Research Article

Verification of the ROSFOND/ABBN nuclear data based on the OECD/NEA benchmark on criticality safety of mox-fueled systems*

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Abstract

The paper presents the results of a computational analysis of the OECD/NEA benchmark conducted to estimate the accuracy of the critical safety parameters of multiplying MOX-fueled systems. The computational test is a set of 15 spherical multiplying systems that differ in their compositions and geometries. According to the test conditions, the k_{eff} values of the analyzed systems are unknown in advance. As part of the computational analysis of the test involving national codes and nuclear data libraries, along with the k_{eff} calculations, it is also necessary to estimate the a priori (due to the accuracy of the nuclear data used) and a posteriori (based on the accumulated experimental information) errors in the calculated k_{eff} values. Based on the benchmark, an updated version of the ROSFOND/ABBN-RF nuclear data was tested. The results of estimating the a priori and a posteriori errors in k_{eff} using the INDECS system for the proposed test models are presented. The analysis of the calculated data shows that (1) the observed spread in the k_{eff} values obtained from the Russian ROSFOND library and foreign evaluated nuclear data libraries (ENDF/B-VII.0, JEFF-3.2, JENDL-4.0) varies from –0.3 up to 0.8%; and (2) the deviation of the calculation results in the k_{eff} values obtained from the ROSFOND library and its group version, ABBN-RF, does not exceed 0.1%. The average a priori error in k_{eff} for all the tested options of multiplying systems is about 1% and, taking into account the selected set of experimental criticality data for MOX-fueled systems, including experiments at the BFS facilities, the average a posteriori error in k_{eff} can be reduced to 0.3%. The performed estimations confirm the high accuracy of the ROSFOND/ABBN-RF nuclear data for calculating the critical safety parameters of multiplying MOX-fueled systems.

Introduction

Following the main objective of the Organization for Economic Cooperation and Development Nuclear Energy Agency (OECD/NEA) to contribute to the safe development of nuclear energy for peaceful purposes in the participating countries through international scientific and technical cooperation, the Agency's various expert and

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working groups, along with collecting, analyzing and improving neutron data libraries, computational methods, programs, and experimental databases, pay considerable attention to the development and computational analysis of various benchmark tests (OECD/NEA 2018). Such tests are the most effective means of testing specialized national codes and neutron data libraries.

Under the auspices of the OECD/NEA, nuclear and critical safety issues are addressed by the Working Party on Nuclear Criticality Safety (WPNCS) Expert Group, which includes a separate Working Expert Group on Uncertainty Analysis for Criticality Safety Assessment (EGUACSA) (Web-page of WPNCS 2018).

The EGUACSA experts were offered a "blind" computational benchmark test for estimating errors in calculating the effective neutron multiplication factor, k_{eff}, (the k_{eff} values of the analyzed systems were unknown in advance) for simplified models of external MOX fuel cycle systems, which makes it possible to test national calculation codes and nuclear data used to substantiate the critical safety of projected reactor plants and external fuel cycle systems. As part of the test, tasks were also set to estimate the accuracy of the calculated predictions, reduce the a priori error by involving the results of previously performed integral and reactor-physical experiments, and adjust the neutron cross-sections.

Based on this benchmark test, a cycle of studies was performed at the JSC "SSC RF-IPPE n.a. A.I. Leipunsky" on verification of the ROSFOND/ABBN-RF nuclear data (Zabrodskaya et al. 2007, Andrianova et al. 2012) and validation of the software and methodological base of the INDECS system of codes and data archives (Manturov 2017, Manturov et al. 2017). The INDECS system includes the covariance neutron cross-sections data from ABBN (Andrianova et al. 2014) and the statistical analysis program of calculational-experimental results, which make it possible to quantify both the a priori (due to the existing errors in the nuclear data) and a posteriori (based on the information from the archives of experimental data) errors in the calculated k_{eff} values.

Critical safety benchmark test specification

The proposed computational test is a simplified model of an external MOX fuel cycle system with a simple spherical geometry (Fig. 1). The spheres of fissile material of different diameters (from 15 to 52.5 cm) and different fuel compositions (mixtures of uranium, plutonium and water) with densities of 3.5, 5.5 and 4.6 g/cm³ are surrounded by a water reflector of a fixed thickness (20 cm). The considered multiplying systems are of the type of systems with an intermediate neutron spectrum.

The ratios of even-odd isotopes of plutonium (^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu) for the proposed fuel compositions (plutonium vector) correspond to the plutonium vector of MOX fuel used in SFR and LWR plants. The task is set in this way because of the interest in studying the influence of plutonium nuclear properties and characteristics due to changes in the plutonium vector in the PuO_2 fuel compositions as well as water slowing properties on the critical mass. Table 1 shows the main characteristics of the benchmark multiplying systems. The corresponding
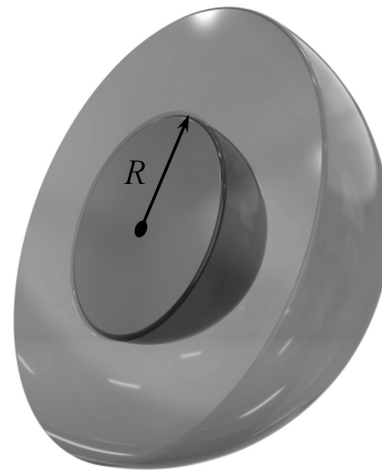

Figure 1. Computational benchmark test geometry

Table 1. Composition and geometry of the multiplying systems

Test option	M_{H2O} / $M_{UO2+PuO2}$	Radius, cm	M_{PuO2}/$M_{UO2+PuO2}$	^{239}Pu/Pu	^{240}Pu/Pu	^{241}Pu/Pu	^{242}Pu/Pu
1	2	3	4	5	6	7	8
1	3%	17.0	100%				
2	3%	22.5	30%	71%	17%	11%	1%
3	3%	46.0	12.5%				
4	3%	17.7	100%				
5	3%	24.1	30%	64%	23%	10%	3%
6	3%	52.5	12.5%				
7	3%	15.0	100%				
8	3%	19.0	30%	96%	4%	0%	0%
9	3%	40.0	12.5%				
10	1%	17.0	100%				
11	1%	22.5	30%	71%	17%	11%	1%
12	1%	46.0	12.5%				
13	5%	17.0	100%				
14	5%	22.5	30%	71%	17%	11%	1%
15	5%	46.0	12.5%				

columns of the table indicate as follows: (1) conventional names of the multiplying systems; (2) fuel moisture (water mass-to-fuel mass ratio); (3) radius of the central part of the sphere shown in Fig. 1, filled with a mixture of MOX fuel and water; (4) PuO_2 content in the fuel; (5–8) relative shares of plutonium isotopes.

The benchmark test specification defines the following design characteristics calculated using the ROSFOND/ABBN-RF nuclear data library:

- Effective multiplication factor, k_{eff}
- One-group integral sensitivity coefficients to k_{eff} of all isotopes that make up the fuel compositions;
- The a priori constant error in k_{eff} due to the uncertainties in covariance nuclear data;
- A list of integral experiments selected to adjust the calculated k_{eff} predictions;
- The a posteriori error in k_{eff} obtained with account of the selected integral experiments by adjusting the nuclear data on the basis of the approaches, methods and codes implemented in the INDECS system.

This benchmark test is primarily aimed at verifying methods for determining displacements and errors in the k_{eff} values and testing libraries of evaluated nuclear data and cross-sections uncertainties. Since the test itself is purely computational (there is no comparison with experimental data), according to the benchmark conditions, the k_{eff} values were assumed to be unknown. This circumstance makes it impossible to focus the calculations on a previously known result; therefore, the emphasis in the analysis shifts from a comparison of the calculated and experimental discrepancies to an analysis of the spread in the calculated data obtained from different libraries (the so-called observed constant error). This task setting allows us to test the computational methods and codes used to improve the accuracy in estimating the a posteriori and a priori constant errors.

Computational methods and results

The a posteriori and a priori constant errors were estimated using the INDEX system of codes and data archives. The basis of computational methods implemented in the INDEX system is the maximum likelihood method (Usachev and Bobkov 1972). The capabilities of this method are verified and demonstrated in (Golovko et al. 2014, Ivanova et al. 2012, Golovko 2012). The method consists in finding the most credible corrections to the variable parameters (neutron cross sections), accounting for which allows us to obtain the best agreement between the calculated and experimental values for the functional of interest (in this case, k_{eff}) in the group of experiments under consideration. This is achieved by finding the maximum of the likelihood function L, which has the form (up to an insignificant factor) $\exp(-Z^2/2)$, where the value of Z^2 in the exponent is determined by the relation

$$Z^2 = \mathbf{S} \cdot \mathbf{W}^{-1} \cdot \mathbf{S}^{\mathrm{T}} + (\Delta\mathbf{k} + \mathbf{H}^{\mathrm{T}} \cdot \mathbf{S}) \cdot \mathbf{U}^{-1} (\Delta\mathbf{k} + \mathbf{H}_{\mathrm{T}} \cdot \mathbf{S})^{\mathrm{T}}, \qquad (1)$$

where $\mathbf{S}$ is the desired vector of corrections to the parameters; $\mathbf{H}$ is the matrix of coefficients of k_{eff} sensitivity to the parameters; $\mathbf{U}$ and $\mathbf{W}$ are the covariance matrices of cross-sections uncertainties of the experimental results (the k_{eff} values) and desired parameters (neutron cross sections); $\Delta\mathbf{k}$ is the vector of discrepancies between the calculated and experimental k_{eff} values.

From expression (1), we can obtain the relation for the desired corrections:

$$\mathbf{S} = \mathbf{W} \cdot \mathbf{H}^{\mathrm{T}} \cdot (\mathbf{U} + \mathbf{H} \cdot \mathbf{W} \cdot \mathbf{H}^{\mathrm{T}})^{-1} \Delta\mathbf{k}, \qquad (2)$$

and also the expression for the covariance matrix of the parameters $\mathbf{W}\mathbf{\phi}$, which takes into account the corrections found:

$$\mathbf{W}' = \mathbf{W} - \mathbf{W} \cdot \mathbf{H} \cdot (\mathbf{U} + \mathbf{H} \cdot \mathbf{W} \cdot \mathbf{H}^{\mathrm{T}})^{-1} \Delta\mathbf{k}. \qquad (3)$$

By means of the matrix ($\mathbf{W}'$), we can estimate the new matrix ($\mathbf{V}'$) of the expected calculated errors using corrected constants, the a posteriori constant calculation error taking into account the data of integral experiments and corrections to the calculated $\Delta\mathbf{k}'$:

$$\mathbf{V}' = \mathbf{H} \cdot \mathbf{W}^{-1} \cdot \mathbf{H}^{\mathrm{T}}, \qquad (4)$$
$$\Delta\mathbf{k}' = \Delta\mathbf{k} + \mathbf{H}^{\mathrm{T}} \cdot \mathbf{S}. \qquad (5)$$

The k_{eff} values for the proposed test options were calculated by the MCNP code (MCNP 2008) using the ROSFOND/ABBN-RF nuclear data library and other libraries of evaluated nuclear data (ENDF/B-VII.0, JEFF-3.2, JENDL-4.0). Table 2 shows the comparison results, based on which (Column 2), it follows that the k_{eff} values obtained from the ROSFOND library of evaluated neutron data and its group version, ABBN-RF, agree within 0.1%. At the same time, the average discrepancies between the calculated k_{eff} values and the evaluated nuclear data obtained from the ROSFOND library and foreign libraries do not exceed 0.25%.

The spread in the k_{eff} values calculated using various libraries of evaluated nuclear data lies in the range from –0.26 to 0.79%. The maximum discrepancies correspond to Option 7, in which only PuO_2 is included in the fuel composition, with a maximum content of the ^{239}Pu isotope equal to 96%.

The analysis of the one-group sensitivity coefficients showed that the options with large values of coefficients of k_{eff} sensitivity to ^{239}Pu neutron cross sections (Fig. 2), in particular, Options 7 and 8, have the greatest discrepancy in the k_{eff} values calculated using different libraries of evaluated nuclear data (the best agreement in the other options can be explained by the error compensation in the constants of other plutonium and uranium isotopes). Since the values of the one-group coefficients of k_{eff} sensitivity to ^{239}Pu neutron cross sections are an order of magnitude higher than the values of the sensitivity coefficients

Table 2. Comparison of calculation results for different nuclear data systems

Test option	ABBN-RF/ ROSFOND	ENDF/B-VII/ ROSFOND	JEF-3.2/ ROSFOND	JENDL-4.0/ ROSFOND
1	0.07%	0.21%	−0.25%	0.21%
2	−0.01%	0.21%	−0.10%	0.04%
3	−0.09%	0.07%	−0.12%	−0.06%
4	0.07%	0.28%	−0.16%	0.21%
5	−0.02%	0.22%	−0.07%	0.04%
6	−0.07%	0.07%	−0.13%	−0.06%
7	0.02%	0.71%	0.36%	0.79%
8	−0.03%	0.48%	0.34%	0.42%
9	−0.08%	0.28%	0.21%	0.22%
10	0.07%	0.18%	−0.26%	0.15%
11	0.05%	0.18%	−0.11%	−0.04%
12	0.04%	0.19%	−0.23%	−0.05%
13	0.06%	0.24%	−0.23%	0.22%
14	−0.07%	0.15%	−0.02%	0.05%
15	−0.12%	0.00%	−0.03%	−0.05%
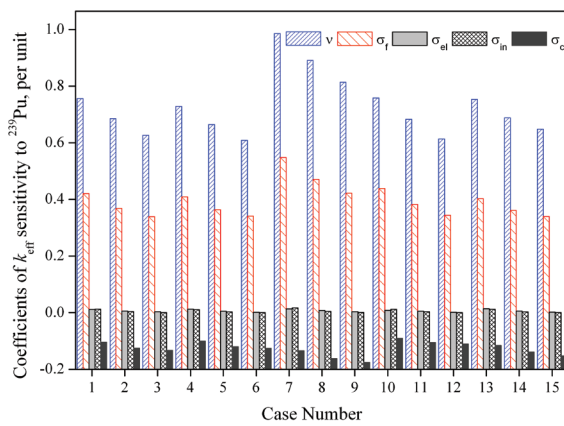
Figure 2. Coefficients of k_{eff} sensitivity to ^{239}Pu cross sections for different benchmark-test models

to neutron cross sections of other fuel isotopes (^{238}U, ^{235}U, $^{240-242}$Pu), it can be concluded that the observed discrepancies in the k_{eff} values are due to the spread in neutron data for the ^{239}Pu isotope presented in various libraries of evaluated nuclear data.

To estimate the a posteriori error of the models under consideration, experiments were selected from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook (ICSBEP 2018). The data of these benchmark experiments were used in (Golovko and Manturov 2017, Golovko et al. 2008, Andrianova et al. 2017, Andrianova et al. 2016) to estimate the accuracy of calculations of external MOX fuel cycle systems. Table 3 presents a list of 101 benchmark experiments that include homogeneous solutions with plutonium (PST-identifier) and mixtures of uranium and plutonium (MST-identifier) as well as benchmark models of experiments performed at the large physical test facilities BFS-1 and -2 (Doulin et al. 2007a, b, c).

Based on the covariance matrices of neutron cross sections for the ABBN group library, according to formula (4), the values of the relative a priori constant error in δk_{eff} calculated for all the 15 benchmark models were obtained (see Table 4).

**Table 3.** List of benchmark experiments

No.	Experiment identifier in ICSBEP	Critical configuration identifier	No.	Experiment identifier in ICSBEP	Critical configuration identifier
1	PST001	1-6	19	PST032	2, 6, 11.
2	PST002	1, 7	20	PMF001	1
3	PST003	1, 5	21	PMF002	1
4	PST004	3, 5, 6, 13	22	PMF011	1
5	PST005	1, 9	23	PMF022	1
6	PST006	2	24	PMF024	1
7	PST009	3	25	PMF027	1
8	PST010	1–3, 9, 11	26	PMF029	1
9	PST011	1, 8	27	PMF031	1
10	PST012	7–13	28	MST002	2, 3
11	PST018	1, 5, 9.	29	MST003	4, 7, 9, 10
12	PST020	3, 5, 8, 9	30	MST004	2, 5, 7.
13	PST021	1, 3, 4.	31	MST005	2, 3, 4, 7
14	PST022	1, 2, 3, 8	32	MST006	1
15	PST023	1, 8, 17, 34	33	MST007	1
16	PST025	3, 10, 17, 22, 31, 36, 42	34	MST010	1
17	PST026	3, 16	35	BFS	31-5, 38-2, 42, 97-1, 97-2, 97-3, 97-4, 99-1, 99-2, 101-1, 101-2, 101-2A, 101-3
18	IMF007	1			

Table 4. Benchmark a priori δk_{eff} and a posteriori $\delta' k_{eff}$ errors caused by the neutron cross section errors

No.	dk_{eff}, %	$\delta' k_{eff}$, %	No.	dk_{eff}, %	$\delta' k_{eff}$, %	No.	dk_{eff}, %	$\delta' k_{eff}$, %
1	0.95	0.31	6	0.95	0.33	11	0.81	0.29
2	0.84	0.32	7	1.16	0.22	12	0.81	0.28
3	0.90	0.32	8	0.95	0.24	13	0.92	0.33
4	0.93	0.31	9	0.95	0.22	14	0.89	0.35
5	0.84	0.32	10	1.01	0.29	15	0.96	0.33

Based on the experimental data (see Tab. 3), the maximum likelihood method was used to estimate the corrections to the k_{eff} values that take into account the most likely displacements of neutron constants obtained as a result of calculations within the limits of errors (corrected constants). The corrected k_{eff} values corresponding to these constants are shown in Fig. 3. The corrected error covariance matrix formed as a result of calculations made it
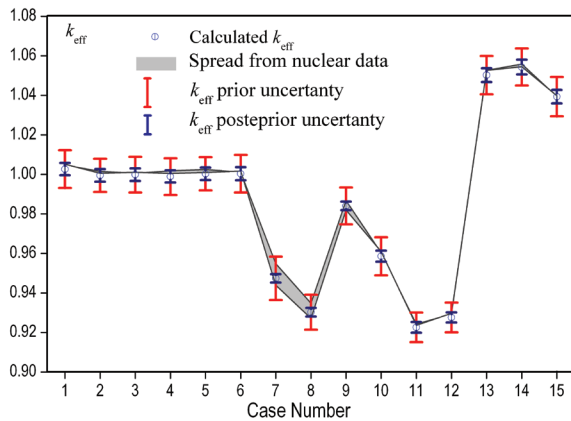
Figure 3. Summary of benchmark test calculation results

possible to calculate the a posteriori constant error in k_{eff}, which is presented in Table. 3 (designated as $\delta' k_{\text{eff}}$) and in Fig. 3 (the figure also shows the a priori constant error and the spread in the k_{eff} values calculated using different libraries of evaluated nuclear data). As can be seen, using the data on previously performed experimental studies of the integral MOX fuel characteristics, it is possible to reduce the constant error in k_{eff} by three times (on average, from 1 to 0.3%) for simple systems with an intermediate neutron spectrum.

Conclusion

In accordance with the calculation program of the OECD/NEA numerical benchmark test to substantiate the critical safety of MOX-fueled systems proposed by the Expert

Group on Uncertainty Analysis for Criticality Safety Assessment (EGUACSA), a series of calculations were performed aimed at verifying the ROSFOND/ABBN-RF nuclear data library. The analysis of the calculated data shows that:

- The maximum deviation in the calculated k_{eff} values obtained using different libraries of evaluated nuclear data (ENDF/B-VII.0, JEFF-3.2, JENDL-4.0), in comparison with the results obtained from the ROSFOND library, reaches 0.8%. The a priori error in the calculated k_{eff} value, caused by the uncertainty in the nuclear data and calculated using the ABBN covariance matrices data, ranges from 0.8 to 1.2%. Thus, the estimated a priori constant error in k_{eff} coincides with the observed spread in the calculated k_{eff} values, which indicates the reliability of the data on the errors in the ABBN neutron cross sections.
- The maximum deviation in the calculated k_{eff} values ~ 0.8% and the maximum a priori error value ~ 1.2% correspond to Option 7 (the highest ^{239}Pu content in the fuel) and are caused by the spread in neutron data for this isotope in different libraries of evaluated nuclear data.
- The deviation in the calculated k_{eff} values obtained from the ROSFOND library and its group version, ABBN-RF, does not exceed 0.1%, which demonstrates the high accuracy of the ROSFOND/ABBN-RF nuclear data for calculating the critical safety parameters of multiplying MOX-fueled systems.
- Using the data on previously performed experimental studies of the integral MOX fuel characteristics, it is possible to reduce the constant error in k_{eff} by three times (on average, from 1 to 0.3%) for simple systems with an intermediate neutron spectrum.

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