ENDF/B-VIII.0-BASED CROSS SECTION LIBRARIES

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Abstract

Cross-section libraries, for 556 isotopes at 11 temperatures (300K, 400K, 500K, 600K, 700K, 800K, 900K, 1000K, 1200K, 1500K and 1800K) have been produced applying the NJOY21 processing code at the ENDF/B-VIII.0 evaluated data files. The aim of this study is the ″validation″ of the above cross-section libraries by benchmarking them (criticality studies) on ″by design″ critical assemblies, as well as on more complex fast systems, and ″point-wise″ comparing the outcome with equivalent results obtained using LANL cross-section libraries produced by the NJOY16 processing code. While the computations have been performed for a larger set of temperatures, a ″point-wise″ comparison is feasible among the sets of cross-section libraries at (300K, 600K, 900K and 1200K), showing a very good agreement on integral and differential neutron parameters.

Keywords: *Nuclear Data, Cross Sections, Criticality, Monte Carlo, Benchmarking*

Background

Nuclear data play an essential role in reactor physics, ensuring safe, reliable and cost effective nuclear systems. Among them, the cross sections are of prime importance for solving the neutrons transport problem, i.e.: critical mass (k_{eff}), safety parameters (e.g. *β_eff*, *Doppler coefficient, Coolant Void Effect*, etc.) along with other neutron parameters evaluations. The accuracy and reliability of the results have direct impact on core design and safety. Hence, there is a need for updated nuclear data that include the latest experimental and theoretical improvements.

Results accuracy and reliability following ″new″ nuclear data and the corresponding cross sections utilization, are affected by the nuclear data processing step, i.e. the assumptions made in the data processing codes which define (and sometime could limit) the accuracy of the results of the reactor physics codes.

Therefore, the need arises for a supplementary step concerning the qualification of the produced nuclear data and cross sections. Usually, this last step refers to benchmarking activities that need to be as accurate as possible.

Introduction

In February 2018, the Cross Section Evaluation Working Group (CSEWG) announced the release of the ENDF/B-VIII.0 evaluated nuclear reaction data library [1], which: "... fully incorporates the new Neutron Data Standards, includes improved thermal neutron scattering data and uses new evaluated data from the Coordinated International Evaluation Library Organisation (CIELO) pilot project for neutron reactions on ^{1}H, ^{16}O, ^{56}Fe, ^{235}U and ^{239}Pu. The evaluations benefit from recent experimental data obtained in the U.S. and Europe, and improvements in theory and simulation..." [2]. The ENDF/B-VIII.0 evaluated nuclear reaction data library refers to a set of 556 isotopes. During the same period (June 2018), the LANL Team announced the release of the Lib80x-Library based on the ENDF/B-VIII.0 evaluated nuclear reaction data, [3], containing ACE files for continuous-energy incident neutrons, processed by the NJOY16 code [4] at 293.6K, 600K, 900K, 1200K, 0.1K and 250K.

For all 556 isotopes, we have produced ACE-formatted cross section libraries, based on the ENDF/B-VIII.0 evaluated nuclear reaction data library, processed by the NJOY21 code, [5] at 300K, 400K, 500K, 600K, 700K, 800k, 900K, 1000K, 1200K, 1500K and 1800K, covering the temperature range of almost any reactor core design, using the corrected $_{5}B^{10}$ evaluated data file [6].

In the frame of the free gas model (i.e. material in thermal equilibrium described by the Maxwell-Boltzmann distribution), for all isotopes and considered temperatures, the following modules of the NJOY21 code have been involved:

- **moder**: to extract/convert neutron evaluated data;
- **reconr**: to reconstruct cross sections for neutrons;
- **broadr**: Doppler broadening of cross sections;
- **heatr**: to add heating kerma and damage energy;
- **gaspr**: to add gas production;
- **thermr**: to add thermal scattering data;
- **purr**: to process unresolved resonance range (if any);
- **acer**: to prepare and check ACE files;
- **groupr**: to prepare multi-group data for neutrons;
- **matxs**: to produce MATXS cross section files for deterministic transport codes.

Therefore, the question arises as to whether the cross-section libraries produced using the NJOY21 code are equivalent to those produced using the NJOY16 code. To this end, the aforementioned benchmarking should refer to the data (cross section libraries) instead of the neutron transport codes as it constitutes a systematic comparison of physical observables, (integral and differential neutron parameters) of the investigated system that has been performed by the Monte Carlo code MCNP5 [7].

While the correct evaluation of the multiplication factor (k_{eff}) is a necessary condition, it is not a sufficient condition to guarantee the data accuracy. Therefore, the benchmarking activity will be performed in two levels:
- comparison of integral and a few differential parameters based on three fast critical assemblies [8];
- comparison of integral and a few reactivity coefficients based on fast systems:
  - sub-critical (Th, U, Pu) Ox / Pb-cooled [9];
  - critical (U, Pu) C / Na-cooled [10].

The choice of fast systems relies on the fact that all fission systems are driven by a source of fast fission neutrons emitted by nucleus fissions. Such a choice doesn't exclude the extension of this type of benchmarking to intermediate and/or thermal spectrum systems.

The three fast assemblies constitute three homogeneous, spherical systems, each one containing primarily one of the following three fuels:
- Godiva (U235): a bare highly enriched uranium sphere of radius 8.7407cm and mass 52.42 kg of U, (average density 18.74/g/cm^3), at: 93.71wt% U^{235}, 1.02 wt%U^{234} and 5.27wt% U^{238}, [11];
- Jezebel (Pu239): a bare sphere of Pu-Ga alloy, 98.98wt%, of radius 6.38493 cm and mass 17.02 kg (average density of 15.61 g/cm^3) at: 95.2 at% Pu^{239}, 4.5 at% Pu^{240} and 0.3 at% Pu^{241}, [12];
- Jezebel23 (U233): a highly enriched uranium-233 sphere of radius 5.0444 cm reflected by natural uranium, of thickness 2.3012 ± 1% cm and masses of:
  - 10.012 kg U^{233} with density 18.621 g/cm^3 at: 98.2 wt% U^{233}, 1.1 wt% U^{234} and 0.7 wt% U^{238},
  - 21.239 kg Unat with density 18.92 g/cm^3 at: 0.72 wt% U^{235} and 99.28 wt% U^{238}, [13].

The fast systems are considered at room temperature (293.6 K), all models being designed to produce k_{eff} close to 1.0.

Concerning the core fast systems, Fig. 1 shows the two core configurations for which details on materials, geometry, operating conditions and neutron performances are given in [9, 10]. Figs. 2a and 2b display the spectral behaviour of the average neutron flux in fuel zones, providing an overview of the neutron differences among the two systems.

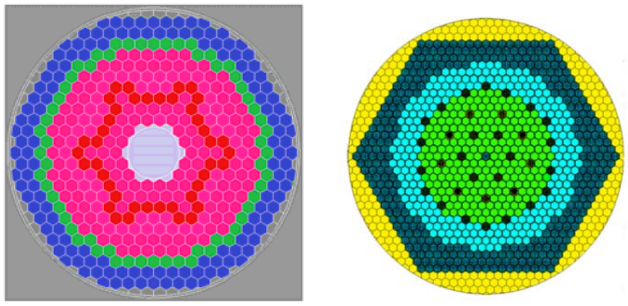


Fig. 1 Sub-critical (Th, U, Pu)Ox ADS/Pb-cooled and Critical (U, Pu)C ESFR/Na-cooled layouts

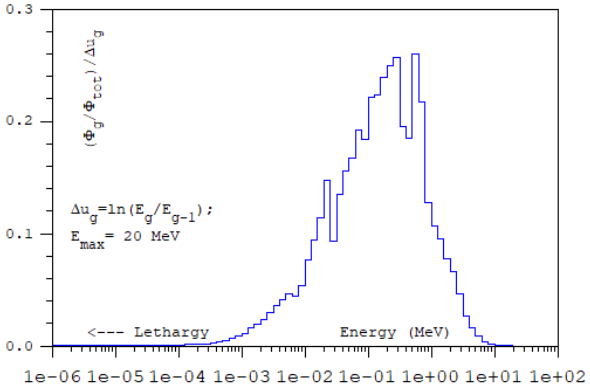


Fig. 2a. Average neutron flux spectrum in (Th, U, Pu)Ox ADS/Pb-cooled fuel zones

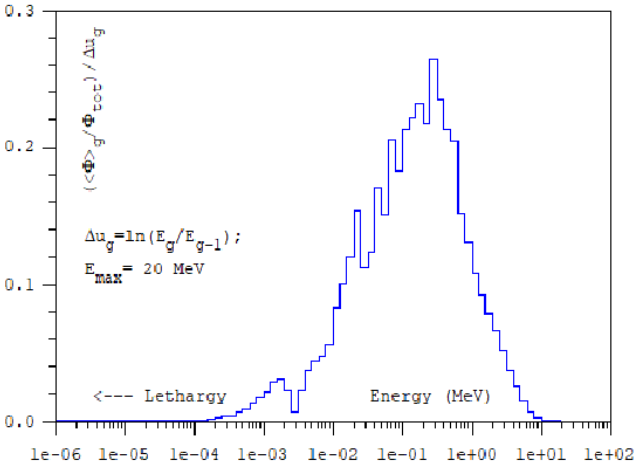


Fig. 2b. Average neutron flux spectrum in (U, Pu)C ESFR/Na cooled fuel zones

Methodology

The aim is to verify, by direct comparison of neutron parameters, whether using cross-sections produced by the NJOY21 code reproduce, with a good accuracy, the same neutron results obtained using cross-sections produced by the NJOY16 code, while both have been applied on the same evaluated data files of ENDF/B-VIII.0.

Replicating the same results means that using cross sections produced by the above two processing codes, lead to "indistinguishable" results, i.e.:

$$\text{Results (xs NJOY21)} \cong \text{Results (xs NJOY16)}$$

Since the considered homogeneous models are designed with a criticality target value of 1.0 ± 0.1% in k_{eff}, the statistical uncertainty should be as much as possible lower than 0.001 in order to:

- satisfy, for instance, the condition:

$$k_{eff}\,(\text{NJOY21}) \cong k_{eff}\,(\text{NJOY16})$$

as well as similar conditions for other neutron parameters,

- no other significant additional uncertainties have been introduced, in the neutron parameters evaluations.

Since the statistical uncertainty is proportional to $1/\sqrt{N}$, where N is the neutron population, for statistical uncertainties of a few pcm (i.e.: ~ 1E-5) the neutrons population should be in the order of a billion neutrons, which is feasible for very simple physical configurations. Such an option would be very costly in CPU time for complex systems like the adopted critical and sub-critical cores. However, a dozen of millions of neutron histories was considered ensuring a statistical uncertainty of a dozen pcm.

Since:

$$\Delta k_{eff} = k_{eff}(NJOY21) - k_{eff}(NJOY16) \pm \sigma$$

$$\sigma^2 = (\sigma^2(NJOY21) + \sigma^2(NJOY16))$$

with estimated 68%, 95% and 99% Δk_{eff} confidence intervals:

$$\Delta k_{eff} \pm \sigma,\ \Delta k_{eff} \pm 2\sigma,\ \Delta k_{eff} \pm 3\sigma$$

and $\sigma \approx$ 1E-5, satisfying the condition:

$$\Delta k_{eff} < 2\sigma \text{ (or } 3\sigma)$$

"indistinguishable" results are assured.

Finally, the MCNP computer code would be useful to verify that analog-capture and implicit-capture results are "indistinguishable" among themselves.

Critical Assembly Results

For all the critical assemblies, the steady state criticality studies have been performed with the MCNP5 code, assuming 200,000 neutron histories per batch, for a total of 5050 active batches, skipping 50 cycles (=10E+6 neutrons) before storing tallies results, for a total of 1 billion "active" neutron histories. Moreover, neutrons from source or collision with $E_n > E_{max}$ =20 MeV are re-sampled, while neutron cross sections outside the range [0 – 20] MeV are expunged. The collected results refer to the neutron integral parameters, as well as a few differential parameters.

First main result, which is common in all configurations studied, is related to the obtained statistical uncertainty, which is significantly lower than potential uncertainties related to other factors. Due to the very low uncertainty value, i.e. the 1E-5 order, it is reasonable to assume that:

$$\text{Result} = \langle\text{Result}\rangle \pm \text{stat. uncertainty} \approx \langle\text{Result}\rangle$$

for every investigated critical assembly.

Tables 1a - 1d display the analog-criticality results and their statistical uncertainties, for all the critical assemblies at four temperatures, as well as the reactivity variation between the NJOY16 and NJOY21 criticality results.

Table. 1a. Steady state criticality results by MCNP5 1.6 at 5050 batches of 2E5n-histories/batch (skipped 50 batches)
T = 300 K

k_{eff} (T=300 K) *	Godiva	Jezebel	Jezebel23
NJOY16	0.99999± 2E-5	0.99979±2E-5	0.99971± 2E-5
NJOY21	1.00006±2E-5	0.99978±2E-5	0.99972± 2E-5
Δk_{eff}	(7±2.8) 1E -5	(-1±2.8) 1E-5	(1±2.8) 1E -5
$\lvert\Delta k_{eff}\rvert < 2\sigma$	no #	yes	yes

* T = 293.6K for NJOY16 results; # $|\Delta k_{eff}| < 3\sigma$

Table 1b. Steady state criticality results by MCNP5 1.6 at 5050 batches of 2E5n-histories/batch (skipped 50 batches)
T = 600 K

k_{eff} (T=600K)	Godiva	Jezebel	Jezebel23
NJOY16	1.00005±2E-5	0.99984±2E-5	0.99979±2E-5
NJOY21	1.00003±2E-5	0.99982± 2E-5	0.99978±2E-5
Δk_{eff}	(-2±2.8) 1E-5	(-2±2.8) 1E-5	(-1±2.8) 1E-5
$\lvert\Delta k_{eff}\rvert < 2\sigma$	yes	yes	yes

Table 1c. Steady state criticality results by MCNP5 1.6 at 5050 batches of 2E5n-histories/batch (skipped 50 batches)
T = 900 K

k_{eff} (T=900K)	Godiva	Jezebel	Jezebel23
NJOY16	1.00006±2E-5	0.99980±2E-5	0.99983±2E-5
NJOY21	1.00003±2E-5	0.99985± 2E-5	0.99983±2E-5
Δk_{eff}	(-3±2.8) 1E-5	(5±2.8) 1E-5	-
$\lvert\Delta k_{eff}\rvert < 2\sigma$	yes	yes	-

Table 1d. Steady state criticality results by MCNP5 1.6 at 5050 batches of 2E5n-histories/batch (skipped 50 batches)
T = 1200 K

k_{eff} (T=1200K)	Godiva	Jezebel	Jezebel23
NJOY16	1.00004±2E-5	0.99980±2E-5	0.99980±2E-5
NJOY21	1.00004±2E-5	0.99982± 2E-5	0.99984±2E-5
Δk_{eff}	-	(2±2.8) 1E-5	(4±2.8) 1E-5
$\lvert\Delta k_{eff}\rvert < 2\sigma$	-	yes	yes

The steady state criticality results, collected in the Tables 1a -1d, satisfy the condition: $|\Delta k_{eff}| < 2\sigma$ or $|\Delta k_{eff}| < 3\sigma$.

In the MCNP stochastic transport code the k_{eff}-result is the least square best estimated average value between the estimated average k_{eff}-values from collisions, absorptions and track length that should behave like the best estimated average k_{eff}-value.

Tables 2a and 2b list the analog-results for estimated average k_{eff}-values from collisions, absorptions and track length. The first one is for all the critical assemblies at 293.6K (and 300K), while the latter lists the findings at 600K, 900K and 1200K with one temperature value per critical assembly.

Table 2a. Steady state criticality results (see Table 1a) for estimated < k_{eff} > of: collisions, absorptions, track length

k_{eff} (T=300 K) *	Godiva	Jezebel	Jezebel23
NJOY16	1.00000± 3E-5 0.99997± 4E-5 1.00001± 3E-5	0.99976±3E-5 0.99984±5E-5 0.99978±2E-5	0.99970±3E-5 0.99975±4E-5 0.99969±3E-5
NJOY21	1.00004±3E-5 1.00010±4E-5 1.00004±3E-5	0.99973±3E-5 0.99978±5E-5 0.99977±3E-5	0.99974±3E-5 0.99968±4E-5 0.99974±3E-5
Δk_{eff}	(4±4.2) 1E-5 (3±5.7) 1E-5 (3±4.2) 1E-5	(-3±4.2) 1E-5 (-6±7.1) 1E-5 (-1±4.2) 1E-5	(4±4.2) 1E-5 (-7±7.1) 1E-5 (5±4.2) 1E-5
$\lvert\Delta k_{eff}\rvert < 2\sigma$	yes	yes	yes

* T = 293.6K for NJOY16 results.

Table 2b. Steady state criticality results (see Tables 1b-1d) for estimated < k_{eff} > of: collisions, absorptions, track length

k_{eff}	Godiva 600 K	Jezebel 900 K	Jezebel23 1200 K
NJOY16	1.00000± 3E-5 1.00007± 4E-5 1.00003± 3E-5	0.99978± 3E-5 0.99973± 5E-5 0.99983± 3E-5	0.99981± 3E-5 0.99986± 4E-5 0.99980± 3E-5
NJOY21	1.00002±3E-5 1.00003±4E-5 1.00002±3E-5	0.99981± 3E-5 0.99980± 5E-5 0.99986± 2E-5	0.99985± 3E-5 0.99984± 4E-5 0.99985± 3E-5
Δk_{eff}	(2±4.2) 1E-5 (-4±5.7) 1E-5 (-1 ±4.2) 1E-5	(3±4.2) 1E-5 (7±7.1) 1E-5 (3±3.6) 1E-5	(4±4.2) 1E-5 (-2±5.7) 1E-5 (5±3.6) 1E-5
$\lvert\Delta k_{eff}\rvert < 2\sigma$	yes	yes	yes

Even in these cases the condition of "indistinguishable" results, i.e.: $|\Delta k_{eff}| < 2\sigma$ or $|\Delta k_{eff}| < 3\sigma$ is found to be met.

It is interesting to note that, between the two sets of cross sections, there are no noticeable differences in many other neutrons parameter, as e.g.:
- average neutron energy causing fission,
- percentages of fissions caused by neutrons,
- average number of neutrons produced per fission,
- the prompt removal lifetime, etc.

For the considered critical assemblies, the percentages of fissions caused by neutrons with $E_n \geq 0.1$MeV exceed 95% of the total number of fissions, a result which justifies the fast critical assembly selection for such a benchmark study.

The same considerations could be applied to neutronic parameters such as fissions, captures, (n, xn) reactions, neutrons production, leakage, etc., where the impact of the different origin of the cross section sets remains essentially within the range of a few pcm. Figs. 3a - 3c display the differential parameters contribution to the total reactivity variation for the transition from NJOY16 to NJOY21, for every temperature considered. The results shown in Figs. 3a-3c confirm the numerical findings from Tables 1a - 1d.

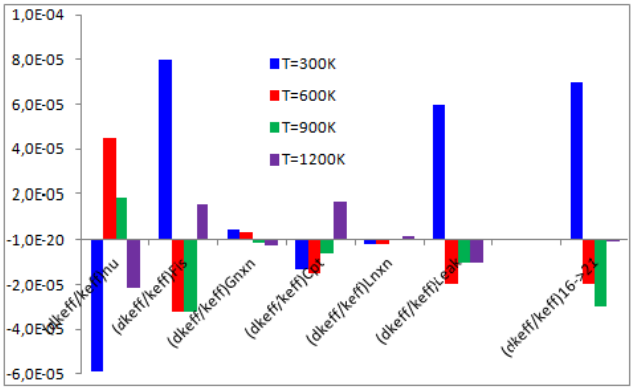


Fig. 3a. The Godiva reactivity variation and its spectral decomposition for the transition NJOY16 to NJOY21

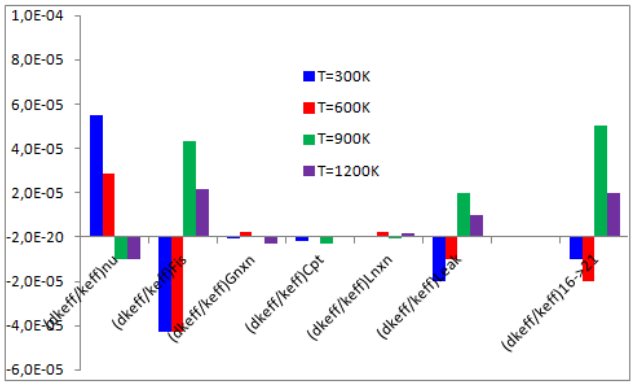


Fig. 3b. The Jezebel reactivity variation and its spectral decomposition for the transition NJOY16 to NJOY21

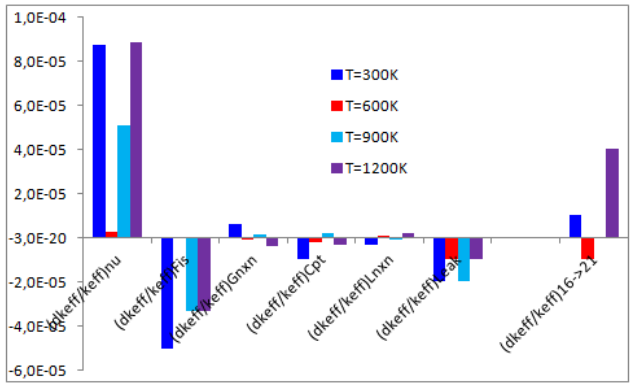


Fig. 3c. The Jezebel23 reactivity variation and its spectral decomposition for the transition NJOY16 to NJOY21

The comparisons between the analog and implicit captures results, at 300K (293.6K) and 1200K for the critical assemblies Godiva and Jezebel, appear to satisfy the condition of "indistinguishable" results. Indeed, assuming 10100 cycles of 1E5 neutrons/cycle and skipping 10 million of neutrons before collecting tallies, it was found for the:

- Godiva assembly:
  - $\Delta k_{eff\ (300K,\ Analog)} = -0.00001 \pm 2.8$ pcm
  - $\Delta k_{eff\ (1200K,\ Analog)} =$ -
  - $\Delta k_{eff\ (300K,\ Implicit)} = -0.00004 \pm 2.8$ pcm
  - $\Delta k_{eff\ (1200K,\ Implicit)} = -0.00002 \pm 2.8$ pcm
- Jezebel assembly:
  - $\Delta k_{eff\ (300K,\ Analog)} = -0.00003 \pm 2.8$ pcm
  - $\Delta k_{eff\ (1200K,\ Analog)} = -0.00002 \pm 2.8$ pcm
  - $\Delta k_{eff\ (300K,\ Implicit)} =$ -
  - $\Delta k_{eff\ (1200K,\ Implicit)} = -0.00003 \pm 2.8$ pcm.

With respect to other differential neutron parameters, such as the neutron fluxes, Fig.4a displays the neutron flux behaviour, normalized per source neutron, for the Godiva critical assembly (at T=1200K) evaluated by both NJOY16 and NJOY21 codes.

Finally, Fig.4b displays the neutron flux behaviour normalized per source neutron, for Godiva, Jezebel and Jezebel23 critical assemblies at the temperature of 1200K, obtained with cross sections from the NJOY21 code.

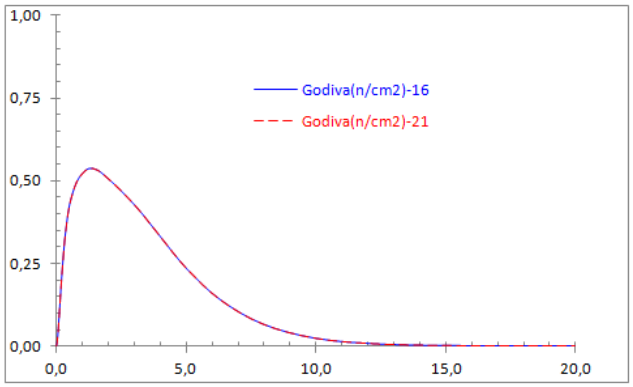


Fig. 4a. The Godiva neutron flux behaviour, in the range of [0, 20] MeV, with cross sections from NJOY16 and NJOY21

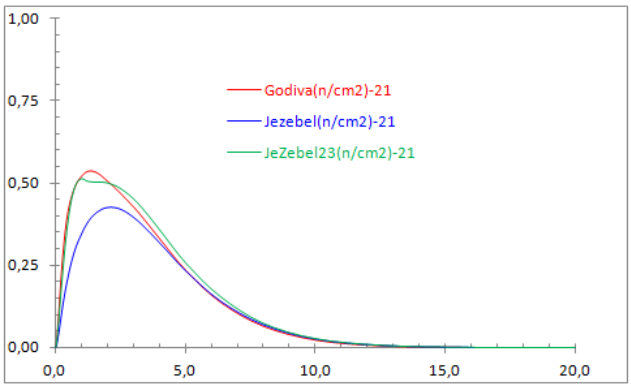


Fig. 4b. The Godiva neutron flux behaviour, in the range of [0, 20] MeV, with cross sections from NJOY16 and NJOY21

In Fig. 4a, the results appear to fully overlap, confirming their "indistinguishable" characteristic. Such behaviour resembles the Watt fission spectrum, with a pick value at 1.2619 MeV.

In Fig. 4b, it is evident the role of the spherical reflector in the Jezebel23 assembly that reduces by more than 12% the neutron leakage, with respect to the bare Jezebel critical configuration. The impact of the natural uranium spherical reflector is also evident on the neutron flux behaviour around the pick value energy.

Moreover, the Watt fission spectrum behaviour is observed with pick values at 1.2619 MeV for the Godiva and Jezebel23 assemblies, and 2.0 MeV for the bare Jezebel assembly.

Reactor Core Results

It was stated that the comparison between the results obtained from the two NJOY code releases, has been extended to a number of integral and differential neutron parameters regarding:

- a sub-critical (Th, U, Pu) Ox / Pb-cooled core [9];
- a critical (U, Pu) C / Na-cooled core [10],

with neutron characteristics and performances ruled by the neutron spectra displayed in Figs. 2a and 2b respectively.

The steady state criticality simulations have been performed with the MCNP5 1.6 stochastic neutron transport code, assuming 100,000 neutron histories per batch, for a total of 201 active batches. Skipping 50 cycles (=5E+6 neutrons) before storing tallies, a total of 20 million "active" neutron histories assure a statistical uncertainty of a dozen pcm.

Sub-critical (Th, U, Pu)Ox / Pb-cooled core

In case of the sub-critical (Th, U, Pu) Ox / Pb-cooled core, Table 3 lists the criticality results obtained using the cross section libraries from NJOY16 and NJOY21, at 300K and 1200K (293.6K in case of NJOY16 cross section library).

Moreover, they are divided into two groups: the first assuming the total neutron (ν_{total}) production per fission, and the second assuming only prompt neutron (ν_{prompt}) production per fission. Such a choice allows the evaluation of differential neutron parameters such as the reactivity variations, effective delayed neutrons fraction, "generalized" Doppler coefficient but not the reactivity variation due to the thermal expansions.

As far as the statement "generalized" Doppler coefficient is concerned, it is to be noted that typically Doppler coefficient expresses the reactivity variation due to fuel temperature variation, without contributions from the thermal expansions. In our case it includes the reactivity variation due to coolant and structural materials Doppler effect (if any) contributions.

Table 3. Sub-critical (Th, U, Pu)Ox / Pb-cooled core steady state criticality results of MCNP5 1.6 at 251 batches of 1E5 n-histories/batch (skipped 50 batches)

	k_{eff} (total ν)	k_{eff} (prompt ν)
NJOY16 293.6K	1.00293 ± 11E-5	0.99843 ± 11E-5
1200K	0.99369 ± 11E-5	0.98974 ± 11E-5
NJOY21 300K	1.00261 ± 13E-5	0.99837 ± 13E-5
1200K	0.99381 ± 12E-5	0.98889 ± 12E-5
Δ k_{eff} 16->21 300K(*)	- 0.00032 ± 17E-5	- 0.00006 ± 16E-5
Δ k_{eff} 16->21 1200K	-0.00012 ± 16E-5	0.00015 ± 17E-5
| Δ k_{eff} | < 2σ	**yes**	**yes**
Δ k_{eff} T1->T2 (16)	- 0.00924 ± 16E-5	- 0.00869 ± 17E-5
Δ k_{eff} T1->T2 (21)	-0.00880 ± 18E-5	0.00848 ± 18E-5
Δ (Δk_{eff} T1->T2)	0.00044 ± 24E-5	-0.00021 ± 25E-5
|Δ (Δ k_{eff})| < 2σ	**yes**	**yes**
d(Δk_{eff} T1->T2)/dT (pcm/K); NJOY16	-1.019E-5±1,76E-7	-
d(Δk_{eff} T1->T2)/dT (pcm/K); NJOY21	-0.978E-5±2.00E-7	-
| Δ (dΔ*keff/dT*) | < 2σ	**yes**	**-**

* T = 293.6K for NJOY16 results.

The results listed in Table 3 show the "indistinguishable" characteristics of the computational findings, while the same conclusion could be reached for the delayed neutrons effective fraction. Based on what it has been demonstrated [14, 15] and including the spectral dependencies of the core, it follows:

$$\beta_{eff} = (k_{eff,\ \nu_total} - k_{eff,\ \nu_prompt}) / k_{eff,\ \nu_total}$$

for the numerical results listed in Table 4.

Table 4. Sub-critical (Th, U, Pu) Ox/Pb-cooled core β_{eff} results of MCNP5 1.6 at 251 batches of 1E5n-histories/batch (skipping 50 batches)

	β_{eff} at 300K*	β_{eff} at 1200K
NJOY16	0.00449 ± 16E-5	0.00398 ± 17E-5
NJOY21	0.00423 ± 18E-5	0.00394 ± 16E-5
Δβ_{eff} 16->21	- 0.00026 ± 24E-5	- 0.00004 ± 23E-5
| Δβ_{eff} | < 2σ	**yes**	**yes**

* T = 293.6K for NJOY16 results.

Even, for this safety parameter, the "indistinguishable" characteristic is kept. Similar behaviour has been observed investigating other neutron parameters, such as the reaction rates, neutron activity, etc.

Concerning the neutron fluxes, Figs. 5a and 5b present their behaviour, normalized per source neutron, at 300K (T=293.6K) and 1200K, respectively, for the NJOY16 and NJOY21 cross section libraries.

For neutron of incident energies higher than 10 meV, a perfect overlapping is observed, re-confirming the concept of "indistinguishable" results. The differences for incident neutron energies lower than 10 meV are observable, but lack physical meaning due to the extremely low neutron population in such an energy range. For the sub-critical (Th, U, Pu) Ox / Pb-cooled core, the percentage of fissions caused by neutrons in the thermal range doesn't exceed 0.07%.

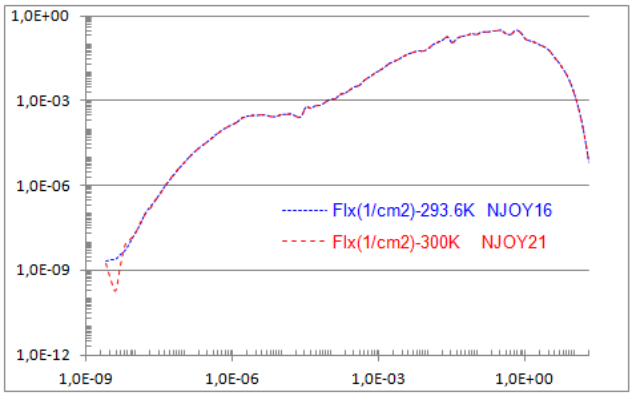


Fig. 5a. The sub-critical (Th, U, Pu)Ox/ Pb-cooled core neutron flux behaviour in the range of [0, 20] MeV at 300K (293.6K)

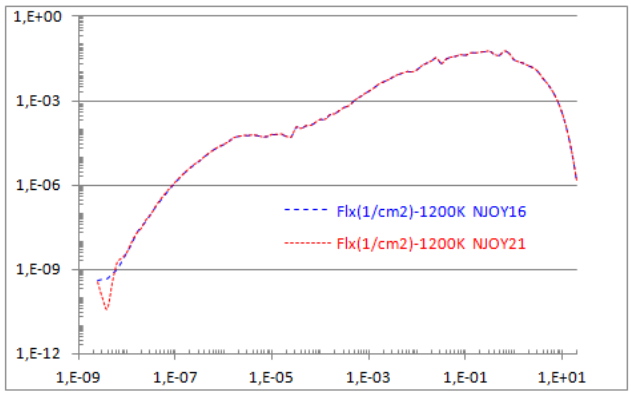


Fig. 5b. The sub-critical (Th, U, Pu)Ox/ Pb-cooled core neutron flux behaviour in the range of [0, 20] MeV at 1200K

Similar observations would be made for evaluations performed using the cross section libraries at 1200K. There is an overlapping for incident neutron energies higher than roughly 10 meV, while for incident neutron energies below the above value, small differences would be observed.

Critical (U, Pu)C / Na-cooled core

As far as a critical (U, Pu)C / Na-cooled core is concerned, criticality evaluations have been performed at both the nominal and coolant voided configurations. The latter configuration is subdivided into two coolant void cases, i.e.: with inner and outer active zones, because of their different enrichments.

Both configurations have been investigated at: 300K (293.6K for NJOY16) and 1200K, allowing also the evaluation of the Doppler coefficient, defined as:

$$dk_{eff}(T)/dT = C_{Dopp}/T^{\alpha}$$

where α ≡ coefficient depending on the neutron spectrum and coolant material; for a Na-cooled fast system: α ≡ 1.

Integrating in the temperature range $[T_1, T_2]$ the outcome is:

$$C_{Dopp} = [k_{eff}(T_2) - k_{eff}(T_1)] / \ln(T_2/T_1)$$

Table 5 lists the criticality results for the nominal state configuration and average reactivity variation per temperature variation (pcm/K) instead of the Doppler coefficients evaluation. This choice relies on the fact that the Doppler coefficient definition is strictly valid only for the fuel isotopes temperature variation, keeping constant the temperature of all other materials/isotopes.

Table 5. Critical (U, Pu)C / Na-cooled core criticality results of MCNP5 1.6 at 251 batches of 1E5 n-histories/batch (skipped 50 batches)

	NJOY16	**NJOY21**
300K *	1.01030 ± 10E-5	1.00998 ± 10E-5
1200K	0.99509 ± 11E-5	0.99498 ± 10E-5
Δk_{eff} 16->21 300K	-	-0.00032 ± 14E-5
$\lvert \Delta k_{eff} \rvert < 2\sigma$	-	**no ($\lvert \Delta k_{eff} \rvert < 3\sigma$)**
Δk_{eff} 16->21 1200K	-	-0.00011 ± 15E-5
$\lvert \Delta k_{eff} \rvert < 2\sigma$	-	**yes**
$\Delta k_{eff} / \Delta T$	-0.000017±1.2E-7	-0.000017 ± 1.1E-7
$\lvert \Delta (\Delta k_{eff}/\Delta T) \rvert < 2\sigma$	-	-

* T = 293.6K for NJOY16 results.

In Table 6, the criticality results for coolant void effect are listed for the NJOY16 and NJOY21 cross section libraries. The different k_{eff} values for T=293.6K and 300K could have an impact on satisfaction of the "indistinguishable" results condition.

As far as the coolant void effect is concerned, the results listed in Table 6 show that even in this case there are no significant differences between the findings, confirming also their "indistinguishable" characteristic.

At the same conclusion leads the comparison of the neutron fluxes, obtained using the above two sets of cross section libraries.

Figs. 6a and 6b display the neutron flux behaviours, normalized per source neutron, at 300K (T=293.6K) and 1200K, respectively, for the NJOY16 and NJOY21 cross section libraries.

It appears that:
- for incident neutron energies lower than 0.1 eV small differences are observed, for a low neutron population, roughly 0.01% of the total;
- for incident neutron energies higher than 0.1 eV, an overlapping can be noticed.

Table 6. Critical (U, Pu)C / Na-cooled core criticality results for coolant void effect of MCNP5 1.6 at 251 batches of 1E5 n-histories/batch (skipped 50 batches)

Coolant Void k_{eff}	**NJOY16**	**NJOY21**
300K * Inner Core	1.01440 ± 11E-5	1.01406 ± 12E-5
($\Delta k_{eff} / k_{eff}$) *Inner*	**0.00406 ± 15E-5**	**0.00404 ± 15E-5**
300K * Outer Core	1.01543 ± 10E-5	1.01517 ± 11E-5
($\Delta k_{eff} / k_{eff}$) *Outer*	**0.00508 ± 14E-5**	**0.00514 ± 15E-5**
1200K Inner Core	0.99995 ± 10E-5	0.99998 ± 10E-5
($\Delta k_{eff} / k_{eff}$) *Inner*	**0.00488 ± 15E-5**	**0.00503 ± 14E-5**
1200K Outer Core	1.00200 ± 10E-5	1.00212 ± 10E-5
($\Delta k_{eff} / k_{eff}$) *Outer*	**0.00694 ± 15E-5**	**0.00718 ± 14E-5**
$\delta(\Delta k_{eff} / k_{eff})$ 300K Inner Core	-	**-0.00002 ± 21E-5**
$\delta(\Delta k_{eff} / k_{eff})$ 300K Outer Core	-	**0.00006 ± 20E-5**
$\delta(\Delta k_{eff} / k_{eff})$ 1200K Inner Core	-	**0.00015 ± 21E-5**
$\delta(\Delta k_{eff} / k_{eff})$ 1200K Outer Core	-	**0.00024 ± 21E-5**
$\lvert \Delta\delta(\Delta k_{eff}/keff) \rvert < 2\sigma$	/	**yes**

* T = 293.6K for NJOY16 results.

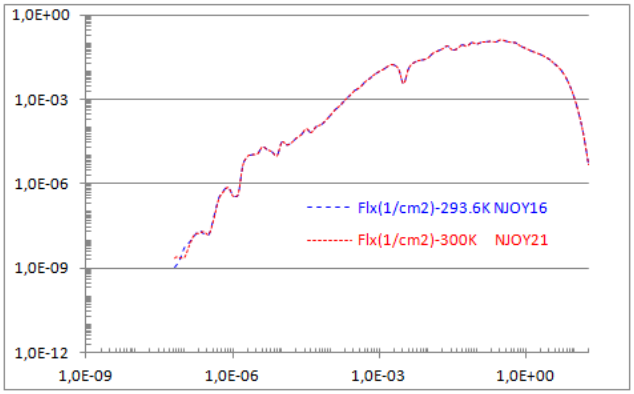


Fig. 6a. The critical (U, Pu)C / Na-cooled core neutron flux behaviour, in the range of [0, 20] MeV at 300K *

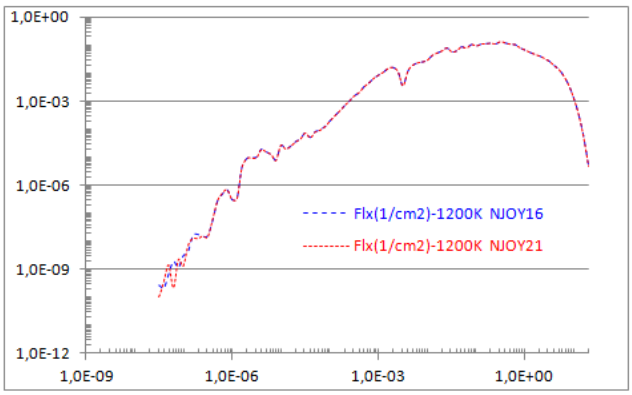


Fig. 6b. The critical (U, Pu)C / Na-cooled core neutron flux behaviour, in the range of [0, 20] MeV at 1200K

Final remarks and Conclusions

The findings of a benchmarking investigation on the cross section libraries, produced by NJOY21 and based on the Evaluated Nuclear Data File: B-VIII.8, for 556 isotopes at 11 temperatures, have been presented.

The benchmarking work examined three fast critical assemblies and two fast system cores (characterized by a diversity of fuel, coolant and structural materials, design concepts and operative conditions), by a point-wise comparison of the results obtained using two sets of cross section libraries produced by NJOY16 and NJOY21 codes.

Steady state criticality results (of MCNP5 code), integral and differential neutron parameters, as well as reactivity coefficients, have been evaluated by applying the two sets of cross section libraries, at four different temperatures, i.e. 300K (293.6 for NJOY16), 600K, 900K and 1200K. These temperatures were used for the three experimental critical assemblies while for the two fast system cores only 300K (293.6 for NJOY16) and 1200K have been used.

The choice of fast assemblies/systems, due to the fact that all fission systems are driven by a source of fast fission neutrons emitted by nucleus fissions, is confirmed and doesn't exclude the extension on analogous type of benchmarking investigation on thermal and/or intermediate spectrum systems.

In general, the results obtained are consistent with the investigated physical systems. Of particular interest is the "indistinguishable" characteristic of the results for both integral and differential parameters.

An important outcome is the overlapping of the neutron fluxes, for most of the energy spectrum, while small differences are observed at the thermal region of the spectrum, i.e. at $E_n \leq 0.625$ eV, independently of the temperature difference of about 6 degrees (only for the case of 293.6K for NJOY16 and 300K for NJOY21). In such a case, the impact on the neutron parameters would be negligible, because of the low neutron population in this region of the spectrum. This behaviour has been observed for all the systems examined. Such a finding could suggest a different treatment of the thermal region physics between the two releases of the NJOY code, as well as different use of tolerances and/or other control parameters in the NJOY code input cards.

Notwithstanding the non-exhaustive character of the current investigation, in terms of the nuclear systems and temperature sets of the cross section libraries, its findings support the extension of the equivalence between the cross section libraries produced by the NJOY21 code and those produced by the NJOY16 code, for similar nuclear systems at the temperatures considered.

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