Actual Status of the Development of Multigroup XS Libraries for the Gas-cooled Fast Reactor in Slovakia

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Abstract. Slovakia is involved in the development of the ALLEGRO reactor, the demonstrator of the unique GFR technology. Since the Gas-cooled Fast Reactor lacks any applicable experimental data, the design and optimization of its core must rely on data from similar reactor concepts and on calculations using Monte Carlo and deterministic methods. Although these two methods differ in their nature, both require appropriate nuclear data libraries. The present paper describes the actual status of the development of multigroup XS libraries, optimized for fast, but precise deterministic calculations of the GFR 2400 reactor. The optimization of the XS library involves in improving the actual XS processing scheme. The improvements are in selecting appropriate energy structure, weight function and nuclear reactions. To select the energy structure the results of sensitivity analysis, based on the Standard Perturbation Theory, implemented in the PORK code, were used. In order to obtain the overall sensitivity profile of the GFR 2400 reactor the previous SBJ V2016 XS library was used. Based on the sensitivity results 186g energy structure of the SBJ V2017 XS library was selected. To minimize the size of the XS library and to remove redundant data, a reaction selection procedure was developed. The SBJ V2017 XS library was tested through 15 benchmarks, selected from the ICSBEP handbook, based on similarity assessment. The selected benchmarks were evaluated in the PARTISN transport code, based on integral parameters. Finally, the SBJ V2017 XS library was applied on the full core GFR 2400 reactor model in DIF3D and on the RZ core model in PARTISN. The results were compared with MCNP5 and with the SBJ V2016 library, based on excess reactivity and core-wide and group-wise distributions of important core parameters.

Key Words: Multigroup XS library, evaluated data, Gas-cooled Fast Reactor, SBJ library.

1. Introduction

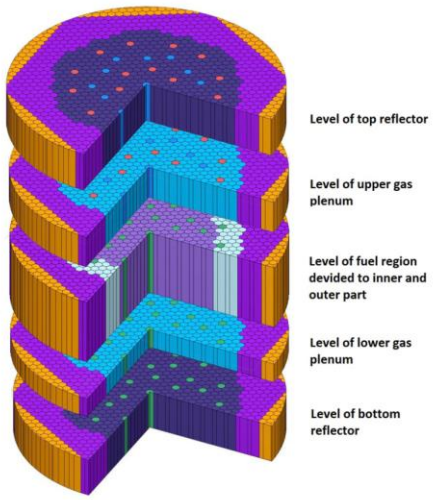
The progress in computer technology in the 21th century gives strong support to the development of modern Monte Carlo codes. Unfortunately, their results are burdened with statistical errors and, due to pointwise cross section (XS) libraries and complex geometry structures, Monte Carlo simulations are costly. For these reasons certain reactor applications require effective deterministic approaches, which imply the development of multi-group XS libraries. There exist several multi-group XS libraries available for fast reactor calculations; however each of them carries a unique fingerprint of a system, for which it was developed and optimized. The best way to optimize a XS library is to use as much experimental data as possible, this could be almost impossible for systems that have never been built, like the GEN IV Gas-cooled Fast Reactor [1]. Slovakia is involved in the development of the ALLEGRO reactor, the demonstrator of the Gas-cooled Fast Reactor (GFR). Since GFR lacks any applicable experimental data, the design and optimization of its core must rely on data from similar reactor concepts and on calculations using Monte Carlo and deterministic methods.

At earlier stages of fast reactor research at the Slovak University of Technology in Bratislava, the Korean KAFAX [2] XS library was used for core calculations. However, since this XS library had been optimized for liquid metal-cooled fast reactor (LMFR) cores, which are characterized by different neutron spectra, requirements were raised to develop a new optimized XS library for GFR. The members of the core physics and nuclear data research group of our institute have been dealing with multi-group XS library development since 2014. The first version of our multi-group XS library (hereinafter the SBJ library) was prepared using standard NJOY processing options (620 SAND-II structure, constant background cross sections and IWT8 weight function). In the next SBJ V2015 library, isotope dependent background XS were used and various neutron spectra, taken from CE MCNP5 [3] calculations of GFR 2400, were investigated (for more detail see [4]). The last version of our library (SBJ V2016) was proposed in 4 fine group (80, 187, 500 and 620) and 2 coarse group (25 and 33) structures. As the analysis presented at [5] shows, the bias of our XS library is comparable with other available XS libraries, but there are still possibilities for improvement, mainly in optimizing the energy group structure and the selection of nuclear reactions. The paper presents the actual development stage of the most recent SBJ V2017 XS library.

2. Overview of the GFR 2400 reactor

As it was mentioned in the introduction part of this paper, the Gas-cooled Fast Reactor, strictly speaking, its GFR 2400 concept, was selected as the target system for XS library optimization. It is a large scale power unit with a thermal power of 2400 MWth. Its design is based on the initial 600 MWth GFR core proposed by CEA [6] and on the concepts and findings of the EU GoFastR project [7]. As primary coolant He at 7 MPa pressure is used. The arrangement of the secondary cycles is based on three main loops (3×800 MWth) [8]. Each loop accommodates an internal heat exchanger and a blower enclosed in a single vessel. In this design the indirect Brayton cycle with the He-N_2 mixture ensures 45 % gross electric efficiency. The cross section of the core and the fuel loading pattern are shown in *FIG. 1*.

a; cross sectional view



b; fuel loading pattern

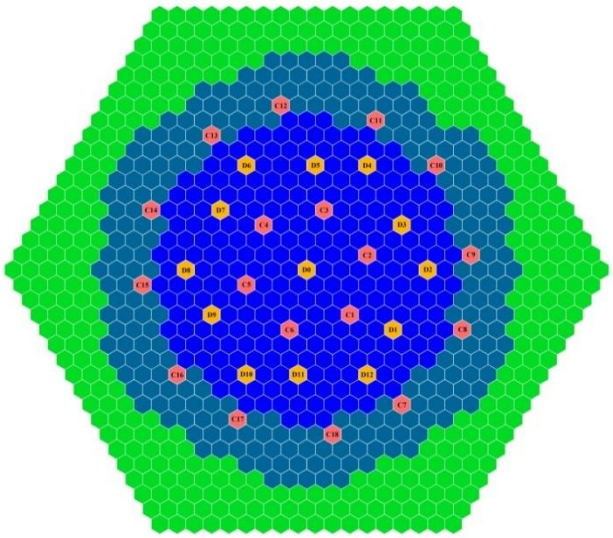


FIG. 1. Cross sectional view of the GFR 2400 reactor and the fuel loading pattern.

The GFR 2400 fuel core is composed of the inner core (IC) and the outer core (OC), with 264 and 252 fuel assemblies respectively. The volumetric content of Pu isotopes in heavy metal in the IC and OC assemblies reach 14.2%, and 17.6%. In both core regions pin type (U,Pu,Am)C fuel is used. Since GFR 2400 has been designed to withstand high temperatures, ceramic structure materials are used in the core. To ensure fission product confinement, the fuel pins are surrounded by refractory liners (W14Re-Re) and with state-of-art SiC/SiC_{fib} cladding. The core fuel region is surrounded by three rings of Zr_3Si_2 reflector assemblies in the radial direction and by a 1 m high axial reflector of the same material placed above and below the fission gas plena. The height of the core, including the gas plenum and reflector, is 5.00 m. The reactivity of the GFR 2400 core is controlled by two systems of control assemblies. The control (CSD) and diverse safety devices (DSD) are concentrically distributed in 4 rings. The numbering scheme of control rods is shown in *FIG. 1.b*, where "C" stands for CSD and "D" stand for DSD assemblies. The absorber part consists of B_4C with 90% weight content of the main absorbing ^{10}B isotope. The rod follower is made of SiC.

3. The SBJ V2017 library

3.1.The processing scheme

The SBJ V2017 multigroup cross-section library is the most recent version of the SBJ multi-group library developed by the STU research team. The main processing engine used in the scheme is the NJOY12 [9] code, which requires a variety of input data. In order to ease the operation of the NJOY12 code and to avoid erroneous input data, the whole scheme has been implemented in an automated C++ utility program. The cross-section processing scheme used for the SBJ V2017 multigroup library is shown in *FIG. 2*.

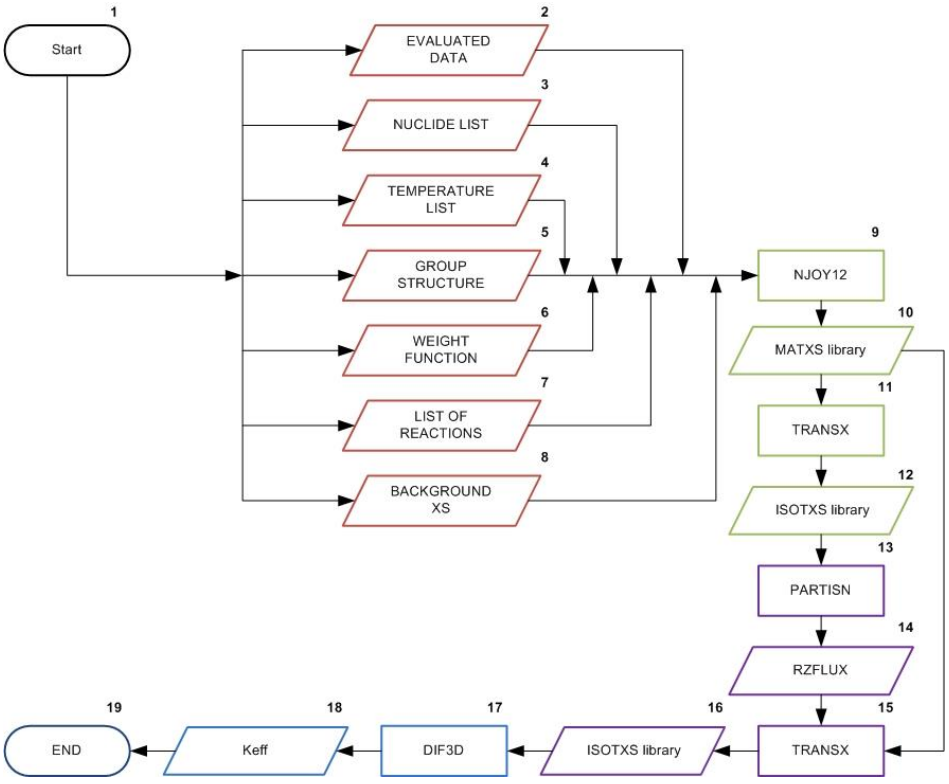


FIG. 2. The SBJ V2017 cross-section processing scheme.

The procedure starts with reading and treating the required input data. These data include evaluated nuclear data (2), list of nuclides (3) list of temperatures (4), energy group structure (5), neutron weight function (6), list of nuclear reactions (7) and background cross sections (8). The list of nuclides and temperatures is defined by the user. The code enables any ENDF6 format evaluated data to be used; however the presented SBJ V2017 library was prepared using ENDF/B-VII.1 [10] data. The selection of the remaining input data is described in the next sections. Based on the specified data the NJOY 2012 code (9) prepares the fine group MATXS XS library (10). These cross-sections are transformed to effective region-wise macroscopic XS data using TRANSX (11) [11] and stored in the ISOTXS library (12). This library can be used in any calculation code supporting CCCC format files. For certain applications, to reduce the calculations costs, group collapsing can be performed. In our case the TRANSX (15) code and the RZFLUX (14) region-wise neutron flux obtained from SN transport calculation in PARTISN (13) were used [12]. Then coarse group ISOTXS library (16) was created based on processing options recommended for fast reactor calculations. The TRANSX calculation was performed for steady state conditions and forward mode. In order to take into account and correct the anisotropy of the scattering matrixes the Bell-Hansen-Sandmeier (BHS) transport correction was used. Since the course group XS library was prepared for the nodal diffusion DIF3D code [13] the XS data was produced only for the zeroth (N) Legendre order, but the transport correction was made for the N+1 Legendre order. The structure of the coarse group library was collapsed from the original 186g structure, taking into account the shape of the neutron spectra in the GFR 2400 reactor core.

3.2.Selection of appropriate energy structure

In the previous versions of the SBJ XS library, standard NJOY energy group structures were used. The achieved precision and computational bias can be considered satisfactory, however to enhance the performance of the XS library, also its energy structure must be linked with the specifics of the target core. For the selection of appropriate energy structure the results of sensitivity analysis based on the Standard Perturbation Theory (SPT) were used. The Sensitivity coefficients can be according to SPT written in a simple form as follows [14]:

$$S_{k,\sigma} = \frac{\sigma}{k}\frac{\Delta k}{\Delta \sigma} \cong \frac{\Delta \sigma}{\sigma}\frac{\langle \Phi^* \left(\frac{1}{k}\frac{\partial P}{\partial \sigma} - \frac{\partial L}{\partial \sigma}\right)\Phi\rangle}{\frac{1}{k}\langle \Phi^* P \Phi\rangle} \quad (1)$$

In the equation above $S_{k,\sigma}$ is the sensitivity coefficient of k_{eff} with respect to σ, which represents nuclear data like cross sections, fission spectrum or nubar. Symbols L and P in Eq. (1) are net loss and production Boltzman operators; $\Phi^*$and Φ adjoint and forward fluxes respectively. The uncertainty of the k_{eff} is then given approximately by Eq. (2):

$$\sigma_k^2 = S_{k,\sigma}.C_{\sigma,\sigma'}.S_{k,\sigma}^T \quad (2)$$

In Eq. (2) $C_{\sigma,\sigma'}$ is the covariance matrix and $S_{k,\sigma}^T$ is the transposed sensitivity profile. The presented theory was implemented in the inhouse PORK code, which uses the DIF3D code as flux solver. The PORK code calculates the sensitivity profiles of the investigated system (sensitivity coefficients vs. neutron energy) for all nuclides and the specified list of nuclear reactions. For the sensitivity calculations the SBJ V2016 XS library was used in 620 group structure. In order to get complex sensitivity information, the absolute values of partial sensitivity profiles of all reactions and nuclides were summarized and the total sensitivity profile of the system was created. The results of the total normalized sensitivity profile are presented in *FIG. 3* in 620 group energy structure.

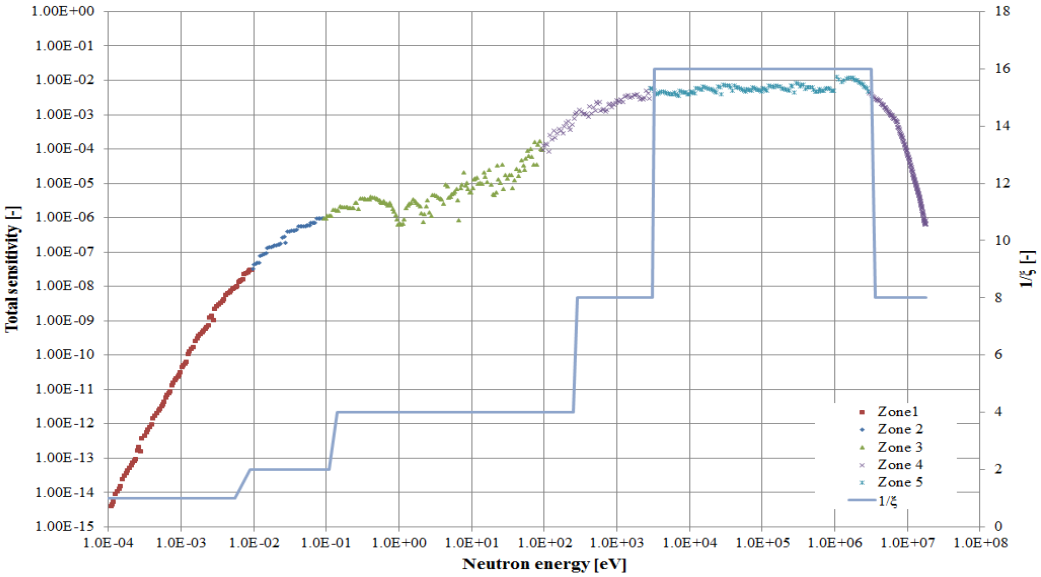


FIG. 3. Results of the sensitivity analysis.

The energy structure of the SBJ V2017 library was created based on the above presented results of sensitivity analysis, however the energy structure of the new 186G library was not created based on the structure of the 620g library, used for the sensitivity calculation. Regarding the sensitivity range specified in TABLE I, the sensitivity profile was divided to 5 energy zones. For each energy zone a constant $1/\xi$ value was specified and the energy bounds of the new 186 group energy structure of the SBJ V2017 library were calculated using Eq. 3. In this equation E_{j+1} and E_j are the upper and lower boundary of the j-th energy group and $1/\xi_i$ is the inverse logarithmic decrement of neutron energy in i-th energy zone.

TABLE I: Description of the energy zones.

Zone	Sensitivity range [-]	Lower energy [eV]	Upper energy [eV]	1/ξ [-]
1	$S_{k,\sigma}$<5e-8	1e-4	1e-2	1
2	5e-8 < $S_{k,\sigma}$ < 1e-6	1e-2	1e-1	2
3	1e-6 < $S_{k,\sigma}$ < 1e-4	1e-1	1e+2	4
4	1e-4 < $S_{k,\sigma}$ < 3e-3	1e+2 / 3e+6	3e+3 /1.8e7	8
5	3e-3 < $S_{k,\sigma}$	3e+3	3e+6	16

$$E_{j+1} = exp\left(\frac{1 + lnE_j/\xi_i}{1/\xi_i}\right) \quad (3)$$

3.3.Weight function

In the XS processing scheme shown in *FIG. 2* the Bondarenko method was used in NJOY12. In addition to the energy structure, the precision of XS processing based on this method is also influenced by the weight function (flux). To maintain the specifics of the target system in the SBJ V2017 library, the core averaged neutron spectrum of the GFR 2400 reactor was used as weight function, calculated by the MCNP5 code. To catch the neutron spectrum in MCNP5 186 group neutron mesh-tallies were used. The neutron weight function is shown *FIG. 4.*

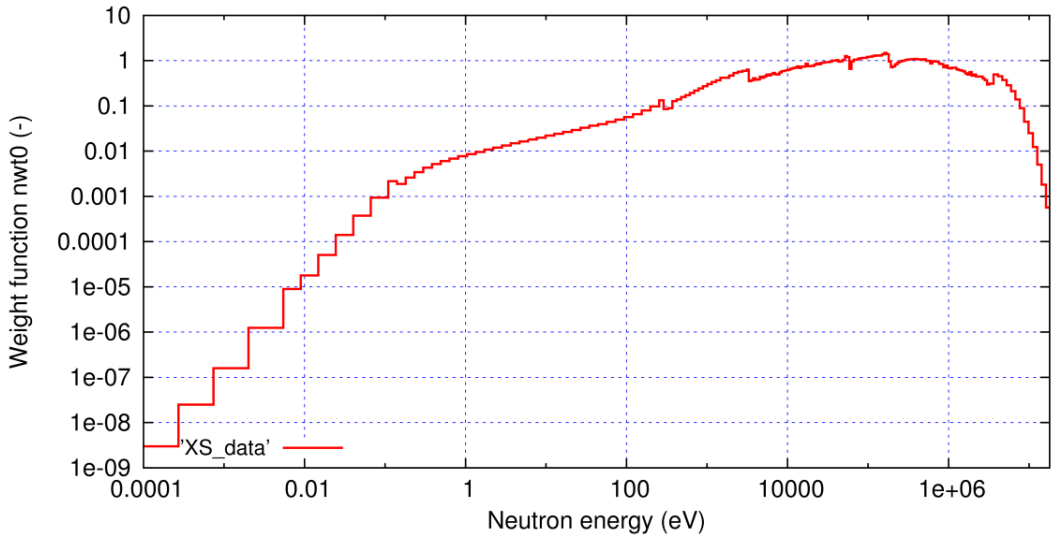


FIG. 4. Neutron weight function of the GFR 2400 core.

3.4.Reaction selection

Another important aspect of multigroup XS processing is the selection of appropriate nuclear reactions. Usually, the pointwise XS data processed by NJOY12 consists of more data than it is required for the processing of region-wise effective cross sections. To minimize the size of the multi-group XS library a new subroutine was implemented in the processing scheme, which selects only those reactions, which are requested by the TRANSX code.

4. Benchmarking

Before using the SBJ_V2017 XS library for the target core it was necessary to estimate its bias through benchmark analyses. The latest edition of the handbook of the ICSBEP project contains 567 benchmark experiments [15]; however, for our purpose it was sufficient to select only ones similar to the target GFR 2400 core.

4.1.Similarity analysis

The most similar benchmark experiments were selected based on the uncertainty and similarity analysis performed by the TSUNAMI-IP program from the SCALE6 [16] package. For similarity assessment 3 integral indices (ck, E and G) were used. Each integral index was normalized such that a value of 1.0 represents complete similarity and 0.0 no similarity between the systems. Based on the similarity assessment performed on 543 benchmark experiments 15 benchmark cases were selected (see *FIG. 5a*). Regarding all 3 integral indices the MIX-COMP-FAST-1, MIX-COMP-FAST-5, MIX-COMP-FAST-6, IEU-MET-FAST-002 and IEU-MET-FAST-007 can be considered as the most important benchmarks, however in terms of the E index, also the remaining PU-MET-FAST experiments could provide valuable results.

4.2.Benchmark results

For the selected 15 benchmark experiments appropriate PARTISN input files were created and the calculations were performed using the 620g SBJ V2016 and 186g SBJ V2017 XS libraries. The C/E-1 (C – calculation, E - experiment) results are shown in *FIG. 5b*. For better understanding of the C/E-1 values, also CE MCNP5 results are shown in the figure.

a; integral indices b; bencmark results

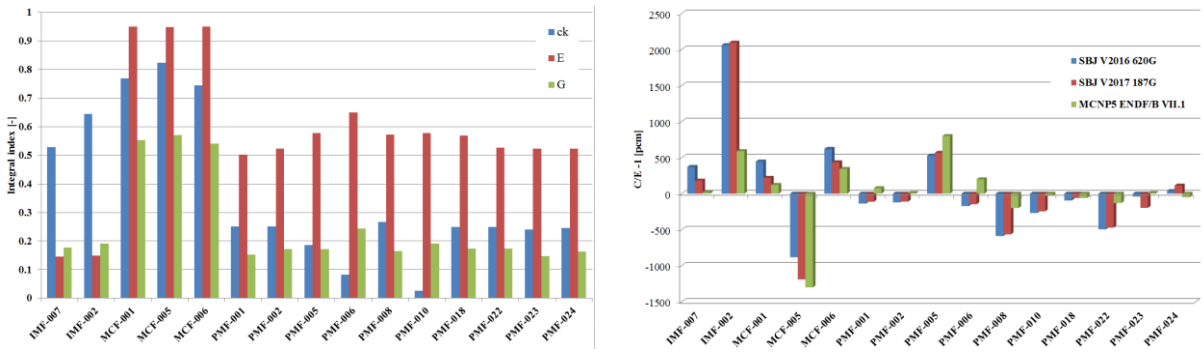


FIG. 5. Results of the integral indices and benchmark calculation

The figure shows very similar results in case of both SBJ V2016 and V2017 XS libraries, with slightly smaller overall bias in case of the SBJ V2017 library. The difference between the two versions of the SBJ library depends on the isotopic composition of benchmark cases. In cases of U systems significant improvement was achieved by using the SBJ V2017 library. On the other hand, in case of Pu systems, the results were almost identical, with slightly smaller bias in case of the SBJ V2017 library. All these results are considered satisfactory, because comparable and slightly smaller bias was achieved by using 187 than 620 energy groups. In the majority of the calculation cases the PARTISN results were comparable with the CE MCNP5 calculations. In the figure we can see two special cases (MIX-COMP-FAST-005 and PU-MET-FAST-005), were the MCNP bias exceeds 1000 pcm. If we consider, that the MCNP5 results are true and the bias is caused by nuclear data, then increased bias of the SBJ V2017 compared to SBJ V2016 can be seen also as improvement of the multi-group library. Among all benchmarks, the largest bias (app. 2000 pcm) was achieved for the IEU-MET-FAST-002 benchmark. The cause of this discrepancy will have to be identified.

5. GFR 2400 application

Since the benchmark cases showed promising results it was justified to use the SBJ V2017 XS library for GFR2400 core calculations and to compare the achieved results with PARTISN and DIF3D calculations, performed using the older SBJ V2016 XS library. The comparison was made based on four main parameters; the bias of excess reactivity from the CE MCNP5 calculation ($\Delta\rho_{MCNP}$), the neutron spectrum, the neutron flux distribution and the power distribution in the core. In terms of excess reactivity 3 calculation cases were compared: the case with fine group structure (620g vs 186g) in PARTISIN on RZ core geometry and two cases with fine and coarse (33g) structures in DIF3D on the full core model using diffusion theory and the nodal method. The results of the comparison of the core excess reactivity are shown in TABLE II. As it can be seen from this table, there is a significant improvement in the RZ PARTISN transport calculation, the bias from MCNP5 decreased from 1118.1 pcm (SBJ V2016) to 304.9 pcm (SBJ V2017). In case of the fine group DIF3D calculation, there is also a slight improvement. The bias from MCNP5 decreased by 135.5 pcm, but it still reaches 1593.9 pcm. However, it should be noted, that the bias is caused not only by the XS library, but also by the diffusion method used in the DIF3D calculation. In the future it will be necessary to evaluate the impact of the diffusion solution on the calculation bias. The coarse group calculations resulted in very similar deviation from MCNP5, the difference between the SBJ V2016 and SBJ V2017 XS library is only 55.1 pcm.

TABLE II: Results of the comparison of excess reactivity.

Code	Core model	XS library	ρ_e [pcm]	$\Delta\rho_{MCNP}$ [pcm]
MCNP5	HEX-Z	ENDF/B-VII.1 CE	1516.6	-
MCNP5	RZ	ENDF/B-VII.1 CE	1577.7	-
PARTISN	RZ	SBJ V2016 620G	2695.9	1118.1
PARTISN	RZ	SBJ V2017 186G	1882.6	304.9
DIF3D	HEX-Z	SBJ V2016 620G	3246.0	1729.4
DIF3D	HEX-Z	SBJ V2017 186G	3115.5	1593.9
DIF3D	HEX-Z	SBJ V2016 33G	1241.6	-275.0
DIF3D	HEX-Z	SBJ V2017 33G	1186.6	-330.1

The average neutron spectrum and the flux distribution were compared only between the SBJ V2016 and SBJ V2017 libraries using the collapsed 33g energy structure. The results of the core-averaged neutron spectrum are shown in *FIG. 6*.

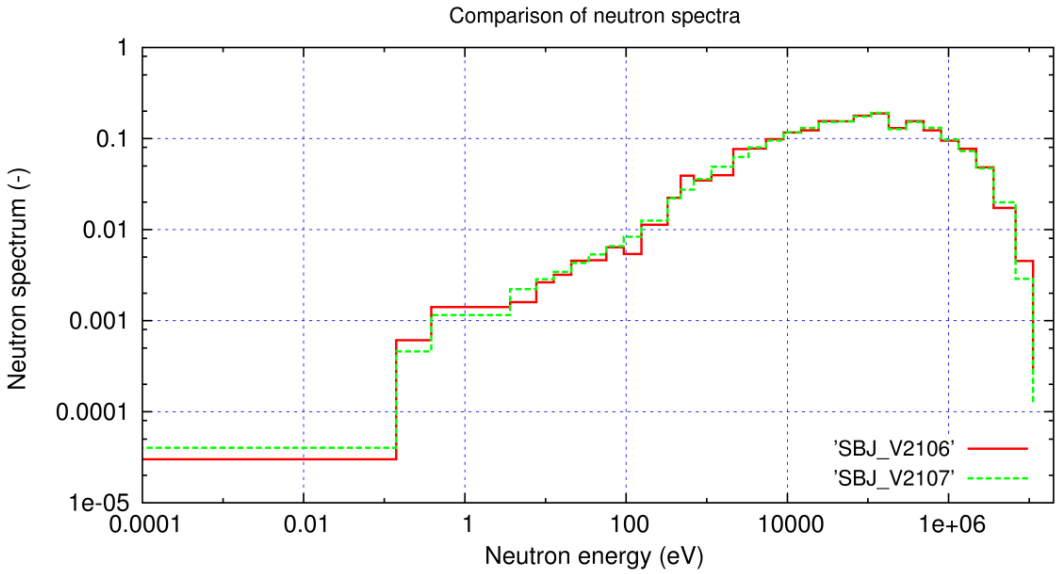


FIG. 6. Comparison of neutron spectra

As it is clear from *FIG. 6*, the shape of the two neutron spectra is very similar, but there are slight deviations between certain energy groups. The biggest deviations can be seen in groups 1-4, 9, 12, 14 and 33 (the numbering starts at the lowest energy). These deviations may have been caused by differences in the original fine group energy structure, which was used for energy group collapsing. In the future, sensitivity analysis will be performed to evaluate the impact of these differences. The comparison of the neutron fluxes and power distributions at the center of core height is shown in *FIG. 7*. The plots were created using the inhouse DIFRES utility. Since the deviations between the results are very small, only the differences were plotted in the figure. In terms of flux distribution the biggest deviations were found at the radial reflector (-3.1 %). This deviation may have been caused by the differences in the neutron spectrum at low energies, which were discussed above. In terms of power distribution, the deviations are much lower (-0.25 % to 0.15%). The biggest negative deviation can be seen in the core center, where the spectrum is the hardest, and the biggest positive deviation at the outer fuel periphery, where low energy neutrons are reflected from the radial reflector.

a; Neutron flux b; Power distribution

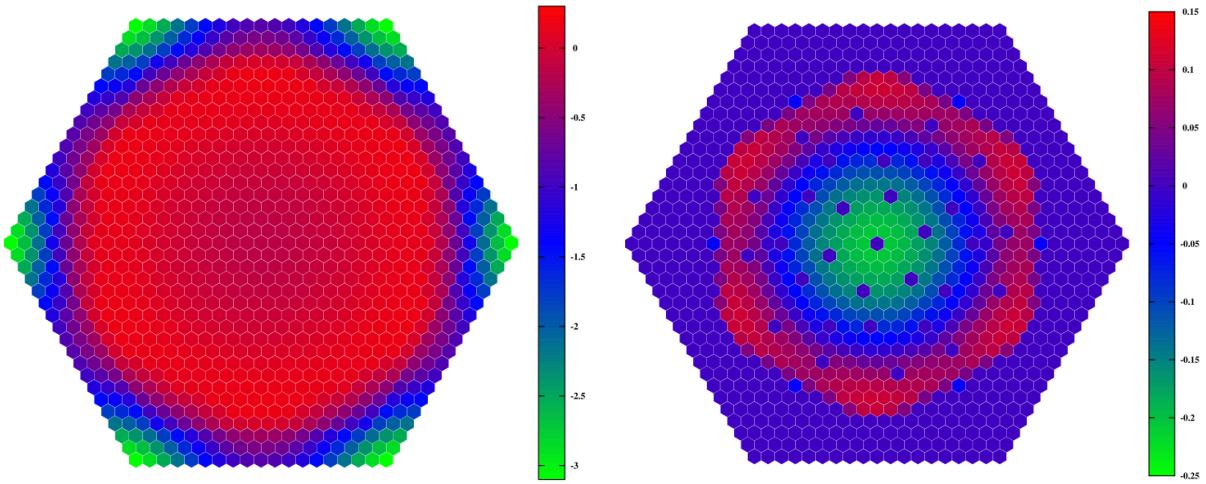


FIG. 7. Comparison of neutron flux and power distribution

Conclusion

Based on ENDF/B-VII.1 evaluated data and the presented calculation scheme the SBJ V2017 multigroup XS library was developed. Its energy group structure (186g) was optimized based on sensitivity and uncertainty analysis of the GFR 2400 reactor. The average neutron spectrum of the GFR 2400 reactor, calculated by MCNP5 was used as the weight function in NJOY12. To minimize the size of the XS library a reaction selection procedure was developed. This procedure was tested on specific benchmark cases and the minimization of reactions did not lead to significant deviations. The SBJ V2017 XS library was tested through 15 benchmarks from the ICSBEP handbook, carefully selected, based on similarity assessment, and compared with the previous SBJ V2016 version. The difference between the two versions of the SBJ library depends on the isotopic composition of the benchmark cases. For U systems, significant improvement was achieved by using the SBJ V2017 library. In case of Pu system the results were almost identical. Except the IEU-MET-FAST-002 benchmark, all cases showed acceptable bias. This discrepancy will have to be identified in the future. The SBJ V2016 and SBJ V2017 libraries were compared also on RZ and HEX-Z models of the GFR 2400 reactor in PARTISN and DIF3D. The SBJ V2017 XS library led to a significant improvement of the RZ PARTISN transport calculation. The bias from MCNP5 decreased from 1118.1 (SBJ V2016) to 304.9 pcm. In case of the fine group DIF3D calculation the bias from MCNP5 decreased by 135.5 pcm, but it still reaches 1593.9 pcm. This bias was caused also by the diffusion method used in the DIF3D calculation. The comparison of neutron spectra showed differences between the XS libraries mainly at low and intermediate neutron energies. These differences led to app. 3 % deviation of the neutron flux distribution and 0.3 % deviation of the power distribution. To better understand these deviations, the core wide distributions will have to be compared with MCNP5. It can be concluded, that SBJ V2017 XS library brought improvements in the benchmark and GFR 2400 calculations, but there are still several issues, which should be identified and fixed in the forthcoming steps of development.

Acknowledgment

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