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Comparison of thermal scattering processing options for S(α,β) cards in MCNP

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ABSTRACT

The MCNP distributions include sets of pre-calculated thermal scattering libraries but these libraries are available for several temperature steps only. In order to achieve reliable results it is suitable to process the cross section libraries for the desired temperature. In general, there are three methods to process these thermal scattering libraries for the desired temperatures. This paper deals with the comparison of these three methods on the basis of several benchmarks and on the basis of a thermal transient experiment of a WWER-440 reactor. The choice is up to the MCNP user but unfortunately very few studies concerning the comparison have been published so far. Therefore conclusions and results presented in this paper may help the user to choose the most appropriate method for his calculation.

1. Introduction

MCNP (X-5 Monte Carlo Team, 2003) is a general-purpose Monte Carlo N-Particle code for steady state radiation safety calculations including the capability to calculate eigen values for critical systems; however it is highly dependent on the used cross section libraries. This dependence is also significant in the case of thermal neutron spectrum calculations, where MCNP uses two different methods to account for the scattering of neutrons. For the most materials it attempts to construct a free-gas scattering model based on the constant elastic cross-section. For important moderator materials, like hydrogen bound in water, it takes the binding of the material in the solid, liquid or gas into account (Brown, 2006). The binding of the scattering nucleus affects the cross-section, the angular and energy distribution of secondary neutrons, as the neutron can give up energy to excitation in the material or it can gain energy. For these reasons the basic nuclear data files are complemented by scattering law S(α,β) files which describe the thermal scattering of bound moderators (Mattes and Keinert, 2005). Nuclear data libraries with treated S(α,β) law are not required but they are absolutely essential to get correct answers in problems involving neutron thermalization (X-5 Monte Carlo Team, 2003).

2. Materials and methods

In order to apply the processed sets of thermal scattering libraries for further work it is essential to make sure that these libraries have been processed correctly. In other words, they have to be validated on the basis of experimental data. For this purpose 7 benchmarks, where each of them contains several cases, have been chosen from the international handbook of evaluated criticality safety benchmark experiments (International Handbook, 2007) and a computational thermal transient criticality experiment has been prepared. Since this paper deals with validation of thermal scattering libraries for the thermal spectrum reactors which are widespread in middle-Europe, it was advantageous to choose benchmarks that have parameters in common with the WWER reactors.

2.1. Description of the benchmarks

The chosen set encompasses 39 cases for the thermal neutron spectrum, for water moderated uranium and uranium–plutonium fuel assemblies with and without boric acid in the coolant and for cases that employ structural materials and absorbers commonly used in WWER reactors. The summary of the basic parameters of the chosen benchmarks is presented in Table 2.1. Apart from the last four tasks, that are closely associated with the WWER reactors, there are another three tasks dealing with MOX fuel. These tasks were chosen to validate the thermal scattering libraries in

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Table 2.1
Summary of the benchmarks (International Handbook, 2007).

Benchmark	Fuel type	^{235}U wt.%	PuO_2 wt.%	Boric acid concentration	Temperature (K)
MIX-COMP-THERM-02 (MCT02)	$PuUO_2$	0.72	1.78	0.9–1090 ppm	295.16
MIX-COMP-THERM-05 (MCT05)	$PuUO_2$	0.72	3.98	–	298.16
MIX-COMP-THERM-11 (MCT11)	$PuUO_2$	44.63	25.8	–	295.16
IEU-COMP-THERM-02 (ICT02)	UO_2	17	–	–	300, 400, 500
LEU-COMP-THERM-19 (LCT19)	UO_2	5.32	–	–	300
LEU-COMP-THERM-21 (LCT21)	UO_2	5.12	–	2.36–3.15 g/l	300
LEU-COMP-THERM-26 (LCT26)	UO_2	4.92	–	–	300, 500

systems containing transuranic fuel as a simplified approach to evaluate the effects of the fuel burnup. A more comprehensive description of the benchmarks can be found in (International Handbook, 2007).

2.2. Thermal transient criticality experiment

The thermal transient experiment was designed to verify the usability of the prepared thermal scattering data for various temperature ranges. A simplified material and geometrical model of reactor WWER-440 was prepared based on the experience of the Institute of Nuclear and Physical Engineering (INPE). This model is described in (Vrban et al., 2012). This model was also used to perform a criticality simulation of the heating up process at minimal control power level during the reactor start-up because this transient process is well-known and runs without any unpredictable k_{eff} fluctuations. The principal scheme of the reactor is shown in Fig. 2.1.

The core heating up, which occurs due to fission during the reactor start up, is a very specific, slow and controlled process. The change of k_{eff} is caused by temperature feedback only, which is in terms of MCNP calculation directly dependent on the nuclear cross section data. The reactor is critical at the minimal control power level throughout the whole process; therefore we can assume that the temperature is changing in all parts of the reactor core uniformly. On the basis of these initial conditions, point-kinetic calculations can be performed in a temperature scale of 200–260 °C with a 2 °C step. This method was partially used for the investigation of thermal reactivity coefficients published in (Vrban et al., 2012), where this method is described in detail.

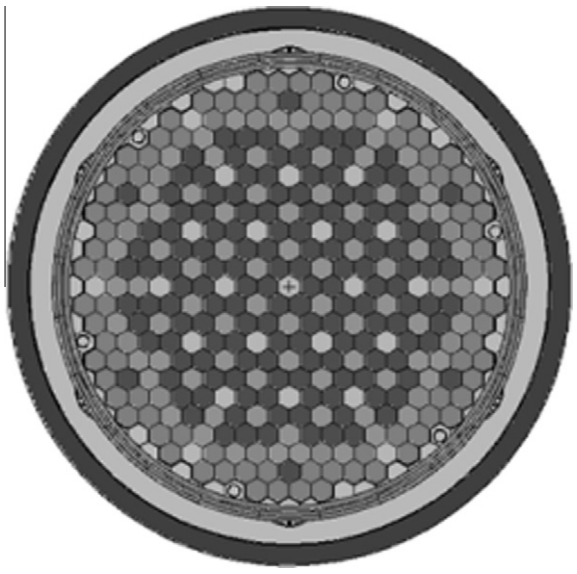

Fig. 2.1. Horizontal section of reactor WWER-440 model.

2.3. Processing of the neutron cross-section and thermal scattering libraries

The NJOY99.364 code was used to process the cross section data for the temperatures required by the benchmark problems and for all states of thermal transient criticality experiment (MacFarlane and Kahler, 2010). The evaluated ENDF/B-VII.0 data files (Chadwick et al., 2006), which are distributed by the IAEA, were used as source data. Three methods were used to process the thermal scattering libraries. They are the following ones:

1. the pre-calculated thermal scattering libraries included in the MCNP5 distribution were used as reference data and interpolated to the desired temperature by the *makxsf* code;
2. the thermal scattering law files distributed in ENDF/B-VII.0 were processed by NJOY for standard temperatures (Mattes and Keinert, 2005) and then they were interpolated to the desired temperature by the *makxsf* code;
3. the scattering law files were computed using the *LEAPR* module of NJOY using parameters interpolated from the IKE (Mattes and Keinert, 2005) model for each desired temperature.

The NJOY code is a modular system, where each module is essentially a separate program performing a well-defined processing task. Processing of the neutron cross-section libraries is comprehensively described in (MacFarlane and Kahler, 2010) and the application of the individual modules, as a standard adjustment used in INPE, is further described in (Lüley et al., 2012). Processing of the thermal scattering libraries requires the use of the *LEAPR* module to prepare the scattering law $S(\alpha,\beta)$ files and related quantities that describe thermal scattering from bound moderators in the ENDF-6 format used by *THERMR* module (MacFarlane, 1994). *LEAPR* requires a uniform grid for the continuous frequency distribution $\rho(\omega)$ for every temperature. The final validated frequency distribution for the standard temperatures was made on the basis of (Mattes and Keinert, 2005).

The *makxsf* code is a utility program to handle the cross-section libraries for the MCNP5 code (X-5 Monte Carlo Team, 2003). The main functions performed by *makxsf* include Doppler broadening and thinning in the resolved resonance range for given temperatures, interpolation of unresolved resonance probability tables to new temperatures, and for our purpose most important feature, interpolation of $S(\alpha,\beta)$ thermal scattering kernel data to new temperatures. The ability to create a nuclide table-set at new temperature was added to *makxsf* by incorporating several routines from the NJOY and DOPPLER codes (Brown, 2006).

3. Theory and calculation

The *LEAPR* module computes the scattering law as a convolution of three models: translation, represented either by a free gas or diffusion model; a continuous, solid-like spectrum $\rho(\omega)$, and discrete oscillators. Parameters used in the models and the resulting thermal scattering cross section libraries are interpolable but

experience has shown that temperature interpolation of S(α,β) is unreliable. It is recommended to compute the cross sections for given moderator temperatures only. Data for other temperatures should be obtained by interpolation between the cross sections. (Herman and Trkov, 2010) Therefore, in methods (1) and (2) described above the thermal scattering libraries were interpolated, and in method (3) the parameters were interpolated. Based on chosen benchmarks and moderator primarily used in our investigations, processing the thermal scattering libraries by mentioned methods was aimed to hydrogen in light water.

3.1. Thermal scattering libraries

The scattering law for hydrogen in light water distributed with ENDF/B-VII is based on the model proposed by (Mattes and Keinert, 2005). In this model, the following parameters are used:

- A free gas model, with temperature dependent mass, to represent translational motion of water clusters.
- Continuous spectrum $\rho(\omega)$, interpolated from the measurements by Haywood and Page (Page and Haywood, 1968) at 294 K and 624 K to represent the librational (hindered rotation) mode. The spectra for 294 K and 624 K are plotted in Fig. 3.1. The spectrum for any intermediate temperatures is a linear interpolation of these values.
- Two discrete oscillators at 205 meV and 436 meV to represent the internal vibrations of the molecule. After computing the weights of the translational and rotational models, the 205 meV takes 1/3 of the remaining weight and represents the scissoring mode, and the 432 meV takes 2/3 of the remaining weight and represents the degenerated stretching mode (symmetric and asymmetric stretching).

These parameters are assumed to be linearly interpolable in the 293–624 K range, and they were used by MacFarlane to evaluate the scattering law at 293.6 K, 350 K, 400 K, 450 K, 500 K, 550 K, 600 K, 650 K, and 800 K, which are distributed in ENDF-6 format as tsl-HinH2O.endf in ENDF/B VII.0. This scattering law file was used to compute thermal scattering cross sections in ACE format at the same temperatures, distributed with MCNP5 as files lwtr.10t to lwtr.18t for each corresponding temperature.

To compute the temperature dependent *LEAPR* models used in method (3), the translational mass was first interpolated from the values used by Mattes and Keinert (2005), and then was used to compute the translational weight:

$$m_T = \frac{m_{624\mathrm{K}} - m_{294\mathrm{K}}}{624\mathrm{K} - 294\mathrm{K}}(T - 624\mathrm{K}) + m_{294\mathrm{K}} \tag{3.1}$$

$$w_T = 1/m_T \tag{3.2}$$

Then, the continuous spectrum $\rho(\omega)$ was interpolated for the desired temperature:

$$\rho_T(E_i) = \frac{\rho_{624\mathrm{K}}(E_i) - \rho_{294\mathrm{K}}(E_i)}{624\ \mathrm{K} - 294\ \mathrm{K}}(T - 624\ \mathrm{K}) + \rho_{294\mathrm{K}}(E_i) \tag{3.3}$$

Finally, the remaining weight was distributed between two discrete oscillators at 205 meV and 436 meV:

$$w_{205\mathrm{meV}} = \frac{1}{3}(1 - w_T - w_{cont}) \tag{3.4}$$

$$w_{436\mathrm{meV}} = \frac{2}{3}(1 - w_T - w_{cont}) \tag{3.5}$$

where w_{cont} is the integral of the continuous frequency spectrum $\rho_T(E_i)$.

3.2. Calculations

To evaluate the results of the benchmark calculations, a bias determination approach was used, which is defined as a measure of the systematic differences between calculation method results and experimental data (Office of Nuclear Material Safety and Safeguards). The partial biases were calculated for each benchmark case using Eq. (3.6), and they represent the absolute deviation between the calculated and the benchmark k_{eff}. σ_i is shown in Eq. (3.7); it is the related standard deviation calculated from the standard deviations of the MCNP calculation and the one provided by the authors of the benchmark experiments. Eq. (3.7) was derived from the chain rule.

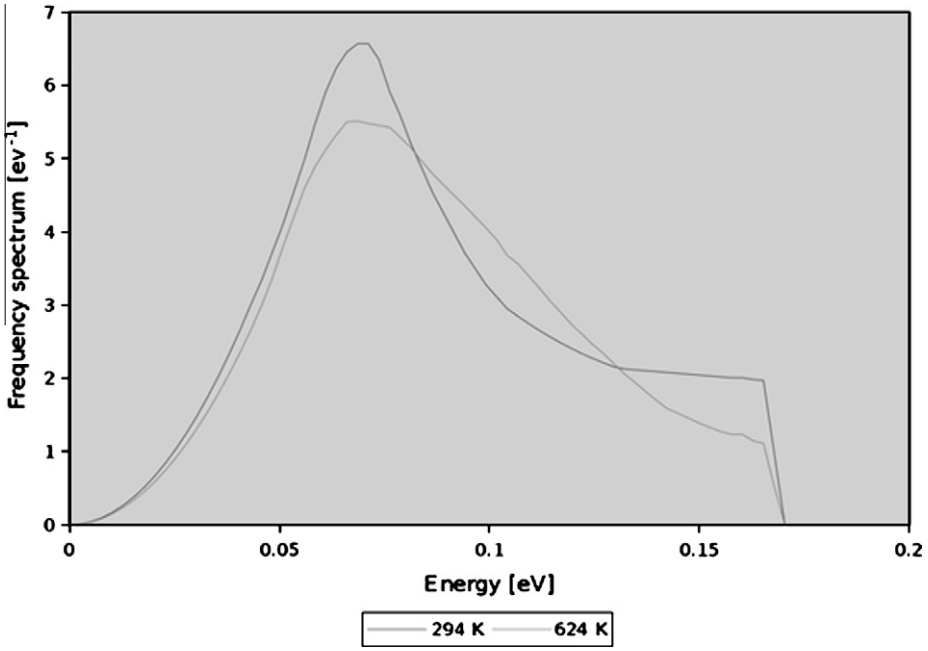

Fig. 3.1. Frequency spectrum at 294 K and 624 (Mattes and Keinert, 2005).

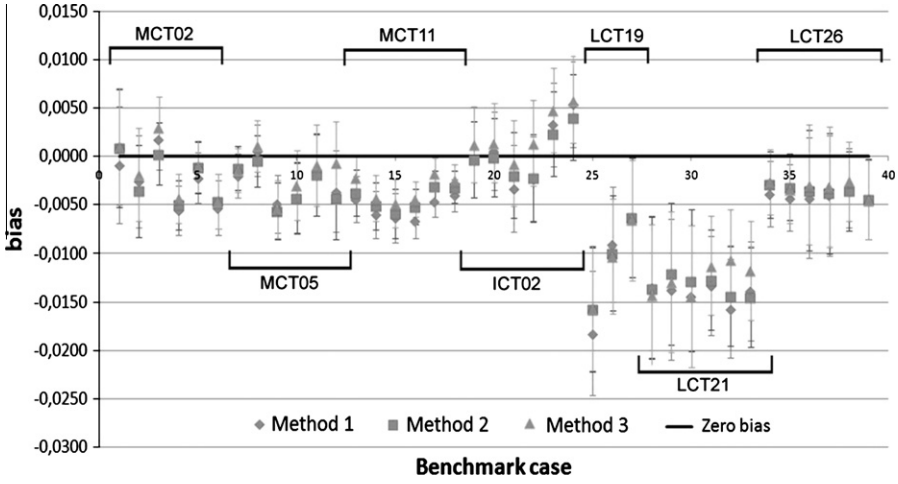

Fig. 4.1. Results of the bias calculations.

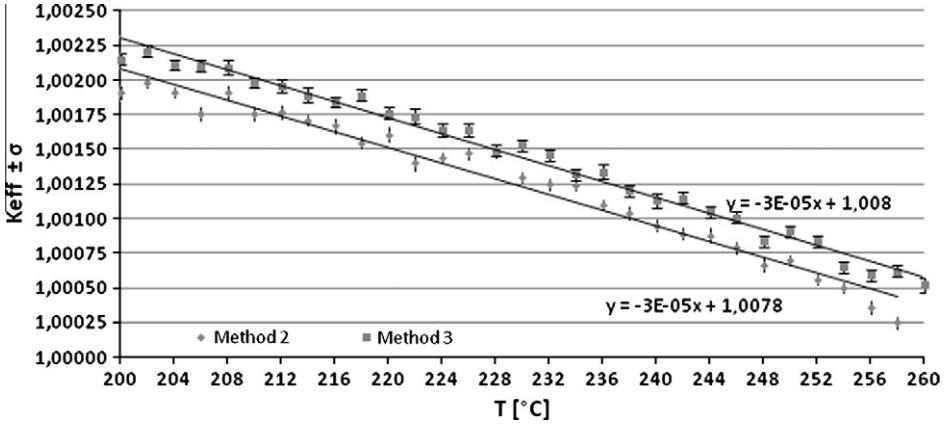

Fig. 4.2. Results of the thermal transient calculation.

$$\text{bias}_i = k_{effi}^{\text{benchmark}} - k_{effi}^{\text{MCNP}} \tag{3.6}$$

$$\sigma_i = \sqrt{(\sigma_i^{\text{benchmark}})^2 + (\sigma_i^{\text{MCNP}})^2} \tag{3.7}$$

The calculation was carried out on a CentOs 6.1 Kernel Linux 2.6.32 x86_64 system across 36 AMD OPTERON 6172 processors. The 1.6 multi-thread version of the MCNP5 code was used with 50,000 neutrons per cycle in 100 inactive and 4000 active cycles.

4. Results

The practical part of this study consists of two types of calculations: the benchmark calculations and the thermal transient calculations. The results of the benchmark calculations are shown in Fig. 4.1. The black center line represents the zero value of the bias which is the value that we would have liked to achieve. The results of the partial biases for every benchmark case and for the three methods are interpreted with their standard deviations.

Since the results of the benchmark calculations for all three methods had been found to be very similar, it was sufficient to perform the transient calculation for the second and the third methods only. The results of the thermal transient calculation shown in Fig. 4.2 are slightly scattered and therefore it was advantageous to use a linear fit of the results. The slope of the curves is the same; the only difference is the slight shift of the tendency of the third methods curve. The average reactivity change caused by this shift was calculated to 21.1 pcm.

5. Conclusion

It can be seen that almost all results of the benchmark calculations, except the cases 14–16 falling within benchmark MCT11 and cases 25–33 falling within benchmarks LCT19 and LCT21, are in very good accordance with the zero bias in the case of all three methods. Although the mentioned cases provided shifted results, these differences were almost the same for all three methods, and since their accuracy was at the same level, we can conclude that all three cases provided results in the same uncertainty range. The comparison of the second and third method in thermal transient calculation showed very good agreement between each other. The tendencies of these curves were almost the same; however, a slight shift of the curve of the third method was observed. Nevertheless, the physical behavior of the system was maintained. Based on these findings it can be concluded that the usability of the third method has been confirmed. All the three methods to obtain temperature-dependent thermal scattering cross sections have been found to be equivalent within the uncertainty of this study and the user can choose the method that best meets his requirements.

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References

Brown, F.B., 2006. The makxsf Code with Doppler Broadening, Los Alamos National Laboratory, Report, LA-UR-06-7002.

Chadwick, M.B. et al., 2006. ENDF/B-VII.0: next generation evaluated nuclear data library for nuclear science and technology. Nuclear Data Sheets vol. 107, 2931–3060.

Herman, M., Trkov, A., 2010. ENDF-6 Formats manual: data formats and procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII. Brookhaven National Laboratory, CSEWG Document ENDF-102, Report BNL-90365-2009 Rev. 1.

International Handbook of Evaluated Criticality Safety Benchmark Experiments, 2007. ECD Nuclear Energy Agency NEA/NSC/DOC(95)03.

Lüley J., et al., 2012. Determination of criticality safety MCNP5 calculation bias by using different libraries of cross section data, Progress in Nuclear Energy, vol. 59. pp. 96–99.

MacFarlane, R.E., 1994. New Thermal Neutron Scattering Files for ENDF/B-VI Release 2, LA-12639-MS (ENDF 356).

MacFarlane, R.E., Kahler, A.C., 2010. Methods for processing ENDF/B-VII with NJOY, Nuclear Data Sheets, vol. 111. Los Alamos National Laboratory Unclassified, Report, LA-RU-10-04652. pp. 2739–2890.

Mattes, M., Keinert, J., 2005. Thermal Neutron Scattering Data for the Moderator Materials H2O, D2O and ZrHx in ENDF-6 Format and as ACE Library for MCNP(X) Codes, INDC(NDS)-0470.

Office of nuclear material safety and safeguards: justification for minimal margin of subcritically for safety, FCSS ISG-10, Rev.0 <http://pbadupws.nrc.gov/docs/ML0616/ML061650370.pdf>. [accessed 15.07.12].

Page, D.I., Haywood, B.C., 1968. The HARWELL Scattering Law Programme: Frequency Distributions of Moderators, AERE-R 5778.

Vrban, B., et al., 2012. MCNP start-up calculation for the first fuel loading of the reactor core of NPP Mochovce-3,4. In: Proceeding of the 21st International Conference Nuclear Energy for New Europe, Ljubljana, No. 708.

X-5 Monte Carlo Team, 2003. MCNP – A general Monte Carlo N-Particle transport code, Version 5, Los Alamos National Laboratory, LA-UR-03-1987 – vol. I. Overview and theory, LA-CP-03-0245 – vol. II. User's guide, LA-CP-03-0284 – vol. III. Developer's guide.