Nuclear data impact on multiplication factor and reactor physics parameters calculation for experiments simulating damp MOX powders

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Abstract. The paper presents calculation results for experiments performed to address needs of the MOX fuel manufacturing process and particularly with low-moderated MOX fissile media. Computation of criticality for eleven configurations and reaction rates ratios for major and minor actinides are performed with CRISTAL french criticality code package, and the reference MCNPX and TRIPOLI-4.3 codes. The multigroup JEF-2.2, JEFF-3.1 and continuous energy JEF-2.2, JEFF-3.1, ENDF/B-VI and ENDF/B-VII neutron cross sections are used for the computations. The results are compared to verify group-wise calculations. Then the obtained calculated values will be used to predict eigenvalue accuracy for applications with damp MOX powder, and to validate ^{238}U, ^{239}Pu, and ^{240}Pu cross sections.

1 Introduction

The experimental program was specifically performed to obtain additional integral benchmark data for the MOX fuel manufacturing process and particularly with low-moderated MOX fissile media[1, 2]. A series of critical configurations was performed at the Institute of Physics and Power Engineering (IPPE), Obninsk, Russia at the BFS-1 critical facility.

The detailed benchmark specifications have been issued for the eleven configurations and published in the ICSBEP and IRPhEP Handbooks [3, 4].

The main goal of this work was the computational analysis of the experiments with the CRISTAL criticality package [5], verification of the CRISTAL results by comparison with the reference MCNPX [6] and TRIPOLI-4.3 [7] codes. The totality of the results, then, will be involved in the "adjustment" procedure in order to 1) predict k_{eff} bias and its uncertainty for applications with damp MOX powder, and 2) validate ^{238}U, ^{239}Pu, and ^{240}Pu cross sections.

2 Description of the experiments

In the experiments damp MOX powders were simulated by assembling tightly packed cylindrical aluminium tubes containing various ratios of metallic plutonium and depleted uranium dioxide fuel pellets. The tubes with outer diameter of 5.0 cm and 0.1 cm wall thickness and 5.1 cm hexagonal pitch were put inside a cylindrical steel vessel with 200.2 cm inner diameter, and 277.5 cm height.

The specified water content was achieved by periodically including polyethylene dowels and/or polyethylene pellets. The composition of fuel material was investigated with two types of plutonium with different content of ^{240}Pu. Axial and radial reflectors were depleted uranium dioxide.

Principal characteristics of the experiments are shown in table 1.

Table 1. Principal characteristics of the BFS assemblies.

BFS	Neutron Spectrum	Pu Content, wt.%	^{240}Pu Content, wt.%	H/Pu	Equiv. Water Content, wt.%
97/1	Fast	22	4.6	0.0	0.0
97/2	Fast	22	4.6	1.0	0.6
97/3	Mixed	22	4.6	4.7	2.5
97/4	Mixed	22	4.6	6.0	3.4
99/1	Mixed	22	10.1	4.7	2.5
99/1A	Mixed	22	10.1	4.7	2.5
99/2	Mixed	22	10.1	6.0	3.4
101/1	Fast	10	4.6	2.5	0.7
101/2	Mixed	10	4.6	4.7	1.3
101/2A	Mixed	10	4.6/10.1*	4.7/7.4	1.3/2.1
101/3	Mixed	10	4.6	7.5	2.1

* Different characteristics shown relate to inner and outer core tubes.

The following measurements performed on the assemblies are analysed in the paper:

 – criticality;
 – spectral indices;
 – central reaction rate ratios measured on the BFS-97/1, -97/3, -99/1, and -101/2 assemblies.

A triple-segment fission chamber with fissile deposits of ^{235}U, ^{238}U, and ^{239}Pu was used for simultaneous measurements of ^{235}U, ^{238}U, and ^{239}Pu fission rates. Measurements at the core center were performed in the empty channel formed by extraction of the central fuel tube.

Ratios of minor actinides (^{237}Np, ^{241}Am, ^{243}Am, ^{244}Cm, and ^{245}Cm) to ^{239}Pu fission rates (F^{MA}/F^{Pu239}) were also measured by absolute fission chambers in the center of the core.

The ^{238}U capture rate to ^{235}U fission rate ratio (C^{U238}/F^{U235}) was measured by activation method. Small square or round foils, placed in the central cell of the assembly either between two hemi cylindrical halves of a dismountable depleted uranium dioxide pellet or between two vertically adjacent depleted uranium dioxide pellets, were used for activation.

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3 Modelling of the experiments

3.1 Criticality

The CRISTAL general-purpose criticality analysis package has been used to compute k_{eff} values for all the configurations. Its standard route is based on JEF-2.2 [8] nuclear data and comprises the following tools:

- APOLLO2 [9] for lattice calculation using multigroup non adjusted cross-section library, and
- MORET 4 code [10] for 3D calculation of neutron transport with Monte Carlo method.

The following approximations are adopted in the APOLLO2 code used for this study:

- 172-energy group structure;
- Anisotropy: P_5 for U, Pu, ^{241}Am and CH_2; P_1 for other nuclides;
- Resonance self-shielding using infinite dilution cross section approach;
- Flux calculation with the collision probability method;
- Use of equivalent theorem for macroscopic cross section preparation.

The JEFF-3.1 library [11] was also used with APOLLO2-MORET 4 route.

Since the calculation of the experiments addressing MOX issue was a first attempt to analyse the critical configurations assembled on the BFS facility, an effect of one-dimensional heterogeneous cell model on the analysis's accuracy was estimated and the k_{eff} results are verified by comparison with the reference TRIPOLI-4.3 and MCNPX codes.

The JEF-2.2, JEFF-3.1, ENDF/B-VI.6 and ENDF/B-VII [12] continuous energy neutron data were used with MCNPX.

The APOLLO2-MORET 4 calculation models are the following: set of infinite plates for lattice computations and detailed description of the core tubes in the MORET 4 inputs. Reflector is presented as homogeneous.

The detailed models of the configurations are created for calculations with references tools.

3.2 Reaction rate ratios

To obtain spectral indices an average neutron energy-dependent flux in the volume of interest was computed and multiplied by the specific cross section as follows: $R_x = \int \bar{\phi}_V(E)\sigma_R^x(E)dE$, where $\bar{\phi}_V$ is the neutron flux averaged on the volume of interest; σ_R^x is the microscopic cross section of reaction R corresponding to isotope x.

Calculations of these rates are performed using the track length estimate of cell flux tally (F4) with the MCNPX. Variance reduction methods are used to compute capture rate for ^{238}U.

The fission rates are calculated with the APOLLO2-MORET 4 route as follows:

$$R_x = \sum_{g=1}^{172} \bar{\phi}_V^g \sigma_{Rx}^g,$$

where $\bar{\phi}_V^g$ is volume-averaged neutron flux estimated on neutron track length, and σ_{Rx}^g is the microscopic cross sections in group g of reaction R corresponding to isotope x, tabulated in multigroup library (without taking into account resonance self-shielding calculation). All the values obtained in such a way are verified by comparison with the MCNPX results. The ^{238}U capture rates are not computed.

The computation of the reaction rate ratios is performed as follows: $R = R_x/R_y$, where R_x and R_y are spectral indices of interest, calculated with the MCNPX or APOLLO2-MORET 4 codes.

The dispersions associated with the mentioned reaction rate ratios are calculated as follows:

$$\Delta\left(\frac{R_x}{R_y}\right) = \sqrt{\left(\frac{\Delta R_x}{R_y}\right)^2 + \left(\frac{R_x \Delta R_y}{R_y^2}\right)^2}.$$

4 Results

The results of the above described criticality and reaction rate ratios calculations are presented in the figures and the tables in this paragraph. The quoted statistical uncertainties are given as single standard deviation.

4.1 Criticality

Table 2. Comparison of JEF-2.2 and JEFF-3.1 k_{eff} results computed with APOLLO2-MORET 4 and MCNPX codes.

BFS	H/Pu	^{240}Pu Content, wt.%	$C^{JEF-2.2}/C^{JEFF-3.1} - 1, \%$	
			APOLLO2 /MORET 4	MCNPX
97/1	0	4.6	−0.47±0.04	−0.08±0.03
97/2	1.1	4.6	−0.49±0.04	−0.07 ±0.03
97/3	4.7	4.6	−0.61±0.04	−0.32±0.03
97/4	6	4.6	-	−0.33±0.03
99/1	4.6	10.1	−0.72±0.04	−0.44±0.03
99/1A	4.6	10.1	−0.79±0.04	−0.48±0.03
99/2	5.9	10.1	−0.74±0.04	−0.36±0.03
101/1	2.4	4.6	−0.65±0.04	−0.04±0.03
101/2	4.7	4.6	−0.38±0.04	−0.15±0.03
101/2A	4.7	4.6/10.1	−0.59 ±0.04	−0.20±0.03
101/3	7.4	4.6	−0.47±0.04	−0.30±0.03

Table 3. k_{eff} values computed with MCNPX code, C/E-1 (%).

BFS	JEF-2.2	JEFF-3.1	ENDF/B-VI.6	ENDF/B-VII	Unc., %
97/1	−0.71	−0.64	−0.10	−0.71	0.29
97/2	−0.47	−0.40	0.03	−0.22	0.26
97/3	−0.19	0.18	0.07	0.32	0.31
97/4	−0.33	0.04	−0.10	0.16	0.27
99/1	0.57	1.06	1.12	1.19	0.28
99/1A	0.45	0.93	0.90	1.00	0.28
99/2	0.54	0.92	0.95	1.08	0.26
101/1	−0.91	−0.86	0.00	−0.57	0.22
101/2	−0.69	−0.43	0.04	−0.23	0.21
101/2A	−0.38	−0.15	0.37	0.09	0.20
101/3	−0.81	−0.42	−0.31	−0.36	0.21
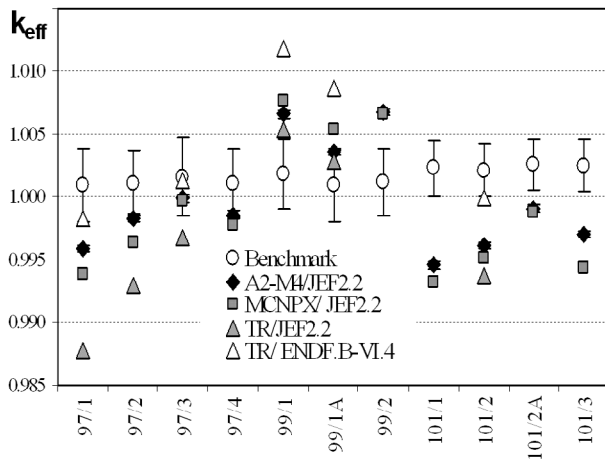
Fig. 1. Results of k_{eff} computations with APOLLO2-MORET 4 (A2-M4), TRIPOLI-4.3 (TR), and MCNPX codes.

4.2 Reaction rate ratios
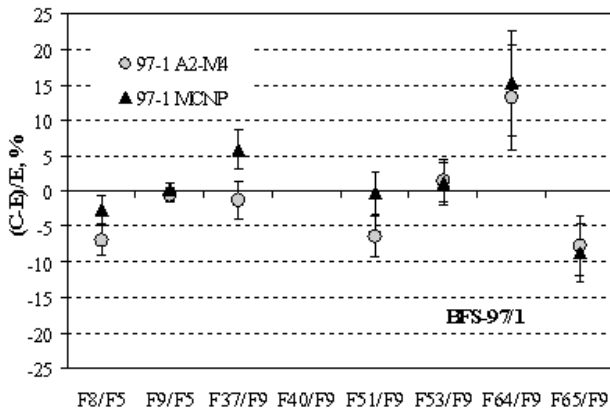
Fig. 2. Comparison of JEF-2.2 fission reaction rate ratios results computed with APOLLLO2-MORET 4 (A2-M4) and MCNPX codes for the BFS-97/1 assembly.

5 Conclusions

The calculated k_{eff} values tend to be lower than the benchmark values for configurations with weapons-grade Pu for all the libraries except ENDF/B-VI.6, and substantially higher for reactor-grade Pu, irrespective of the library used (see table 3, and fig. 1). Sensitivity study shows that this overestimate may hardly be due to error of ^{240}Pu content in Pu pellets (isotopic composition of Pu pellets corresponds to those indicated in passport data but was not measured).

Table 3 depicts that all the libraries produce good agreement for "small" configurations (BFS-97) with relatively high equivalent water content (> 2 wt.%).

The JEFF-3.1 k_{eff} results are systematically superior to the JEF-2.2 results (see tables 2 and 3).

Table 4. Minor actinides to ^{239}Pu fission rates computed with MC-NPX, C/E-1 (%).

	JEF-2.2	JEFF-3.1	ENDF/B-VII
	BFS-97/1		
F^{Np237}/F^{Pu239}	0.3 ± 2.7	5.9 ± 2.7	5.0 ± 2.7
F^{Am241}/F^{Pu239}	-3.3 ± 2.9	-0.3 ± 3.0	-0.7 ± 3.0
F^{Am243}/F^{Pu239}	5.25 ± 3.0	1.1 ± 3.0	1.1 ± 3.0
F^{Cm244}/F^{Pu239}	15.0 ± 7.4	15.3 ± 7.4	13.2 ± 7.4
F^{Cm245}/F^{Pu239}	-9.2 ± 4.2	-8.7 ± 4.2	-8.4 ± 4.2
	BFS-97/3		
F^{Np237}/F^{Pu239}	-2.6 ± 3.0	1.3 ± 2.9	1.9 ± 2.9
F^{Am241}/F^{Pu239}	-5.3 ± 3.3	-2.2 ± 3.2	-6.4 ± 3.2
F^{Am243}/F^{Pu239}	-3.4 ± 3.8	-5.3 ± 3.7	-4.5 ± 3.7
F^{Cm244}/F^{Pu239}	43.9 ± 2.0	38.7 ± 1.5	32.3 ± 1.5
F^{Cm245}/F^{Pu239}	-4.0 ± 5.1	1.5 ± 5.0	3.7 ± 5.0
	BFS-99/1		
F^{Np237}/F^{Pu239}	-5.3 ± 3.0	1.9 ± 3.3	4.3 ± 3.2
F^{Pu240}/F^{Pu239}	3.4 ± 3.2	-0.1 ± 3.5	6.0 ± 3.4
F^{Am241}/F^{Pu239}	-7.7 ± 3.3	0.6 ± 3.4	-1.5 ± 3.5
F^{Am243}/F^{Pu239}	-6.0 ± 3.8	-7.1 ± 4.1	-4.4 ± 4.0
	BFS-101/2		
F^{Np237}/F^{Pu239}	-5.1 ± 3.8	-2.6 ± 3.2	-1.6 ± 3.2
F^{Pu240}/F^{Pu239}	6.8 ± 3.9	-1.4 ± 3.3	0.1 ± 3.3
F^{Am241}/F^{Pu239}	-2.1 ± 4.0	-0.5 ± 3.5	-5.4 ± 3.5
F^{Am243}/F^{Pu239}	-9.7 ± 3.6	-13.9 ± 3.1	-11.8 ± 3.1

Table 5. ^{238}U and ^{239}Pu fission to ^{235}U fission rate computed with MCNPX, C/E-1 (%).

	JEF-2.2	JEFF-3.1	ENDF/B-VII
	BFS-97/1		
F^{U238}/F^{U235}	0.6 ± 2.0	-2.6 ± 2.0	-2.0 ± 2.0
F^{Pu239}/F^{U235}	1.3 ± 1.0	0.2 ± 1.0	0.0 ± 1.0
	BFS-97/3		
F^{U238}/F^{U235}	-4.1 ± 2.5	-4.8 ± 2.5	-7.5 ± 2.5
F^{Pu239}/F^{U235}	-3.6 ± 2.3	-1.3 ± 2.1	-6.4 ± 2.2

Table 6. ^{238}U capture rate to ^{235}U fission rate computed with MCNPX/JEF-2.2, C/E-1 (%).

Foil Position →	1	2	3
BFS-97/1	3.7 ± 2.7	7.1 ± 3.3	-
BFS-97/3	7.0 ± 3.3	9.7 ± 3.2	8.5 ± 2.7
BFS-99/1	7.1 ± 5.0	10.2 ± 4.3	7.3 ± 2.9
BFS-101/2	0.4 ± 2.8	0.2 ± 3.5	2.0 ± 4.1

Overall, ENDF/B-VI.6 produces better agreement with k_{eff} benchmark values than other libraries do for 8 configurations with weapons-grade Pu: majority of the ENDF/B-VI.6 results are within one standard deviations of the corresponding benchmark value, but only 3 ENDF/B-VII and JEFF-3.1 results, and 1 JEF-2.2 result are (see table 3).

The JEFF-3.1 and ENDF/B-VII libraries recently released produce big spread of the k_{eff} results (about 1.9%) for totality of the BFS configurations, while JEF-2.2 and ENDF/B-VI.6 libraries do 1.5% (see table 3).

Comparison of the multigroup APOLLO2-MORET 4 and continuous energy MCNPX results based on the same evaluated nuclear data files, are in a good agreement for both criticality and reaction rates computation with JEF-2.2 for all the configurations and for majority of the cases calculated with JEFF-3.1 (see table 2 and fig. 2). Discrepancy observed for k_{eff} obtained with JEFF-3.1 (see table 2) for configurations with fast neutron spectrum requires analysis of both point- and group-wise cross section preparation.

Most of the results for the fission reaction-rate calculations are within the evaluated uncertainty of the experimental values and statistical uncertainty of computations (see tables 4 and 5).

F^{Cm244}/F^{Pu239} ratios are significantly superior (up to 44%) to the measured values for all the libraries used (see table 4).

Systematic overestimation of the C^{U238}/F^{U235} ratio is discovered for "small" configurations computation based on JEF-2.2 library (see table 6).

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