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# Processing of the multigroup cross-sections for MCNP calculations

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**Abstract:** Stochastic Monte Carlo (MC) neutron transport codes are widely used in various reactor physics applications, traditionally related to criticality safety analyses, radiation shielding and validation of deterministic transport codes. The main advantage of Monte Carlo codes lies in their ability to model complex and detail geometries without the need of simplifications. Currently, one of the most accurate and developed stochastic MC code for particle transport simulation is MCNP. To achieve the best real world approximations, continuous-energy (CE) cross-section (XS) libraries are often used. These CE libraries consider the rapid changes of XS in the resonance energy range; however, computing-intensive simulations must be performed to utilize this feature. To broaden our computation abilities for industrial application and partially to allow the comparison with deterministic codes, the CE cross section library of the MCNP code is replaced by the multigroup (MG) cross-section data. This paper is devoted to the cross-section processing scheme involving modified versions of TRANSX and CRSRD codes. Following this approach, the same data may be used in deterministic and stochastic codes. Moreover, using formerly developed and upgraded cross-section processing scheme, new MG libraries may be tailored to the user specific applications. For demonstration of the proposed cross-section processing scheme, the VVER-440 benchmark devoted to fuel assembly and pip-by-pin power distribution was selected. The obtained results are compared with continues energy MCNP calculation and multigroup KENO-VI calculation.

**Keyword:** *MCNP, Multigroup calculation, VVER, criticality*

## I. INTRODUCTION

A lot of effort has been spent on the development of techniques to effectively compute sensitivity coefficients and cross-section induced uncertainties (S/U) by Monte-Carlo codes and continues-energy libraries. MCNP6 and SCALE6.2 have currently implemented approaches to calculate the adjoint weighted tallies, which allow both codes to carry out S/U analyses related to criticality safety calculations using CE libraries. Although, it is no necessary for CE libraries to calculate flux moments from mesh flux, implicit sensitivity coefficients or adjoint flux and to perform cell treatment, S/U calculation can be still memory and time expensive and special attention must be given to the preparation of the covariance matrix. [1,2,3] Alternatively, the multigroup option is still an effective method for other applications and in case of cross-section adjustment, it can also extend the applicability of S/U calculation. The

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main advantage of multigroup calculation is not only in the reduction of the calculation time but also offers to an engineer utilization of the adjoint calculations in problems where the forward transport calculation is not efficient. [4]

Effective use of the multigroup approach is depending on the appropriate and target tailored cross-section library. To achieve a required accuracy of the multigroup MC calculation, the problem specific cross-sections have to be available. Currently, there are four VVER-440 reactor units in operation and two other units are under construction in Slovakia, thus there is a clear need of improvement in our calculation abilities. The VVER-440 reactors belong to PWR family, where thermal scattering treatment has to be taken into account during cross-section data processing. In many industrial applications, a validation of deterministic codes requires that the MC code utilize the same data as a deterministic code [5]. Optimized cross-section library applicable to both types of calculation is therefore the basic requirement for the current neutronic analyses and allows us to implement various methods to the multigroup constants processing scheme.

## II. THE MULTIGROUP CROSS-SECTION PROCESSING

### A. Cross-section library

Within this analysis the SBJ_V2019T multigroup cross-section library, which is updated version of SBJ_V2018T library presented in [5], was utilized as source data file. The library is based on the ENDF/B-VII.1 evaluated data [6], includes thermal scattering data for hydrogen in $H_2O$ based on IKE S(α,β) [7, 8] and CAB [9] models; and is stored in MATXS format. The cross-section library was prepared in 238 group structure, the same as in SCALE6 libraries [10], where the core averaged neutron spectrum of the VVER-440 reactor was used as a weighting function. Utilization of the SBJ_V2019T library is a part of long term complex validation process of developed cross-section processing scheme.

### B. Computational scheme

The fundamental part of the problem oriented MG constants processing scheme is a universal code which is able to prepare MG constant in various formats. In our previous analyses, the TRANSX code [11] was standardly utilized. The TRANSX code is able to work with cross-section library in general MATXS format and region-wise flux files in CCCC format. It can process cross-section data with an appropriate cell treatment; infinite homogeneous mixture incorporating self-shielding effects by Bondarenko Method or lump materials incorporating Dancoff correction for several geometrical configurations (slab or cylinders in triangular or square lattice). Some modifications were made in the TRANSX source code to enhance its versatility, like considering cladding within Dancoff correction calculation, enabling utilization of dummy materials, extraction of scattering matrixes for individual reactions (elastic, inelastic and n2n) and others. The TRANSX code prepares problem oriented MG constants (micro or macroscopic) standardly in ISOTXS format, which can be directly used by deterministic codes PARTISN [12] or DIF3D [13]. To process MG constants for MCNP calculation the CRSRD [4] modules were implemented to the TRANSX code. The CRSRD code was designed to translate deterministic MG cross-section to the format suitable for MCNP.

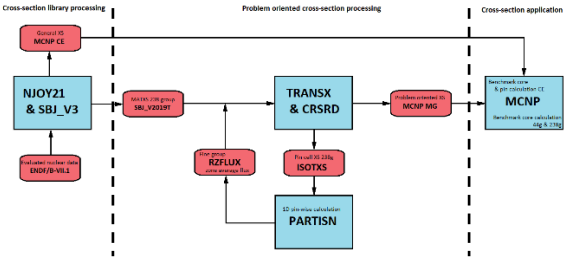


**Fig. 1.** Computational scheme.

The computational scheme applied in this analysis is shown in Fig. 1. The left side is devoted to the processing of the SBJ_V2019T library which is describe in [5]. The right side is aimed to the transport calculations and is described in following sections. The mid part is schematically describing the data flow and the utilized codes. In the first round the SBJ_V2019T library is directly used to prepare two sets of MG cross-sections. The first set was prepared in the way that all materials were processed as an infinitely diluted, in 238 group structure and in MCNP MG format, later denoted as **238 gH**. The second set was prepared in the way that all structural materials were processed as infinitely diluted, in 238 group structure and in MCNP MG format. Fuel, cladding and coolant were processed through the cell treatment considering cylindrical shape of lump in triangular lattice and in 238 group structure in MCNP MG format, later denoted as **238 g** and in ISOTXS format for spectral pin calculation. In the second round the region averaged flux spectra calculated for each fuel enrichment was used to collapse MG cross-sections. The 44 group structure, same as used in SCALE6 libraries, was used due to its compatibility with 238 energy group structure. The third set is later denoted as **44 g**. All three cross-section sets comprise of isotope-wise constants (microscopic cross-section) and homogenized material-wise constants (macroscopic cross-sections). Calculations, which utilized homogenized constants are later denoted with abbreviation HM as **238 gHHM**, **238 gHM** and **44 gHM** respectively to the individual sets.

All the TRANSX calculations were performed with the same set of input parameters. Legendre polynomial expansion for scattering matrixes was set to 3. Consistent-P approximation was used for transport correction and 95 thermal groups were defined in the 238 group calculation. In the 44 group calculation, for transport correction, the Bell-Hansen-Sandmeier approximation was used and 23 thermal groups were defined. In case of CRSRD translation part, the absorption cross-sections were kept with negative values, if occurred, and scattering matrixes were processed with the factor $2\ell+1$ to 32 equi-probable bins by the Maximum Entropy approach. Since this process was managed by the TRANSX code with implemented modules from CRSRD, the data flow and the formats from the MATXS through TRANSX and CRSRD procedures to MCNP MG cross-section file were controlled. More information with the data flow scheme is presented in [14].

All MCNP MG calculations were validated by the MCNP calculation in CE mode and KENO-VI [10] MG calculation using 238 group library. In case of MCNP CE calculation the cross-section data processing is quite straightforward. Regarding to KENO-VI calculation all parameters related to the cross-section data processing were selected similarly as much as it was possible, like 238 group library, cell treatment, Legendre expansion, material definition, etc.

### C. VVER-440 benchmark overview

The VVER-440 benchmark devoted to fuel assembly and pip-by-pin power distribution was selected to demonstrate the proposed cross-section data processing capabilities. Benchmark definition is based on zero power state with uniform temperature 543.15 K. The geometry was simplified to two-dimensional definition with 30-degree symmetry. All internal parts like core barrel, core basket and core rim called “vygorodka” were included. The outer boundary of the benchmark is defined by the outer edge of reactor pressure vessel with vacuum boundary condition. The geometry definition is presented

in Fig. 2, based on the SCALE6 model. The core is composed of three types of fuel assemblies with enrichment 1.6, 2.4 and average 4.25 % and two fully inserted Emergency Reactor Control Assembly (ERC) of 6th working group. The fuel assembly with average enrichment 4.25 % consists from fuel pins with four different enrichments where one type of pin contains combination of the $UO_2$ and gadolinium absorber. All fuel assemblies are considered as a fresh fuel. [15]

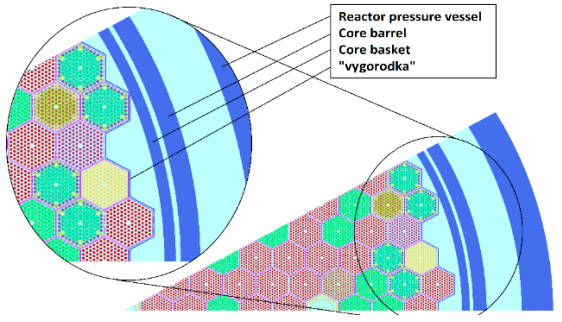


**Fig.2.** VVER-440 benchmark geometry model [16].

## II. RESULTS AND DISCUSSION

The first type of calculation was carried out at the level of fuel pin to obtain neutron flux spectra for cross-section collapsing. These calculations were performed by the PARTISN code in simplified 1D geometry where the hexagonal lattice cell was represented by the radius of equivalent cylinder. Due to direct utilization of flux files (RZFLUX shown in Fig. 1) and capabilities of the TRANSX code, helium volumes were omitted in the geometry model. The same geometry definition, except hexagonal to cylindrical approximation, was used also in the comparative MCNP and KENO-VI calculations. MCNP as well as KENO-VI was run with 10 mil. histories in 1000 generation and 30 generations were skipped.

The main part of the research is focused on the validation of proposed cross-section processing scheme utilizing in-house prepared cross-section data and software application on benchmark calculation, where not only integral parameter $k_{eff}$ is evaluated, but also local parameters like relative fuel assembly (FA) power distribution and relative fuel pin (FP) power distribution are available. Within this paper only results of $k_{eff}$ and FA power distribution are presented and discussed. Geometrical and material model of the benchmark core was prepared for MCNP and KENO-VI codes as it is described in the previous part and shown in Fig. 2. All MCNP calculations were performed by the MCNP5 1.6 version [17] with 750 mil. neutron histories within 5 000 generations. The KENO-VI calculation was performed using the version distributed within the SCALE6.1.3 system with 100 mil. neutron histories during 500 generations.

Due to the relatively small difference between the results of IKE and CAB thermal scattering models (in maximum it was 63 pcm) only the results of CAB model are presented in the next chapter. All comments and conclusions presented in this paper are relevant and applicable for the results of IKE model.

### A. Results

The results of the FP spectral calculations are presented in Table I. Six different enrichments represent three types of FA where the last four belong to the FA with average enrichment 4.25 %. The results of spectral calculation carried out by PARTISN code are supplemented by the MCNP CE and KENO-VI MG calculation due to only partial validation of the SBJ_V2019T library and the part of cross-section processing dedicated only to deterministic codes. The first value presented for each code is the infinite multiplication factor $k_{inf}$, instead of $k_{eff}$, due to reflective boundary conditions on geometric model edges. The second value in case of MC codes stands for the standard deviation of $k_{inf}$.

**Table I.** Comparison of fuel pin (FP) calculation

| FP enrichment | PARTISN | MCNP CE | | KENO-VI MG | |
|---|---|---|---|---|---|
| % of $U^{235}$ | $k_{inf}$ | $k_{inf}$ | $\sigma$ | $k_{inf}$ | $\sigma$ |
| 1.6 | 1.06290 | 1.07071 | 0.00018 | 1.06392 | 0.00015 |
| 2.4 | 1.18125 | 1.18943 | 0.00019 | 1.18228 | 0.00019 |
| 3.6 | 1.27898 | 1.28595 | 0.00020 | 1.27894 | 0.00020 |
| 4.0 | 1.30090 | 1.30790 | 0.00020 | 1.30036 | 0.00018 |
| 4.0+3.35$Gd_2O_3$ | 0.39722 | 0.39874 | 0.00008 | 0.39647 | 0.00009 |
| 4.4 | 1.31954 | 1.32602 | 0.00021 | 1.31864 | 0.00019 |

Values of $k_{eff}$ from the MC VVER-440 benchmark calculation are presented in Table II. The first three values can be considered as a reference due to their independence on the demonstrated cross-section scheme processing and the previous validation. The next six values represent the current capabilities of the cross-section processing scheme and possibilities of future use.

**Table II.** Results of $k_{eff}$ of the VVER-440 benchmark

| Computational case | $k_{eff}$ | $\sigma$ |
|---|---|---|
| MCNP ref [15] | 1.06827 | 0.00005 |
| KENO-VI 238g [16] | 1.06343 | 0.00006 |
| MCNP CE | 1.06478 | 0.00002 |
| MCNP MG 238gHM | 1.05447 | 0.00006 |
| MCNP MG 44gHM | 1.05498 | 0.00008 |
| MCNP MG 238g | 1.05161 | 0.00002 |
| MCNP MG 44g | 1.05015 | 0.00002 |
| MCNP MG 238gH | 1.08597 | 0.00002 |
| MCNP MG 238g HHM | 1.08831 | 0.00006 |

The relative FA power distribution calculated by the KENO-VI and MCNP in CE and MG mode with their relative change from the reference MCNP calculation are presented in Fig. 3, Fig. 4 and Fig.5 respectively. MCNP MG case is represented by the calculation with 44g collapsed data, since it is the most perspective one for application in future analyses.

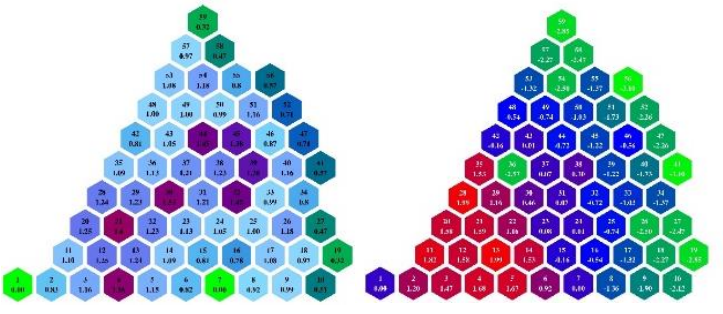

**Fig. 3.** Relative FA power distribution of KENO-VI (left) calculation and relative change in % from MCNP reference values (right).

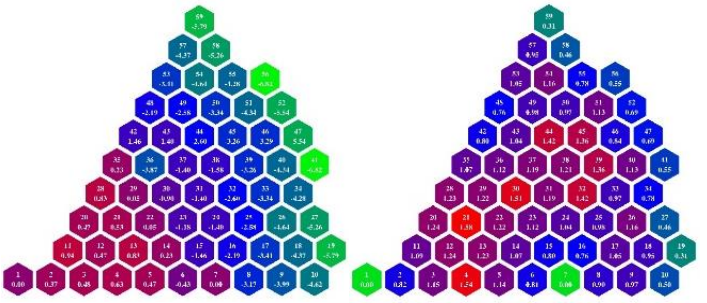

**Fig. 4.** Relative FA power distribution of MCNP CE (left) calculation and relative change in % from MCNP reference values (right).

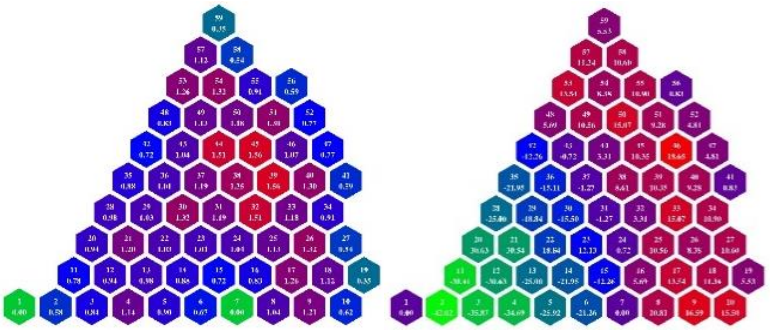

**Fig. 5.** Relative FA power distribution of MCNP MG 44g (left) calculation and relative change in % from MCNP reference values (right).

### D. Discussion

Comparison of the fuel pin calculation demonstrates the validity of the SBJ_V2019T library for thermal applications and the fact that the whole functionality of TRANSX code has been maintained after the implementation of CRSRD modules. Special attention should be given to the comparison of MG calculations (PARTISN vs. KENO-VI, see Table 1) where the relative difference in almost all cases is less than 100 pcm. Only for calculation of the FP consisting Gd the relative difference was higher, but 479 pcm is still quite reasonable due to comparison of very low $k_{eff}$. Relative difference between PARTISN and MCNP CE calculation is also acceptable because relative difference in average is just 570 pcm and PARTISN calculations systematically underestimated the MCNP CE calculations.

Within the criticality calculation of the VVER-440 benchmark, the first inconsistency in the results presented in Table 2 was obtained at the level of reference calculations. The relative difference between the reference MCNP and KENO-VI or MCNP CE is in both cases more than 300 pcm. The obtained difference has been caused by the different nuclear evaluated data used during libraries processing. Reference MCNP calculation was carried out with the library processed from ENDF/B-VI data, while the KENO-VI library is based on ENDF/B-VII.0 and MCNP CE library is based on ENDF/B-VII.1 data. Therefore, it is more suitable to compare calculated values of MCNP MG with KENO-VI or MCNP CE values, at least at the level of $k_{eff}$.

The relative difference between MCNP MG and MCNP CE calculations vary from 872 pcm to 2031 pcm in absolute values. The closest $k_{eff}$ was obtained for cases where the homogenized macro-constants were used with appropriate cell treatment (44gHM and

238gHM). Relatively comparable values were obtained from calculation with isotope-wise constants (44g and 238g). Significant difference is in the calculated standard deviation. While the computational time of cases with homogenized macro-constants is around 10 % faster than in cases with micro-constants, the obtained standard deviation is more than three times higher. Therefore, all promising benefits from a utilization of homogenized macro-constants is vanishing in this stage of development. Generally, utilization of MG constants shortened the computational time about 30 %. The worst results were obtained for the cases with materials which were all treated as infinitely diluted.

In case of calculation of relative FA power distribution, inconsistent results were obtained. While the relative change between KENO-VI or MCNP CE values and reference MCNP values is in maximum 3.1 % for KENO-VI and 6.8 % for MCNP CE, the relative FA power distribution of MCNP MG calculations compared with reference MCNP is unacceptable. The relative change varies from -42 % to 17 % which is suggesting that the MG constants are not properly prepared. Revision of all input files and source code of the TRANSX/CRSRD code did not reveal any formal or technical problem. But collected information are pointing to different interpretation of the absorption cross-section in TRANSX and MCNP.

## III. CONCLUSIONS

This paper demonstrates the first result of cross-section processing scheme aimed to preparation of the problem oriented MG cross-section constants for MCNP calculation. The first stage of research activities involved development of the new code able to prepare MG constants for deterministic as well as MC codes, which is almost done. Although, the first result of benchmark calculation with complex geometry identified relevant problems with the cross-section interpretation, quite good experience with TRANSX code itself and experience with cross-section processing for deterministic codes give us opportunity to solve this problem in near future. The achieved reduction of computational time about 30 % is promising for next applications, but significant difference between 238g and 44g was not observed. The following analysis will be therefore focused on this phenomenon and optimal coarse group structure will be sought. The performance of the SBJ_V2019T library fulfilled all requirements and its applicability at least within deterministic calculations was clearly demonstrated on pin spectral calculations. Next step will be the final validation on the complex set of criticality safety benchmarks.

## ACKNOWLEDGEMENT

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