IRPhE DUKE Depletion Benchmark Analyses by McCARD and PRAGMA with Various ENDF/B Evaluated Nuclear Data Libraries

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1. Introduction

With advanceds in computing resources and the applications in GPU programming, Monte Carlo (MC) based transport codes have been used more frequently in nuclear core design analyses. Accordingly, MC depletion and thermal feedback analyses, which had long been challenging due to the limitations from the drawback of the MC methodology, are now being actively conducted. The accuracy of MC calculations is highly dependent on the fidelity and accuracy of the nuclear reaction cross sections used. MC codes have been thoroughly validated against reactor physics benchmark problems derived from various critical experiments. However, reactor physics benchmark problems specifically addressing MC depletion analyses remain scarce, and corresponding studies are limited.

The IRPhE (International Handbook of Evaluated Reactor Physics Benchmark Experiments)/DUKE benchmarks [1] are among the few available benchmark problems that provide reference values for reactor depletion analyses.

In this study, the IRPhE/DUKE depletion benchmark will be performed and evaluated using the McCARD [2] MC code with various evaluated nuclear data libraries (i.e., ENDF/B-VIII.1 [3], ENDF/B-VIII.0, ENDF/B-VII.1, and ENDF/B-VI.8). In addition, the depletion analysis capability of PRAGMA [4], a recently developed GPU-based MC code, is cross-validated.

2. Depletion Benchmark and Methods

2.1 IRPhE/DUKE FA depletion benchmark

The DUKE fuel assembly (FA) depletion benchmark problem (DUKE-PWR-POWER-001) [1] was introduced by K. Smith. Especially, it provides reference reactivity decrements during burnup for validation of depletion analysis capability. K. Smith inferred the reference reactivity decrements using measured ^{235}U fission rate distributions taken from operating commercial reactors (i.e., McGuire and Catawba nuclear power plants). The DUKE benchmark fuel assembly (FA) has a 17×17 WH fuel assembly configuration consisting of 4.25 wt. % enriched UO_2 fuel rods with a typical pressurized water reactor (PWR). In addition, the FA includes 104 integral fuel burnable absorber (IFBA) rods with ZrB_2 coating. This benchmark includes reference benchmark reactivities and their uncertainties at 6 burnup points (10, 20, 30, 40, 50, and 60 MWd/kgU). It also provides the sample benchmark results by SCALE 6.1 with 238-group ENDF/B-VII.0 evaluated cross section library.

2.2 Doppler Broadening Scattering Model

In general, MC neutron transport codes consider a thermal motion between a neutron and a target atom to adopt scattering transport mechanism. However, temperature-dependent variations in the scattering kernel are not adequately reflected in the cross sections generated by the cross section processing code such as NJOY. In order to correct this problem, on-the-fly Doppler broadening is implemented by sampling the target nucleus's velocity vector and using the relative neutron energy in the MC simulation of the collision kernel. Most MC neutron transport codes provide various modules or capabilities to accurately model scattering transport mechanisms with Doppler broadening effects. The McCARD includes an approximate approach, known as the Constant Cross Section (CXS) Model derived from the free monoatomic gas model, as well as the Doppler Broadening Rejection Correction (DBRC) method [5,6], which enables accurate treatment of Doppler broadening effects. The PRAGMA code provides Relative Speed Tabulation (RST) Scheme as Rejection-free Target Velocity Sampling method.

Recently, a few studies [7] have examined the influence of accurately treating Doppler broadening effects on burnup-dependent analysis results. In this study, DUKE depletion benchmark calculations will be performed to evaluate the differences between the default Constant CXS case and the DBRC or RST cases.

2.3 Evaluated Nuclear Cross Section Library

Some recent studies [8,9] have reported a clear negative reactivity swing of several hundred pcm in PWR fuel pin reactivity analyses using ENDF/B-VIII.0 compared to ENDF/B-VII.1 at near end of cycle (EOC). As a result, many institutions and academic researchers have become hesitant to immediately adopt the

ENDF/B-VIII.0 evaluated nuclear data library in reactor design or analysis. The recently released ENDF/B-VIII.1 shows a reduction in the negative reactivity swing, and the magnitude of this improvement will be assessed using the DUKE depletion benchmark. In addition, ENDF/B-VI.8 depletion analyses will be performed to examine overall trends in burnup characteristics across the ENDF nuclear data libraries.

2.4 Depletion Solver and QE/QI Predictor-Corrector

For depletion analysis, a burnup matrix discretized in time must be constructed and solved. To solve the burnup matrix, Matrix Exponential Method (MEM) and Chebyshev Rational Approximation Method (CRAM) have been widely adopted. Furthermore, discretization of the burnup matrix with respect to depletion time step (DTS) interval inevitably introduces numerical errors. Such errors can become non-negligible in reactor burnup analyses with a substantial number of burnable absorbers such as Gd_2O_3. To reduce these errors, a variety of higher-order predictor–corrector (P-C) methods (time integration method) have been proposed, and the quadratic extrapolation/quadratic interpolation (QE/QI) [10] scheme implemented in the McCARD, KARMA, and PRAGMA has been widely recognized as an effective solution. In the DUKE depletion benchmark, there are IFBA burnable absorber fuel pins. In the McCARD DUKE benchmark analyses, the MEM burnup matrix solver with sub-step treatment and the QE/QI time integration method will be applied by default. In the PRAGMA code, the QE/QI method based on CRAM will also be employed for the benchmark analysis.

3. DUKE Depletion Benchmark Results

3.1 Depletion Reactivity Results with ENDF/B-VII.1

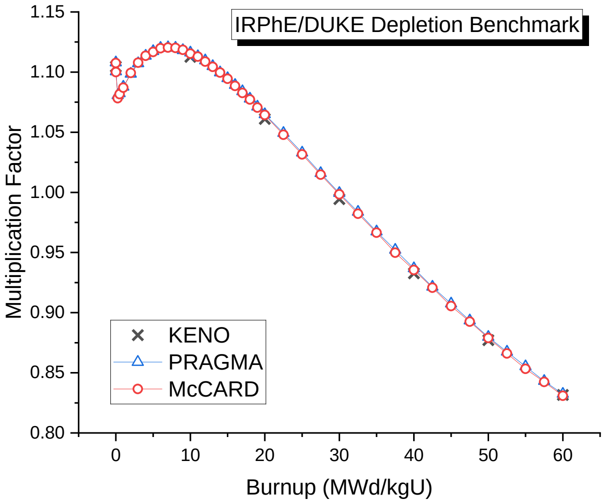

Fig. 1. IRPhE/DUKE depletion benchmark k_{eff} results by KENO, PRAGMA, and McCARD using ENDF/B-VII.1 evaluated nuclear data library.

First, DUKE MC depletion benchmark calculations were performed using the ENDF/B-VII.1 evaluated nuclear data library. In these calculations, the DBRC- or RST-based Doppler-broadening scattering model and the QE/QI high-order P-C modules were applied by default. Figure 1 shows the k_{eff} results by KENO, PRAGMA, and McCARD MC codes with the ENDF/B-VII.1 evaluated nuclear data library. As the ZrB_2 ring region of the IFBA depletes, the reactivity initially increases and subsequently decreases, following the depletion of the absorber. Figure 2 compared the reactivity gain and loss results over burnup calculated by KENO, PRAGMA, and McCARD MC codes with the ENDF/B-VII.1. The DUKE benchmark book provides the reference values and their uncertainties. The results of KENO code were taken from the reference [1].

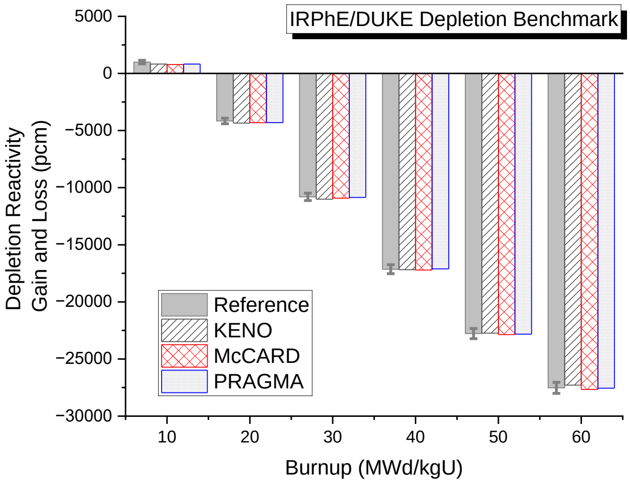

Fig. 2. Comparison of reactivity gain and loss results over burnup by KENO, PRAGMA, and McCARD Monte Carlo code using ENDF/B-VII.1 evaluated nuclear data library.

Table I: Difference in depletion reactivity between reference and two MC codes with ENDF/B-VII.1

Burnup (MWd/kgU)	Unc. of Ref.* (pcm)	Difference in reactivity from Reference (pcm)	
		McCARD	PRAGMA
10.0	151	-213	-170
20.0	245	-158	-149
30.0	325	-109	-50
40.0	392	-68	29
50.0	446	-82	-43
60.0	484	-138	-31

* Uncertainties of reference depletion reactivity (pcm)

Table I presents differences in depletion reactivity between reference and two MC codes (i.e., McCARD and PRAGMA). It also provides the uncertainties in reference depletion reactivities in units of pcm. Both the McCARD and PRAGMA codes demonstrate agreement with the reference within the uncertainty range, except at 10 MWd/kgU.

3.2 Effect of Doppler Broadening Scattering Models

Recently, several studies [3,7] have reported on the effects of applying accurate Doppler-broadening scattering models to compensate for the negative reactivity swing observed with ENDF/B-VIII.0. Table II and Figure 3 show the depletion reactivity differences between the reference and the MC codes for different Doppler-broadening scattering model treatments. For McCARD, the results obtained using the DBRC method were compared with those calculated using the default CXS model without DBRC. For PRAGMA, the results obtained with the RST method were compared with those calculated using the default CXS model. The McCARD DBRC correction and PRAGMA RST correction lead to a reactivity gain of about 180 pcm and 230 pcm at EOC, respectively. Accordingly, it is confirmed that accurate Doppler broadening scattering models are capable of alleviating the negative reactivity swing over burnup associated with ENDF/B-VIII.0.

Table II: Difference in depletion reactivity between reference and McCARD w/ and w/o DBRC doppler broaden scattering with ENDF/B-VII.1

Burnup (MWd/kgU)	Difference in reactivity from Reference (pcm)			
	McCARD		PRAGMA	
	DBRC	CXS	RST	CXS
10.0	-213	-184	-170	-138
20.0	-158	-174	-149	-118
30.0	-109	-187	-50	-94
40.0	-68	-151	29	-150
50.0	-82	-242	-43	-167
60.0	-138	-325	-31	-265

***** Uncertainties of reference depletion reactivity (pcm)

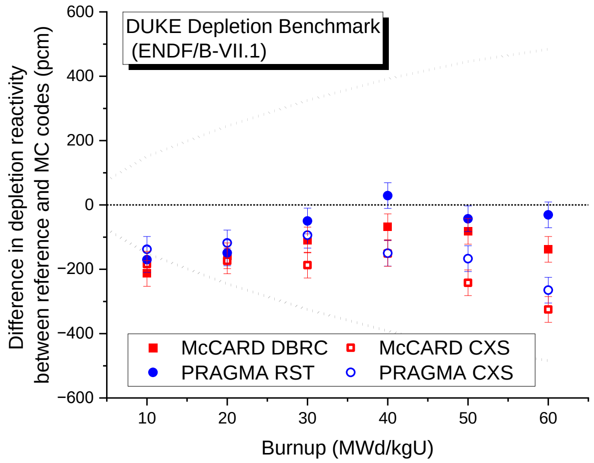

Fig. 3. Comparison of depletion reactivity between reference and MC codes with various Doppler broadening scattering models using ENDF/B-VII.1.

3.3 Effect of Evaluated Nuclear Data Library

Figure 4 compares the McCARD depletion reactivity results calculated by different evaluated nuclear data libraries. The ENDF/B-VI.8, ENDF/B-VII.1, ENDF/B-VIII.0, and the ENDF/B-VIII.1 are compared with the reference depletion reactivities. In agreement with results reported in some studies [8,9], ENDF/B-VII.1 provides the best agreement with the reference solution, while ENDF/B-VIII.0 shows the largest error over burnup. With the DBRC effect considered, the maximum discrepancy between the ENDF/B-VIII.1 and ENDF/B-VII.1 decrease to approximately 230 pcm. Notably, the ENDF/B-VI.8 results show only minor discrepancies, with the exception of the 10 and 20 MWd/kgU burnup points.

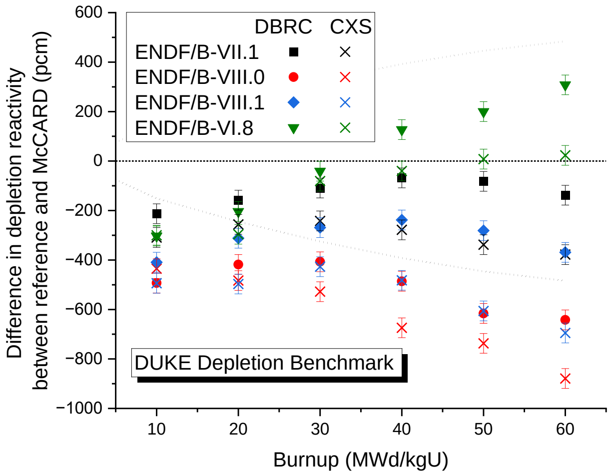

Fig. 4. Comparison of depletion reactivity between reference and McCARD using various evaluated nuclear data libraries.

3. Conclusions

In this study, the IRPhE/DUKE depletion benchmark calculations were performed by McCARD and PRAGMA MC codes using various Doppler broadening scattering models and evaluated nuclear data libraries. For ENDF/B-VII.1, both McCARD and PRAGMA show good agreement with the benchmark reference bounds, except at 10 MWd/kgU. From these results, it was confirmed that the burnup capabilities of both MC codes work correctly and reliably. Noted that PRAGMA adopts multi-level spectral collapse (MSC) approximation for burnup analysis, and the results indicate that this approximation has no significant impact on the accuracy of the burnup calculations.

Furthermore, it is demonstrated that whether an exact Doppler broadening scattering model (e.g., DBRC or RST) is applied can lead to reactivity differences on about several hundred pcm over burnup. It is also reconfirmed that the negative reactivity swing observed in ENDF/B-VIII.0 is mitigated in ENDF/B-VIII.1.

Because reactivity errors can be compensated by the combined effects of these two factors, a detailed comparison of number densities and one-group reaction rates will be performed as the next study.

Acknowledgment

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