Calculation and experimental analysis of benchmark experiments with a fast neutron spectrum and models of sodium and lead cooled fast reactors using different evaluated nuclear data libraries

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Abstract

The paper presents the results of a comparative analysis of criticality calculations using a Monte-Carlo code with the BNAB-93 and BNAB-RF neutron group constants, as well as with evaluated neutron data files from the Russian ROSFOND evaluated nuclear data library and other evaluated nuclear data libraries (ENDF, JEFF, JENDL) from different years. A set of integral experiments on BFS critical assemblies carried out in different years at the Institute of Physics and Power Engineering (60 different critical configurations) was analyzed. The considered integral experiments are included in the database of evaluated experimental neutronic data used to justify the neutronic performance of sodium and lead cooled fast reactors, to verify codes and nuclear data as well as to estimate uncertainties in neutronic parameters due to the nuclear data uncertainties. It has been shown that the ROSFOND evaluated nuclear data library is a library that minimizes the calculation and experimental discrepancies for the considered set of integral experiments. The paper also presents the results of criticality calculations for models of sodium and lead cooled fast reactors based on different evaluated neutron data libraries and provides estimates for the uncertainty in criticality associated with nuclear data.

Keywords

Integral experiments, BFS facilities, ENDF, JEFF, JENDL, ROSFOND, BNAB-93, BNAB-RF, sodium cooled fast reactor, lead cooled fast reactor

Introduction

Refining the neutron data for the isotopes playing a crucial role in achieving the target level of accuracy when predicting analytically the neutronic performance of Generation IV reactors is an issue receiving a great deal of attention. The most prominent efforts were undertaken as part of the international project CIELO (Collaborative International Evaluated Library Organisation) (Chadwick et al. 2018). The results of the project have
been new versions of the US ENDF/B-VIII evaluated nuclear data library (released in 2018) (Brown et al. 2018) and the European JEFF-3.3 evaluated nuclear data library (JEFF-3.3) (released in late 2017). These evaluated nuclear data library versions have become another stage in the process of regularly updating national libraries of evaluated nuclear data the intensity of which varies among countries and which takes into account national priorities in the field of nuclear reactor engineering. The leader in updating evaluated neutron data files is the USA where a new version of the ENDF library is released every five to seven years (ENDF/B-V.2 (1994), ENDF/B-VI.8 (2001), ENDF/B-VII.0 (2006), ENDF/B-VII.1 (2011), ENDF/B-VIII.0 (2018)) (Evaluated Nuclear Data File).

ROSFOND, the commonly available official version of the national library of evaluated neutron data, (Zabrodskaya et al. 2007) dates back to 2010 (in this paper, the ROSFOND library shall be understood to mean the official release of the library publicly accessible on IPPE’s website at [https://www.ippe.ru/reactors/reactor-constants-datacenter/rosfond-neutron-database](https://www.ippe.ru/reactors/reactor-constants-datacenter/rosfond-neutron-database)). This library version has been tested in detail and local library versions are built on its basis for individual applications and projects. The ROSFOND evaluated nuclear data library files are composed of data selected from files of the national libraries BROND-2.2 (1992) and FOND-2 (1993), as well as of nuclear data evaluations from the ENDF/B, JEFF, JENDL, and CENDL libraries. ROSFOND was formed with regard for the results obtained in a critical analysis of similar U.S., European and Japanese evaluated nuclear data libraries from the same time period, which have undergone several updating stages for the past nine years. Despite the fact that ROSFOND was repeatedly tested based on different analytical and experimental benchmarks, it demonstrates consistently good results as compared with alternative counterparts. However, the practice of using it (or its group version, BNAB-RF, (Koshcheyev et al. 2014) being in the process of introduction into fast reactor neutronic and radiation protection calculations at the industry’s enterprises) in neutronic calculations in the Russian Federation is not commonplace. Despite fairly obvious advantages of using updated constants, BNAB-93 (1993 release), a group neutron data library, has been used most extensively in the Russian Federation for neutronic calculations of fast reactors (BN, BREST, SVBR, MBIR, and others) and the processes taking place in the closed nuclear fuel cycle (CNFC) facilities (Manturov et al. 1996). The BNAB-93 system of neutron constants was formed in 1993 based on evaluated neutron data of the FOND-2 library with regard for the experience of computational-ly analyzing integral experiments on critical assemblies. Such delays in introducing and using an improved system of neutron constants and data for neutronic calculations discourage the evolution of the national system of neutron data.

One of the factors that hampers the introduction of updated neutron data library versions is the fear of discrepancies to be detected in the reactor performance calculations based on an updated library of neutron data and the predecessor library. At the same time, there is no surprise that such discrepancies can be observed, this being proved by analyzing the world experience in introducing updated versions of evaluated neutron data in the process of which the causes for potential inconsistencies are demonstrated and discussed.

The predictive capability and the efficiency of updated neutron data library versions are compared by matching the results of the performance calculations for critical assemblies with experimental data. In the paper, respective performance indicators were calculated and compared to identify high-priority activities on further enhancing the ROSFOND/BNAB-RF nuclear data libraries. It was used a representative set of experimental data measured on the BFS-1 and BFS-2 critical facilities. Experimental calculations were performed using different versions of Russian (ROSFOND, BNAB-RF and BNAB-93) and other evaluated nuclear data libraries (ENDF, JEFF and JENDL) from different years (ENDF/B-V.2 (USA, 1994), ENDF/B-VII.1 (USA, 2011) and ENDF/B-VIII (USA, 2018), JEFF-3.2 (Europe, 2014), JEFF-3.3 (Europe, 2017) and JENDL-4.0u2 (Japan, 2012)) (Shibata et al. 2011). To demonstrate the discrepancies in the criticality calculations for models of sodium and lead cooled fast reactors performed based on different evaluated neutron data libraries, the paper also presents the results of comparative calculations of criticality for three models of fast reactors with different coolants and fuel types, as well as the uncertainty in criticality associated with nuclear data.

### Brief description of experiments on BFS critical assemblies

Worldwide, the results of integral experiments are used for estimating and improving the accuracy of predictive calculations for reactor facilities and fuel cycle systems under design, planning new experiments, estimating the efficiency of experimental programs, etc. (Andrianova et al. 2016, 2017). The nuclear data, constants and software tools for the analytical support of power and research reactors under design or in operation are improved based on the calculation analysis of data from experiments on BFS critical assemblies (IPPE). Experimental investigation programs based on the BFS critical assemblies encompass such fields of research as neutronic performance of sodium and lead cooled fast reactors and thermal reactors with MOX fuel, minimum critical masses in fabrication of MOX fuel, nuclear safety of nuclear waste disposal systems, etc. As part of the international project to establish the framework for critical safety experiments in (ICSBEP) and reactor experiments in (IRPhEP), some of the experiments performed in different years on the BFS-1 and BFS-2 critical facilities were described in detail. Altogether, international IRPhEP and ICSBEP handbooks
include eight reviews of benchmark experiments conducted on about 30 types of the critical core configurations. Table 1 presents brief characteristics of 60 considered core configurations assembled at the BFS-1 and BFS-2 critical facilities in the period of 1974 through 2009. Large, all cores of the considered critical assemblies were formed of mixed uranium-plutonium fuel and had fast or intermediate neutron spectra. The exclusion is the series of BFS-57 and BFS-59 critical assemblies, which simulated different fuel configurations for light water reactors. Work has been initiated to form the databank for integral experiments based on BFS critical assemblies so that to systematize the accumulated information and enable its use for testing and adjusting evaluated nuclear data files, verifying codes, and estimating the accuracy of predicting the neutronic performance of fast reactors. This databank is designed to supplement the existing information and enable its use for testing and adjusting evaluated nuclear data files, comparing the evaluated nuclear data libraries (Golovko et al. 2019). The procedures to calculate BFS critical assemblies using Monte Carlo codes in a group approximation are described in (Andrianova et al. 2019b).

A statistical analysis was carried out using the calculation and experimental discrepancies for different versions of Russian and other evaluated nuclear data libraries, which makes it possible to conclude on the accuracy of calculations and the efficiency of describing a set of N integral experiments by the given system of constants L. Table 2 presents values of the following quantities which can be considered as performance indicators when comparing the evaluated nuclear data libraries (Golovko et al. 2014, Andrianova et al. 2019a).

1. Average value of deviations of estimated multiplication factors from experimental values expressed as a percentage:
   \[ \Delta_{av} = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{C_{av}^L - E_n}{E_n} \right) \times 100, \]
   where \( C_{av}^L \) is the calculated value obtained using library L for assembly n assigned to \( E_n \) (experimental value).

2. Root-mean-square deviation of calculation and experimental relations for multiplication factors expressed as a percentage:
   \[ \delta_{rms} = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} \left( \frac{\Delta_{rms}^L}{E_n} \right)^2}, \]
   where \( \Delta_{rms}^L = \left( \frac{C_{av}^L}{E_n} - 1 \right) \) is the calculation and experimental deviations in percentage terms obtained using library L for assembly n.

3. Number of standard deviations between the experiment and the criticality calculation, average for the set of N integral experiments, for the system of constants:
   \[ \mu = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{C_{av}^L - E_n}{E_n} \right)^2 \frac{1}{\left( \delta_{rms}^L \right)^2 + \delta_{av}^L}}. \]
where $\delta_e$ is the relative deviation of the experimental error, %; and $\delta_c$ is the relative value of the calculated (statistical) error, % (Usachev and Bobkov 1972).

All values of the performance indicators in Table 2 have been calculated for three categories: assemblies with a fast neutron spectrum, assemblies with an intermediate neutron spectrum, and assemblies with a fast neutron spectrum and an intermediate neutron spectrum. Rows 3 through 10 list libraries using which $k_{eff}$ was calculated for the BFS critical assemblies. No data on the performance indicators is provided for BNAB-RF since it coincides with ROSFOND (Table 2, row 3).

Table 3 presents the maximum and the average values as a percentage of the criticality magnitude ratio, calculated using library $L(C_i)$, to the criticality magnitude calculated using ROSFOND ($C_{ROSFOND}$): 

$$\Delta C_{ROSFOND}^L = \frac{1}{N} \sum_{n=1}^{N} \frac{C_i^L}{C_{ROSFOND}} - 1 \cdot 100\%.$$ 

Fig. 1 shows deviations of the criticality values, expressed as a percentage, during the transition from the library’s older version to the new one. The blue segments connecting the blue markers show the relation of the $k_{eff}$ calculation based on BNAB-93 to the calculation based on BNAB-RF, and the green segments connecting the green markers show the relation of the $k_{eff}$ calculation based on ENDF/B-V to the calculation based on ENDF/B-VIII. The range of representative neutron spectra in the considered assemblies is highly extensive. The vertical dash lines show the regions corresponding to the types of the experimental configurations listed in Table 1. Fig. 2 presents data on the maximum and the minimum values of deviations in calculations based on different libraries in percentage terms – $(C_i/C_j - 1) \cdot 100\%$, where $i$ and $j$ are the library index as shown in Table 2 (ENDF, JEFF, JENDL, and ROSFOND).

### Criticality calculations for fast reactor models

Table 4 presents data on deviations of the calculated $k_{eff}$ values for sodium-cooled fast reactors with mixed oxide and nitride nuclear fuel, as well as for a lead cooled fast reactor. The deviations of the $k_{eff}$ values have been calculated as the ratio of the $k_{eff}$ calculation using the evaluated neutron data libraries to the $k_{eff}$ calculation using ROSFOND:

$$\frac{C_i}{C_{ROSFOND}} - 1 \cdot 100\%.$$ 

### Table 2. Average deviations of calculated multiplication factors from experiment

| Neutron spectrum | Fast | Intermediate | All |
|------------------|------|--------------|-----|
| ROSFOND          | -0.21 | 0.31 | 1.12 | 0.13 | 0.83 | 2.09 | -0.10 | 0.54 | 1.53 |
| ENDF/B-VII       | -0.27 | 0.53 | 1.51 | 0.23 | 1.00 | 2.51 | -0.09 | 0.72 | 1.92 |
| ENDF/B-VIII      | -0.22 | 0.40 | 1.31 | 0.37 | 0.88 | 2.70 | -0.02 | 0.60 | 1.91 |
| ENDF/B-V         | -0.29 | 0.82 | 2.39 | 0.47 | 1.16 | 3.00 | -0.03 | 0.94 | 2.61 |
| JEFF 3.2         | -0.18 | 0.41 | 1.47 | 0.30 | 0.85 | 2.46 | -0.01 | 0.59 | 1.87 |
| JEFF 3.3         | -0.15 | 0.35 | 1.22 | 0.26 | 0.83 | 2.14 | -0.02 | 0.55 | 1.76 |
| JENDL-4.0        | -0.02 | 0.47 | 1.11 | 0.46 | 0.87 | 2.34 | 0.15  | 0.63 | 1.64 |
| BNAB-93          | -0.09 | 0.63 | 1.98 | 0.30 | 1.12 | 2.87 | 0.05  | 0.83 | 2.33 |

### Table 3. Average deviations of calculated multiplication factors in transition from ROSFOND to other libraries

| Indicator | BNAB-RF | ENDF/B-VII | ENDF/B-VIII | ENDF/B-V | JEFF 3.2 | JEFF 3.3 | JENDL-4.0 | BNAB-93 |
|-----------|---------|------------|-------------|----------|----------|----------|-----------|---------|
| Average   | 0.11    | 0.23       | 0.33        | 0.66     | 0.26     | 0.24     | 0.39      | 0.44    |
| Maximum   | 0.34    | 0.86       | 0.66        | 2.35     | 0.70     | 0.84     | 0.90      | 1.66    |

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Figure 1. Deviations in calculated criticality values caused by the transition from the evaluated nuclear data library’s older version to the new one: 1) magnitude $(C_i/C_{ROSFOND} - 1)$ in percentage terms; 2) magnitude $(C_i/C_{ENDF/B-V} - 1)$ in percentage terms. Regions shown by dashed lines: a) sodium cooled fast reactor; b) lead cooled fast reactor; c) fabrication of MOX fuel; d) waste disposal in sand; e) CNFC facilities.
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The calculated nuclear data libraries shown in column 1 to the $k_{\text{eff}}$ calculation using the library shown in column 2. The $k_{\text{eff}}$ calculations for fast reactor models were performed at the temperatures of the materials corresponding to the operating status of the reactor facility.

Based on covariance matrices and sensitivity coefficients of $k_{\text{eff}}$ to the variation of the neutron cross-sections, the $k_{\text{eff}}$ uncertainty were calculated for fast reactor models which have been found to be 1.9% for sodium cooled fast reactors and 2.0% for lead cooled fast reactors.

**Discussion of results**

Based on analyzing the results of the $k_{\text{eff}}$ calculations for the entire set of the BFS critical assemblies, the following conclusions can be made.

Present-day Russian evaluated nuclear data and constants make it possible to calculate strongly heterogeneous BFS critical assemblies using precise Monte Carlo codes with high accuracy. The transition from ROSFOND to its group version, BNAB-RF, for the considered BFS critical assemblies leads to a deviation of the $k_{\text{eff}}$ calculations equal to ~ 0.1% (see Table 3).

The transition from BNAB-93 to BNAB-RF leads to an increased accuracy of predicting $k_{\text{eff}}$ for the BFS critical assemblies both with a fast neutron spectrum and with an intermediate neutron spectrum. On the average, the calculation and experimental discrepancies have decreased by a factor of one and a half to two; the criticality calculation values having changed by not more than 0.44% on the average. The maximum deviation of the $k_{\text{eff}}$ calculations of up to 2% is observed for assemblies with an intermediate neutron spectrum and plutonium fuel. The maximum deviation value does not exceed the constant uncertainty for systems with an intermediate neutron spectrum, which varies in the limits of 2 to 3% depending on the assembly composition.

The transition from BNAB-93 (1993) to BNAB-RF (2010) leads to deviations of the criticality calculation results for fast reactors with nitride fuel in the limits of 0.5 to 0.9%. The spread in the calculated $k_{\text{eff}}$ values obtained based on state-of-the-art U.S., European and Japanese evaluated nuclear data libraries from 2017–2018 is not less than ~ 1%.

The transition from JEFF3.3 and ENDF/B-VIII of the 2010 and 2011 versions to the 2017 and 2018 versions did not lead to a more accurate description of the BFS critical assemblies and major deviations in the $k_{\text{eff}}$ calculations for fast reactor models. However, when comparing the deviations in the BFS critical assembly $k_{\text{eff}}$ calculations (see Fig. 1) in the event of the transition from the ENDF/B-V.2 (1994) and ENDF/B-VIII (2018) libraries, these are the same as the deviations in the results observed in the event of the transition from BNAB-93 (1993) to BNAB-RF (2010).

The observed spread in the calculated $k_{\text{eff}}$ values for the BFS critical assemblies and fast reactor models as a result of using different evaluated neutron data libraries does not exceed the uncertainty of the calculations caused by the neutron cross-section uncertainties.


## Conclusion

The results of the calculation and experimental analysis presented in this paper for a set of experiments on BFS critical assemblies make it possible to conclude the following. The results of the $k_{\text{eff}}$ calculations based on the ROSFOND evaluated nuclear data library may differ from the results obtained using certain versions of U.S., European and Japanese evaluated nuclear data libraries by about 1%. The differences between the calculated $k_{\text{eff}}$ values obtained using JEFF 3.3 and ENDF/B-VIII are also at a level of ~1%. When comparing different versions of the same library (e.g. ENDF/B-V.2 (1994) and ENDF/B-VIII (2018)) similar deviations are observed in the calculation-experiment results as in the event of the transition from BNAB-93 (1993) to BNAB-RF (2010). It has been shown for the entire set of the considered experiments that the calculation and experimental discrepancies are smaller when updated versions of the evaluated neutron data libraries are used, as compared with the results obtained based on earlier versions of the respective evaluated nuclear data libraries.

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