DETERMINATION OF THE ISOTOPIC COMPOSITION OF NEUTRON IRRADIATED NUCLEAR FUEL MATERIALS BY MCNPX

Štefan Čerba[1], Vladimír Nečas[1]

[1] *Institute of Nuclear and Physical Engineering FEIIT SUT in Bratislava*
E-mail: stefan.cerba@stuba.sk

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1. Introduction

Since the beginnings of nuclear science there have existed several deterministic codes applicable for fuel depletion calculation; however, these tools employ a variety of approximations about system physics in order to achieve a quick result. In some cases the implementation of inadequate assumption may have lead to a drawing of false system physics. As advanced reactor concepts challenge the accuracy of current modeling technologies, a higher fidelity depletion calculation is crucial to properly model advanced reactor concepts [1]. This study deals with the verification of the burnup capabilities of the MCNPX code. For such a purpose the IV-B phase of the OECD NEA Burnup credit benchmark has been chosen. Before the verification was carried out, it was necessary to declare the value of the system bias for MOX fuel. To do so several tasks from [2] were carried out.

2. Calculation method

MCNPX is a stochastic Monte-Carlo steady-state reaction rate calculator code that links the MCNP code with CINDER90. MCNPX solves the Ludwig-Boltzman transport equation by randomly sampling the occurring physical events. CINDER90 is a zero dimensional deterministic number density calculator code. The CINDER90 computation process involves utilizing linear Markovian chains to determine the time dependent nuclide densities. The CINDER90 depletion algorithm is placed within the MCNPX code package. The coupled depletion process involves a Monte-Carlo steady-state reaction rate calculation linked to a deterministic depletion calculation. MCNPX runs a steady state calculation to determine the system eigenvalue collision densities, recoverable energies from fission and neutrons per fission events. In order to generate number densities for the next time step the CINDER90 code takes the MCNPX generated values and performs a depletion calculation. MCNPX then takes the new number densities and caries out a new steady-stated calculation. The process repeats itself until the final time step. The MCNPX transmutation process is capable of tracking 3400 isotopes; however the current ENDF/B VII distribution only contains transport cross sections for 393 isotopes. For nuclides containing tabulated cross section data in the MCNPX data library the codes uses the generated continuous energy flux, for the rest MCNPX uses theoretically models to generate cross sections. MCNPX generates a 63 group Monte-Carlo flux and matches to 63 group cross sections from the CINDER data file. MCNPX calculates continuous energy integral reaction rates only for the following reaction rates: (n, fission), (n, γ), (n, 2n), (n, 3n), (n, p) and (n, α). For the remaining reaction rates MCNPX calculates a 63 group Monte-Carlo flux and matches to a generalized 63 group CINDER cross-section set. Executing a successful depletion process involves accounting for the reactivity effects of as many fission products as possible. CINDER90 contains energy dependent fission yields for 1325 fission products. Depending on the neutron energy and the fissionable isotope MCNPX selects the most appropriate fission product yield [1].

The NJOY code is a modular computational system. Each of the modules solves a specific part of the given problem. The combination of its modules makes NJOY an effective tool for cross section library processing. For basic neutron cross section library processing the

following modules are to be used: MODER, RECONR, BRODR, LEAPR, PURR, GASPR and ACER [3]. The modules of the NJOY code can be easily automated using the ".bash" scripting language in order to save time and to obtain results in MCNP usable form.

3. Description of a calculation

3.1 Bias calculation

The bias represents the systematic error of the calculation, which is the deviation from the experiment. This error depends on the used computation code, on methodology, on the used cross section libraries and also on other significant effects. The "Handbook of international evaluated criticality safety benchmark experiments" [2] provides benchmark tasks in order that different users can validate their codes. This handbook, made on the basis of real criticality safety experiment, encompasses benchmark tasks applicable for various reactor and fuel types. Since the aim of this study was to evaluate the bias for MOX fuel the following tasks were performed: MIX-COMP-THERM-002, MIX-COMP-THERM-005 and MIX-COMP-THERM-011 [2]. The first two cases represent fresh MOX fuel in light-water thermal reactors and the third one is a pool storage of irradiated MOX fuel from sodium fast reactors. Each of the tasks consists of 6 subtasks and the calculations were performed for 3 cross section library evaluations: ENDF/B-VII.0 [4], JEFF-3.1.1 [5] and JENDL-4.0 [6].

3.2 Burnup calculation

The IV-B phase of the OECD Burnup Credit Benchmark [7] is addressed to a MOX fuel in light water reactors. The benchmark task encompasses 6 cases, 3 geometry specifications and 2 different fuel compositions. This study deals with the CASE3 of the IV-B benchmark task, which is a calculation of a single LWR fuel assembly with LWR discharged Pu in fresh fuel. The considered fuel assembly consists of 289 fuel pins placed in 17x17 square lattices. Each fuel pin is surrounded by Zircaloy-2 cladding and the remaining part of the lattice is filled with borated water (600 ppm). The desired burnup is 48 GWd/t_{HM}. The aim is to compare the k_{eff} and the isotopic composition at three burnup steps (16, 32 and 48 GWd/t_{HM}) and after 5 years of cooling. Additional information about this benchmark can be found in [7].

4. Calculation results

4.1 Bias calculation

The bias calculations were carried in MCNP5 1.6 on a CentOs 6.1 Kernel Linux 2.6.32 x86_64 system across 36 AMD OPTERON 6172 processors. Since the input files were included in [2], it was not necessary to model the geometries. To fully utilize the temperature dependence of the problem a new set of cross section libraries has been processed using the NJOY99 code system. Considering the number of results it was advantageous to perform statistical evaluation. 3 main and 4 auxiliary parameters were investigated (eq.1-4).

$$bias_i = k_{eff\,i}^{benchmark} - k_{eff\,i}^{MCNP} \quad (1)\ [8]$$

$$\sigma_i = \sqrt{\left(\sigma_i^{benchmark}\right)^2 + \left(\sigma_i^{MCNP}\right)^2} \quad (2)\ [8]$$

$$\sigma_{bias} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(bias_i - \overline{bias}\right)^2} \quad (3)\ [8]$$

$$\sigma_{comb} = \sqrt{\left(\sum_{i=1}^{n} \sigma_i^2\right) + \sigma_{bias}^2} \qquad (4)\ [8]$$

The bias represents the absolute deviation between the calculated and the benchmark $k_{eff,}$ and σ_i is the related combined standard deviation calculated from the standard deviations from MCNP and the one provided by the authors of the benchmark task. $\overline{bias}$ is the average of the calculated partial biases and σ_{bias} is its corresponding standard deviation. The main parameter that determines the true uncertainty of the calculation is σ_{comb}. It is the combined standard deviation of σ_i and σ_{bias} and it reflects the variance of $k_{eff\,i}^{MCNP}$ and σ_i^{MCNP} either. The comparison of the calculation results is shown in Tab. 1.

Tab. 1. *Results of the bias calculation*

	ENDF/B VII.0	JEFF 3.1.1	JENDL 4.0
$\overline{bias}$	-0.003499	-0.001623	-0.003932
σ_{bias}	0.002307	0.001978	0.002649
σ_{comb}	0.013886	0.013829	0.013943

Concerning the average bias, the JEFF-3.1.1 libraries provided the most accurate results, however their partial variances were a little higher than in the case of ENDF/B VII.0 and JENDL 4.0 libraries, therefore the difference in σ_{comb} was not so significant as in the case of $\overline{bias}$. The results are clearly showing that the system bias and the combined standard deviation are low enough to conclude that all 3 cross section library sets have been processed correctly and they can be used for further applications.

4.2 Burnup calculation

Since the cross section libraries prepared in NJOY99 had been benchmarked and the bias had been found to be appropriate, it was possible to perform the burnup calculation. The tasks were carried out in MCNPX 2.7 with point neutron sources defined in every pin, with 100 inactive and 300 active cycles and using 10 000 neutron histories per cycle. In order to achieve conditions of infinite lattice reflective boundaries were used. The desired final burnup level of 48 GWd/t_{HM} was achieved in 32 successive burnup steps. The total system power was calculated to be 17.9 MW_{th}. The comparison of the k_{eff} is shown in Fig.1.

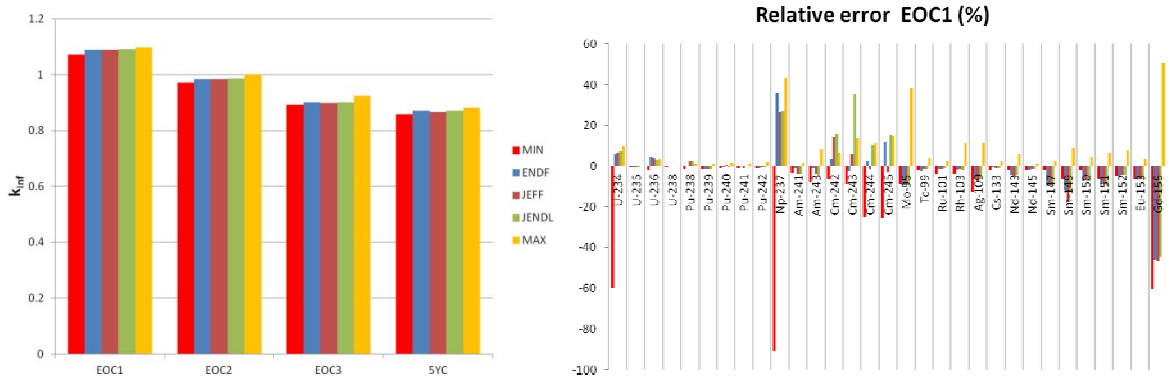

Fig.1: *Comparison of the calculated k_{eff} per cycles and the isotopic composition*

The results are showing very good agreement in the calculation of k_{eff}. All the 3 libraries provided results within the range of other codes. There were some differences between them; however there were small enough to be considered as negligible. The comparison of the concentrations of the most important isotopes is also in Fig.1. The relative error represents the relative deviation of the calculated results from the average values

obtained from other participants. In low burnup levels the agreement was very good. The relative errors were within 1 % for almost all nuclides. The largest deviations were observed in the case of 234-U, 237-Np, 242-Cm, 243-Cm, 244-Cm, 95-Mo, 109-Ag and 149-Sm. The differences in the cases of 234-U, 237-Np and 244-Cm might have been caused by the wide range of results from other code. The other discrepancies might not have been necessarily caused by the inaccuracy of the program but rather by the different cross section evaluations. In high burnup levels the deviations were slightly increased, but the agreement was still satisfactory. The best agreement was found in the case of ENDF/B VII cross section libraries.

5. Conclusions

The aim of this study was to examine whether the MCNPX code can provide acceptable results in fuel depletion calculation. There sets of cross section libraries have been process with the NJOY code on the basis of three different cross section evaluations. These libraries had been validated and the statistical evaluation of the results showed that all three sets had been processed correctly and they are applicable for the burnup calculation. To verify the burnup capabilities of the MCNPX code the third case of the IV-B phase of the OECD NEA Burnup credit benchmark [7] has been chosen, which is a code to code validation**.** The main task was to compare the k_{eff} and the isotope concentrations at 4 burnup steps. The comparison of the calculation results clearly showed that the results obtained by MCNPX were in the range of other codes used in nuclear research. There were some discrepancies between the calculated and the benchmark data, but it was not possible to definitely conclude whether they were caused by the accuracy of the program or not. On the one hand, the results showed that some discrepancies may have been caused by the different cross section evaluations used in the calculation. On the other hand we cannot determine, how accurate the results from the other codes were; thus the deviations that at the first glance seemed to be high might not have necessarily meant inaccuracies in the calculation. Despite the fact that the MCNPX code is still in development, we can conclude that the code is capable of obtaining relevant results.

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