SELECTION OF APPROPRIATE ENERGY STRUCTURE OF THE MULTI-GROUP CROSS SECTION LIBRARY FOR FAST REACTOR CALCULATIONS

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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.

1.1. Development of multi-group XS libraries at the home institution

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 first version of our multi-group XS library (hereinafter the SBJ library) was prepared in 2014 using standard NJOY processing options. In the next versions, isotope dependent background XS were implemented and various neutron spectra were investigated (for more detail see [3]). 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 [4] showed, 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.

2. XS processing for fast reactors

2.1. The general processing scheme

The SBJ V2017 multi-group 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 for this library is the NJOY12 [5] code, which requires a variety of input data. In order to ease the operation of the NJOY12 code at our university as well as 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 multi-group library is shown in Fig. 1.

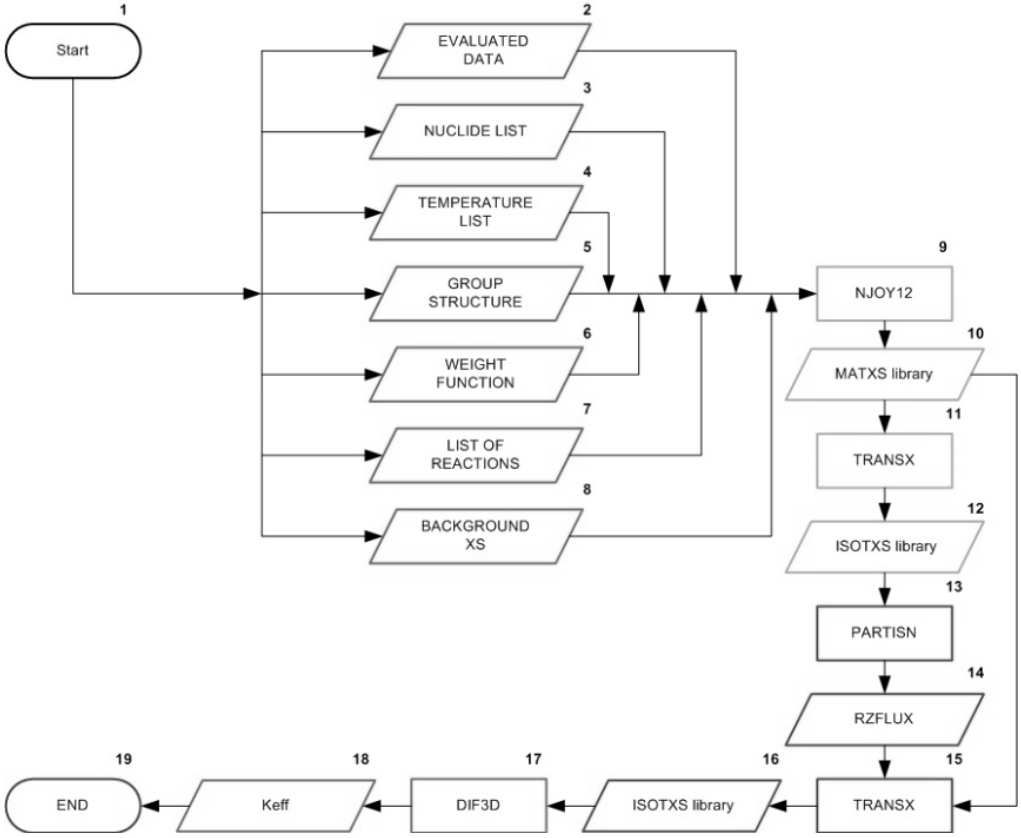

Fig. 1: The SBJ XS processing scheme

The XS processing 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 [6] data. Based on the input parameters the NJOY 2012 code (9) prepares the fine group MATXS XS library (10). For practical applications, the MATXS library is subsequently transformed to effective region-wise macroscopic XS data using TRANSX (11) [7] and stored in the ISOTXS library format (12). This library can be used in any calculation code able to treat CCCC format files. For certain applications, to reduce the calculations costs, group collapsing can be performed. Usually the TRANSX (15) code and the RZFLUX (14) region-wise neutron flux obtained from SN transport calculation in PARTISN (13) are used [8]. In the present analysis no group collapsing was performed.

2.2. Selection of appropriate energy structure

In the previous versions of the SBJ XS library, standard NJOY energy group structures were used. There were the LANL 80g, LANL 187g, SAND-II 500g and the SAND-II 620g.The achieved precision and computational bias can be considered satisfactory, however analyses pointed out, that the quality of the final XS library may be influenced by its energy structure, which also depends on the given application. It is clear, that an appropriate energy structure must carry the fingerprint of the target core. In other words, the structure of the XS library must maintain the sensitivity of the reactor core on key isotopes in various

energy ranges. If this condition is not valid and the structure is not fit to the target core, the most important characteristics of the system may be altered.

As it was mentioned, to enhance the performance of the SBJ XS library, its energy structure must be linked with the specifics of the target core. Since the majority of fast reactor calculations performed at the STU had been related to the Gas-cooled Fast reactor, the GFR 2400 reactor was selected for the optimization of the SBJ V2017 library. For XS optimization two major philosophies were adopted. In the first philosophy it was assumed, that if the logarithmic decrement of the XS library structure is maintained constant the precision of the XS library depends only on the number of energy groups. In the second philosophy we assumed that the quality of the XS library depends also on the sensitivity of the target core on key isotopes, thus the energy structure must be made based on the magnitude of the total sensitivity profile of the core. In both cases the structure of the SBJ XS library was created using Eq. (1):

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

where 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. In the first philosophy constant $\boldsymbol{\xi_i}$ were used over the whole energy range, and in the second philosophy $\boldsymbol{\xi_i}$ was constant only over a specified energy range, selected based on the total sensitivity profile. Putting these two philosophies into practice and using Eq. (1) 5 different energy structures were created. The constant 155g, 207g, 311g and 415g and the energy dependent 186g. The main parameters of these energy structures are presented in *Tab. 1*, where $S_{k,\sigma}$ is the total sensitivity of the k_{eff} of the system on nuclear data.

Tab. 1: Description of the energy zones

Number of energy groups	**1/ξ [-]**	**Sensitivity range**	**Energy range [eV]**
186	1	$S_{k,\sigma}$<5e-8	1e-4 – 1e-2
	2	5e-8 < $S_{k,\sigma}$ < 1e-6	1e-2 – 1e-1
	4	1e-6 < $S_{k,\sigma}$ < 1e-4	1e-1 – 1e+2
	8	1e-4 < $S_{k,\sigma}$ < 3e-3	1e+2 / 3e+6 – 3e+3 /1.8e7
	16	3e-3 < $S_{k,\sigma}$	3e+3 – 3e+6
155	6	-	1e-4 – 3e+6
207	8	-	1e-4 – 3e+6
311	12	-	1e-4 – 3e+6
415	16	-	1e-4 – 3e+6

The calculation of the sensitivity profile of GFR 2400 was performed using the in-house PORK code and the implemented Standard Perturbation Theory (SPT) [9]. The results of the total normalized sensitivity profile are presented in Fig. 2 in 620 group energy structure.

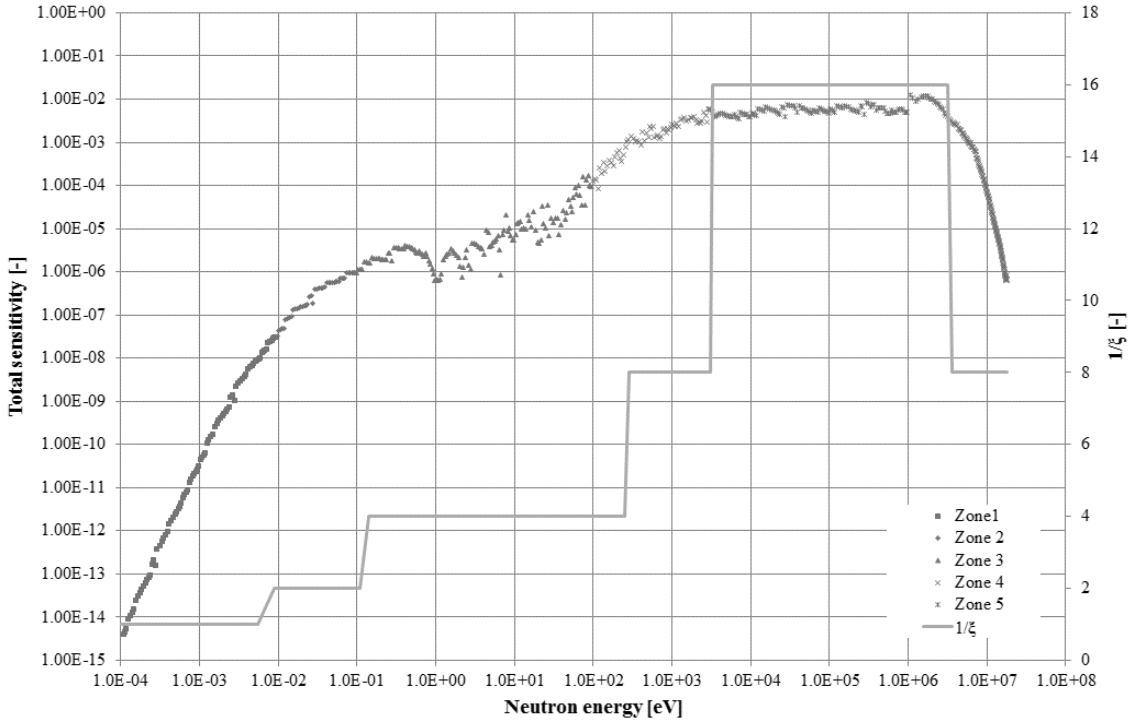

Fig. 2: Results of the sensitivity analysis.

2.3. Selection of the weight function, reaction and background XS

In our XS processing scheme the Bondarenko method was used in NJOY12. In addition to the energy structure, which was discussed above, the precision of XS processing is also influenced by the weight function (flux). To maintain the specifics of the GFR 2400 reactor in the SBJ V2017 library, the core averaged neutron spectrum of our target system was calculated in MCNP5 code using 186 group neutron mesh-tallies. The obtained neutron weight function is shown in *Fig. 3*. Another important aspect of multi-group 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 to create region-wise effective cross sections. To minimize the size of the multi-group XS library and get rid of unused data a new subroutine was implemented in the processing scheme. The subrutine selects only those reactions, which are requested by the TRANSX code. Selection of isotope dependent background XS is also an important issue. In our case, the required background XS data were extracted from the KAFAX E70 library [2].

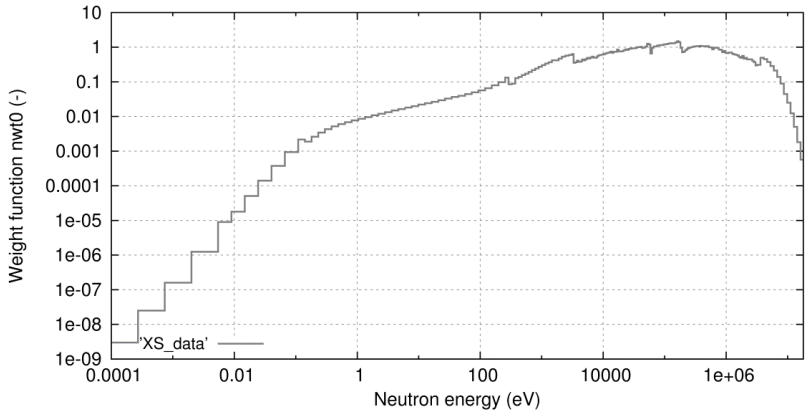

Fig. 3: Neutron weight function of the GFR 2400 reactor.

3. Benchmarking

3.1. Selection of appropriate benchmark tasks

Prior to using the SBJ_V2017 XS library routinely for the target core, it is necessary to estimate its bias by benchmark analyses. The latest edition of the handbook of the ICSBEP project contains 567 benchmark experiments [10]; however, for our purpose it was sufficient to select only ones similar to the target GFR 2400 core. The most similar benchmark experiments were selected based on the uncertainty and similarity analysis performed by the TSUNAMI-IP program from the SCALE6 [11] package. For similarity assessment 3 integral indices (ck, E and G) were used. Based on these results, 14 benchmark experiments were selected. The methodology and the results of the similarity assessment can be found in [12].

3.2. Evaluation methodology

For the selected 14 benchmark experiments PARTISN input files were created and the calculations were performed using all investigated energy structures, i.e. 186g, 150g, 207g, 311g and 415g. In PARTISN 4th order of Legendre polynomials was used. To evaluated the calculation bias and to compare the results between energy structures and with continuous energy MCNP5 calculations the Δ_k (C/E-1) parameter was calculated using Eq. (2):

$$\Delta_k = \frac{C}{E} - 1 = 1e5 * \left(\frac{k_{eff}^{calc}}{k_{eff}^{bench}} - 1 \right) \quad (2)$$

where k_{eff}^{calc} is the calculated (C) and k_{eff}^{bench} is the benchmark or experimental (E) value of the multiplication factor of the system. In order to get the results in units of pcm, the C/E-1 values were multiplied by 1e5.

3.3. Benchmark results

The results of the selected 14 benchmark experiments, in case of all investigated energy structures and CE MCNP5, are shown in *Fig. 4*. In this figure the titles on the x-axis represent the abbreviated unique IDs of the benchmark tasks from the handbook [10] and the zero line represents the experimental (benchmark) value of k_{eff} in units of pcm. The results are presented with error bars, representing statistical uncertainties (±1σ standard deviation of the benchmark value of k_{eff} derived from the handbook).

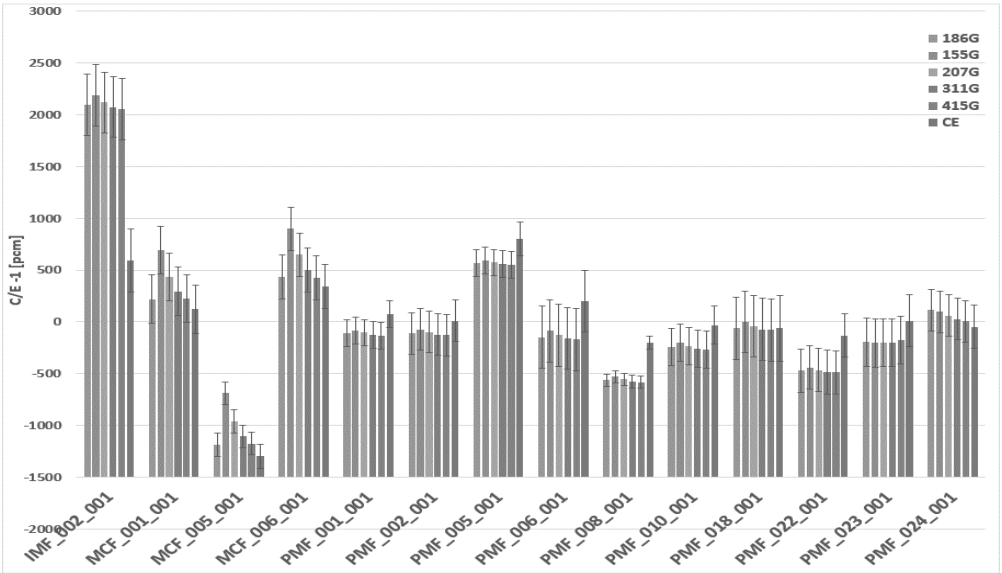

Fig. 4: Results of the benchmark calculations.

From the general point of view, the 186g XS library provided the lowest computational bias. The results of the benchmark calculations indicate strong dependence of computational bias on the isotopic composition of the tasks. Since the energy structure of the 186g XS was optimized for the GFR reactor, the best results in the benchmark calculations were achieved for mixed U-Pu systems. In such cases the bias of the 186g XS library is visibly smaller than the ones for the 155g, 207g and 311g. Among the uniform structures only the 415g library provided comparable results with the 186g library, while the computational time was longer and more iterations were required to achieve convergence. In case of pure Pu systems, the difference between the libraries was not significant, but still the optimized 186g and the uniform 415g structures provided the best results. In the majority of the cases the MG results were comparable with the CE MCNP5 calculations. Among all benchmarks, the largest bias (approx. 2000 pcm) was achieved for the IEU-MET-FAST-002 benchmark, which is a pure U system. Since this system is characterized with relatively high CK value (0,52) compared to GFR, the cause of this error must be further analyzed.

4. Application for complex full-core calculation

Since the benchmark cases showed promising results it was justified to use the SBJ V2017 XS library for the calculations of the target core (GFR2400) in PARTISN and DIF3D. In DIF3D 3D HEX-Z geometry was used and the calculations were performed using the nodal method and diffusion solver. On the other hand, transport solution (SN method, 4^{th} Legendre polynomials) in PARTISN was used, however the geometry of the system had to be modeled as a cylindrical R-Z model. The comparison was made based on the bias of the excess reactivity from the CE MCNP5 calculation ($\Delta\rho_{MCNP}$) in units of pcm. The results are shown in *Fig. 5*.

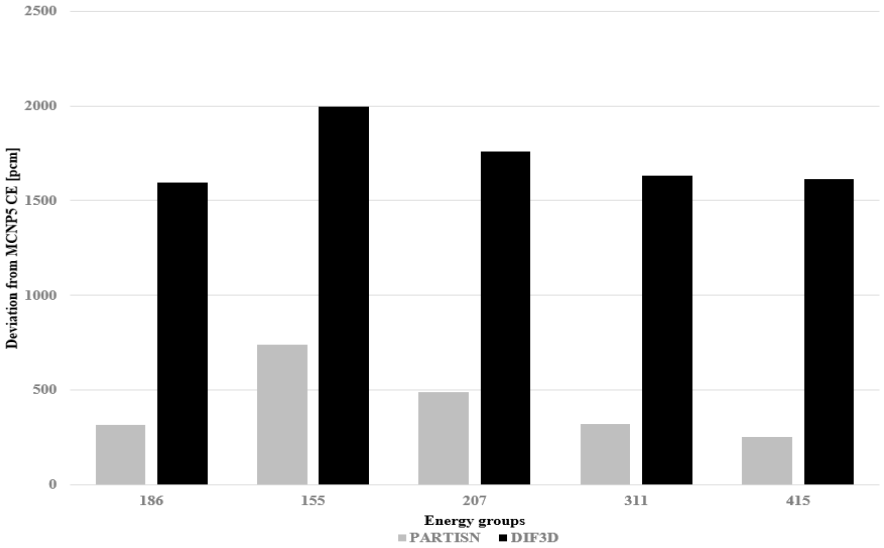

Fig. 5: Results of the GFR calculation.

As it can be seen from the figure, the lowest bias between MCNP5 and the deterministic calculations (PARTISN and DIF3D) was achieved in case of the optimized 186g and the uniform 415g structures and the highest bias in case of the uniform 155g structure. Concerning PARTISN, the difference in the bias between the 186g and 155g structures was 423 pcm (316 pcm Vs. 740 pcm). Although the difference between the 186g and 415g structures was only 62 pcm (316 pcm Vs. 254 pcm) with slightly lower bias for the 415g structure, therefore the shorter calculation time and faster convergence favor the 186g structure. Due to the diffusion solution in DIF3D, the computational bias was much higher,

compared to the RZ transport calculation in PARTISN. Among the investigated libraries, the 186g structure provided the best results (1594 pcm). Similar results were achieved using the 415g structure (1612 pcm) but the remaining libraries resulted in 150 – 300 pcm higher bias.

5. Conclusion

Based on ENDF/B-VII.1 evaluated data and the presented calculation scheme the SBJ V2017 multi-group XS library was developed. Five energy structure options were investigated, the 186g structure, optimized based on sensitivity analysis, and the uniform 155g, 207g, 311g and 425g structures. In all cases the average neutron spectrum of the GFR 2400 reactor was used as the weight function and to minimize the size of the XS library a reaction selection procedure was developed. The SBJ V2017 XS library was tested through 14 benchmarks from the ICSBEP handbook, carefully selected, based on similarity assessment. The difference between the SBJ libraries with different structure depends on the isotopic composition of the benchmark cases. For mixed U-Pu systems, significant improvement was achieved by using the optimized 186g structure. In case of pure Pu systems, the difference between libraries was smaller but the largest bias (2000 pcm) was achieved in case of a pure U system. The libraries were compared also on RZ and HEX-Z models of the GFR 2400 reactor in PARTISN and DIF3D. In both codes, the best results were achieved by using the optimized 186g structure. Although the uniform 415g library provided comparable results, the convergence of the calculations was slower and the calculation time several times longer. It can be therefore concluded, that the 186g structure of the SBJ V2017 XS library brought improvements in both the benchmark and GFR 2400 calculations, but there are still several issues, which should be identified and fixed in the forthcoming steps of development. The major issue is to decrease the large bias for pure U systems.

Acknowledgement:

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