Testing the multigroup, group and subgroup options of the CONSYST / ABBN-RF system on criticality calculations of fast reactor models with MNUP fuel

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Abstract. The unified code CONSYST-2020 for neutron constants preparation and the ABBN-RF-2020 neutron data library are being tested as part of the new generation codes development for neutronic calculations of fast reactors with mixed nitride uranium-plutonium fuel (MNUP). Testing was carried out on prototype models of fast reactors with MNUP fuel. The errors of the multigroup, group and subgroup approximation are analyzed in comparison with the calculations performed using point-wise cross-sections libraries. The results obtained with point-wise cross-sections libraries are accepted in the final cross-verification as reference results. An assessment was made of the influence of approximations associated with averaging and preparing group cross-sections, and methodological errors determined by the selected spatial and angular computational grids. It was shown that the transition to the direct use of 299-group blocked constants reduces the error to 0.1 – 0.2%. The assessment of the efficiency of using the subgroup approximation shows the possibility of reducing the constant component of the error below 0.05%.

1. Introduction
The development of new-generation codes for calculations of fast reactors with MNUP fuel is being actively pursued within the framework of the PRORYV project. Such codes include the unified constants preparation code CONSYST-2020 for neutronic calculations of fast reactors and the ABBN-RF-2020 constants system. An updated subgroup option and an option with a detailed description of neutron cross-sections became a significant expansion of the system’s capabilities. This work is a continuation of works on solving test problems for fast reactors with MNUP fuel [5] – [11].

The CONSYST-RF program with the ABBN-RF data libraries (CONSYST / ABBN-RF-2020 system) [12] – [15] is designed to provide constants for multigroup neutronic calculations of reactors and radiation protection, as well as nuclear and radiation safety problems during production, transportation and nuclear fuel storage at fuel cycle enterprises and nuclear power plants. The ABBN constants can be used both for performing neutronic calculations and directly, for example, for calculating the transmutation of nuclides or the accumulation of long-lived fission products. The CONSYST-RF program (CONSYST / ABBN-RF-2020 system) provides the calculation of multigroup homogenized neutron constants based on the initial ABBN-RF cross-sections libraries, taking into account:
• resonant self-shielding of cross sections included in the composition of the nuclides environment;
• heterogeneous environment;
• neutrons thermalization;
• scattering anisotropy in the approximations provided by the capabilities of the initial constants library (for neutron constants up to the P5 approximation).

The created constant support is adapted to modern computational methods – deterministic (engineering, grid and DSN methods) and stochastic (Monte Carlo method). The CONSYST-RF program is designed for linking the ABBN constants with such neutronic calculation codes as ANISN, TWODANT, DORT. It also allows to use the ABBN data through the ANISN format in Monte Carlo calculations in the Russian MMKK program, the American KENO and MCNP programs. The program allows to prepare medium constants for neutron-physical calculations in 28 or 299 group approximations, taking into account the scattering anisotropy in the approximations provided by the capabilities of the original library of constants (for neutron constants up to the P5 approximation). The microconstants prepared using the CONSYST program were calculated taking into account the resonant self-shielding of the cross-sections, i.e. so-called blocked environment micro-constants.

Testing of the multigroup, group and subgroup options and option with a detailed description of the ABBN-RF neutron cross-sections on the test models of the BN-1200 and BREST reactors in the criticality calculations was carried out on the latest version of the unified CONSYST-RF code. The CONSYST / ABBN-RF system includes a new nuclear data library ABBN-RF, obtained on the basis of ROSFOND data, and a package of CONSYST-RF support programs, which task is converting the ABBN-RF constants (resonant blocking of cross-sections) and preparing them for the neutronic calculations of nuclear installations (reactor core, radiation protection, etc.).

2. Methods and algorithms
The ideology of the problem solving is based on the separation of the constant and computation errors in the multiplication factor calculations.

The following calculations chains were built for the implementation.

ROSFOND (continuous) ---» MCU–FR
This calculation chain is based on the use of continuous dependences of neutron cross-sections and uses to obtain results by the Monte Carlo method. It makes the possible to exclude approximations related with averaging and preparation of group cross-sections and methodological errors determined by the selected spatial and angular computational grids. The results obtained by the ROSFOND (continuous) – MCU–FR chain are accepted in the final cross-verification as reference results.

ABBN-RF (group) ---» CONSYST ---»
---» blocked cross-sections (299, 28 or 26 groups) ---» KENO
This calculation chain is based on the use of ABBN multigroup neutron constants and uses to obtain results by the Monte Carlo method. The chain allows to exclude the methodological errors determined by the selected spatial and angular computational grids. The results obtained by the ABBN - CONSYST - KENO chain make it possible to separate the component of the calculated error related with the preparation of the initial 229-group library of ABBN constants, with averaging of the cross-sections to 28 or 26 groups.

A three-dimensional algorithm for calculating the criticality KENO-VI, based on the Monte Carlo method using a continuous or multi-group representation of neutron cross sections is used in this work. KENO-VI is one of the main criticality safety analysis tools in SCALE 6.2 package. The KENO-VI code from SCALE 6.2 is used to construct a calculation chain based on the use of ABBN multigroup blocked neutron constants to obtain the Monte Carlo results. It must be notes that the MCU – FR code does not allow calculations using the ABBN multigroup blocked neutron constants at present time. The chosen approach makes it possible to exclude methodological errors determined by the chosen spatial and angular estimated grids. The results obtained by the ABBN - CONSYST - KENO chain will allow us to isolate the component of the calculated error associated with the preparation of the
original 229-group library of ABBN constants and averaging the cross-sections during convolution in 28/26 groups.

All calculations using the KENO-VI code were carried out with the following parameters: the number of histories – 106, the number of batches – 203, the statistical error of Keff calculation – no more than 0.00005. All calculations by the MCU-FR code were carried out on the NRNU MEPhI BASOV multiprocessor computing cluster with a total number of simulated histories equal to 100 million. This number of neutron histories allows to calculate the effective multiplication factor with a standard deviation not exceeding 0.007%.

Horizontal sections of the BN-1200 and BREST reactor models are shown in figures 1 and 2.
3. Results

The consistency of the BN-1200 and BREST reactor models developed in the MCU-FR and KENO-VI codes was controlled by calculating the materials volume. The maximum deviation of the materials volumes in the models does not exceed 1%, the average deviation is 0.01%.

Testing results of a multi-group, group options and options with a detailed description of the ABBN-RF neutron cross-sections on the BN-1200 and BREST reactor models in criticality calculations are presented in table 1.

Table 1. \( K_{\text{eff}} \) and \( \varepsilon(\text{Keff}) \) of the test models with the connection of CONSYST / ABBN-RF-2020 multi-group and group options for cross-verification with MCU-FR code.

| Variant     | Keff (group option) | \( \varepsilon(\text{Keff}) \) |
|-------------|---------------------|-----------------|
|             | 299 | 28 | 26 | 299 | 28 | 26 |
| BN-1200_v1  | 1.00332 | 1.00107 | 0.99835 | -0.19 | -0.42 | -0.69 |
| BN-1200_v2  | 1.00409 | 0.99971 | 0.99930 | -0.24 | -0.68 | -0.72 |
| BN-1200_v3  | 0.95841 | 0.95506 | 0.95471 | -0.19 | -0.54 | -0.58 |
| BREST       | 0.98151 | 0.99065 | 0.99083 | -0.06 | 0.27 | 0.29 |

Note that the differences between the CONSYST / ABBN-RF-2020 system in comparison with a detailed description of the neutron cross-sections ABBN-2020 in calculations of the effective multiplication factor in all considered versions of the BN-1200 reactor models are about 0.2% for the multi-group option and not exceed 0.8% for the group option. The same values for BREST reactor model are about 0.06% for the multi-group option and do not exceed 0.3% for the group option.

The ABBN-RF system of constants includes data of the Bondarenko factors, which make it possible to take into account the effect of the cross-section structure on the neutron flux structures and current, with the weight of which the group constants are averaged. The ABBN-RF system contains the so-called "subgroup parameters" presented as a function of a temperature for a more correct accounting of the resonant self-shielding effects (with strong heterogeneity of the medium). The subgroup approximation [3] was primarily used in calculating of BFS critical assemblies to take into account heterogeneous resonance effects that are very significant in this case. As a result, in the subgroup parameters preparing process for taking into account the structure of cross sections in the region of unresolved resonances, a two-subgroup method was used with its suitability verification for all those dilution cross sections that are encountered in a given specific task. If two subgroups are insufficient, a more complex algorithm is used [4]. In the unresolved resonant region, where the subgroup method is the only way to take into account the resonant self-shielding, the two-subgroup approximation turned out, as practice has shown, to be suitable in all cases.

There is a limitation of the maximum number of groups in criticality calculations of BN-1200 and BREST reactor models during the constants preparation with the connection of subgroup options by CONSYST program in chain:

\[
\text{ABBN} \rightarrow \text{CONSYST} \rightarrow \text{KENO}
\]

This number is equal 999. Therefore, we analyzed the number of groups in the created library of constants for KENO code. The number of groups depends on nuclides and numbers of wide ABBN groups, for which subgroup parameters are taken into account. The results are shown in table 2.

The relative fission reaction rates (Sf) and capture reaction rates (Sc) in MNUP fuel were obtained with the aim of selecting the most significant groups. Results are presented in table 3.
Table 2. Number of groups in the created library of constants (subgroup options).

| Wide groups | For $^{238}$U and $^{239}$Pu | For $^{238}$U, $^{239}$Pu and $^{240}$Pu |
|-------------|-------------------------------|--------------------------------------|
| All groups (9 – 28) | 1101 | 2447 |
| 9 – 15 | 495 | 738 |
| 9 – 16 | 578 | 1106 |
| 9 – 22 | 978 | – |
| 9 – 23 | 1000 | – |
| 10 – 28 | 1008 | – |
| 11 – 28 | 999 | – |
| 16 – 18 | 482 | 967 |
| 15 – 18 | – | 1431 |

Table 3. Relative reaction rates by groups in MNUP fuel of BN-1200.

| Group | Sf | Sc | Group | Sf | Sc |
|-------|----|----|-------|----|----|
| 1 | 0,000 | 0,000 | 15 | 0,016 | 0,032 |
| 2 | 0,001 | 0,000 | 16 | 0,031 | 0,057 |
| 3 | 0,012 | 0,006 | 17 | 0,025 | 0,040 |
| 4 | 0,036 | 0,023 | 18 | 0,014 | 0,020 |
| 5 | 0,072 | 0,048 | 19 | 0,007 | 0,010 |
| 6 | 0,125 | 0,073 | 20 | 0,004 | 0,004 |
| 7 | 0,092 | 0,061 | 21 | 0,000 | 0,002 |
| 8 | 0,124 | 0,100 | 22 | 0,000 | 0,001 |
| 9 | 0,119 | 0,096 | 23 | 0,000 | 0,000 |
| 10 | 0,102 | 0,094 | 24 | 0,000 | 0,000 |
| 11 | 0,084 | 0,098 | 25 | 0,000 | 0,000 |
| 12 | 0,059 | 0,094 | 26 | 0,000 | 0,000 |
| 13 | 0,044 | 0,080 | 27 | 0,000 | 0,000 |
| 14 | 0,030 | 0,059 | 28 | 0,000 | 0,000 |

Table 4 presents the results of testing the subgroup option and option with a detailed description of the ABBN-RF neutron cross-sections on the BN-1200 and BREST reactor models in criticality calculations.

Differences between calculations with CONSYST / ABBN-RF-2020 sub-group option in comparison with a detailed description of ABBN-2020 neutron cross sections in calculations of the effective multiplication factor in all considered models of the BN-1200 reactor are about 0.2% for the multi-group option and do not exceed 0.07 % for the subgroup option with the number of calculation groups not exceeding 999. However, it must be noted that the number of groups is directly related to the calculation time in programs which implement engineering grid and DSN methods.
Table 4. $K_{\text{eff}}$ and $\varepsilon(K_{\text{eff}})$ of the test models with the connection of CONSYST / ABBN-RF-2020 sub-group option for cross-verification with MCU-FR code.

| Variant        | $K_{\text{eff}}$ (sub-group option) | $\varepsilon(K_{\text{eff}})$ |
|----------------|-------------------------------------|-------------------------------|
|                | 299       | 28    | 26    | 299  | 28    | 26    |
| BN-1200_v1     | 1.0056    | 1.0066| 1.0054| 0.04 | 0.13  | 0.02  |
| BN-1200_v2     | 1.0070    | 1.0052| 1.0073| 0.05 | -0.13 | 0.07  |
| BN-1200_v3     | 0.9605    | 0.9590| 0.9605| 0.03 | -0.14 | 0.02  |
| BREST         | 0.9823    | 0.9829| 0.9828| 0.02 | 0.09  | 0.07  |

4. Conclusions

It has been confirmed that the use of CONSYST / ABBN-RF-2020 group (26 or 28 groups) library makes it possible to obtain criticality parameters of reactors with MNUP fuel with an error of about 0.5%. It is shown that the transition to the direct use of 299-group blocked constants reduces the error to 0.1 – 0.2%. The assessment of the efficiency of using the subgroup approximation shows the possibility of reducing the constant component of the error below 0.05%.

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