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Cross Section Library Based Discrepancies in MCNP Criticality Calculations

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ABSTRACT

In nuclear engineering several reactor physics problems can be approached using Monte Carlo neutron transport techniques, which usually give reliable results when properly used. The quality of the results is largely determined by the accuracy of the geometry model and the statistical uncertainty of the Monte Carlo calculation.

There is, however, another potential source of error, namely the cross section data used with the Monte Carlo codes. It has been shown in several studies that there may be significant discrepancies between results calculated using cross section libraries based on different evaluated nuclear data files. These discrepancies are well known to the evaluators of nuclear data but less acknowledged by reactor physicists, who often rely on a single cross section library in their calculations.

In this study, discrepancies originating from base nuclear data were investigated in a systematic manner using the MCNP4C code. Calculations on simplified UOX and MOX fuelled LWR lattices were carried out using cross section libraries based on ENDF/B-VI.8, JEFF-3.0, JENDL-3.3, JEF-2.2 and JENDL-3.2 evaluated data files. The neutron spectrum of the system was varied over a wide range by changing the ratio of hydrogen to heavy metal atoms. The essential isotopes underlying the discrepancies were identified and the roles of fission and absorption cross sections of the most important nuclides assessed.

The results confirm that there are large systematic differences up to a few per cent in the multiplication factors of LWR lattices. The discrepancies are strongly dependent on material compositions and neutron spectra, and largely originate from U-238 and the primary fissile isotopes. It is concluded that these discrepancies should be taken into account in all reactor physics calculations, and that reactor physicists should not rely on results based on a single cross section library.

1 INTRODUCTION

The MCNP [1] Monte Carlo particle transport code is used for various neutron transport problems in nuclear engineering. Reactor physics, and especially criticality calculation is one of the most common applications. In fact, when compared to experimental results, criticality calculation has shown to be one of the most succesful applications of Monte Carlo neutron transport techniques.

The MCNP code uses continuous energy cross section data based on the standard Evaluated Nuclear Data Files. In order to be accessed by MCNP, the data is converted from the ENDF-format into point-wise libraries (ACE-format) typically using the NJOY [2] nuclear data processing system. Standard cross section libraries based on the American

ENDF/B-VI are provided along with the code itself. In addition there are several libraries based on different evaluated data files available through public channels, such as the OECD/NEA Data Bank.

It is generally known among scientists working in the data evaluation projects, that there are significant discrepancies between the major evaluated nuclear data files (ENDF/B, JEFF and JENDL), even for the most common isotopes, such as U-235 and U-238. Discrepancies in the cross section data are inevitably reflected to the applications using it. This issue is not allways acknowledged by nuclear engineers and reactor physicists, who often rely on a single (default) cross section library in their calculations.

It has been shown in several studies that discrepancies in base nuclear data may result to differences in the order of 1% in k_{eff}. Such differences are observed using MCNP [3-6] and orther Monte Carlo neutron transport codes [7], and should be compared to the statistical uncertainty of the criticality calculation (typically less than 0.1%). The differences are not always self-explanatory, and seem to depend on several factors, such as material composition (UOX vs. MOX fuel) and flux spectrum (fast vs. thermal).

In this study, library-based discrepancies in the cross sections of fuel isotopes are investigated in a systematic manner. MCNP4C criticality calculations were carried out using ENDF/B-VI, JEFF-3.0, JENDL-3.3, JEF-2.2 and JENDL-3.2 based cross section libraries in geometries representing UOX and MOX fuelled LWR arrays with varying neutron moderation. The complexity of the system is reduced to minimum using infinite "sandwich" slab arrays to model the heterogenious reactor core. The sources of the observed discrepancies are studied, and the essential isotopes and cross sections identified. In this paper, only the UOX case is discussed in detail. The theory can be directly generalised to the MOX fuel cases, and the results of the MOX study are briefly reviewed in section 4.1.

2 GEOMETRY AND NUCLEAR DATA

The geometry consists of a repeated structure of infinite fuel slabs surrounded by light water moderator. Such model was chosen because it is the simplest representation of a heterogeneous reactor lattice. For the purpose of this study this model does not significantly differ from other simplified models, such as the infinite pin-cell array. The thickness of the fuel slab is fixed to 5 mm, and the level of neutron moderation adjusted by varying the slab spacing. Fuel-to-moderator ratio is used as a measure of spectrum hardness. In this study, this ratio is defined as the ratio of heavy metal to hydrogen atoms. For a typical LWR lattice this value varies from about 0.24 (a cold reactor at normal pressure) to about 1.65 (a BWR core with 80% void fraction).

Three types of fuel materials are studied – a simplified low-enriched uranium oxide fuel (UOX) and two types of mixed oxide fuels (MOX) with different plutonium compositions (reactor- and weapons-grade plutonium). All cladding and structural materials were omitted since their contribution to the discrepancies was assumed to be insignificant compared to the fuel materials. The simplified UOX fuel consists of uranium and O-16 in a 1:2 atomic ratio, the uranium being enriched to 4.0 at-% with respect to U-235. The gram density of the oxide is 10.970 g/cm^3. The moderator is pure light water at 1.000 g/cm^3 density. All materials are at 300 K temperature.

The ACE format cross section libraries used by MCNP were generated with NJOY-99 nuclear data processing system. The base nuclear data for the fuel was taken from 5 commonly used evaluated data files: ENDF/B-VI.8, JEFF-3.0, JENDL-3.3, JEF-2.2 and JENDL-3.2. All libraries were generated using similar parameters in the NJOY input files. The cross sections of the moderator isotopes as well as the S(α,β) thermal scattering data for light water were taken from ENDF/B-VI.8 in all cases.

3 TOOLS AND METHODS

The fuel-to-moderator ratio was varied from 0.02 to 100 spanning the neutron spectrum from well over-moderated thermal spectrum to practically unmoderated spectrum dominated by the energy distribution of fission neutrons. All calculations were carried out in the criticality source (KCODE) mode of MCNP, which automatically gives an estimate for the multiplication factor of the system.

The calculated k_∞ for UOX fuel varied from about 0.7 to 1.5 (from 1.0 to 1.4 in the LWR regime of the spectrum). It should be pointed out that in order to produce physically reasonable results, the system should be sufficiently close to criticality. If this is not the case, the simulated flux spectrum is distorted, and the actual flux is either exponentially growing in time ($k_\infty > 1$), or dominated by the intrinsic spontaneous fission source ($k_\infty < 1$). Since the purpose of this study was merely to compare different cross section libraries in similar reactivity conditions, this restriction was not taken too seriously.

The library comparison calculation consists of three phases. At first, full cross section library comparison was carried out in order to estimate the total magnitude of differences resulting from discrepancies in the base nuclear data. Infinite multiplication factors as a function of fuel-to-moderator ratio were calculated for each library. Results based on ENDF/B-VI.8 are taken as the reference case.

The second phase involved replacement calculations using the ENDF/B-VI.8 library with one isotope at a time taken from the library under study. Comparison to reference results reveals which isotopes are the most significant sources of discrepancy.

In the third phase all significant isotopes are taken for more detailed analysis. Group constants, such as spectrum-averaged cross sections $\overline{\Sigma}_i$ of isotope i were calculated using the standard cell flux (f4) tallies of MCNP. These tallies give estimates for the corresponding reaction rates R_i integrated over space, time and energy. From these results, the group-averaged cross sections can be calculated simply by dividing with the corresponding group flux Φ_i:

$$\overline{\Sigma}_i = \frac{R_i}{\Phi_i} = \frac{\int_t \int_V \int_E \Sigma_i(E)\phi(t,\vec{r},E)\,dE\,dV\,dt}{\int_t \int_V \int_E \phi(t,\vec{r},E)\,dE\,dV\,dt}. \tag{1}$$

The average number of fission neutrons $\overline{\nu}_i$ can be calculated in a similar manner, by dividing the total fission neutron production rate with the corresponding fission rate. In this study, all parameters are treated as time-independent one-group constants and averaged over the entire flux spectrum and the volume of the material region.

Since the geometry is infinite in all directions, there is no neutron leakage, and the core multiplication is essentially determined by the total rates of fission and absorption. The infinite multiplication factor can be written as

$$k_\infty \approx \frac{\Phi_f V_f \sum_i \overline{\nu}_i \overline{\Sigma}_{fi}}{\Phi_f V_f \sum_i \left(\overline{\Sigma}_{fi} + \overline{\Sigma}_{ci}\right) + \Phi_m V_m \overline{\Sigma}_{am}}, \tag{2}$$

where $\overline{\Sigma}_f$ and $\overline{\Sigma}_c$ are the spectrum-averaged macroscopic fission and total capture cross sections and the summations extend to all isotopes in the fuel. All isotopes in the moderator are included as a single absorption cross section $\overline{\Sigma}_{am}$. Volumes and one-group fluxes of fuel and moderator region are denoted as V_f and V_m, and Φ_f and Φ_m, respectively.

The total capture cross section includes all reactions in which the incident neutron is lost without generating new neutrons. For heavy metal isotopes (and obviously hydrogen) this implies almost exclusively the (n,γ) reaction, since the energy thresholds of the other (n,0n) reactions are high, and fission becomes the predominant interaction at such high energies.

The microscopic absorption cross section of O-16 is relatively low. The large content of this isotope, however, makes this contribution noticeable (0.5-1.0% of neutron absorption in fuel). The absorption mainly consists of (n,α), which has an energy threshold in the order of few MeV. For this reason O-16 is essentially an absorber of fast neutrons. The rest of the neutron absorption reactions constitute less than 1% of total absorption in fuel O-16.

Equation (2) gives a good description of neutron multiplication in the system. When compared to the MCNP criticality calculation, the multiplication factor is underestimated by some 0.5% or less. This difference results mainly from the absence of (n,xn)-reactions in equation (2). If (n,2n) reactions in uranium are included, the differences are narrowed to approximately 0.1%, which is about the same order in magnitude as the statistical uncertainty. The contribution of (n,3n) reactions is negligible, as is all neutron multiplication in O-16.

The definition (2) of the multiplication factor can be used for estimating the effects of small deviations in single group constants. If parameter $\bar{x}$ is deviated from its initial value $\bar{x}_0$ by some small amount $\Delta\bar{x}$, the corresponding (linear) change Δk_∞ in k_∞ is given by

$$\Delta k_\infty = \Delta\bar{x}\frac{\partial k_\infty}{\partial\bar{x}}\bigg|_{\bar{x}_0} . \tag{3}$$

It should be pointed out that the use of this first order series expansion only gives a formal and rather simplified estimate of the actual difference. The partial derivatives are evaluated in the reference spectrum and the differences in the group constants taken as small deviations from the reference values. In reality, small difference in any cross section also implicates small deviation in the flux spectrum, which in turn implicates small differences in all group constants in the system. For the purpose of this study it is assumed, however, that these spectral couplings are sufficiently weak to justify the independent treatment of the parameters and the use of equation (3).

In the third phase of the comparison the spectrum-averaged one-group constants of all essential isotopes were calculated. The contribution of each parameter discrepancy (relative to ENDF/B-VI.8) was estimated using equation (3), and the predicted total differences in the multiplication factors compared to the observed results (phase I).

4 RESULTS

Figure 1 shows the differences in k_∞ compared to the reference results calculated using ENDF/B-VI.8 data. In the LWR regime of the spectrum both older libraries (JEF-2.2 and JENDL-3.2) give multiplication factors some 0.5 to 1.0% higher than the corresponding reference values. For the recently published JEFF-3.0 and JENDL-3.3 the consistency is better, although the discrepancies grow significantly towards the fast end of the spectrum.

The isotope replacement calculations show that the differences in k_∞ originate almost exclusively from U-235 and U-238. The results of U-235 replacement are plotted in Figure 2. It can be seen that the increased reactivity for JEF-2.2 and JENDL-3.2 in the LWR regime arise from U-235. Similar calculations on U-238 show that this isotope is responsible of the decreasing k_∞ towards the fast end of the spectrum for all libraries. The replacement of fuel oxygen gives small increase for the JENDL-libraries and slight decrease for JEF-2.2 and JEFF-3.0. These differences, however, are insignificant compared to the uranium isotopes.

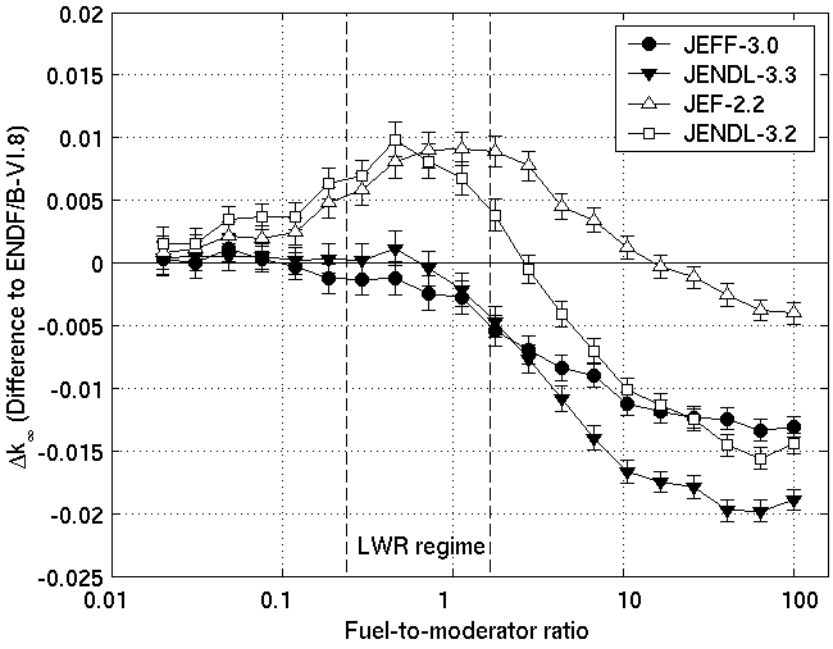

Figure 1**:** Results of phase I calculations – the library-based differences in k_∞ as a function of fuel-to-moderator ratio. The error bars show 95% confidence intervals.

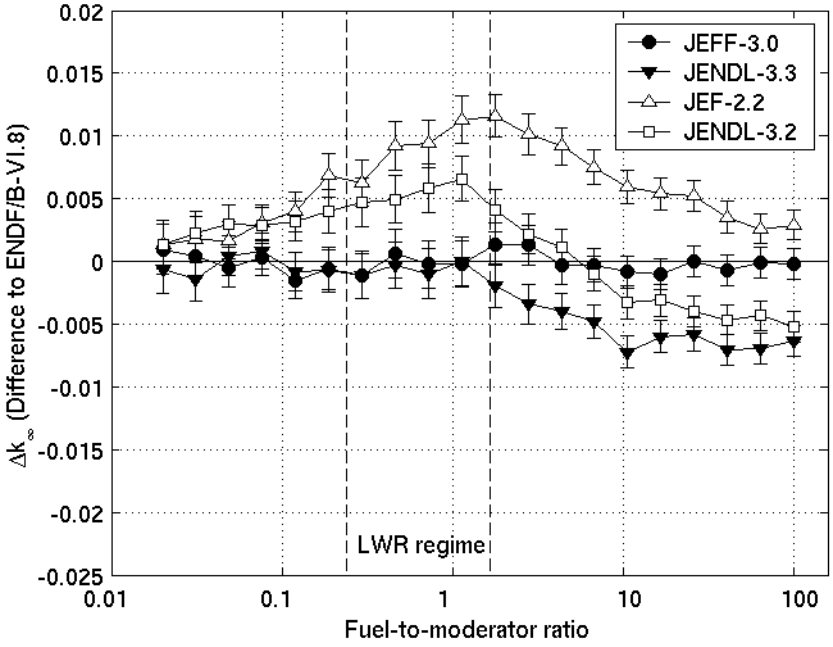

Figure 2**:** Results of phase II calculations – differences in k_∞ when only the cross sections of U-235 are taken from the library under study.

In the third phase of the study, all group constants were calculated for all libraries. The differences in $\bar{\nu}$ are small, less than 0.5% in all cases. The fission and absorption cross sections of U-235 and U-238, on the other hand, differ up to several per cent from the

reference results. The discrepancies in the absorption cross section of O-16 are even greater. The JEF-2.2 and JEFF-3.0 libraries give values 10-15% higher and the two JENDL libraries 25-35% lower compared to ENDF/B-VI.8.

When the differences in the group constants are combined with the corresponding partial derivatives according to equation (3), the contribution of each parameter can be assessed. It was discovered that there are several parameters causing considerable differences in both directions. The most significant contributors are the fission cross section of U-235 and the absorption cross section of U-238. The contributions of fuel oxygen are relatively minute (in the order of 0.1% or less) despite the large differences in the group constants.

Figure 3 illustrates the contributions of the most significant individual discrepancies between JEF-2.2 and ENDF/B-VI.8. It can be seen that the total contribution is very close to that in Figure 1. This, in fact, is true for the other three libraries as well, which certifies that equations (2) and (3) can be used for estimating the impact of discrepancies in single group constants. The overall consistency between two libraries seems to depend not so much on the magnitude of differences in individual cross sections, but rather on how well these differences cancel out each other.

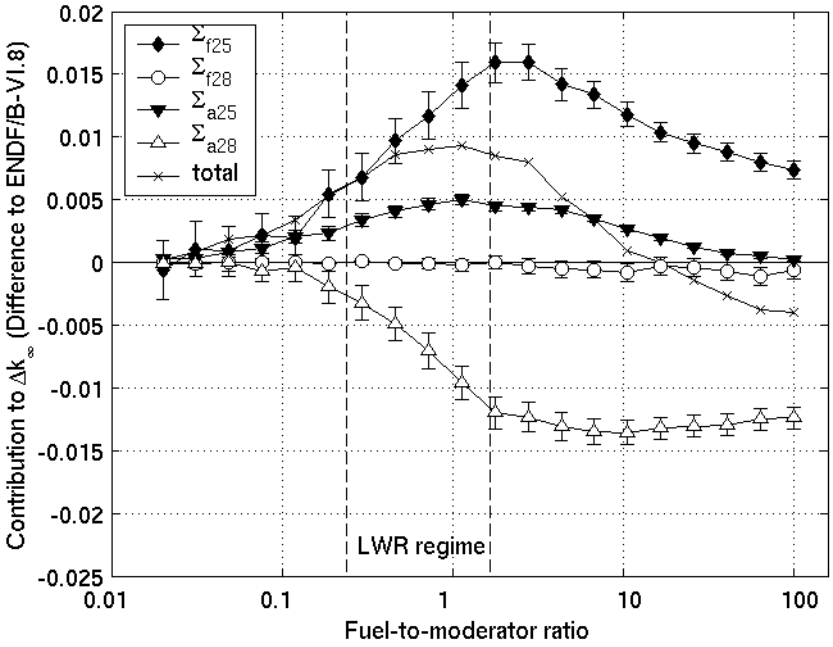

Figure 3**:** Results of phase III calculations – the contributions of individual group constant discrepancies on Δk_∞. Comparison between JEF-2.2 and ENDF/B-VI.8 data.

The results of phase III are consistent with the results of the previous phases. It should, be noted, however, that since equation (2) only deals with the total rates of neutron generation and absorption, all spectral dependencies remain "hidden" in the integrals of equation (1). In addition to the spectral couplings between reaction rates there are other effects, such as discrepancies in scattering cross sections, that can not be assessed in detail using the introduced methods. These hidden contributions can be very significant in some cases. Further, this study covers only the discrepancies in the cross sections of fuel isotopes, and therefore reveals nothing about similar differences in the moderator.

4.1 MOX Fuels

Some of the introduced results can be generalised to the two MOX fuels that were also studied. Compared to the UOX case, the consistency in k_∞ is slightly better for JEF-2.2 and JENDL-3.2 in the LWR regime. In the fast end of the spectrum, all four libraries give significantly lower values compared to ENDF/B-VI.8. The differences between the two MOX fuel types are relatively small.

As would be expected, the discrepancies originating from U-238 are almost identical to the UOX case. Of the plutonium isotopes, Pu-239 has clearly the most significant impact on the results. The contributions of other plutonium isotopes are far less significant. Despite the small contributions, there are some significant discrepancies up to 10% in the group constants of the minor plutonium isotopes.

4.2 Validity in general LWR calculations

The calculations using different cross section libraries reveal several discrepancies originating from the base nuclear data. Before these results can be extrapolated to general LWR lattices, some sensitivity studies have to be carried out on the model in order to demonstrate that the observed discrepancies are not too seriously affected by small variations in the basic parameters.

The sensitivity study was done for the UOX slab array using the same cross section libraries as in the previous calculations. The parameters of the slab were varied within ranges typical for different types of light water reactors. The following parameters were varied: fuel enrichment (2.0, 3.0, 4.0 and 5.0 at-% U-235), fuel temperature (300, 600, 900 and 1200 K), slab thickness (1.25, 2.5, 5.0, 10.0 and 20.0 mm), and moderator boron concentration (0, 650 and 1300 ppm boron). One set of calculations was carried out using square-lattice pin-cell models with similar material compositions and fuel-to-moderator ratios.

Increasing the fuel enrichment enhances the discrepancies originating from U-235. As it turned out, this isotope is the dominant source of discrepancy for JEF-2.2 and JENDL-3.2 in typical LWR spectra. For the enrichments of common LWR fuels, this variation is not very significant.

For heavy elements, the Doppler-broadening of resonance peaks is the most significant difference between cross section libraries generated from the same base data at different temperatures. For the given temperatures this comparison showed that there are neither systematic nor particularly significant changes in the observed discrepancies.

Varying the slab thickness changes the level of heterogeneity of the system. This effect should be most significant in the thermal end of the spectrum, where the neutron mean free path is short enough to distinguish the details of the geometry. Within the given limits, this variation has no effect on the library-based differences. Changing the geometry from the one-dimensional slab lattice to the two-dimensional pin-cell lattice had no effect on the results.

Chemical shim lowers the absolute value of the multiplication factor when fuel-to-moderator ratio is low. Boron-10 is a $1/v$-absorber, so that increasing the boron concentration also has a hardening effect on the neutron spectrum. With the given concentrations, this seems to have no effect on the results.

5 SUMMARY AND CONCLUSIONS

Cross section library based discrepancies in MCNP criticality calculations were studied in a systematic manner. The NJOY-99 nuclear data processing system was used for generating cross section libraries from ENDF/B-VI.8, JEFF-3.0, JENDL-3.3, JEF-2.2 and JENDL-3.2 evaluated nuclear data files. A large number of MCNP4C criticality calculations

were carried out using different cross section libraries in similar reactivity conditions. Simplified infinite slab array models were used to represent heterogeneous UOX and MOX fuelled LWR cores. Fuel-to-moderator ratios were varied within a wide range by adjusting the slab spacing.

The observed differences were studied in detail. The essential nuclides were identified by repeating the reference calculations (ENDF/B-VI.8) with one isotope at a time taken from the library under study. The deviations in spectrum-averaged fission and absorption cross sectios were used for estimating the corresponding contributions to the discrepancies in k_∞.

On the basis of the results, several conclusions can be made. There are some large discrepancies up to nearly 2% in the multiplication factors of UOX and MOX fuelled LWR lattices calculated using cross section libraries of different origin. The discrepancies are strongly case-dependent, and related to the hardness of the neutron spectrum and the isotopic composition of the fuel. Moderator isotopes were not included in the comparison.

The origin of the reactivity differences can be traced to the cross sections of individual isotopes. The most significant contributors are the absorption cross section of U-238 and the fission cross section of the primary fissile isotope, U-235 or Pu-239. The disadvantage of the analysis using spectrum averaged group constants is that the detailed structure of the flux spectrum is lost, and there is no information on scattering reactions or spectral couplings between the reaction rates.

Rather than being particularly dependent on the magnitudes of individual differences between two cross section libraries, the resulting discrepancies depend on how well these differences are averaged out. This, on the other hand, implies that good consistency in criticality calculation is not necessarily an evidence of good consistency in the underlying cross section data.

These issues should be taken into account in all reactor physics calculations, and results based on a single cross section library used with caution.

REFERENCES

[1] J. F. Briesmeister, Editor, “MCNP – A General Monte Carlo N-Particle Transport Code, Version 4C”, Los Alamos National Laboratory Report LA-13709-M, 2000.

[2] R. E. MacFarlane, D. W. Muir, “The NJOY Nuclear Data Processing System Version 91”, Los Alamos National Laboratory Report LA-12740-M, 1994.

[3] J-D. Kim, C-S. Gil, “Validation of ENDF/B-VI.2, JEF-2.2 and JENDL-3.2 Through MCNP Analysis of BWR-simulated Critical Experiments”, *Ann. Nucl. Energy*, **24**, 1997, pp. 197-204.

[4] O. P. Joneja et al., “Validation of an MCNP4B whole-reactor model for LWR-PROTEUS using ENDF/B-V, ENDF/B-VI and JEF-2.2 cross-section libraries”, *Ann. Nucl. Energy*, **28**, 2001, pp. 701-713.

[5] W. Bernnat et al., “Validation of Nuclear Data Libraries for Reactor Safety and Design Calculations”, *J. Nucl. Sci. Technol.*, **Supp. 2**, 2002, pp. 884-887.

[6] S. C. van der Marck, A. Hogenbirk, “The new releases JEFF-3.0, ENDF/B-VI.8 and JENDL-3.3”, JEF/DOC-955, OECD/NEA, 2003.

[7] H. Takano et al., “Validation of JENDL-3.3 by Criticality Benchmark Testing”, *J. Nucl. Sci. Technol.*, **Supp. 2**, 2002, pp. 847-851.