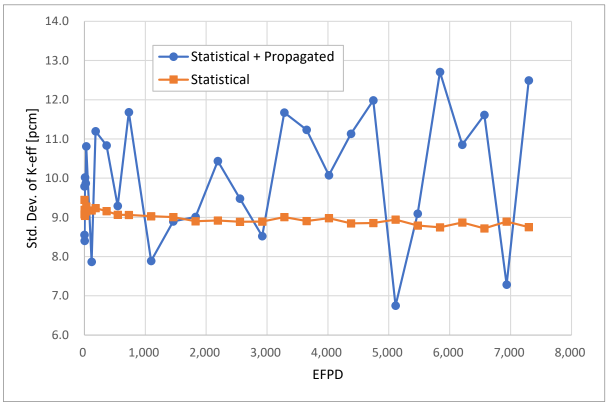

Fig. 9 Comparison of $\widehat{s_j}$ (Statistical + Propagated) and $\overline{s_j}$ (Statistical) in SALUS MC Depletion calculation

5. Conclusions

In this paper, number density uncertainty on SALUS MC burn-up calculation were estimated and its effect on criticality was examined. The number density uncertainty was estimated 0.1% at maximum in U-235 and about 0.01% in U-238. The uncertainty of U-235 and U-239 showed a tendency to increase as the nuclear fuel was burned, while the uncertainty of newly generated Pu-239 showed a tendency to decrease with fuel depletion.

As a result of considering the number density error, the criticality showed increased uncertainties up to 30% compared to the case where the number density error was not considered. Accordingly, it should be considered conservatively that the MC Depletion calculation on SALUS would have up to 30% greater uncertainty than the sample standard deviation.

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REFERENCES

[1] T. Takeda, N. Hirokawa, and T. Noda, "Estimation of error propagation in Monte-Carlo burnup calculations," journal of Nuclear Science and Technology, Vol. 36, no. 9, pp. 738-745, 1999.

[2] M. Tohjoh, T. Endo, M. Watanabe, and A. Yamamoto, "Effect of error propagation of nuclide number densities on Monte Carlo burn-up calculations," Annals of Nuclear Energy, Vol. 33, no. 17-18, pp. 1424-1436, 2006.

[3] H. J. Park, H. J. Shim, and C. H. Kim, "Uncertainty propagation in Monte Carlo Depletion Analysis," Nuclear Science and Engineering, Vol 167, pp. 196-208, 2011.

[4] M. J. Lee, J. H. won, Y. I. Kim, J. Y. Lim, "Comparison of REBUS-3 and McCARD Depletion Calculations on a Long-term Sustainable Small Modular Reactor, SALUS," Trans. Korea Nucl. Soc. Spring Meeting, Jeju, Korea, May 19-20, 2022.

[5] H. J. Shim, B. S. Han, J. S. Jung, H. J. Park and C. H Kim, "McCARD: Monte Carlo code for advanced reactor design and analysis," Nuclear Engineering and Technology, Vol.44, 2012.