Improvements of MCOR: a Monte Carlo depletion code system for fuel assembly reference calculations

Chanatip Tippayakul, Kostadin Ivanov
The Pennsylvania State University, University Park, USA
cut110@psu.edu, kni1@psu.edu

Stefan Misu
AREVA NP GmbH, Erlangen, Germany
An AREVA and SIEMENS Company
Stefan.Misu@areva.com

Abstract

This paper presents the improvements of MCOR, a Monte Carlo depletion code system for fuel assembly reference calculations. The improvements of MCOR were initiated by the cooperation between the Penn State University and AREVA NP to enhance the original Penn State University MCOR version in order to be used as a new Monte Carlo depletion analysis tool. Essentially, a new depletion module using KORIGEN is utilized to replace the existing ORIGEN-S depletion module in MCOR. Furthermore, the online burnup cross section generation by the Monte Carlo calculation is implemented in the improved version instead of using the burnup cross section library pre-generated by a transport code. Other code features have also been added to make the new MCOR version easier to use. This paper, in addition, presents the result comparisons of the original and the improved MCOR versions against CASMO-4 and OCTOPUS. It was observed in the comparisons that there were quite significant improvements of the results in terms of k_{inf}, fission rate distributions and isotopic contents.

KEYWORDS: Monte Carlo depletion, MCOR, fuel assembly reference calculations, MCNP, KORIGEN

1. Introduction

A new Monte Carlo depletion code system was initially developed at the Penn State University (PSU) when a simple script was written to transfer data between MCNP5 [1] and ORIGEN-S [2] for LWR fuel depletion analysis. Subsequently, the script was further developed into a working code, which was then named as MCOR (MCnp-ORigen). When the cooperation between PSU and AREVA NP has been established, the MCOR code has been further improved to enhance its capabilities and accuracy in order to be used as a new Monte Carlo depletion analysis tool. Several improvements have been performed during the course of the cooperation. Currently the new MCOR code system utilizes the ORIGEN based KORIGEN [3], a depletion code of the research center in Karlsruhe, as the depletion module instead of ORIGEN-S. This paper will mainly discuss several aspects of the introduced improvements of the MCOR code system from

the previous PSU version to the new AREVA NP version. In addition, the paper presents the comparisons between the results calculated by the original MCOR version and the results calculated by the improved MCOR version as well as the comparisons of the MCOR results against CASMO-4 [4] and OCTOPUS [5], a Monte Carlo depletion system developed at NRG. Finally, the improved MCOR version is further verified against the TRIPOLI-PEPIN Monte Carlo depletion system, HELIOS and CASMO-4 in two pin cell benchmark problems.

2. Descriptions of original PSU-MCOR

The original PSU-MCOR is basically a coupling code between MCNP5 and ORIGEN-S. In the coupling scheme, MCNP5 performs the steady-state calculation to determine the fission rate distribution for the subsequent depletion calculation by ORIGEN-S. After the depletion calculation is complete, the output material compositions are fed back to the next MCNP calculation and so on. Major features of the original PSU-MCOR are described as follows:

2.1 Interfacing functions

2.1.1 Automatic generation of MCNP input

One of the main features of the MCOR code is the capability to generate automatically the MCNP input from the MCNP input skeleton. The MCOR code does this by translating some symbolic links in the MCNP input skeleton to the corresponding burnup dependent parameters (e.g. material composition, moderator density or etc.). Thus, these burnup dependent parameters are updated in every MCNP calculation to account for the burnup effects.

2.2.2 Automation of MCNP execution and output extraction

This feature allows the calculation and the transfer between two codes to be performed in an automatic manner. The MCOR code is capable of executing the MCNP calculation and also extracting tally results from one of the MCNP output files automatically. The results are then printed into the output and also kept in the computer memory for the subsequent depletion calculation.

2.2.3 Calculations of fission rate distributions and power levels

Once the tally results from MCNP calculation are extracted, the MCOR code calculates the normalized fission rate distribution and the power levels for the succeeding depletion calculations. The normalized fission rate distribution and power levels are computed by

$$fis_i = \frac{(T_i V_i)}{\sum_{i=1}^{all} (T_i V_i)} \quad (1)$$

$$pow_i = (PW)(fis_i) \quad (2)$$

when: fis_i = normalized fission rate distribution of material zone i

T_i = fission rate tally of material zone i from MCNP output

V_i = volume of material zone i (cm^3)

pow_i = power level of material zone i (MW)

PW = total power (MW)

2.2.4 Automatic generation of ORIGEN-S input

The capability to generate ORIGENS input is another main feature of the MCOR code. The ORIGEN-S input for the depletion calculation is generally quite generic since the input requires no geometry descriptions. One ORIGEN input is generated for each material zone by the MCOR code so that each material can be depleted separately.

2.2.4 Automation of ORIGEN-S execution and output extraction

Like the MCNP calculation, the ORIGEN-S calculation for each burnup zone is executed automatically by the MCOR code. In the depletion calculation, ORIGEN-S determines the changes of the material composition using the initial material composition and the power level of each material zone. The MCOR code subsequently extracts material composition after burnup of each material zone when the ORIGEN-S calculation is completed. The material composition of each material zone is then fed back for the next MCNP calculation.

2.2 Utilization of continuous cross sections for Monte Carlo calculations

In order for the MCOR code to correctly represent the temperature dependent neutron interactions, the continuous cross sections to be used with MCNP5 must be pre-processed at temperatures of interest. These continuous cross sections are processed externally and prior to the Monte Carlo depletion calculation. In essence, the MCOR code has a feature to automatically select the most appropriate cross sections for the temperature of the calculation from the cross section directory file. This ensures that the cross sections used in the Monte Carlo calculation are the most suitable.

2.3 Utilization of burnup dependent cross sections

In addition to the initial material composition and the power level, the depletion calculation by ORIGENS requires one-group burnup cross sections to estimate the reaction rates, which eventually determines the changes of isotopic contents. These one-group burnup cross sections are usually dependent on the neutron spectrum which, in fact, changes with burnup. To account for the changes of the one-group cross section, the MCOR code utilizes the pre-calculated one-group burnup dependent cross section library, which is created by the TRITON control module [6]. The generated one-group cross sections are tabulated as a function of burnup and are specific to each fuel assembly design. The MCOR code is capable of integrating the one-group burnup dependent cross section library into the ORIGEN-S input generation process.

3. Improvements from PSU-MCOR to AREVA-MCOR

When the cooperation between PSU and AREVA NP was established, several improvements from PSU-MCOR to AREVA-MCOR were foreseen to enhance the simulation features. The major introduced improvements are described as follows:

3.1 Utilization of KORIGEN as the depletion module

The first upgrade to the PSU-MCOR code was to decouple ORIGEN-S and to adopt KORIGEN as the depletion module since KORIGEN is a standard tool for depletion analysis at AREVA NP. The KORIGEN code is a depletion code, which was developed at the research center in Karlsruhe starting from original ORIGEN coding. Basically, in MCOR, the ORIGEN-S input generation and output extraction subroutines were removed and replaced with the KORIGEN input generation and output extraction subroutines. Also, the depletion code execution subroutine was modified since the ORIGEN-S code is executed through SCALE driver while KORIGEN is executed as a stand-alone code.

3.2 Utilization of thermal flux for the depletion calculation

KORIGEN requires three-group spectral coefficients and thermal flux in order to perform the depletion calculation while the previous PSU-MCOR scheme uses power level in the depletion calculation. Since the power level was no longer used, new subroutines were then added to calculate the thermal flux and the three-group spectra namely: THERM, RES and FAST.

In general, the flux level is calculated based on the total fission power provided in the MCOR input. Since the MCNP code typically normalizes the output result per one source, the number of neutron sources which is dependent on the total fission power is first to be determined in order to calculate the actual flux level. The number of neutron sources is computed by

$$S = \frac{PW(CV)}{\sum_{i=1}^{all}\left(fis_i V_i\right)} \tag{3}$$

Where: S = Number of neutron sources (sources)
PW = Total fission power (MW)
fis_i = Fission rate tally of material zone i (MeV/source-cm^3)
V_i = volume of material zone i (cm^3)
CV = Conversion factor (6.242x10^{18} MeV/MW)

Once the number of neutron sources is obtained, the actual neutron flux level is calculated by

$$\phi_{g,i} = FT_{g,i} S \tag{4}$$

Where: $\phi_{g,i}$ = Neutron flux level of group g of material zone i
$FT_{g,i}$ = Neutron flux tally of group g of material zone i
S = Number of neutron sources (sources)

3.3 Online burnup cross section generation by the Monte Carlo calculation

The next improvement was the implementation of the online burnup dependent cross section calculated by the Monte Carlo calculation itself instead of the pre-calculated burnup cross section by TRITON. This methodology is supposedly superior to the previous pre-calculated burnup cross section since the burnup cross sections are derived based on the Monte Carlo calculation, which reflects the most current conditions in the most accurate way. The current AREVA-MCOR implementation determines the one-group burnup cross sections from the

reaction rate tally of the MCNP calculation by

$$\sigma_x = \frac{\text{Reaction "x" rate tally value}}{\text{Total flux tally value}} \quad (5)$$

To compromise between the computational time and the accuracy of AREVA-MCOR, eighty-eight isotopes, which one-group cross sections are updated by the Monte Carlo calculation, are selected from an importance ranking procedure performed by CASMO-4. The burnup cross sections of other isotopes not in this list are taken directly from the standard KORIGEN libraries pre-calculated for each fuel assembly type.

3.4 Predictor-Corrector depletion algorithm

The MCOR code is further improved to utilize a predictor-corrector depletion algorithm to account for the neutron spectrum changes from the beginning of the time step to the end of the time step. The implementation of the predictor-corrector depletion algorithm practically allows relatively larger burnup steps to be used for the Monte Carlo depletion calculation.

3.5 Expansion of the maximum number of tallies

The maximum number of tallies of MCNP5 used with the AREVA-MCOR version is expanded from 100 to 1000 so that AREVA-MCOR can be used with a problem having a number of burnup zones larger than 100 which is typical for cases with Gd_2O_3 fuel pins.

3.6 Input card enhancement and optimization

In the AREVA-MCOR version, several input cards were improved and some input cards were eliminated to streamline the input generation. Also, some input cards were added to the AREVA-MCOR version to provide more information needed with the new implementation.

3.7 Automatic restart capability

The restart capability is practically crucial and must be implemented in the Monte Carlo coupled depletion code. Although the previous PSU-MCOR code can be restarted by preparing a new set of inputs to continue from the earlier-terminated burnup step, this task is very error-prone since one must check the terminated burnup step and get the current burnup information from the previous run output. Thus, the automatic restart capability was implemented in the AREVA-MCOR code to enhance the simulation features. In the restart mode, the current AREVA-MCOR code automatically checks for the earlier terminated-burnup step, extracts the current burnup and rereads input from the input echo section in the output file. This automatic restart capability continues the earlier-terminated calculation without having to create a new set of inputs like the previous PSU-MCOR code.

4. AT10MOX calculation model

The Atrium-10 MOX fuel assembly (AT10MOX) [7] was used as the computational model for the comparisons in this paper. The fuel assembly was modeled in half symmetry with all reflective boundaries as shown in Figure 1. Each fuel pin was treated as a fuel zone. For PSU-

MCOR and AREVA-MCOR, the fuel pin with Gd_2O_3 was divided into 10 equal-volume rings. The simulation of the same model was performed with CASMO-4 and OCTOPUS except that the Gd_2O_3 fuel pin was not divided into rings in the OCTOPUS model. Furthermore, the PSU-MCOR code requires the pre-calculated one-group burnup dependent cross sections, which were generated by the TRITON code as shown in Figure 2. In the burnup dependent cross section generation, the fuel assembly was simulated in full symmetry since this geometry was easier to model in rectangular coordinates in TRITON. Also, small approximations were applied to the geometry, i.e., square corners are used instead of the round corners, due to the geometry limitation of the TRITON code. For PSU-MCOR and AREVA-MCOR, continuous cross sections were generated from ENDF/B-VI data by using the nuclear data processing code NJOY99.81 while the OCTOPUS model was simulated with continuous cross sections derived from JEF2.2 with an exception that the cross section of ^{235}U was taken from ENDF/B-VI.

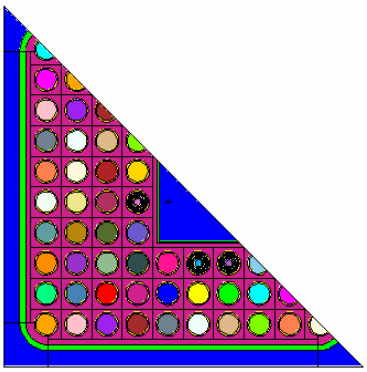

Figure 1: AT10MOX model

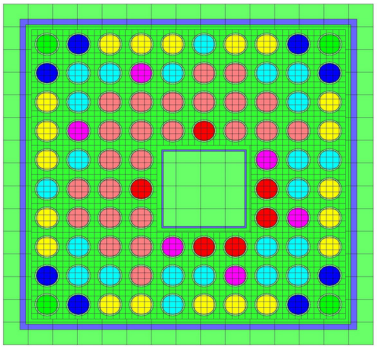

Figure 2: The AT10MOX model utilized by TRITON code to generate burnup dependent cross sections

5. Results

Table 1 and Figure 3 present the comparison of the k_{inf} as a function of burnup of each model. In addition, the root mean square (RMS) of the fission rate differences among each pair of codes is plotted in Figure 4. Finally, the normalized ratios of isotopic contents at the discharge exposure of 70GWD/MTU of each pair of codes are tabulated in Table 2.

Table 1: Comparison of AT10MOX results for k_{inf} as a function of burnup

BU (GWD/MTU)	OCTOPUS	AREVA-MCOR	PSU-MCOR	CASMO4
0.0	1.13954 ± 0.0049	1.13811 ± 0.0032	1.13810 ± 0.0047	1.14047
0.5	1.11706 ± 0.0048	1.11603 ± 0.0028	1.11637 ± 0.0042	1.11733
5.0	1.11558 ± 0.0046	1.11513 ± 0.0038	1.11897 ± 0.0046	1.11661
10.0	1.10775 ± 0.0045	1.10589 ± 0.0027	1.11302 ± 0.0042	1.10960
15.0	1.08164 ± 0.0045	1.07948 ± 0.0029	1.08494 ± 0.0042	1.08345
20.0	1.05517 ± 0.0045	1.05170 ± 0.0034	1.05719 ± 0.0043	1.05694
30.0	1.00635 ± 0.0044	1.00325 ± 0.0033	1.00579 ± 0.0043	1.00874
50.0	0.92668 ± 0.0045	0.92042 ± 0.0031	0.91923 ± 0.0041	0.92531
70.0	0.86558 ± 0.0042	0.85700 ± 0.0027	0.85084 ± 0.0038	0.85661

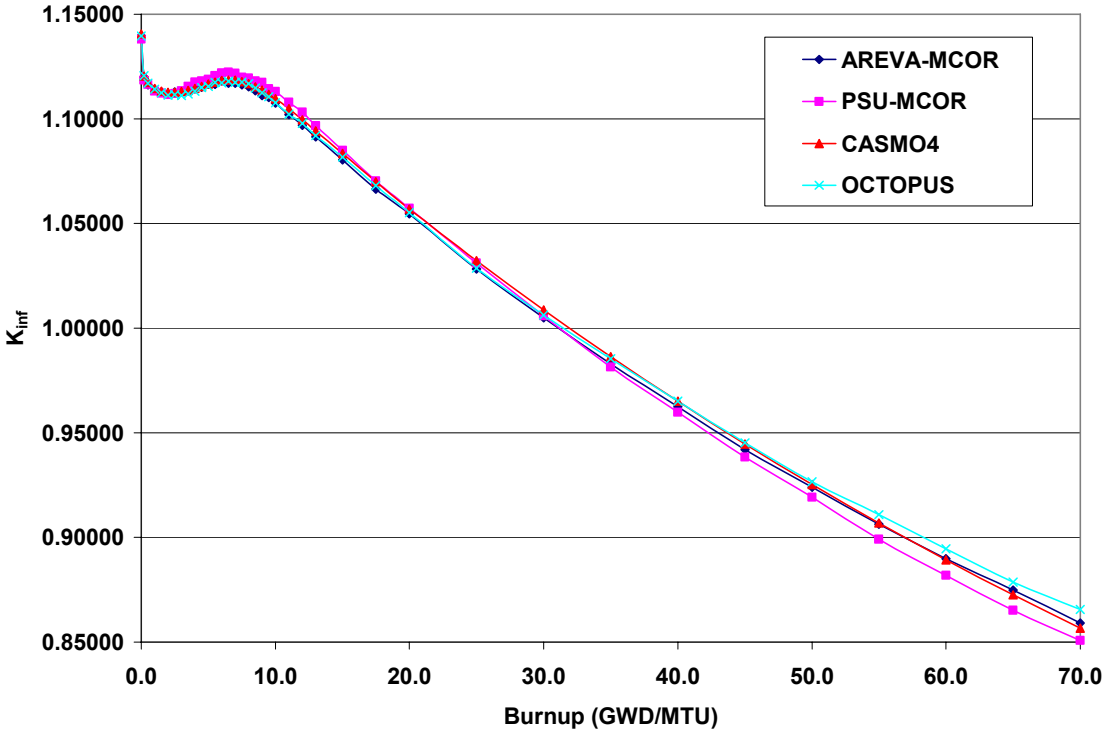

Figure 3: Comparison of k_{inf} as a function of burnup

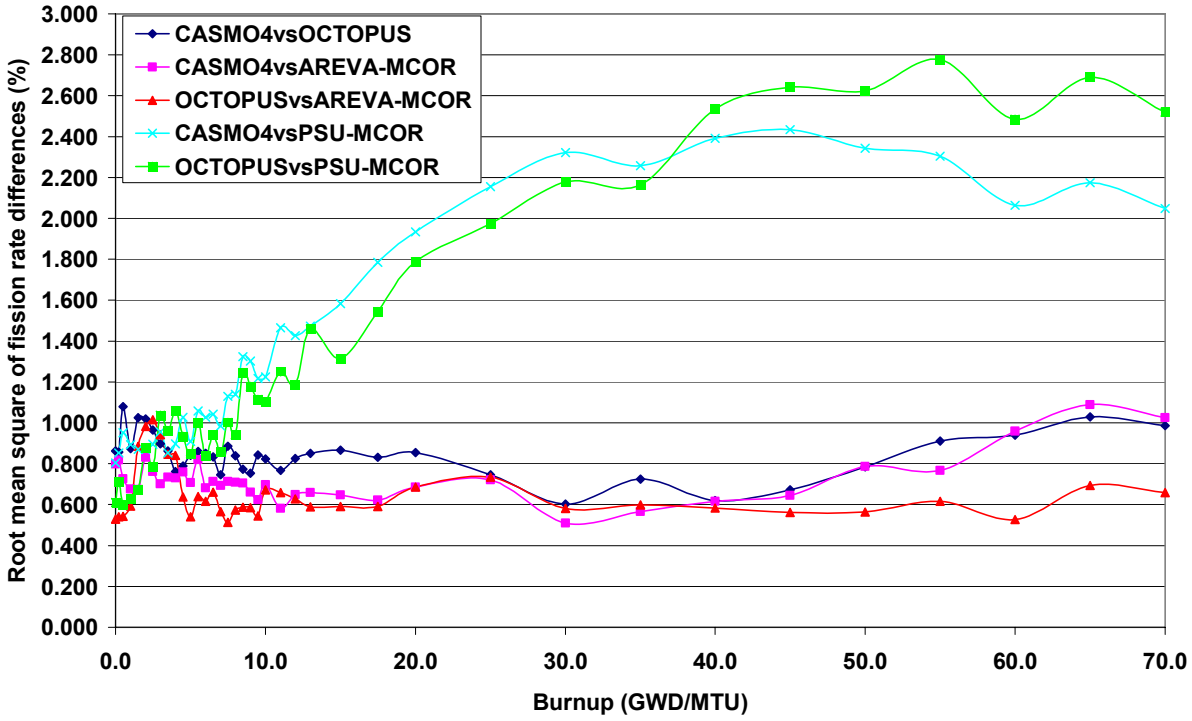

Figure 4: Comparison of fission rate distribution as a function of burnup

Table 2: Comparison of normalized ratios of isotopic contents at 70 GWD/MTU

Isotope	Normalized ratios of isotopic contents at 70 GWD/MTU				
	P-MCOR / OCTOPUS	P-MCOR / CASMO4	A-MCOR / OCTOPUS	A-MCOR / CASMO4	CASMO4 / OCTOPUS
Cs-135	0.988	1.022	0.954	0.992	1.034
Nd-143	0.821	0.822	0.991	0.997	1.001
Nd-145	1.003	1.001	0.983	0.991	0.998
Nd-148	1.020	1.009	0.900	0.901	0.989
Sm-147	0.796	0.824	0.988	1.020	1.036
Sm-148	0.812	0.794	0.962	0.957	0.977
Sm-149	0.982	0.949	0.974	0.938	0.966
Sm-150	0.929	1.008	0.998	1.096	1.086
U-234	0.954	1.040	0.996	1.070	1.09
U-235	0.831	0.849	0.993	0.988	1.022
U-238	0.998	0.997	1.005	1.003	0.999
Pu-238	0.894	1.083	1.016	1.223	1.212
Pu-239	0.950	0.986	0.994	1.018	1.037
Pu-240	0.930	0.977	1.004	1.046	1.051
Pu-241	0.931	0.951	1.001	1.013	1.021
Pu-242	1.087	1.068	1.006	0.991	0.982
Am-242m	1.402	1.303	1.397	1.268	0.929
Cm-244	1.090	1.174	0.981	1.079	1.077
Cm-245	0.719	0.770	0.963	1.055	1.071

As it can be seen, slight improvements of AREVA-MCOR over PSU-MCOR in k_{inf} values as a function of burnup are observed when comparing against CASMO-4 and OCTOPUS. Nevertheless, the comparisons of fission rate distributions illustrate more clearly the improvements of AREVA-MCOR over PSU-MCOR. In the PSU-MCOR results, the RMS difference propagates to 2%-2.5% as the burnup increases while the RMS difference generally remains less than 1%-1.5% in the AREVA-MCOR results. The evidence of the improvements is even clearer when considering the isotopic content comparison. The main actinides of the AREVA-MCOR results agree well (<1%-2%) with those from OCTOPUS and CASMO-4. Relatively greater isotopic content deviations are observed when comparing the PSU-MCOR results with OCTOPUS and CASMO4. It is also noted that, since the fuel pins with Gd_2O_3 are not divided into rings in the OCTOPUS model, one can observe practically larger differences between AREVA-MCOR and OCTOPUS at low exposure (<10 GWD/MTU) than at higher exposure. However, the deviations from the effects of Gd rings are considered relatively low in the AT10MOX model since the fuel pins with Gd_2O_3 are using only 1.5% Gd concentration. It is absolutely important in a higher concentration Gd model that the fuel pins with Gd_2O_3 be divided into rings.

In addition, the propagations of the isotopic content differences of some main actinides

between AREVA-MCOR and OCTOPUS as well as between AREVA-MCOR and CASMO-4 are shown in Figure 5 and Figure 6.

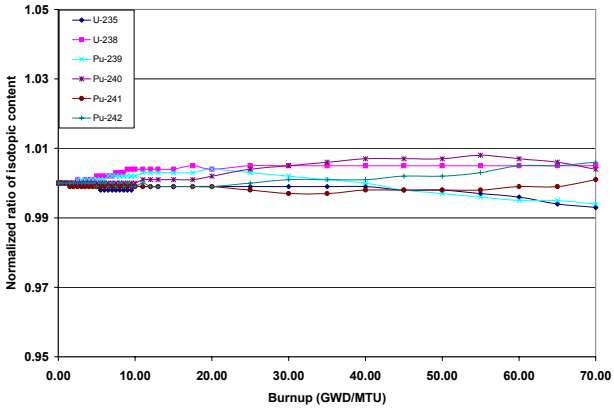

Figure 5: Normalized ratio $[\frac{A-MCOR}{OCTOPUS}]$ of main actinides as a function of burnup

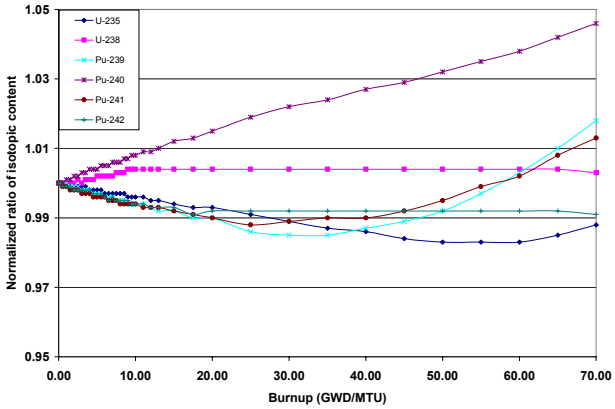

Figure 6: Normalized ratio $[\frac{A-MCOR}{CASMO-4}]$ of main actinides as a function of burnup

The results in Figure 5 and Figure 6 assure that the differences in isotopic contents of these main actinides are relatively low throughout burnup. Better agreements are generally observed for the isotopic content differences between AREVA-MCOR and OCTOPUS than the isotopic content differences between AREVA-MCOR and CASMO-4. As one can see from Figure 6, the largest isotopic content difference between AREVA-MCOR and CASMO-4 is ^{240}Pu. Although this deviation is quite noticeable and seems to increase linearly with exposure, it is still within reasonable bound (<5%) and does not occur when comparing with OCTOPUS.

6. Pin cell benchmark models

To further verify the accuracy of AREVA-MCOR, two pin cell models from the benchmark problem suite for reactor physics study of LWR next generation fuels [8] were simulated. These models were the UO_2 pin cell at hot temperature and the MOX pin cell at hot temperature. The UO_2 pin cell model is basically a pin cell model with 6.5% w/o ^{235}Uenriched fuel with the discharge exposure of 70 GWD/MTU. The fuel is at the hot temperature of 900K during burnup. Similarly, the MOX pin cell model has the same geometry as the UO_2 pin cell model. The Pu-fissile content in this model is 11% w/o. Also, the fuel is at the hot temperature and the discharge exposure is at 70 GWD/MTU. Table 3 presents the normalized ratio of the isotopic content comparisons at the 70 GWD/MTU discharge exposure of AREVA-MCOR against CASMO-4, HELIOS [9], and TRIPOLI-PEPIN [10] (a Monte Carlo depletion system developed at CEA).

Table 4: Comparison of normalized ratios of isotopic contents at 70 GWD/MTU

Isotopes	AREVA-MCOR TRIPOLI-PEPIN	AREVA-MCOR HELIOS	AREVA-MCOR CASMO4
U235	1.00	1.04	0.99
U238	1.00	1.00	1.00
Np237	1.17	1.09	1.09
Pu238	1.17	1.13	1.14
Pu239	1.00	1.02	1.01
Pu240	1.01	1.05	1.06
Pu241	1.00	1.04	1.01
Pu242	1.02	1.07	1.01
Am242m	0.83	0.70	0.87
Tc99	1.00	1.01	1.05
Rh103	1.00	0.98	1.00
Cs133	1.00	0.93	1.05
Sm149	0.99	1.00	0.95
Sm150	0.99	1.12	1.09
Nd143	0.99	1.01	1.00
Nd145	0.99	1.02	1.00
Eu153	1.00	0.95	0.91
Gd155	1.01	2.07	1.67

The comparisons in Table 4 demonstrate that the agreements between AREVA-MCOR and other codes are good in general. Particularly, AREVA-MCOR and TRIPOLI-PEPIN, which is another Monte Carlo depletion code, agree very well for most isotopes (<1%).

7. Conclusions

Several improvements were performed in order to upgrade the PSU-MCOR code version to the AREAVA-MCOR code version. Additionally, the handling of AREVA-MCOR is now more user-friendly and thus easy to use. In general, the improved version has shown significant increase in the accuracy of the results of k_{inf}, fission rate distributions and isotopic contents when compared against CASMO-4 and OCTOPUS in the AT10MOX model. Further, the comparisons of the UO_2 and MOX pin cell models also show good agreements with other commercial codes, as well as with the TRIPOLI-PEPIN Monte Carlo depletion code.

References

1) "MCNP - A General Monte Carlo N-Particle Transport Code, Version 5", Los Alamos National Laboratory, April 2004.
2) O. W. Hermann, and R. M. Westfall, "ORIGEN-S: SCALE system module to calculate fuel depletion, actinide transmutation, fission product buildup and decay, and associated radiation source terms", Oak Ridge National Laboratory, March 2000.
3) U. Fischer and H. W. Wiese, "Improved and Consistent Determination of the Nuclear Inventory of Spent PWR Fuel on the Basis of Cell-Burnup Methods Using KORIGEN",

KFK-3014; ORNL-tr-5043, January 1983.
4) M. Edenius, B. H. Forssen and C. Gragg, "The Physics Model of CASMO-4", Proc. Adv. in Math., Comp. & Reactor Physics, Vol. 10-1, Pittsburgh (1991)
5) J.L. Kloosterman, J.C. Kuijper, and P.F.A. de Leege, "The OCTOPUS Burnup and Criticality Code System", Report ECN-RX—96-032, Netherlands Energy Research Foundation ECN, June 1996
6) M. D. DeHart, "TRITON: a two-dimensional depletion sequence for characterization of spent nuclear fuel", Oak Ridge National Laboratory, May 2004.
7) "Physics of Plutonium Recycling Vol. VII: BWR MOX Benchmark Specification and Results", NEA OECD 2003 ISBN 92-64-1995-0
8) A. Yamamoto, T. Ikehara, et. al., "Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels", Journal of Nuclear Science and Technology, Vol. 39. No. 8, p.900-912, August 2002
9) Studsvik^{TM}Scandpower, "HELIOS Documentation", April 1, 2000.
10) Y. Lee, B. Roesslinger, and A. Tsilanizara, "TRIPOLI-PEPIN Depletion Code and Its First Numerical Benchmarks for PWR High-Burnup UO2 and MOX Spent Fuel", Proceedings of the M&C 2005 Conference, September 2005, Avignon, France