DEVELOPMENT OF MULTIGROUP NEUTRON CROSS SECTION LIBRARY FOR FAST REACTOR CALCULATIONS

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Received 05 May 2016; accepted 16 May 2016

1. Introduction

The key issue in the design and analysis of any nuclear reactor is to accurately predict the space, angle, energy, and time distribution of neutrons.The transport of neutrons through matter is well described by the transport equation, a linear version ofBoltzmann's equation originally developed in the kinetic theory of gases. Unfortunately, analytic solution of the Boltzmann equation can be obtained only for simple problems, thus in real applications often its numerical solutionsare used. The history of computational transport basically follows the development of two competing methods, commonly called stochastic and deterministic[1]. Although these methods use fundamentally different approaches, their common feature is their strong dependence on nuclear data. Stochastic or Monte Carlo methods are widely used because of their relative ease of implementation, they complex geometry treatment and their ability to solve problems with extremely complex energy dependence. Apart from the statistical nature of obtained results, due to continues energy cross section libraries and complex geometry of the investigated system, Monte Carlo simulations can be costly. In these situations, Monte Carlo codes are not a "black box"into which a user can simply specify the problem, press the "start" button, and expect reliableanswer in a short time[1]. For these reasons certain reactor applications require effective deterministic approaches to be used, which however imply the development of multi-group cross section libraries. In this paper the development of cross section libraries optimized for fast reactor applications is presented.

2. Nuclear data for reactor calculations

2.1. Theoretical background

Multi-group cross sections in a form of multi-group constants are used by computer codes that calculate thedistributions of neutrons in space and energy, and that computevarious responses, such as k_{eff}. The multi-group constants are the energy dependences of the total macroscopic cross section, of the macroscopic cross section of the most important nuclear reactions and of the scattering matrix. These distributions are obtained by solving the neutron transport equation presented in Eq.(1)[2]:

$$\mu\frac{\partial}{\partial x}\phi(x,\mu,E)+\Sigma_t(X,E)\phi(x,\mu,E)= \\ =\int d\Omega'\int dE'\Sigma_x(x,E'\to E,\Omega'\to\Omega)\phi(x,\mu',E')+Q(x,\mu,E) \tag{1}$$

The importance of a given group constant is represented by its weighting flux ϕ. In general, the weighting flux is not known. However, it is often possible toobtain fairly accurate group constants for a particular application if the shape of the flux is reasonably well known over the broad energy ranges of a particularfew-group structure. One of the possible

options is to use the Bondarenko model. In this approach the real particle weight function is replaced by a smooth function $C(E)$ and the resonance self-shielding is treated as an effect separable for 2 components, the total macroscopic cross section $\Sigma_t^i(E)$ and the background cross section $\Sigma_0^i(E)$. The Bondarenko approximation of the l-th Legendre expansion of the weighting flux is show in Eq. (2)[2]:

$$\phi_l^i(E) = \frac{C(E)}{\left[\Sigma_t^i(E) + \Sigma_0^i(E)\right]^{l+1}} \tag{2}$$

2.2. Nuclear data formats

As a result of development of computation codes, there exist several internationally recognized data formats. In principle, nuclear cross sections come from precise experimental measurements. Theses raw data are then evaluated and stored in accordance with the ENDF (Evaluated Nuclear Data Files) format[3]. This file format has undergone a long historical development; the current version is labelled as ENDF-6. If desired, XS data in the ENDF format can be transformed to the desired file format. To obtained continuous energy XS data for the stochastic MCNP5[4] code, the ENDF evaluated data is transformed through PENDF (Pointwise ENDF) to the ACE (A Complex ENDF) format. For deterministic codes such as DIF3D[5] or PARTISN [6]first GENDF (Group-wise ENDF) cross section data are produced by the NJOY[7] code which is subsequently transformed to effective macroscopic cross section data MATXS and ISOTXS.

3. Cross section processing for fast reactor calculation

3.1. Description of the target reactor core

Although the aim was to develop a cross section library applicable for arbitrary fast neutron systems, several parameters of the XS library have to lean on an exact reactor system. Since the authors of this paper are involved also in the Gas-cooled Fast Reactor development in Slovakia, the GFR 2400 reactor has been chosen for XS data optimization. The sectional and top view of the GFR 2400 reactor core is shown in Fig.1.

a; b;

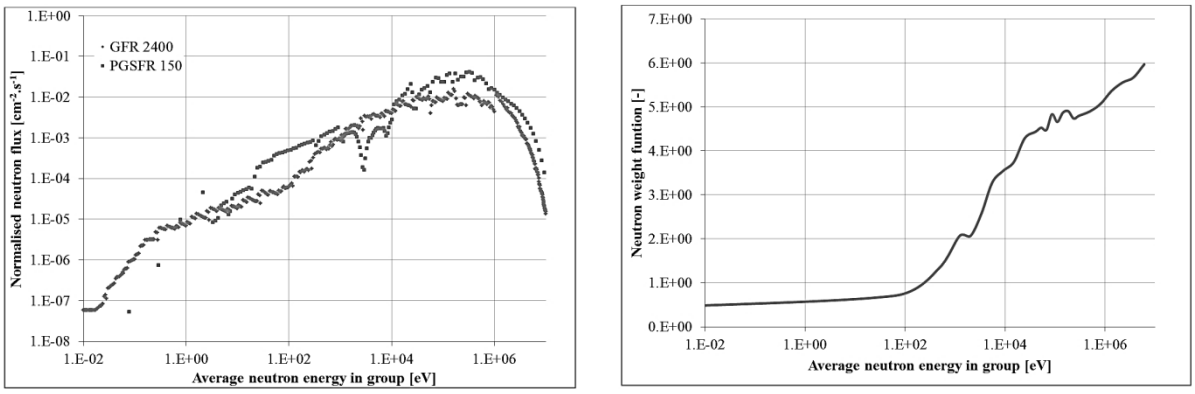
Fig.1:*Sectional and top view of the GFR 2400 reactor core*

GFR 2400 is a large scale power unit with a thermal power of 2400 MW_{th}.The reactor core consists of two zones, the inner fuel (IF) and outer fuel core (OF).The inner and outer fuel cores consist of 264 and 252 (U,Pu,Am)C fuel assemblies with SiC-SiC_{fib} cladding and W14Re-Re refractory liner. The volumetric content of Pu isotopes in heavy metal in the IC and OC fuel assemblies reach 14.2%, and 17.6%. The core fuel region is surrounded by six

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 reactivity of the GFR 2400 GFR 2400 core is controlled through the system of control rods, CSD and can be sufficient shut down by the additional system of DSD assemblies. Both systems accommodate B_4C absorbers with 90% weight content of ^{10}B isotope[9].

3.2. Available cross section libraries for fast reactor calculations

There are several multi-group cross section libraries available for fast reactor calculations. Before starting a development of a new cross section library it is important to find out, if and how the available ones are applicable for the selected target system and what their limitations are. One of the possible candidates for evaluation is the ZZ-KAFAX-E70[10]library, which was developed by KAERI (Korea Atomic Energy Research Institute)based on ENDF/VII.0 [11] evaluated data and is available at the OECD NEA website[12]. It is a 150 group MATXS library optimized for KALIMER 150 (Korean Advance LIquidMEtal Reactor)[13]. The comparison of the GFR 2400 and KALIMER 150 neutron spectra is shown in Fig.2a; and the KALIMER 150 adjoint flux in Fig.2b;. The GFR 2400 spectrum is presented in 620 group structure and the KALIMER 150 spectrum in 150 group structure.



a; b;

Fig.2:*a - GFR 2400 and KALIMER 150 neutron spectra b- KALIMER 150 adjoint flux*[14]

Due to different fuel (carbide vs. metallic), coolant (helium vs. sodium) and cladding (SiC vs. metallic) materials as well as the absence of refractory liners in the KALIMER 150 reactor core, the neutron spectra are slightly shifted. To identify the most important areas of the neutron spectrum the KALIMER 150 adjoint flux can be used (Fig.2b.). It can be seen that the difference between the two neutron spectra are in two main areas, below 100 eV and above 100 keV. As a result of the low importance of slowed neutrons the differences in the 100 eV energy range can be considered as negligible. On the other hand, high energy neutrons are of the major importance, thus the differences above 100keV energy might influence the precision of GFR 2400 calculations performed using the ZZ-KAFAX-E70 cross section library. Based on the above mentioned it can be concluded that the ZZ-KAFAX-E70 cross section library is not optimal for deterministic GFR 2400 calculations.

3.3. The cross section processing scheme

Precise deterministic calculations of the GFR 2400 reactor require a new set of cross section libraries to be created. It is a complex process which requires both experimental and calculation data and multiple computer codes to be used. To develop and optimize the new set of cross sections a new calculation scheme was developed, which is shown in Fig.**3**.

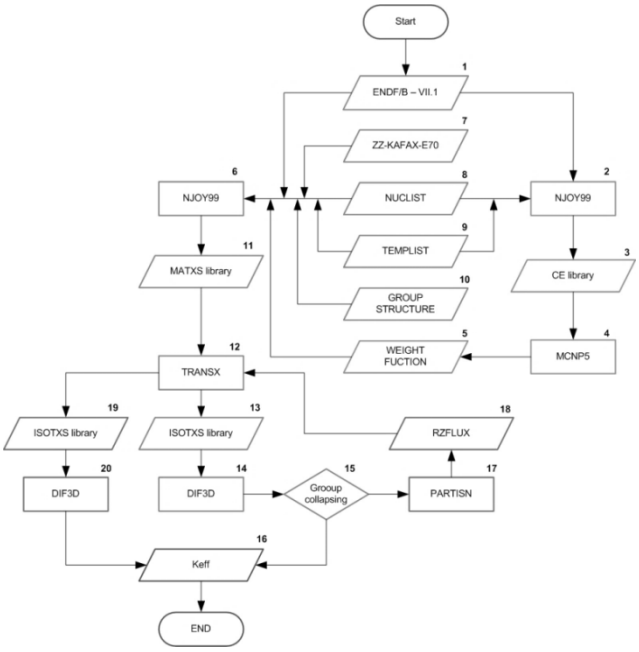


Fig.3:*The cross section processing scheme*

The scheme starts with the processing of ENDF/B-VII.1 evaluated data (1) using the NJOY99 code (2). The produced continuous energy cross section library (3) is used in the Monte Carlo MCNP5 code (4). The MCNP5 calculation requires detailed geometry and material model of the GFR 2400 core to be created. In addition to basic neutron physical parameters the 620 group weight flux is produced (5) using superimposed mesh tallies. The weight flux, the ENDF/B-VII.1 [15]evaluated data, the ZZ-KAFAX-E70 background cross sections (7) and the NUCLIST (8), TEMPLIST (9) and GROUP STRUCTURE (10) files are subsequently evaluated in NJOY99 (6) to produce 620 group MATXS libraries (11).These microscopic cross section data are then transformed to effective region-wise macroscopic cross sections using the TRANSX code (12). The cross sections data are stored in the ISOTXS library (13), which can be directly used to 3D perform full core calculations in DIF3D (14). In order to accelerate the core calculations group collapsing (15) can be performed, based on the RZFLUX (18) region-wise neutron flux obtained from RZ transport calculation carried out using PARTISN (17). The region-wise neutron flux is used as weight function in TRANSX and 25 group ISOTXS library (19) is created. This cross section library is used again in DIF3D (20) to calculate neutron physical parameters of the system, such as k_{eff} (21). According to the used group structure and collapsing scheme, the final ISOTXS cross sections are labelled as SBJ_E71_620G or SBJ_E71_25G.

4. Optimization of cross section libraries

The performance of the cross section library directly depends on its input parameters and functions. It was found out, that the precision of the implemented Bondarenko model ismainly influenced by the weighting function and the background cross sections.

4.1. *Selection of appropriate weight function*

The weight function represents the smooth $C(E)$ function in Eq. (2). In the optimization process various GFR 2400 neutron spectra were analysed. Since the neutron spectrum is not dominant in the axial direction, thus only radial distributions were found to be interesting. Four cases were investigated,the constant weight function (CONST) the core averaged spectrum (AVG), the inner fuel averaged spectrum (IF) and the outer fuel averaged spectrum (OF). The spectra are compared in Fig.4.

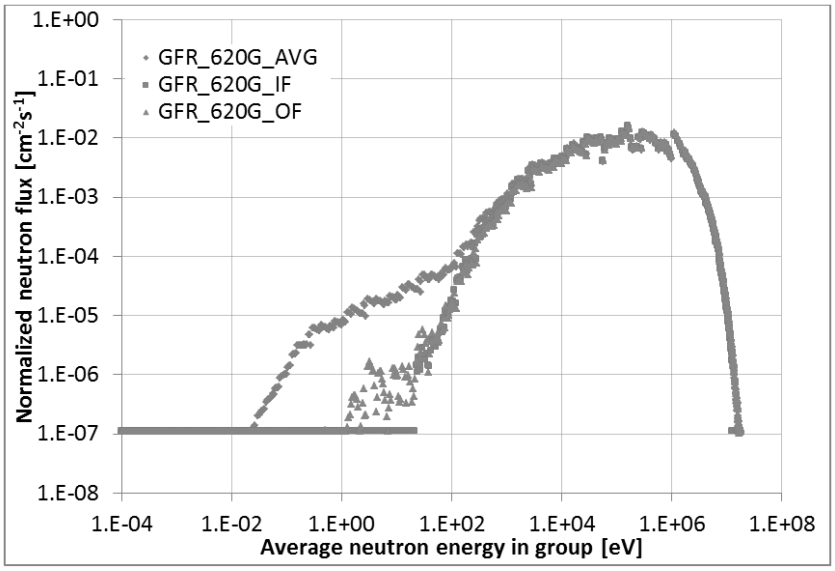


Fig.4: *Comparison of neutron spectra at various positions in the GFR 2400 core*

The analysis was performed using several versions of the SBJ_E71_620G cross section library on the RZGFR 2400 model in DIF3D. The results were compared with theCERZ MCNP5 calculation and are shown in Tab. **1**.In the table below $\rho_e$is the excess reactivity of thesystem and $\delta\rho_{MCNP}$ is the absolute reactivity deviation from MCNP5.

Tab. 1.*Comparison of various weight spectra*

Calculation case	ρ_e [pcm]	$\delta\rho_{MCNP}$ [pcm]
MCNP_CE_RZ	1577.7 ± 3.9	-
DIF3D_620G_RZ_CONST	206.3	-1371.4
DIF3D_620G_RZ_IF	637.8	-939.9
DIF3D_620G_RZ_OF	629.0	-948.7
DIF3D_620G_RZ_AVG	637.2	-940.5

The results show significant dependence of calculation precision on the weight function. Due to the -1371.4 pcm deviation from MCNP5 the constant weight function option in DIF3D was excluded from further analyses. As it can be seen the IF, OF and AVG cases showed very similar performance. Since the difference between these three cases did not exceed the Monte Carlo statistical uncertainty, it can be concluded, that all three versions can be used to obtain results with approximately the same precision.

4.2. Influence of background cross sections on calculation precision

The second investigated parameter is the background cross section, which represents the $\Sigma_0^i(E)$parameter in Eq. (2). The background cross section determines the self-shielding of the system and it is an isotope and energy dependent parameter. In the optimization process two methods were investigated, the basic NJOY99 (S0) and the KAFAX method (SKF). In case of the basic S0method the same set of background cross sections was used for all of the investigated isotopes. In case of the SKFmethod unique background cross sections were used for every isotope. The analysis was performed for the 620g and 25g versions of the SBJ_E71 cross section library on the RZ DIF3D core model. The results were compared with the continuous energy RZ MCNP5 calculation and are shown in Tab. **2**. In the table below $\rho_e$is the excess reactivity of thesystem, $\delta\rho_{sig}$ is the reactivity deviation due to background cross sections and $\delta\rho_{MCNP}$ is the absolute reactivity deviation from the MCNP5.

Tab. 2.*Comparison of various background cross sections*

Calculation case	ρ_e [pcm]	$\delta\rho_{sig}$[pcm]	$\delta\rho_{MCNP}$ [pcm]
DIF3D_620G_RZ_S0	637.2	-	-940.5
DIF3D_620G_RZ_SKF	887.0	246.8	-690.7
DIF3D_25G_RZ_S0	902.6	-	-675.1
DIF3D_25G_RZ_SKF	1158.2	255.6	-419.5

The results clearly show, that the implementation of the SKF method brought positive impact on calculation precision. In case of the 620g calculation the deviation from MCNP5 decreased from 940.5 to 690.7 pcm an in case of the 25g calculation from 675.1 to 419.5. It can be seen that the effect of background cross section is approximately 250 pcm, regardless the group structure. Based on these results the SKF method was selected for the processing of the final SBJ_E71_620G and SBJ_E71_25G libraries.

5. Results

5.1. Benchmarking on integral experiments

The next step of the evaluation of the precision of cross section libraries is their benchmarking on integral experiments. The aim was to compare the reactivity deviation of various calculation caseswith the detailed heterogeneous MCNP5 calculation. Based on the recommendations of WPEC Subgroup 33 (SG33)[16] 8 integral experiments were selected. The results are also compared with the results of SG33 and are shown in Fig.5

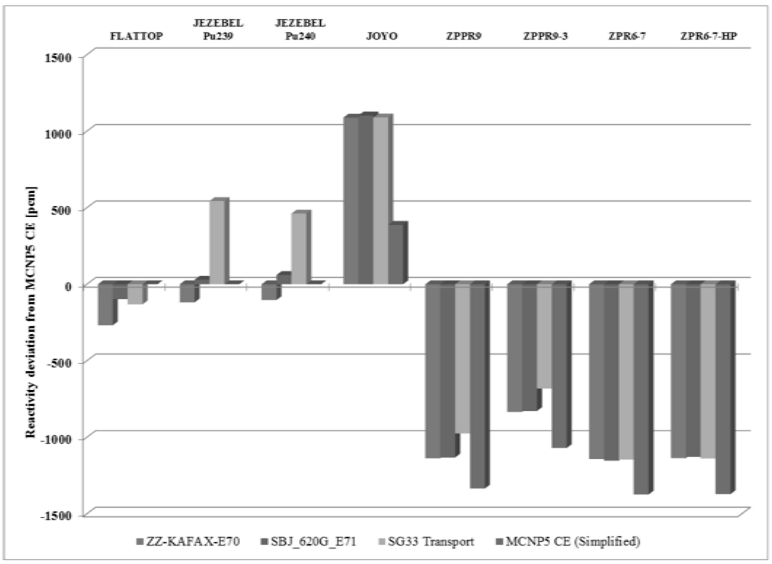


Fig.5:*Comparison of the results of integral experiments*

The benchmark results show very similar performance of the SBJ_E71_620G and ZZ-KAFAX-E70 libraries. Their precision is comparable and in several cases better than the results provided by SG33. It was found out that the precision of cross section libraries depends on the complexity of geometry models and required simplifications. In case of complex systems, such as JOYO and ZPPR9, all cross section libraries were burdened by approximately 1000 pcm uncertainty, caused by the homogenization effect. In case of simple systems (FLATTOP, JEZEBEL) the reactivity deviation of the SBJ_E71_620G is less than 300 pcm. It can be concluded that the precision of developed cross section libraries is comparable with available multigroup cross section libraries for both simple and complex geometries.

5.2. Verification against MCNP5 on GFR 2400

The final step in the development process is the evaluation of the cross section libraries on the target reactor core. For this study the 3D HEX full core model of GFR 2400 was created in DIF3D and the results were compared with the heterogeneous CE MCNP5 calculation. In addition to the excess reactivity ρ_e, also the worth of control rods $\Delta\rho_{CR}$ was calculated. The results are shown in Tab. 3, where "ALL UP" represents the case with all control rods above the core, "ALL DOWN" the case with all control rods inserted, and "CSD DOWN" and "DSD DOWN" the cases with the CSD or DSD systems inserted.

Tab. 3.*Comparison based on GFR 2400 excess reactivity*

Calculation Case	MCNP5 CE HEX		DIF3D 25G HEX		$\Delta\rho_{MCNP}$ [pcm]
	ρ_e [pcm]	$\Delta\rho_{CR}$ [pcm]	ρ_e [pcm]	$\Delta\rho_{CR}$ [pcm]	
ALL UP	1577.8	-	1334.2	-	-182.4
ALL DOWN	-10707.6	12229.1	-10656.8	-11991.0	-238.1
CSD DOWN	-6410.2	7931.6	-6419.1	7753.3	-178.3
DSD DOWN	-2764.4	4285.8	-2892.5	4226.8	-59

The agreement between the DIF3D and MCNP5 results fulfilled our expectations. The reactivity deviation for the "ALL UP" case was -182.4 and for the "ALL DOWN" case –it was 238.1 pcm. Taking into account the total worth of control rods (12229.1 pcm) these deviations are less than 2 % of the total worth. The difference of $\Delta\rho_{MCNP}$ between the calculation cases could have been caused by the weighting function used for cross section processing. The average neutron spectrum of the core changes after the insertion of control rods, but this effect was not implemented in our cross section processing scheme.

6. Conclusion and discussion

The design and the safety requirements of GEN IV fast reactors require special approach to be used. Although Monte Carlo methods are widely used and can achieve promising results, due to their stochastic naturethe results are burdened by statistical uncertainties. To obtain more accurate insight into the physical nature of unique reactor systems the stochastic calculations must be supported by deterministic methods. These methods require precise and reliable nuclear data, optimized for a given application. This paper deals with the development of multi-group cross section libraries for the GFR 2400 reactor. A new cross section processing scheme was developed, based on ENDF/B-VII.1 evaluated data, the combination of computer codes and ZZ-KAFAX-E70 background cross sections. Two versions of cross section libraries were created, the fine group SBJ_E71_620G and the coarse structure SBJ_E71_25G. These cross sections were benchmarked on integral experiments and compared with data provided by the WPEC Subgroup 33. The precision of theSBJ_E71libraries is comparable with available multi-group cross section libraries, however in the future more benchmark experiments will have to be evaluated. Finally both versions of the SBJ_E71 XS library were used on the full core 3D HEX model of GFR 2400 in DIF3D. The results were compared with MCNP5 were the reactivity deviation was -182 pcm for the non-roded and -238 pcm for the roded case. The most important finding of this analysis is that using the SBJ_E71_620G and SBJ_E71_25G reliable results can be obtained in approximately 1 min calculation time, while the same MCNP5 analysis requires 24 hours of execution on a cluster system.

Acknowledgement

This work was financially supported by grant of Science and Technology Assistance Agency no. APVV-0123-12.

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