Consideration of heterogeneous effects in preparing neutron multigroup constants in the CONSYST/BNAB-RF system*

Olga N. Andrianova¹, Gennady M. Zherdev¹, Gleb B. Lomakov¹, Yevgeniya S. Teplukhina¹

¹ JSC “SSC RF-IPPE n.a. A.I. Leypunsky”, 1 Bondarenko Sq., Obninsk, Kaluga Reg., 249033, Russia

Corresponding author: Olga N. Andrianova (o.n.andrianova@yandex.ru)

Abstract

The need for building mutually self-agreed computational models for high-precision and engineering neutronic codes is defined by requirements to certification and verification of software products and nuclear data in accordance with the Regulations for Verification and Expert Examination of Neutronic Calculation Software Tools (RB-061-11). The key requirement in RB-061-11 is that there shall be a methodically transparent and reproducible procedure to estimate the methodological and nuclear data component of the neutronic parameter uncertainties to be implemented only if there are mutually self-agreed computational neutronic models. Using an example of a series of measurements carried out on three critical BFS-61 configurations, factors are discussed which need to be taken into account when building such types of neutronic models and the peculiarities of their application for calculating the neutronic parameters of BFS-61 assemblies. Improved functional capabilities of updated software tools and nuclear data for the computational and experimental analysis of integral BFS experiments (ROSFOND/BNAB-RF, CONSYST and MMK-RF) have been demonstrated, allowing a much shorter time and the smallest risks of errors in preparing mutually self-agreed computational models for various neutronic codes, as well as correct estimation of the methodological and nuclear data components of the uncertainties in neutronic parameters in accordance with RB-061-11. The results of estimating the uncertainty in neutronic parameters with respect to the group approximation approach, are presented. It has been shown based on an analysis of the obtained results that the discrepancies in the calculations of the BFS-61 configurations in the transition from the ROSFOND evaluated neutron data library to its group version, BNAB-RF, does not exceed 0.3% in criticality (heterogeneous effects uncertainty of 0.2 to 0.8 %). The estimated spectral index data biases lie in the limits of the Monte Carlo statistical error. Based on the results of a computational and experimental analysis for the entire set of measurements performed on a series of BFS-61 assemblies, the ROSFOND library is the optimal nuclear data library.

Keywords

Integral experiments, BFS, effective neutron multiplication factor, nuclear data uncertainty, Monte Carlo, ROSFOND, BNAB-RF, spectral indices.

* Russian text published: Izvestiya vuzov. Yadernaya Energetika (ISSN 0204-3327), 2019, n. 4, pp. 58–70.
Introduction

The purpose of the paper is to demonstrate the improved functional capabilities of updated software products and nuclear data to support the computational and experimental analysis of integral experiments based on BFS assemblies (using BFS-61 critical assemblies as the example). These capabilities make it possible to reduce considerably the time and to minimize the risks of errors in preparation of models, to build mutually self-agreed models for precision and engineering codes, and to estimate the methodological and nuclear data components of uncertainties in neutronic parameters required for verification and qualification of codes in accordance with the Regulations RB-061-11 (RB-061-11). The uncertainties in engineering calculations, as specified in RB-061-11 (par. 13–15), are determined by comparing the calculation results against the respective results obtained based on precision (reference) neutronic codes (par. 22). One of the world’s most commonly used codes of the kind is MCNP, a US code (MCNP 2008). The MCU code is an extensively used Russian analog (Gomin et al. 2000). Both codes are specific in that they are fitted with a versatile geometrical module. This versatility however leads to more time spent, so it is reasonable to use an adapted and optimized geometrical module to accelerate calculations of standard neutron multiplying systems and media.

The MMKK code developed at IPPE (Blyskavka et al. 2001) (referred to as MMKKENO in early publications) features a much greater (several-fold) speed of response thanks to a specialized geometrical module with extensive capabilities covering the basic needs of describing the layouts of both reactor and BFS critical facilities. The capabilities for recording the neutron flux and computing the flux-averaged neutron cross-sections for an independent geometrical grid (similarly to MCNP), implemented in the latest code version known as MMK-RF (Zherdev et al. 2018, 2018a), make it possible to cut the post-processing time for the BFS experiment calculation results. Thanks to the optimized functional capabilities, the MMK-RF code has a much better speed of response than its foreign and Russian analogs when used in computational and experimental studies based on BFS critical facilities.

The constant component of an error should be estimated based on comparing the results of the benchmark experiment calculations, performed with the use of the codes implementing the Monte Carlo method, in detailed and group representations of neutron cross-sections. A computational description of experiments performed on the BFS facilities in a group representation of neutron cross-sections is associated with the problem of taking into account, in a correct manner, the effects of the cross-section resonance self-shielding due to the heterogeneous arrangement of materials (Abagyan et al. 1964, Nikolayev et al. 1984). The neutron group constants preparation system, CONSYST, (Manturov et al. 2000) implements approximate and comparatively user friendly methods of preparing group constants allowing the spatial heterogeneity effects to be taken into account correctly.

Specification of benchmark experiments on the BFS-61 assemblies

Critical assemblies of the BFS-61 series were set up in 1990 at the BFS-1 facility to investigate the characteristics of lead cooled nuclear reactors. In 2009, the experiments conducted based on the BFS-61 critical assemblies were evaluated for international handbooks of evaluated benchmark experiments (Rozhikhin et al. 2006, 2008).

The BFS-61 assemblies (Fig. 1) had a standard configuration and were composed of steel tubes filled with plutonium metal pellets, depleted uranium metal, lead, graphite, etc. The BFS-61-0 assembly (Fig. 1a) had a three-layer side reflector consisting of lead (lead pellets of two types), steel and depleted uranium dioxide. The
BFS-61 assembly (Fig. 1b) used a two-layer reflector consisting of lead and uranium dioxide. The BFS-61-2 assembly (Fig. 1c) reflector had two layers and consisted of depleted uranium dioxide. Thin, cylindrical stainless steel bars were inserted between the tubes in the reflector.

The program of experimental studies based on the BFS-61 assemblies included measuring the ratios of the neutron interaction cross-sections (\( \langle \sigma_i \rangle / \langle \sigma_j \rangle \)) averaged by the spectrum at a certain point of the critical assembly (spectral indices) containing ample information on the properties of the fast neutron reactor composition under investigation (Andrianova et al. 2016, 2017, Andrianova 2017). By definition,

\[
\frac{\langle \sigma_i \rangle}{\langle \sigma_j \rangle} = \int \int \frac{\varphi(E)\sigma_i dE}{\varphi(E)\sigma_j dE},
\]

where \( \varphi(E) \) is the spectral density of the neutron flux; \( \langle \rangle \) is the symbol of averaging by energy; \( i, j \) are the isotope type; and \( x \) is the reaction type (e.g., \( f \) is fission). The ratio of the average fission cross-section for the isotopes \( ^{232}\text{Th}, ^{233}, ^{238}\text{U}, \) and \( ^{239}\text{Pu} \) to the average fission cross-section for \( ^{235}\text{U} \), and the ratio of the average fission cross-section for the minor actinides \( ^{238}, ^{240}, ^{241}, ^{242}\text{Pu}, ^{241}\text{Am}, \) and \( ^{237}\text{Np} \) to the average fission cross-section for \( ^{239}\text{Pu} \) were measured on the BFS-61 assemblies using a small-size fission chamber (SFC).

The SFC design is described in (Rozhikhin et al. 2006). The chamber body is a stainless-steel tube of the diameter 6 mm and the length 140 mm with a wall thickness of 0.5 mm. Inside the chamber there is another tube of the diameter 4 mm and the length 40 mm with a wall thickness of 0.2 mm, which has a 30 mm high layer of a fissile material applied to its inner surface. The chamber is filled with argon pressurized to 10 atm.

To measure the spectral indices, the chamber is installed such that the middle of the fissile material layer inside the chamber coincided with the median plane of the assembly core (with the middle of the fuel composition in the central tube). Fig. 2 shows the standard arrangement of the small-size fission chamber in the space between tubes.

**Figure 2.** SFC arrangement diagram.

### Estimation of the methodological and nuclear data components of the calculation uncertainty in neutronic parameters

The experiment evaluation procedure suggests that the description of a mathematical model in the calculated value shall include estimated contributions from all of the adopted assumptions and approximations of the methods in use. A practicable way to estimate these assumptions and approximations is to do this successively while relying on the results of the calculations based on a high-precision neutronic models. Schematically, the calculation procedure for the uncertainty evaluation is shown in Fig. 3.

A computational neutronic model is prepared at the initial stage for the precision Monte Carlo code that allows performing calculations with a pointwise representation of the neutron cross-sections without introducing any approximations and simplifications associated with the description of the actual geometry and the material composition of the neutron multiplying system.

Based on the above computational model, neutron multigroup calculations are proceeded to at the second stage while estimating the nuclear data component of the uncertainty by comparing the results of two calculations. The methodological component of the uncertainty, associated with the implementation of the neutron group approximation in another particular code using the Monte Carlo method, can be also estimated at this stage (Andrianova 2017). And the computational models for these codes should be fully identical and have a single computational task for preparing neutron macro-constants.

One can proceed from the precision specification of the assembly configuration and composition to homogenized compositions at stage 3 while making changes to the geometry description in the computation neutronic model.

Comparing the results of the Monte Carlo calculations with the detailed representation of the neutron cross-sections for the homogeneous model and for the heterogeneous model makes it possible to estimate the computational adjustment factor for heterogeneity. The following
uncertainty components can be determined using precision codes: a nuclear data component, a methodological component (associated with the applied neutron group approximation) and the uncertainty caused by the transition to the homogeneous neutronic model.

When comparing the results of the calculations for homogeneous models, based on various engineering neutronic codes, with the results of the calculation for the same model, using a high-precision neutronic code with a single nuclear data basis, it is possible to estimate the uncertainties of the approximations the engineering neutronic codes.

**Consideration of heterogeneous effects in the CONSYST system**

The CONSYST processing system implements various methods to take into account heterogeneous effects when preparing neutron multigroup macroscopic cross-sections based on the principle of equivalence of homogeneous and heterogeneous media (theorem of equivalence):

- “manual” introduction of corrections – the user can calculate the corrections for the dilution cross-section manually: a) by introducing the fictitious isotope of the δ-scattering, b) by identifying additional material blocking zones;
- automatic calculation of corrections – the system is capable to compute automatically the values of the corrections if the user has described the actual heterogeneous structure using the GETER module.

The concentrations of fictitious materials need to be calculated in the “manual” mode of introducing the corrections to take into account the spatial heterogeneity.

First, if the dimensions of the uniform region are comparable with the length of the free path and it includes isotopes with resonances, a fictitious isotope named “D-SC”, the so-called δ-scattering that does not change the

---

**Figure 3. Flowchart for the uncertainty quantification of neutronic parameters.**
neutron transport process but influences the way the resonance self-shielding of neutron cross-sections is taken into account, can be introduced in this region. The full cross-section of the δ-scattering is equal to 1 barn, and the average cosine of the scattering angle is equal to unity. The concentration of the δ-scattering is selected as equal to 1/\(l\), where \(l = 4V/S\) is the mean chord or the average value of the neutron path length in a zone without regard for collisions; \(V\) is the volume; and \(S\) is the surface area.

Second, the CONSYST system comprises two classes of material zones having different nuclide compositions – material blocking zones and physical zones. The blocking zones serve to calculate the resonance self-shielding factors, and the neutron fields are calculated in a system consisting of physical zones each of which is assigned a blocking zone. A zone with a homogeneous composition, including a set of physical zones (a tube, pellets of various materials, etc.), can be chosen as the blocking zone.

Heterogeneous effects can be taken into account by delivering information on the actual cell structure of the medium into the CONSYST. In this case, the program will recalculate the dilution cross-sections of the resonance isotopes with regard for the particular geometry of the heterogeneous cell with the following corrections computed in the dilution cross-section:

- the Dancoff correction that takes into account the interactions of blocks in an infinite periodic array;
- the Bell factor depending on the block thickness (Nikolayev et al. 1984).

The concentration of the δ-scattering for all of the materials will be computed automatically.

Another important change in the CONSYST system is that the system determines independently for which zones and how the anisotropy of the full cross-section needs to be taken into account. To do this, it is enough for the user to set the respective indicator.

**Calculation results and their comparison**

The neutronic parameters were calculated for the three BFS-61 configurations using the MMKK, MMK-RF, and MCNP codes. Table 1 presents the values and the statistical error of the criticality calculations (the values in brackets are the absolute statistical error multiplied by \(10^4\)) for each BFS-61 assembly configuration. The neutron multigroup blocked constants for the MMKK and MCNP codes were prepared using the CONSYST-RF system (Koshcheyev et al. 2016, Manturov et al. 2013) with the inclusion of the GETER module. The calculations were performed using the subgroups for \(^{235}\text{U},\ ^{239}\text{Pu}\), and the natural Fe mixture, the total number of the groups being 1520. Additional calculations were performed using the MCNP and MMK-RF codes with the pointwise representation of the ROSFOND neutron cross-sections (ROSFOND 2019) and the BNAB-RF neutron group library (Koshcheyev et al. 2014, Andrianova et al. 2012).

The values shown in columns 5 and 6 of Table 1 demonstrate that taking into account heterogeneous corrections in the CONSYST-RF system in the ‘manual’ mode and in the automatic mode does not lead to changes in the calculation results. The table’s final line shows the time of a calculation based on a single-core processor (one and the same computer), using the MCNP, MMKK, and MMK-RF codes, required to achieve the statistical error \(k_{eff}\) equal to ± 0.00020, which corresponds to 10 million active histories of neutrons. Thanks to the specialized geometrical module, the MMKK and MMK-RF codes have three to four times as high computational speed as the MCNP code or higher in some cases.

The results of the calculations shown in the table formed the basis for estimating the value of the nuclear data component for the uncertainty in neutronic parameters caused by the transition from the pointwise representation of neutron cross-sections to the group approximation (this makes ~0.3% for the considered systems). Taking into account the spatial heterogeneity when preparing the macroscopic constants leads to a 0.8% finer criticality calculation.

The spectral characteristics measured by the SFC in the tube gap to the right of the BFS-61 assembly central tube in the core median plane were calculated (see Fig. 2). In the computation model, the SFC was represented as a cylinder of the diameter 4 mm and the height 3 cm in accordance with the height of the applied layer of the fissile material in the actual SFC description (Rozhikhin et al. 2008).

Apart from the criticality calculation results, the base version of the MMKK code is capable to produce a flux in the preset zone with the same energy structure with which the CONSYST system prepared the macroscopic cross-sections. Therefore, unlike the MCNP code, the MMKK code does not include capabilities for computing integrals of the \(\int \phi(E)dE\) and \(\int \phi(E)\sigma(E)dE\) form. Calculating such integrals requires extra programs for post-processing of calculation results. Apart from the capability to

<table>
<thead>
<tr>
<th>BFS-61 configuration</th>
<th>MMK-RF</th>
<th>MCNP</th>
<th>MMKK</th>
<th>MMK-RF</th>
<th>Model (Kozhikhin et al. 2008)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ROSFOND</td>
<td>BNAB-RF</td>
<td>ROSFOND</td>
<td>GETER</td>
<td>GETER</td>
</tr>
<tr>
<td>BFS-61-0</td>
<td>0.99661(20)</td>
<td>0.9931(21)</td>
<td>0.9966(21)</td>
<td>1.0000(20)</td>
<td>0.9966(21)</td>
</tr>
<tr>
<td>BFS-61-1</td>
<td>0.9946(19)</td>
<td>0.9909(21)</td>
<td>0.9947(20)</td>
<td>0.9997(20)</td>
<td>0.9967(21)</td>
</tr>
<tr>
<td>BFS-61-2</td>
<td>0.9939(19)</td>
<td>0.9906(20)</td>
<td>0.9937(20)</td>
<td>0.9973(20)</td>
<td>0.9950(21)</td>
</tr>
<tr>
<td>Time, min</td>
<td>56</td>
<td>50</td>
<td>262</td>
<td>156</td>
<td>48</td>
</tr>
</tbody>
</table>
compute any types of convolution with the flux, MMK-RF, an improved version of the MMKK, (Zherdev et al. 2018, 2018a) is fitted with an independent grid for identifying the cylindrical or spherical regions of the neutron flux recording.

Fig. 4 shows the results of the neutron flux calculations for the cylindrical region matching the recording region in the SFC, based on the MCNP code with the pointwise representation of nuclear cross-sections (ROSFOND library) and the neutron data group representation of constants (BNAB-RF library, 1520 groups), and based on the MMKK code with the group representation of constants (BNAB-RF library, 1520 groups).

As can be seen from the diagram, the results of the neutron spectra calculations in the neutron cross-section group and detailed representations agree well in the limits of the statistical calculation error. Spectral indices can be calculated based on these energy distributions of neutron fluxes.

Table 2 presents the results of calculating the spectral indices measured by the SFC using the BFS-61-0 assembly, namely: the ratio of the average fission cross-section for the isotopes $^{232}$Th, $^{233}$U, and $^{238}$U to the average fission cross-section for $^{235}$U, and the ratio of the average fission cross-section for the minor actinides $^{240, 241, 242}$Pu and $^{241}$Am to the average fission cross-section for $^{239}$Pu. The MMK-RF calculations were performed using an independent grid and an automated convolution of the neutron flux with the cross-section $\int \phi(E) \sigma_x(E) dE$.

The data presented in the table demonstrate a good agreement of the spectral indices calculation results obtained based on the MCNP and MMK-RF codes using the ROSFOND library.

### Table 2. Calculated values of the fission rates measured at the BFS-61-0 assembly.

<table>
<thead>
<tr>
<th>Index</th>
<th>Experiment</th>
<th>Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_f$ $^{232}$Th/$\sigma_f$ $^{235}$U</td>
<td>$0.00947 \pm 0.00003$</td>
<td>$0.00730 \pm 0.00003$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{233}$U/$\sigma_f$ $^{235}$U</td>
<td>$1.513 \pm 0.03$</td>
<td>$1.4666 \pm 0.0035$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{238}$U/$\sigma_f$ $^{235}$U</td>
<td>$0.0320 \pm 0.0008$</td>
<td>$0.0307 \pm 0.0001$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{239}$Pu/$\sigma_f$ $^{235}$U</td>
<td>$1.057 \pm 0.015$</td>
<td>$1.037 \pm 0.003$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{240}$Pu/$\sigma_f$ $^{239}$Pu</td>
<td>$0.2575 \pm 0.007$</td>
<td>$0.2674 \pm 0.0008$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{241}$Pu/$\sigma_f$ $^{239}$Pu</td>
<td>$1.259 \pm 0.03$</td>
<td>$1.2936 \pm 0.003$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{242}$Pu/$\sigma_f$ $^{239}$Pu</td>
<td>$0.1883 \pm 0.005$</td>
<td>$0.1908 \pm 0.0007$</td>
</tr>
<tr>
<td>$\sigma_f$ $^{241}$Am/$\sigma_f$ $^{239}$Pu</td>
<td>$0.1963 \pm 0.005$</td>
<td>$0.1935 \pm 0.0006$</td>
</tr>
</tbody>
</table>

### Discussion

The quality of the criticality calculation results obtained using different libraries (ROSFOND, BNAB-RF, and BNAB-93) and the spectral indices measurements can be judged from the data presented in Table 3. The table’s
columns present the following data: column 3 – experimental data, column 4 – experimental error value (δ \( \sigma \)), columns 5 through 7 – relative deviations between the calculated data C and the experimental data E, column 8 – relative value of the calculated (statistical) error (\( \delta \)).

As can be seen from the table, the calculation/experiment discrepancies for most of the spectral indices lie within the experimental error limits of 3σ for all of the libraries. The exception is the calculation/experiment discrepancies for the ratio of the \( { }^{238}\text{Pu} \) fission cross-section to the \( { }^{239}\text{Pu} \) fission cross-section, the values of which are several times as great as the experimental error value. Such large discrepancy values are explained by technical aspects of the fission cross-section measurements for these isotopes. The experimental data for these spectral indices were ignored for the subsequent computational and experimental analysis.

The data shown in Table 3 makes it possible to conclude that the nuclear data uncertainty component caused by the group approximation (the transition from the ROSFOND library to its BNAB-RF group version) does not exceed 2.5% for the integral fission cross-sections, this being comparable with the statistical calculation error. And the transition from the BNAB-93 library to the BNAB-RF library does not lead to a bias in the fission rate calculation results \( \langle \sigma \rangle \) (variations in the values \( \langle \sigma \rangle \) within the statistical calculation error limits) for most of the spectral indices, except the \( { }^{241}\text{Am} \) and \( { }^{243}\text{Am} \) isotopes for which the discrepancies in the \( \langle \sigma \rangle \) calculation results reach 14 to 23%. No experiments with measuring the relative fission rate using the SFC were conducted based on the BFS-61 assemblies.

Table 3 presents the value of the integral efficiency indicator \( \mu_2 \), the quantitative efficiency measure in the description by the nuclear data library \( k \) for the set of integral experiments \( N \), which is defined by the following relation (Usachev and Bobkov 1972):

\[
\mu_2 = \frac{1}{N} \sum_{n=1}^{N} \left[ \left( \frac{C_n}{E_n} - 1 \right) \cdot 100 \right]^{2} \left[ \delta_{n}^{2} + \delta_{E_n}^{2} \right]^{1/2},
\]

where \( N \) is the number of the experiments; \( n \) is the experiment number; and \( k \) is the identifier of the nuclear data library.

L.N. Usachev defines an optimized system of nuclear data that does not need to be adjusted to describe a set of \( N \) experimental data as the system of nuclear data, for which the value of the integral efficiency indicator \( \mu_2 \) lies in the interval of zero to unity.

As shown by the results of the calculation and experimental analysis (see the closing line in Table 3), the minimum value of \( \mu_2 \) for \( k_{61-2} \) is observed only for the BNAB-93 library since the BFS-61 experiments were planned using the calculation results obtained using this nuclear data group library. However, the ROSFOND nuclear data library is the optimal nuclear data library based on the results of the calculation and experimental analysis for the entire set of measurements performed on a whole series of the BFS-61 assemblies.

**Conclusion**

Peculiarities have been considered of preparing mutually self-agreed computational models for precision and engineering neu- tronic codes and calculating, on the basis of these, the neutronic parameters of the three critical BFS-61 assembly configurations.

The improved functional capabilities of updated software products and nuclear data have been demonstrated to support the computational and experimental analysis of integral experiments based on the BFS assemblies which make it possible to reduce considerably the time for and to minimize the probability of errors in preparing models and building mutually self-agreed neutronic models for high-precision and engineering neutronic codes. The new capabilities of the CONSYST-RF system allow simplifying to a great extent and automating the preparation of computational tasks for taking into account the heterogeneous self-shielding effects, while avoiding the need for additional codes to be involved. The updated version of the MMK-RF code includes a superimposed grid function which permits computations of spectral characteristics and spatial distributions of the BFS-measured reaction rates. Besides, the MMK-RF code can be used for calculations in a neutron multigroup approximation with a pointwise representation of nuclear cross-sections and using a combined technique. Since the MMK-RF code has a better calculation rate than the MCNP code thanks to a specialized geometrical module, it can be chosen as the Russian high-precision neutronic code for the computational support of experiments on the BFS critical facilities.

The procedures have been tested for preparing neutron multigroup constants with regard for the effects of the spatial heterogeneity implemented in the CONSYST-RF code. It has been shown that the difference between the group approach and the pointwise representation of neutron cross-sections in the criticality calculations does not exceed 0.3% in criticality for the BFS-61 assemblies.
The biases in the results for the spectral indices are in the limits of the statistical calculation error. Based on the results of the computational and experimental analysis for the entire set of measurements performed based on a series of the BFS-61 assemblies, the ROSFOND library is the optimal nuclear data library.

References