DEVELOPMENT OF MULTI-GROUP XS LIBRARIES FOR THE GFR 2400 REACTOR

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ABSTRACT

GFR 2400 is considered as a conceptual design of the large scale GEN IV Gas-Cooled Fast Reactor. In general, the GEN IV technologies are seen as reliable but also very challenging reactor concepts. Since GFR 2400 lacks any experimental data, the questions on its safety are even more complex and the assessment of its performance could be made only based on computational experience. The paper deals with the development process of multi-group XS libraries based on a hybrid deterministic-stochastic methodology, using the NJOY99, TRANSX, DIF3D, PARTISN and MCNP5 codes. A new optimized 25 group SBJ_E71_25G cross section library was developed based on ENDF/B-VII.1 evaluated data, ZZ-KAFAX-E70 background cross sections and GFR 2400 neutron spectrum. The created library was validated through integral experiments evaluated on the HEX-Z deterministic models in DIF3D. The results were also compared with MCNP5 calculations.

Key words: multi-group XS library, GFR 2400, NJOY99, DIF3D, SBJ_E71_25g

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 of Boltzmann'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 solutions are used. The history of computational transport basically follows the development of two competing methods, commonly called stochastic and deterministic. Although these methods use fundamentally different approaches, their common feature is their strong dependence on nuclear data. Both use nuclear data in a form of special cross section libraries. 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 (CE) 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 reliable answer 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.

Theoretical background

Multi-group cross sections in a form of multi-group constants are used by computer codes that calculate the distributions of neutrons in space and energy, and then compute various 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]:

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

The neutron flux $\phi(x,\mu,E)$ is defined as a function of position x, polar cosine μ and energy E. The left side of this equation represents the destruction and the right side the production of neutrons. The importance of a given group constant is represented by its weighting flux. In general, the weighting flux is not known. However, it is often possible to obtain fairly accurate group constants for a particular application if the shape of the flux is reasonably well known. The key to using the multi-group method effectively is balancing the trade-offs between the choice of weight function and the number of groups. One of the possible options is to use the Bondarenko model, the method with narrow resonance approximation, to obtain [2]:

$$\phi_l^i(E) = \frac{W_l(E)}{\Sigma_t(E) + \sigma_0^{i+1}} \quad (2)$$

where $\phi_l^i(E)$ is the l-th Legendre component of the angular flux, $W_l(E)$ is a smooth function of energy (such as 1/E) and $\Sigma_t(E)$ is the total macroscopic cross section for the desired material. If one makes $W_l(E)$ equal to an arbitrary smooth function $C(E)$ and assumes that the self-shielding effect can be obtained for isotope i by representing all the other isotopes with constant background cross section $\Sigma_0^i(E)$ Eq. (5) can be written as follows [2]:

$$\phi_l^i(E) = \frac{C(E)}{\Sigma_t^i(E) + \Sigma_0^i(E) + \sigma_0^{i+1}} \quad (3)$$

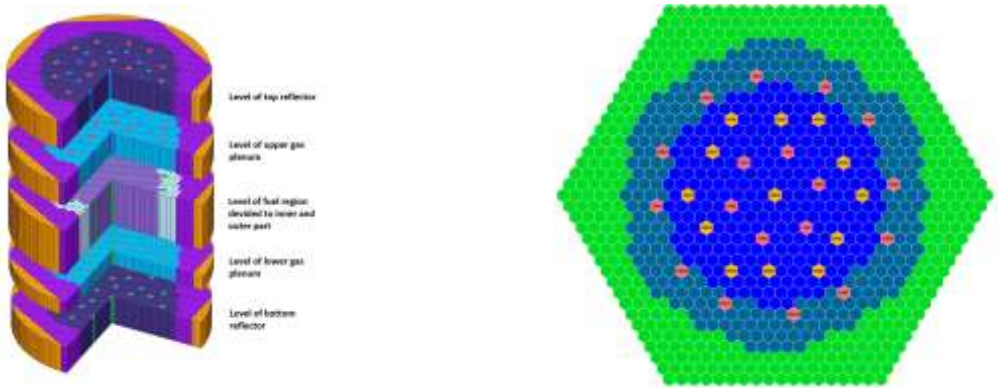
Description of the target core

As the target core for cross section processing and optimization the GFR 2400 reactor was selected. The Gas-cooled Fast reactor is one of the GEN IV nuclear reactors selected by the GIF (Generation IV International Forum) and supported by the SNETP (Sustainable Nuclear Energy Technology Platform) for further development in the EU. 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 IF and OF 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 below and above the fission gas plena. The reactivity of the GFR 2400 core is controlled through two systems of control rods, CSD and DSD assemblies. Both systems accommodate B_4C absorbers with 90% weight content of ^{10}B isotope [3]. The basic design parameters of the GFR 2400 reactor are summarized in Tab. 1. The sectional and top view of the GFR 2400 reactor core is presented in Fig. 1.

Tab. 1. *Basic design parameters of the GFR 2400 reactor core* [3]

Parameter	Value	Parameter	Value
Reactor thermal power	2400 MW_{th}	Fuel pin diameter	3.335 mm
Gross electric efficiency	45 %	Cladding diameter	4.550 mm
Primary coolant	100% He	Fuel pin pitch	11.570 mm
Secondary coolant	20% He + 80% N_2	Fuel assembly can thickness	2.000 mm
Primary pressure	7 MPa	Fuel assembly pitch	8.915 cm
Mass flow rate	1213 kg/s	Number of pins per fuel assembly	217 pcs
Core inlet/outlet temperature	400/780 °C	Number of fuel assemblies	516 pcs
Core pressure drop	0.143 MPa	Number of CSD CR assemblies	18 pcs
Secondary pressure	6.5 MPa	Number of CSD CR assemblies	13 pcs



a; b;

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

Cross section processing scheme

Computational codes require the cross section data to be stored in libraries of an appropriate structure. 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 [4]. This file format has undergone a long historical development; the current version is labelled as ENDF-6. If desired, XS data in the ENDF form can be transformed to various file formats. To obtain continuous energy XS data for the stochastic MCNP5 [5] code, the ENDF evaluated data is transformed through PENDF (Pointwise ENDF) to the ACE (A Complex ENDF) format. For deterministic codes such as DIF3D [6] or PARTISN [7] first GENDF (Group-wise ENDF) cross section data are produced by NJOY [2]. The data are subsequently transformed to effective macroscopic cross sections in MATXS and ISOTXS format.

Precise deterministic calculations of the GFR 2400 reactor require a new XS library to be created. It is a complex process which requires both experimental and computational data and multiple computer codes. To develop and optimize the cross section library a new calculation scheme was developed, which is shown in Fig. 2. 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 target core to be created. In addition to basic neutron physical parameters available at the MCNP5 output file the 620 group weight flux is produced (5) using superimposed mesh tallies. Although there are several options for the weighting flux, a previously performed optimization study showed that the best option is to use the average neutron spectrum from the inner and outer fuel core of GFR 2400. The weight flux, the ENDF/B-VII.1 [8] evaluated data, the ZZ-KAFAX-E70 [9] background cross sections (6), the NUCLIST and TEMPLIST files (7) and the GROUP STRUCTURE (8) files are subsequently evaluated in NJOY99 (9) to produce 620 group MATXS libraries (10). These microscopic cross section data are then transformed to effective region-wise macroscopic cross sections using the TRANSX code (11). The cross sections data are stored in the IXOTXS library (12). This XS library can be directly used to perform 3D full core calculations in DIF3D, however in order to effectively accelerate the simulations group collapsing (15) is carried out. It is done based on the RZFLUX (14) region-wise neutron flux binary data file obtained from the RZ transport calculation carried out using PARTISN (13). The region-wise neutron flux is used as weight function in the second TRANSX run (15) and 25 group ISOTXS library (16) is created. The final ISOTXS cross section library is labelled as SBJ_E71_25G. This cross section library is used in DIF3D (17) to calculate neutron physical parameters of the system, such as k_{eff} (18).

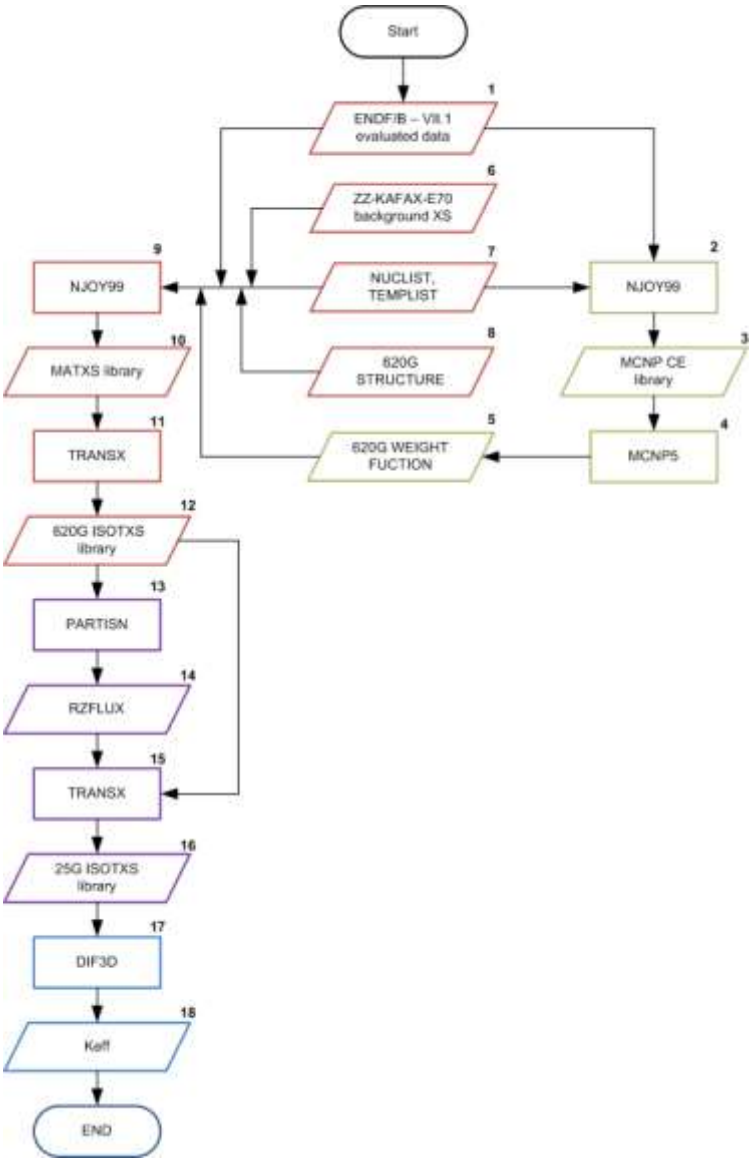


Fig. 2. *The cross section processing scheme.*

Benchmarking on integral experiments

The precision of the produced cross section libraries can be evaluated through benchmarking on integral experiments. The aim is to compare the reactivity deviation of various calculation cases from the detailed heterogeneous MCNP5 calculation. Based on the recommendations of WPEC Subgroup 33 [10] 8 integral experiments were selected. The calculations were performed using the fine group version (without group collapsing) of the SBJ_E71_620G library. The results are shown in **Fig. 3**.

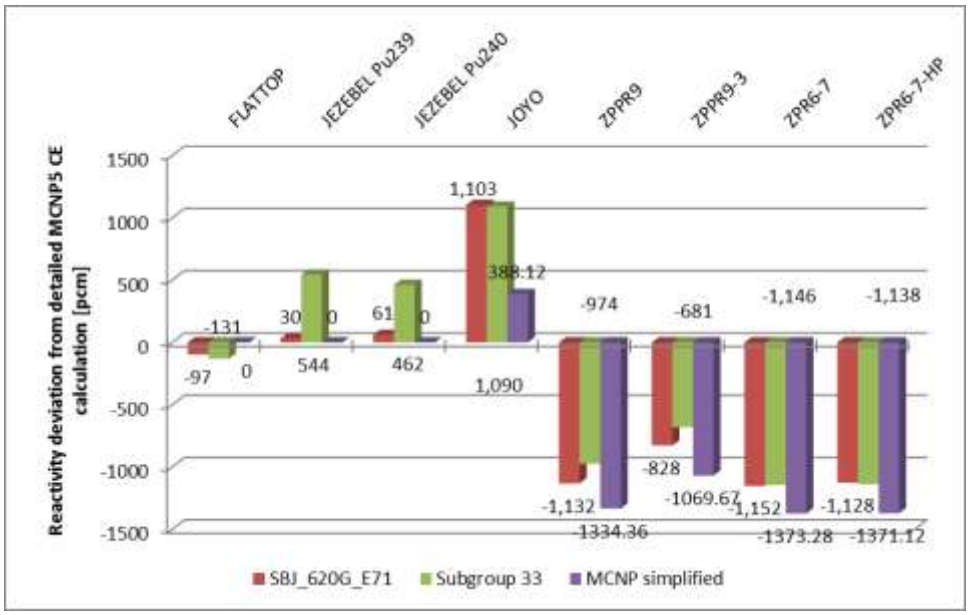


Fig. 3: *Results of integral experiments.*

The benchmark results showed very similar performance of the SBJ_E71_620G libraries and the results provided by Subgroup 33. 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 was less than 300 pcm. It can be concluded that the precision of the developed XS library is comparable with available multi-group cross section libraries for both simple and complex geometries.

Application for GFR 2400

Since the benchmarks showed promising results it was justified to apply the developed cross section library on the target GFR 2400 reactor core. The analyses performed on GFR 2400 focused on two major aspects. Basically, the main goal was to compare the deterministic results with MCNP5 in order to validate the performance of our library. The second aspect was to apply the XS library for modelling and symulation areas which are due to their computational costs not reliable for stochastic methods. The comparison between MCNP5 and DIF3D was made based on three parameters, the excess reactivity of the system without control rod insertion, the worth of control rods and the interference of control rods. All calculations were performed on the full core homogeneous 3D GFR 2400 model in both MCNP5 and DIF3D. The calculation of control rod (CR) worth was performed based on a twostep approach. First the excess reactivity of the system was calculated. The comparison of the excess reactivity fulfilled our expectations; the reactivity deviation was only -182 pcm (1578±4 pcm in MCNP5, 1334 pcm in DIF3D). In the second step, the investigated CR was fully inserted in its position in the reactor core and the calculation was repeated.
The worth of i-th CR was calculated using the following equation:

$$\Delta\rho_{CR}^{i} = \rho_{e} - \rho_{CR}^{i} \tag{4}$$

where ρ_e and ρ_{CR}^{i} are the values of excess reactivity before and after the CR insertion. The CR interference was calculated using Eq. (5):

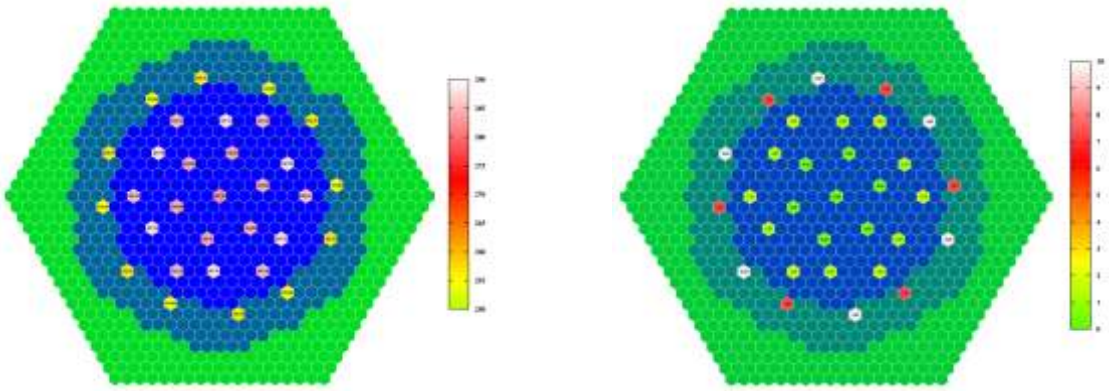
$$A_{CR}^{i} = \frac{\Delta\rho_{CR}^{1..N} - \Delta\rho_{CR}^{1..N \setminus i}}{\Delta\rho_{CR}^{i}} \quad (5)$$

In the equation above $\Delta\rho_{CR}^{1..N}$ stands for the worth of all CRs, $\Delta\rho_{CR}^{i}$ for the worth of the investigated CR and $\Delta\rho_{CR}^{1..N \setminus i}$ for the total worth of CRs expect the investigated one. If $A_{CR}^{i} < 1$ shadowing effects and if $A_{CR}^{i} > 1$ anti-shadowing effects occur, otherwise the control rods are not influenced by each other. The results of the CR worth and interference are shown in Tab. 2.

Tab. 2. *Results of control rod worth and interference*

Control rod ID	$\Delta\rho_{CR}^{i}$ [pcm]		$\delta\rho_{MCNP}^{i}$ [pcm]	A_{CR}^{i} [-]		δA_{MCNP}^{i} [%]
	MCNP5	DIF3D		MCNP5	DIF3D	
CSD+DSD	12229	11991	-238	-	-	-
CSD	7932	7753	-179	1.001	1.001	0.01
DSD	4286	4227	-59	1.003	1.003	0.01
CSD 1 ring	1419	1409	-10	0.822	0.821	0.18
CSD 2 ring	4592	4559	-33	1.494	1.610	-7.78
DSD0	282	282	0	0.295	0.260	11.98
DSD4	289	285	-4	1.719	1.721	-0.09
CSD2	287	284	-3	0.418	0.415	0.64
CSD10	261	284	23	10.083	9.687	3.93

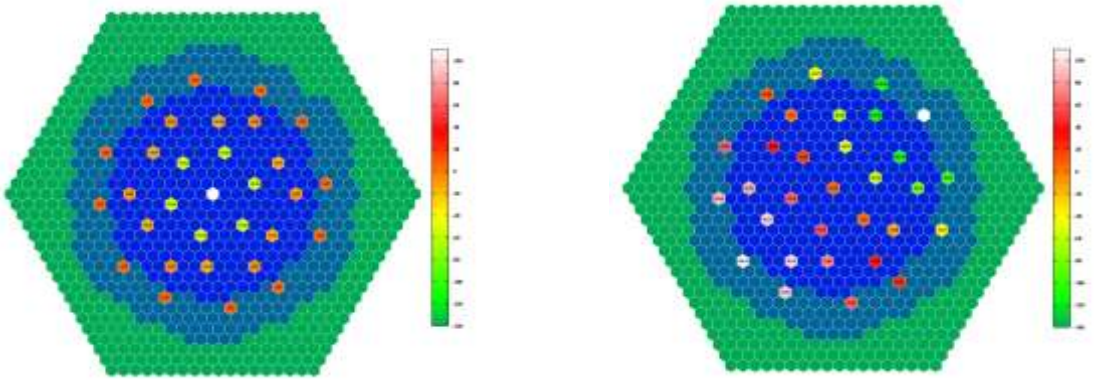
The reactivity deviation in case with all inserted control rods is slightly above the case without CRs in the core, but -238 pcm can be still considered as a good value. The worth of individual CRs is almost identical in both codes, however it can be seen that the difference between MCNP5 and DIF3D is a function of CR position (neutron flux distribution) in the core. The comparison of CR interference also showed good agreement to stochastic results. The amplification factor was smaller than several percent in case of the majority of calculation cases. The biggest difference (11.98%) was found in case of the central DSD0 assembly. The differences 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. Although the deterministic approach caused several pcm deviations in the CR results, the biggest advantage of this method is the extremely short calculation time. A DIF3D calculation on a single CPU did not take more than 1 minute, while the similar MCNP5 calculation required more than 24 hours calculation time on a cluster system. This big advantage allowed us to create a full core map of CR worth and interference, which are shown in **Fig. 4**. In the results presented in Fig. 4 we can identify the CR symmetry. It can be seen that the symmetry of GFR 2400 control rods changes from centre to periphery. In the core centre, the symmetry is ideal 360°, while at the core boundary the symmetry was disturbed to 60°.



a; CR worth ***a; CR interference***

Fig. 4. *Worth and interference of control rods.*

In order to better understand the CR interactions the analysis of CR pairs was performed. In this analysis all control rod pair combinations were subjects of investigation. The results for the central DSD0 assembly and the outermost CSD10 assembly are shown in **Fig. 5**.



a; DSD0 interference ***b; CSD10 interference***

Fig. 5. *Interference of CR pairs*

In the figure above it can be seen that the central DSD0 device is attenuated mainly by the flux depression resulting from the insertion of the first CSD ring. The attenuation of DSD0 decreases by distance. Due to the maximum of neutron flux, the outer ring of the CSD system increases the worth of DSD0. The effect of neutron flux can be seen also in **Fig. 5**b. Although the CSD10 assembly is attenuated by the surrounding control rods, the final reactivity worth is significantly increased due to the influence of the farthest assemblies. This is an interesting finding since the distance between these assemblies is several meters. It can be concluded, that in terms of control rod interactions the neutron flux in the place of CR insertion is more important than the distance between CRs.

Conclusion

The design and the safety requirements of GEN IV fast reactors require special approaches. Although Monte Carlo methods are widely used and can achieve promising results, due to their stochastic nature the results are burdened by statistical uncertainties (in addition to XS data uncertainty). 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 the given application. This paper deals with the development of the SBJ_E71_25G multi-group cross section library and its application for the GFR 2400 reactor. A new cross section processing scheme was developed, based on ENDF/B-VII.1 evaluated data, combination of computer codes and ZZ-KAFAX-E70 background cross sections. These XS library was benchmarked on integral experiments and compared with data provided by the WPEC Subgroup 33. The precision of the SBJ_E71 libraries is comparable with available multi-group cross section libraries, however in the future more benchmark experiments will have to be evaluated. Finally, the SBJ_E71_25G XS library was 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 in the non-roded and -238 pcm in the roded case. The most important finding of this analysis is that using 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. This extremely short calculation time opens research areas which are difficult for Monte Carlo calculations, such as calculations of sensitivity coefficients and higher mode harmonics of eigenvalues and neutron fluxes. Using the SBJ_E71_25G XS library and the DIF3D code core wide maps of CR worth, CR amplification factors and CR pair interaction were prepared and analysed.

Acknowledgement

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References

[1] D. G. Cacuci. Handbook of Nuclear Engineering, Springer, 2010
[2] R.E. MacFarlane, D.W. Muir, R.M. Boicourt, A.C.Kahle. The NJOY Nuclear Data Processing System, Version 2012, Los Alamos National Laboratory, USA, 20122
[3] M. Zabiego at. all. Overview of CEA´s R&D on GFR Fuel Element Design: From Chalanges to Solutions, Progress in Nuclear Energy, 2014
[4] M. Herman, A. Trkov. ENDF-6 Formats Manual, DataFormats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII, BNL, Brookhaven, USA, 2009
[5] LANL. MCNP - A General N - Particle Transport Code, Los Alamos National Laboratory, Los Alamos, USA, 2003
[6] ORNL. DIF3D: Code System Using Variational Nodal Methods and Finite Difference Methods to Solve Neutron Diffusion and Transport Theory Problems. RSIC, 2011
[7] ORNL. PARTISN: Multi-Dimensional, Time-Independent or Time-Dependent, Multigroup, Discrete Ordinates Transport Code System, RSIC, 2009
[8] M.B Chadwick et. al.. ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data, Nuclear Data Sheets, vol. 112, no. 2, pp. 2887-2996, 2011
[9] D.H. Kim, C.S. Gil, Y.O. Lee. ZZ KAFAX-E70, 150 and 12 Groups Cross Section Library in MATXS Format based on ENDF/B-VII.0 for Fast Reactors, Korea Atomic Energy Research Institute, Nuclear Data Evaluation Laboratory, Daejeon, 2008
[10] OECD NEA. Methods and Issues for the Combined Use of Integral Experiments and Covariance Data, OECD, Paris, 2013