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Research Article

Generating a system of group constants for neutron-physical calculations of fast reactors based on ROSFOND-2020.2 library files*

Elizaveta P. Averchenkova[1], Yana V. Dyachenko[1], Svetlana V. Zabrodskaya[1], Gennady N. Manturov[1], Vyacheslav A. Mishin[1], Daria V. Panova[1], Anton A. Peregudov[1], Mikhail Yu. Semenov[1], Ivan V. Tormyshev[1], Evgeny P. Lyapin[2]

1 *IPPE JSC, Bondarenko Sq, 249033, Obninsk, Kaluga Reg., Russia*
2 *Beloyarsk NPP, 624251 Zarechny, Sverdlovsk Reg., Russia*

Corresponding author: Daria V. Panova (dvpanova@ippe.ru)

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Abstract

The subject of constant support development is currently becoming increasingly important in connection with the national strategy of transition to a closed nuclear fuel cycle. At the same time, the importance of the tasks of refining calculation models and minimizing methodological, statistical, and constant errors is increasing. In this connection, the idea of creating a universal system of constants describing with equal accuracy both uranium loading and loading with mixed oxide uranium-plutonium fuel and the possibility to perform on its basis both precision Monte Carlo calculations (data format – ACE) and multigroup calculations (formats – ABBN and ANISN) was laid in the basis of this work. In this paper we analyze the freely available libraries of evaluated nuclear data in order to justify the choice of source files for the formation of a new system of group constants for neutron-physical calculations of fast reactor cores, describe the process of formation of a new library of reactor constants, and verify the obtained system on computational test models of BN-800 reactor and critical systems. The process of formation of the new system of group constants included selection of initial neutron data files, updating of data tables of basic neutron cross-sections, self-shielding factors and Doppler coefficients, as well as data on fission spectra for the main fuel nuclides. The methodological component of the error for test models of the BN-800 core was evaluated. Using the ABBN-RF22 system of group constants it was possible to estimate the correction in the 299 groups calculation, which amounted to 0.3%. Previously, when using the ABBN-93 library, there was no such possibility due to the lack of continuity between the files of evaluated neutron data and the group constants used.

Keywords

BN-800, ROSFOND-2020.2, evaluated data, constant error, group constants, mixed oxide uranium-plutonium fuel

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Introduction

Design of and computational support for nuclear power plants require estimating, mandatorily, the uncertainty of the design parameters. One way to minimize this uncertainty is to use reliable and proven set of constants.

Computational studies into the neutronic performance of fast neutron reactors are based on using three-dimensional diffusion codes, such as JAR-FR (Yaroslavtseva 1983), GEFEST (Belov and Seleznev 2010), GEFEST800 (Asatryan et al. 2015), TRIGEX (Seregin and Kislitsyna 1997), FACT-BR (FACT BR 2018) and codes based on the Sn-method, including TWODANT (Alcouffe et al. 1984), KATRIN (KATRIN-2.5 2014) and CASCADE (CASCADE-3.0 2019). These codes have been extensively used in practical calculations, since they do not require heavy computational costs and much calculation time.

Increased productivity and reliability of computer equipment over the past decade have made it possible to calculate a reactor using complex detailed models in codes based on the Monte Carlo method. The most common of these are MCNP5 (MCNP 2003), a US code, and Russian codes such as MMKKENO (Blyskavka et al. 2001) and MCU-FR (MCU-FR 2020).

Cross verification based on all of the above codes, as well as estimating the methodological component of the calculation error require using a unified set of constants, which is currently provided via the CONSYST constant preparation system (Manturov et al. 2000) with the ABBN-93 library (Manturov et al. 1996; ABBN-93 2014). Using this system of constants for uranium reactor systems has made it possible to determine the constant component of the error in the criticality value at a level of ~ 0.2%. The ABBN-93 library does not offer, however, continuity of the evaluated neutron data files and the group constants used, this making it impossible, consequently, to estimate the correction in the group calculation.

Currently, the composition of effective fast reactor cores has begun to change. Thus, in the autumn of 2022, the BN-800 reactor reached criticality following the tenth refueling with a core, which had a 93% share of fuel assemblies (FA) with uranium-plutonium. The eleventh cycle between refueling is usually looked upon as the initial interval of the BN-800 operation fully loaded with mixed oxide uranium-plutonium fuel. It needs to be noted that this is the first experience of commercially operating a reactor core with such type of fuel. It is planned that minor actinides will be added to the fuel composition at the next stage in the framework of the national strategy for closing the nuclear fuel cycle. As a result, the share of plutonium and the mass of minor actinides in the core will increase. This means that the established balance of the constant set will move into the increased uncertainty area. Fig. 1 shows the change in the k_{eff} values obtained in the process of the BN-800 calculation during the period of conversion to the full loading with mixed uranium-plutonium oxide fuel (between refueling cycles 8 and 11).

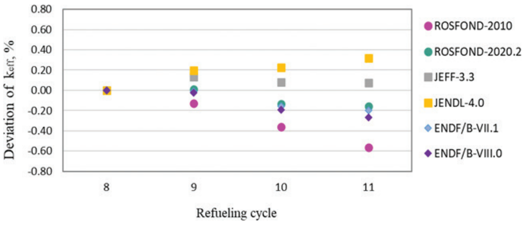

Figure 1. Change in k_{eff} values relative to refueling cycle 8.

The increase in the share of plutonium in the core has led to the constant error scatter increased to ~ 1% in the k_{eff} estimation using various libraries of reactor constants. With minor actinides involved in the fuel cycle, the constant component of the error will increase still greater.

In this connection, it is essential to develop a new version of the group library of constants, capable to describe equally accurately both the uranium and mixed uranium-plutonium fuel loads in reactor cores. It will be reasonable to introduce the new constant library, similarly to the existing ABBN-93 library, in codes used by different organizations for the fast reactor calculations.

Selection of initial data for verification

To form a unified verification, in terms of calculating uranium and plutonium systems, one needs to analyze the currently available libraries of evaluated nuclear data. The following versions of evaluated neutron data libraries were used for verification calculations: ENDF/B-VII.1 (Chadwick et al. 2011), ENDF/B-VIII.0 (Brown et al. 2018) (in the USA), JEFF-3.3.1 (The JEFF-3.3.1 2018) (in Europe) and JENDL-4.0 (Shibata et al. 2011) (in Japan), as well as a Russian library of group constants, ABBN-93, and files of Russian evaluated neutron data libraries, ROSFOND-2010 (Zabrodskaya et al. 2007) and ROSFOND-2020.2 (Manturov et al. 2022).

The ROSFOND-2010 data library accumulates current estimates of neutron cross-sections for more than 680 primary and secondary materials (nuclides). It contains complete sets of neutron data for all stable periodic system elements (for individual isotopes as a rule). A complete set means a set of data sufficient to take into account the interaction of neutrons with nuclei in the process of the neutron propagation in the medium.

The ROSFOND-2020.2 estimates for fuel and structural materials were updated and taken from the CIELO (Collaborative International Evaluation Library Organization) project results (Chadwick et al. 2018). The data on the cross-sections for calculating the damaging doses of structural materials, the constants of delayed neutrons, and the fission neutron spectra were determined more exactly. The database of covariance matrices for the nuclear constant errors was extended.

The verification of the above constant libraries was conditionally divided into two stages, including verification based on a set of benchmark models from the ICSBEP Handbook (NEA/NSC/DOC(95)/03 2016) and test models of the BN-800 core.

The benchmark models were calculated at the initial verification stage. The models were selected based on the extent of consistency with real reactor systems in terms of the composition and characteristics of the energy spectrum. They were conditionally divided into two groups.

Compact metal assemblies (CMA) with highly enriched uranium (GODIVA, FLATTOP-25) and plutonium (JEZEBEL, FLATTOP-Pu) were used to verify the constants of the key fissile nuclides in the fast energy spectrum of neutrons. Structurally, the assembly is either a metal sphere with no reflector or a metal sphere surrounded by a metal reflector made of depleted uranium. Also used was a cylindrical assembly with uranium metal (10% enrichment) with a reflector of depleted uranium metal (BIG TEN) and an experiment in the form of an infinite cell with $k_\infty = 1$, which determined the critical content of ^{235}U in the mixture with ^{238}U (ZEBRA 8B). Additionally, an artificial model was used, which represented an infinite medium consisting of ^{235}U and ^{238}U with $k_\infty = 1$ (SCHERZO556).

To verify nuclear data and methods for preparing constants, critical assemblies were used with characteristics more consistent with real fast reactor systems (RS). Benchmark models were selected such that their composition correlated with models of the BN-type reactor cores both with uranium loads (ZPR-type assemblies) and with oxide uranium-plutonium fuel loads (ZPPR-type assemblies). Thus, assemblies were selected which met the conditions of testing a set of constants for calculations of fast neutron reactors.

Test models of the BN-800 critical states were used for the second verification stage. Refueling cycles (8 through 11) were selected for the BN-800, which characterized the 100% increase in the share of mixed uranium-plutonium fuel.

All test models were developed in the framework of the BNcode (Peregudov et al. 2019) from the reactor fuel assembly archive, which contained information on all reactor lifecycle states.

Neutron data library verification results

To verify the set of constants, a series of calculations was undertaken using benchmark models based on the libraries described above. Figs 2, 3 shows discrepancies in the criticality calculation results for the series of CMA and RS benchmark models respectively.

The following conclusions can be made from the presented calculated data of the constant set verification for the series of benchmark models:

1. the deviation of the calculated values from experimental data does not exceed 1% for all libraries of evaluated nuclear data;
2. the most accurate description of the selected critical systems was provided by the ROSFOND-2020.2 library: the average deviation for the CMA systems was –0.06 ± 0.10%, and the average deviation for the RS systems was 0.05 ± 0.14%.

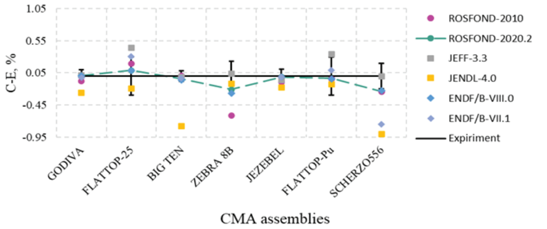

Figure 2. Discrepancies in the criticality calculation results for the CMA-type benchmark models.

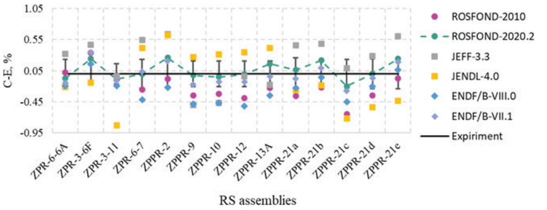

Figure 3. Discrepancies in the criticality calculation results for the RS-type benchmark models.

To verify the set of constants using a set of the BN-800 test models, a series of calculations was undertaken based on the above libraries.

Fig. 4 shows the changes in the k_{eff} values relative to refueling cycle 8 obtained in the calculation of the BN-800 test models.

The following conclusions can be made based on the reactor neutronic performance calculation results:

- the results of the BN-800 calculations using the ROSFOND-2010 and JENDL-4.0 systems of constants have shown a trend towards a decreased/increased criticality value with mixed oxide uranium-plutonium fuel loaded into the core;
- the results of the BN-800 calculations using the ROSFOND-2020.2 library of constants describe the criticality in the event of transition to mixed oxide uranium-plutonium fuel with an accuracy of ~ 0.2%.

Therefore, it has been recommended that the ROSFOND-2020.2 files of evaluated neutron data should be used to form a group library of constants and its further implementation in practical computational support for the Beloyarsk NPP units.

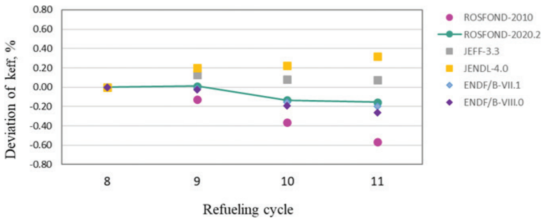

Figure 4. Changes in k_{eff} values relative to refueling cycle 8.

Formation of a new group constant system

The process of forming a new system of group constants consists in establishing a library of 28-group and

299-group constants of a versatile format based on the ROSFOND-2020.2 neutron data.

The data in this constant system should be presented in a format with an increased accuracy, which has the same content as the ABBN-93 format.

The process of forming a new group library of neutron data in a format with an increased accuracy was divided into a number of stages:

1. compiling the list of nuclides from the ROSFOND-2020.2 library files required for calculating the neutronic performance of fast neutron reactors and justifying safety;
2. preparation of the key neutron cross-sections for 28 and 299 groups;
3. preparation of self-shielding factors and Doppler coefficients for the same group breakdown;
4. formation of a constant system in a format with an increased accuracy;
5. conversion of the library to a binary form.

At the initial stage, nuclides were selected from the ROSFOND-2020.2 library files, the data of which are required in the process of calculating the key neutronic characteristics of operating reactors:

- fuel nuclides (^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu);
- structural materials (Al, Cr, Fe, Mo, Nb, Ni, Zr);
- coolant materials (Nd and Pb).

The next stage used the NJOY program (MacFarlane et al. 2019) to convert the ROSFOND-2020.2 library files from the ENDF-6 format (Herman and Trkov 2010), which stores all key END libraries, to a group format.

Further, after the ROSFOND-2020.2 files were processed using the NJOY program, two types of files were formed (for the 28- and 299-group breakdowns). This step formed files containing tables of the key neutron cross-sections and files containing data on self-shielding factors (MF = 4/304) and Doppler coefficients (MF = 5/305). The files were prepared at temperatures of 300 K, 900 K, and 2100 K in a fast spectrum approximation. The output files were integrated then on a group basis.

Tables MF = 5/305 are presented for the key and reactor nuclides, the contributions of which to the Doppler effect are decisive.

Data for natural mixtures have been obtained for those materials where possible, including Fe, Cr, Ni, Pn, Mo, and Zr. The process of obtaining constants for natural mixtures is based on the calculation of pointwise data for each stable isotope (Peregudov et al. 2011).

The process of convoluting neutron data of stable isotopes into microconstants for a natural mixture has two constituents.

Initially, data with an additive property are convoluted which include interaction cross-sections and their energy-angular dependencies.

This is followed by convoluting data which do not have an additive property: these include data on the resonant self-shielding of cross-sections, the so-called Bondarenko factors, or self-shielding factors.

Based on the list of the nuclides selected from the ROSFOND-2020.2 and ROSFOND-2010 neutron data libraries, a new system of group constants, called ABBN-RF22, was formed and converted to a binary form.

BN-800 calculation with a new system of group constants

The criticality of the BN-800 test model was calculated using the MMKKENO code as of the refueling cycle (RC) start time for the “cold” reactor state between refueling cycles 8 and 11. The statistical error was ± 0.00003.

Fig. 5 shows the changes in k_{eff} values relative to refueling cycle 8 when calculated using the design ABBN-93 library and the new system of group constants (ABBN-RF22). One can see that the results obtained using the ABBN-93 and ABBN-RF22 libraries of constants are not mutually contradictory.

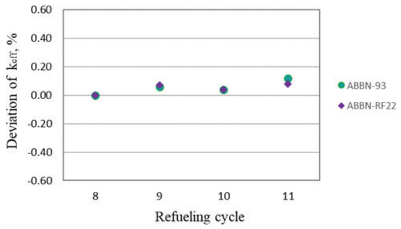

Figure 5. Changes in k_{eff} values relative to refueling cycle 8.

The methodological component of the error was estimated for the test model of the BN-800 reactor core for the case of its conversion to a mixed oxide uranium-plutonium fuel load (cycles 8 through 11). The calculation was undertaken using the design ABBN-93 library of constants and a new system of group constants (ABBN-RF22).

The criticality value was calculated in a P_5 approximation using the MMKKENO code (299 groups) for a homogeneous test model and a heterogeneous test model. The statistical error of the k_{eff} calculation using the MMKKENO and MMKC codes (MMKC 2019) is equal to 10^{-4}.

Table 1 shows the result of the k_{eff} calculation using the TRIGEX code and the methodological allowances obtained for this result.

Based on the results presented in the table, conclusions can be made on the methodological allowances for the diffusion calculation:

- the kinetic allowance of the diffusion calculation, along with the allowance for the 299-group calculation, was about +0.7%;
- the heterogeneous allowance changes as the result of conversion to mixed oxide uranium-plutonium fuel and was +0.7% for the conversion region, and +0.9% for the core with MOX fuel;
- the allowance for the 299-group calculation does not depend on the type of fuel used and is about +0.3%.

Table 1. TRIGEX k_{eff} calculation results and the methodological allowances obtained for this result

	RC 8		RC 9		RC 10		RC 11	
	ABBN-93	**ABBN-RF22**	**ABBN-93**	**ABBN-RF22**	**ABBN-93**	**ABBN-RF22**	**ABBN-93**	**ABBN-RF22**
k_{eff}								
TRIGEX_6p	0.9821	0.9844	0.9817	0.9840	0.9802	0.9823	0.9814	0.9834
Methodological allowance, %								
TRIGEX_1p	1.2	1.2	1.2	1.3	1.3	1.3	1.3	1.3
MMKK (hom.)	0.7	0.6	0.7	0.7	0.7	0.7	0.6	0.6
MMKK (het.)	1.4	1.3	1.5	1.5	1.6	1.5	1.5	1.4
MMKC (het.)	–	1.6	–	1.8	–	1.8	–	1.7

The complete methodological allowance for the diffusion calculation was +1.6% for the conversion region, and 1.7% for the core with mixed oxide uranium-plutonium fuel.

Based on the results of the computational studies, the following should be noted:

- the change in the methodological allowance of the diffusion calculation for the case of conversion to mixed oxide uranium-plutonium fuel is not significant;
- the allowances introduced to the design ABBN-93 library of constants and the new system of group constants (ABBN-RF22) are consistent;
- using the ABBN-RF22 system of group constants made it possible to estimate the allowance associated with the 299-group calculation (0.3%); it was not possible to do this when the ABBN-93 library was used due to the lack of continuity of the evaluated neutron data files and the group constants used;
- using a solution with one point per assembly in the diffusion calculation led to a +0.4% smaller methodological allowance.

Conclusions

In connection with the BN-800 conversion to a full load with mixed uranium-plutonium oxide fuel and plans for minor actinides to be involved in the fuel cycle, the resultant balance in the set of constants shifts to the increased uncertainty region, this leading to an increase in the error's constant component.

To minimize the methodological and constant errors, a unified system of group constants, ROSFOND-2020.2, was developed based on the ABBN-RF22 evaluated neutron data files, which describes equally accurately both the uranium load and the load with mixed oxide uranium-plutonium fuel. The process of forming a new system of group constants included updating data in the tables of the key neutron cross-sections, self-shielding factors and Doppler coefficients, as well as data on the fission spectra for the key fuel nuclides.

The key advantage of the ABBN-RF22 constant library, as compared with its earlier counterpart (ABBN-93), is as follows:

- current estimates of neutron cross-sections are used for fuel and structural materials;
- 299-group data on the cross-sections are available for all nuclides contained in the library (there are only 16 nuclides presented in the ABBN-93 in a 299-group breakdown);
- there are neutron data for both isotope mixtures and mixtures (the ABBN-93 does not include data for individual isotopes of structural materials);
- due to the continuity of the evaluated neutron data files and the prepared group constants, it was possible to estimate correctly the methodological component of the error associated with the group representation of neutron cross-sections; it was not possible altogether to do this in the ABBN-93 constant system;
- it is possible to promptly add other neutron data estimates to the ABBN-RF22 group library of constants;
- there is a matrix fission spectrum for each fuel nuclide.

In the process of the study, the methodological component of the error for the BN-800 core test models was estimated as part of the calculation with a new system of group constants, which has shown the following:

- the change in the methodological allowance of the diffusion calculation for the case of conversion to mixed oxide uranium-plutonium fuel is not significant;
- the allowances introduced to the design ABBN-93 library of constants and the new system of group constants (ABBN-RF22) are consistent;
- using the ABBN-RF22 system of group constants made it possible to estimate the allowance associated with the 299-group calculation (0.3%); it was not possible to do this when the ABBN-93 library was used due to the lack of continuity of the evaluated neutron data files and the group constants used;
- using a solution with one point per assembly in the diffusion calculation led to a +0.4% smaller methodological allowance.

It is planned to update further other neutron data estimates for the remaining sections. The obtained version of the ABBN-RF22 group constant system is planned to be added to the design codes and to the GEFEST-M unified coupled code for the computational support of the BN-600 and BN-800 reactors at the Beloyarsk NPP.

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