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Chapter

A Criticality Study of Fast Critical Experimental Benchmarks Using MCNP Code to Qualifying Different Evaluations

Sanae El Ouahdani, Hamid Boukhal, El Mahjoub Chakir, Ahmed Gaga, Houda Elyaakoubi, Mustapha Makhloul, Abdelaziz Ahmed, Abdessamad Didi and Mohamed Bencheikh

Abstract

In this chapter we present our MCNP modeling, concerning fast critical experimental benchmarks, about qualifying our libraries of cross-sections deduced from the evaluations ENDF/B-VII, JEFF-3.1, JENDL-3.3, JENDL-4 processed by the code NJOY. The benchmarks analyzed are characterized by simple geometries which help to have a precise calculation. In our neutron calculation, we used the MCNP code (version 5), the reference code for the neutron transport calculation with the Monte Carlo method. It is also very efficient for criticality calculation. The cross-section data for all the isotopes that make up the material of the studied benchmarks are processed in ACE format at 300 K temperature using the NJOY 99.9 modular system. A detailed comparison of the criticality results of our simulation was carried out to highlight the influence of these evaluations on the $k_{eff}$ calculations.

Keywords: benchmark, MCNP code, NJOY code, ENDF/B-VII, multiplication factor, criticality

1. Introduction

The effective multiplication factor $k_{eff}$ is an important parameter in the design, control and safety of reactors. For safety considerations, the $k_{eff}$ is desired to be very close to one throughout the core life. The calculation of the $k_{eff}$ is rather a complicated problem due to the contributions of different physical phenomena related to the neutron's population change. That is why it is important to validate any reactor calculation tool and any nuclear data library with an accurate prediction of this parameter.

The main objective of the present work is to perform the qualification and analysis of the most recent nuclear data libraries available to the scientific community, in particular; ENDF/B-VII [1], JENDL-4.0 [2], JENDL-3.3 [3], and JEFF-3.1 [4], to check the accuracy of cross-section libraries for the criticality calculations. For this objective
a set of critical fast benchmarks highly enriched uranium and with $^{233}\text{U}$ and with $^{239}\text{Pu}$ fuel rods were used to consider as closely as possible all types of geometries to simulate the criticality coefficient of interest. The continued energy cross sections necessary for the present work were processed by the NJOY system (version 99.9, update 364) [5] in the ACE format. The analysis and the interpretation of the results were reinforced by a comparison study of the parameter with the experimental values excerpt from the literature [6]. These experiments have already been analyzed by the Monte Carlo code MCNP using the American nuclear data ENDF/B-V continuous [6] and other codes.

The first part of the paper is reserved to explain the methodology and the materials used. The materials used are the MCNP code and the NJOY code and the JANIS code. The second part cites the characteristics of the different benchmarks selected for the present study. In the third part, we develop our results obtained about the simulation of the $k_{\text{eff}}$ parameter and their interpretations concerning the qualification of the used libraries. We finished with a conclusion.

2. Methods and materials

2.1 MCNP code

The MCNP code [7] (Monte-Carlo N Particle transport), is a code that deals with the transport of neutrons, photons and electrons or coupled/photon/electron by the Monte-Carlo method, including the possibility of calculating the values clean for critical systems. The code deals with an arbitrary three-dimensional configuration with materials in geometric cells delimited by surfaces.

The code takes into account the processed cross-sections, for neutrons, all reactions, which are proposed in particular data evaluations (for example, ENDF/B-VI), thermal neutron scattering which is treated both by the model of the free gas and $S (\alpha, \beta)$, for photons the code takes into account incoherent and coherent diffusions, the possibility of fluorescence emission after the photoelectric effect, absorption in the production of pairs with a local broadcast of annihilation radiation. It can also treat the braking radiation emitted. In this way, MCNP is qualified as a three-dimensional, continuous energy code, thus it has been proven to simulate physical phenomena correctly. The series of important features that make MCNP very flexible and easy to use code is that it includes a powerful general source, criticality source, surface source, geometry and output pointing plotters, a rich collection of variance reduction techniques, the desired result structure called “tally” and has a large collection of cross-section data.

2.2 NJOY code

The NJOY nuclear data processing code [5] is a system developed at the Los Alamos laboratory in the USA since 1974. It is a modular code allowing, from the assessments of so-called basic nuclear data, to create specific or multigroup parameters (multigroup cross sections, fission spectra, etc...) because the information contained in these files is, such as it cannot be, exploited directly by the various transport codes MCNP, WIMS, APPOLLO, EPRI-CELL... etc. The role of the NJOY system is to process this information and make it usable by these codes. The data processed by this system are then stored in files in a standardized ENDF (Evaluated Nuclear Data File) format.
2.3 JANIS

The enormous amount of data stored in the standard ENDF format files as well as the different versions or evaluations do not always allow easy access to the information desired by the user for a particular application. JANIS (Java-based Nuclear Information Software) [8] is a program designed to facilitate the visualization and manipulation of nuclear data. It was developed by the “OECD Nuclear Energy Agency”, the “CSNSM-Orsay” and the University of Birmingham as an extension of the JEF-PC program. The main objective of this program is to allow the user to access the numerical values and the graphic representation of the various data without any prior information on the ENDF format. It gives maximum flexibility for the comparison of different types of nuclear data.

3. The fast critical benchmarks

3.1 The benchmarks

The benchmarks are fixed points of reference used to test the results of modeling and theoretical calculations and to validate nuclear data.

There are two types of benchmarks:

- Theoretical benchmarks: Are exact references with great precision, obtained by solving mathematical equations describing physical phenomena and processes. They are used primarily to conduct a rough and inherent validation of algorithms widely used in computer codes.

- Experimental benchmarks: Are experiments using measuring instruments dedicated to a good description of physical aspects and phenomena. They are mainly used for the qualification of nuclear data.

3.2 Characteristics of the fast benchmarks used

The benchmarks analyzed cover different and simple geometries (spherical, cylindrical, and parallelepiped), with or without reflector, and concern the three main fissile nuclei $^{235}\text{U}$, $^{233}\text{U}$, $^{239}\text{Pu}$ in metallic form.

Fast benchmarks use a fast neutron spectrum that covers the energy range greater than 100 keV, and are therefore characterized by very high fission and capture percentages in the fast energy domain.

By way of example, Tables 1–3 give the average percentages of the flux as well as the fission and capture rates in the following three energy intervals [6]:

- Thermal energy interval, characterized by neutron energies below 0.625 eV.
- Epithermal energy interval between 0.625 eV and 100 keV.
- Fast energy interval, for neutrons with energy greater than 100 keV.
Qualitative and Computational Aspects of Dynamical Systems

3.3 Description of the fast benchmarks studied

As we mentioned before, to qualify our cross-section libraries as well as the modeling method, we have chosen a series of critical fast experimental benchmarks which cover different geometries and relate to the three main fissile nuclei $^{235}\text{U}$, $^{239}\text{Pu}$ and $^{233}\text{U}$. These benchmarks are derived from the International Handbook of Critical Benchmarks published by the nuclear energy agency AEN [6].

### 3.3.1 Fast benchmarks highly enriched in U-235 (HEU-MET-FAST)

We have processed a series of 20 highly enriched benchmarks known with HEU-MET-FAST that is chosen carefully with simple geometries. It includes GODIVA, TOPSY, FLATTOP and HEU-MET-FAST-xxx.

**HEU-MF-001**: GODIVA (1950–1959, LANL, USA), sphere containing metallic uranium highly enriched in the isotope $^{235}\text{U}$ (93.71% wt*).

*wt = mass fraction.

**HEU-MF-002**: TOPSY-8 (1950, LANL, USA), assemblages of different geometry (depending on the case) containing uranium highly enriched in the $^{235}\text{U}$ isotope (93.55% wt) reflected by natural uranium, (6 cases).

**HEU-MF-003**: ORALLOY (1950, LANL, USA), spherical assemblies containing metallic uranium highly enriched in $^{235}\text{U}$ (93.5% wt), reflected by reflectors of different types and thicknesses depending on the case (12 cases): seven spheres are reflected by 5.08, 7.62, 10.16, 12.7, 17.78, 20.32, 27.94 cm of natural uranium, four

---

<table>
<thead>
<tr>
<th>Benchmarks</th>
<th>&lt;0.625 eV</th>
<th>0.625 eV–100 keV</th>
<th>&gt;100 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>HEU-MET-FAST</td>
<td>0.005%</td>
<td>≈6.74%</td>
<td>≈93.255%</td>
</tr>
<tr>
<td>PU-MET-FAST</td>
<td>0.00%</td>
<td>≈4.41%</td>
<td>≈95.5%</td>
</tr>
<tr>
<td>U233-MET-FAST</td>
<td>0%</td>
<td>≈3.55%</td>
<td>≈96.48%</td>
</tr>
</tbody>
</table>

Table 1. Average percentages of flux in the three energy intervals.

<table>
<thead>
<tr>
<th>Benchmarks</th>
<th>&lt;0.625 eV</th>
<th>0.625 eV–100 keV</th>
<th>&gt;100 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>HEU-MET-FAST</td>
<td>0.75%</td>
<td>10.035%</td>
<td>89.215%</td>
</tr>
<tr>
<td>PU-MET-FAST</td>
<td>1.64%</td>
<td>≈5%</td>
<td>93.36%</td>
</tr>
<tr>
<td>U233-MET-FAST</td>
<td>0%</td>
<td>4.82%</td>
<td>95.19%</td>
</tr>
</tbody>
</table>

Table 2. Average percentages of fissions caused by neutrons in the three energy fields.

<table>
<thead>
<tr>
<th>Benchmarks</th>
<th>&lt;0.625 eV</th>
<th>0.625 eV–100 keV</th>
<th>&gt;100 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>HEU-MET-FAST</td>
<td>0.815%</td>
<td>23.32%</td>
<td>75.865%</td>
</tr>
<tr>
<td>PU-MET-FAST</td>
<td>5.72%</td>
<td>25%</td>
<td>69.38%</td>
</tr>
<tr>
<td>U233-MET-FAST</td>
<td>0.00%</td>
<td>10%</td>
<td>90%</td>
</tr>
</tbody>
</table>

Table 3. Average percentages of neutron capture in the three energy domains.
spheres are reflected by 4.826, 7.366, 11.43, 16.51 cm of Tungsten carbon, one sphere is reflected by 20.32 cm of nickel.

**HEU-MF-028**: FLATTOP-25 (1964–1966, LANL, USA), a sphere containing metallic uranium highly enriched in the $^{235}$U isotope (93.24% wt) reflected by natural uranium.

### 3.3.2 Fast benchmarks in U-233 (U233-MET-FAST)

- **U233-MF-001**: JEZEBEL-23 (1961, LANL, USA), sphere containing metallic uranium highly enriched in the $^{233}$U isotope (93.24% wt).
- **U233-MF-002**: (1958, LANL, USA), sphere containing metallic uranium highly enriched in the $^{235}$U isotope (50.59% wt) reflected by a layer of 235 U, (2 cases, in both cases the mass varies critical).
- **U233-MF-003**: (1958, LANL, USA), sphere containing metallic uranium highly enriched in the $^{233}$U isotope (98.89% wt) reflected by natural uranium, (2 cases, in both cases the critical mass varies).
- **U233-MF-004**: (1958, LANL, USA), sphere containing metallic uranium highly enriched in the $^{233}$U isotope (98.2% wt) reflected by tungsten, (2 cases, in the 2 cases varies the critical fatigue and the reflector thickness).
- **U233-MF-005**: (1958, LANL, USA), sphere containing metallic uranium highly enriched in the $^{233}$U isotope (98.2% wt) reflected by beryllium, (2 cases, varies the critical mass).
- **U233-MF-006**: FLATTOP-23 (1964, LANL, USA), sphere containing metallic uranium highly enriched in the $^{233}$U isotope (98.13% wt) reflected by natural uranium.

### 3.3.3 Fast benchmarks in Pu-239 (Pu-MET-FAST)

- **Pu-MF-001**: JEZEBEL-39 (1950, LANL, USA), metallic plutonium sphere enriched in the $^{239}$Pu isotope (95.17%), (4.5 at% $^{240}$Pu, 1.02 wt% Ga), without a reflector.
- **Pu-MF-002**: JEZEBEL-40 (1964, LANL, USA), metallic plutonium sphere enriched in the $^{239}$Pu isotope (20.1 at% $^{240}$Pu, 1.01 wt% Ga), without a reflector.
- **Pu-MF-005**: (1958, LANL, USA), metallic plutonium sphere enriched in the $^{239}$Pu isotope (94.76%), reflected by tungsten.
- **Pu-MF-006**: FLATTOP-39 (1964–1966, LANL, USA), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (94.84% wt) reflected by natural uranium.
- **Pu-MF-008**: THOR (1960–1961, LANL, USA), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (94.54% wt), reflected by thorium.
- **Pu-MF-009**: (1960, LANL, USA) plutonium metallic sphere highly enriched in the $^{239}$Pu isotope (94.8% wt), reflected by aluminum.
- **Pu-MF-010**: DELTA-PHASE (1958, LANL, USA): metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (94.76% wt), reflected by natural uranium.
- **Pu-MF-011**: ALPHA-PHASE (1968, LANL, USA), metallic plutonium sphere highly enriched in $^{239}$Pu (94.4% wt) reflected by light water.
- **Pu-MF-018**: DELTA-PHASE (1958, LANL, USA), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (94.7% wt) reflected by beryllium.
- **Pu-MF-023**: (1962, VNIIEF, Russia), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (98.19%), reflected by the graphite.
- **Pu-MF-024**: (1964, VNIIEF, Russia), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (98.19%), reflected by polyethylene.
Pu-MF-025: (1964, VNIIEF, Russia), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (98.19%), reflected by stainless steel (1.55 cm).

Pu-MF-026: (1962, VNIIEF, Russia), metallic plutonium sphere highly enriched in the $^{238}$Pu isotope (98.19%), reflected by stainless steel (11.9 cm).

Pu-MF-027: (1965, VNIIEF, Russia), metallic plutonium sphere highly enriched in the $^{239}$Pu isotope (98.19%), reflected by stainless steel (1.55 cm).

Pu-MF-028: (1965, VNIIEF, Russia), spherical assembly in metallic plutonium highly enriched in the $^{239}$Pu isotope (89.66%), reflected by polyethylene.

Pu-MF-029: (1965, VNIIEF, Russia), spherical assembly in metallic plutonium highly enriched in the $^{239}$Pu isotope (88% wt), without a reflector.

Pu-MF-030: (1965, VNIIEF, Russia), spherical assembly in metallic plutonium highly enriched in the $^{239}$Pu isotope (88% wt) reflected by stainless steel.

Pu-MF-031: (1965, VNIIEF, Russia), spherical assembly in metallic plutonium highly enriched in the $^{239}$Pu isotope (88% wt) reflected by polyethylene.

Pu-MF-032: (1965, VNIIEF, Russia), spherical assembly in metallic plutonium highly enriched in the $^{239}$Pu isotope (88% wt) reflected by stainless steel.

4. Results and interpretations

For the calculation of the $k_{eff}$ parameter, we used the MCNP code based on the Monte Carlo method. The Monte Carlo method solves the transport equation in integral form. The latter is based on the random selection of several variables and after the estimation of their mathematical expectation which is equivalent to the value of the physical quantity sought. It simulates the history of each neutron through the different interactions it can have in the media where it propagates.

In the present calcul, we simulated 1500 cycles of 30,000 neutrons each, the first 50 cycles are used to ensure the homogeneity of the source distribution. With this number of simulated stories, all $k_{eff}$ results are obtained with a standard deviation between ±9 and ±12 pcm.

5. Case of fast benchmarks highly enriched in $^{235}$U

The experimental values obtained for the various Benchmarks concerning the effective multiplication factor $k_{eff}$, as well as the average deviations from experience are shown and compared to the experience in Figures 1 and 2.

Figure 1 represents the variation of $k_{eff}$ according to the cases for the fast benchmarks very highly enriched in $^{235}$U, from this figure we notice that for the majority of the cases studied, the ENDF/B-VII and JEFF-3.1 evaluations give results that are in good agreement with experience. The average deviation from experience is in the order of 0.42% for ENDF/B-VII and 0.39% for the JEFF-3.1 evaluation: all the libraries keep the same difference between themselves and the same behavior for the benchmarks reflected by natural uranium, except for the benchmarks from HEU-MF-008 to HEU-MF-011 which are reflected by tungsten carbide and HEU-MF-012 reflected by nickel. We also note that the JENDL-3.3 evaluation underestimates the criticality in most cases, with an average deviation from experience equal to 0.6%. However, there is a marked improvement when upgrading the evaluation from JENDL-3.3 to JENDL-4. Although, we still have an underestimation compared to the other evaluations of JENDL-3.3 and JENDL-4. We notice an overestimation of $k_{eff}$ for all the evaluations.
Figure 1. $k_{\text{eff}}$ depending on the case for the fast benchmarks very highly enriched in $^{235}\text{U}$.

Figure 2. The $|C-E|/E$ ratio of $k_{\text{eff}}$ for each evaluation.

Concerning the benchmarks reflected by the Tungsten carbide which contains the carbon, the problem probably stems from a poor underestimation of the carbon capture cross-sections especially in the energy interval of 5 keV to 5 MeV of the capture cross-section where JENDL-4 overestimates ENDF/B-VII and JEFF-3.1.

### 5.1 Fast benchmarks in U-233

Figures 3 and 4 represent the variation of $k_{\text{eff}}$ according to the cases for the fast benchmarks in $^{233}\text{U}$ isotope as well as the average deviations from the $k_{\text{eff}}$ experiment.
From Figures 3 and 4 we find that the best results of criticality are given by JENDL-4 with a deviation from the experience of 0.16%, secondly, we find ENDF/B-VII with a deviation by compared to the experience of 0.26% we note an improvement during the transition from JENDL-3.3 to JENDL-4. We also notice an overestimation of JEFF-3.1 of the criticality with a deviation from the experience of 0.39%.

5.2 Fast benchmarks in Pu-239

Figures 5 and 6 represent the variation of $k_{\text{eff}}$ according to the cases for the fast benchmarks in $^{239}$Pu isotope as well as the average deviations from the experience. In Figures 5 and 6, the variation of $k_{\text{eff}}$ shows that the process based on ENDF/B-VII and JEFF-3.1 gives results that are in good agreement with the experimental values, the deviations from the experiment are 0.34% and 0.33% respectively, with...
the exception of JENDL-3.3 and JENDL-4 which have deviations from criticality greater than the other libraries of 0.39% and 0.38% respectively. Apparently, JENDL-3.3 gives $k_{\text{eff}}$ far from 1 compared to other libraries in the Pu-MF-006 and Pu-MF-008 and Pu-MF-010 benchmarks as we notice that the problem is corrected in JENDL-4, and JENDL-4 far from 1 compared to other libraries in benchmarks Pu-MF-026, Pu-MF-28 and Pu-MF-32. We note that there is a deterioration during the transition from JENDL-3.3 to JENDL-4 in these three benchmarks. At the three benchmarks Pu-MF-11, Pu-MF-27 and Pu-MF-31 all the libraries have criticality estimates.

The Pu-MF-26, 28 and 32 benchmarks use stainless steel as a reflector, so the JENDL-4’s underestimation of criticality compared to other libraries and due to the overestimation of JENDL-4 to other libraries in the cross-section of carbon capture.

Figure 5.
$k_{\text{eff}}$ depending on the case for the fast benchmarks in Pu-239.

Figure 6.
The $|C-E|/E$ ratio of $k_{\text{eff}}$ in the case of fast benchmarks in Pu-239.
6. Conclusions

In this work we were able to model rapid critical benchmarks using the main fissile nuclei which are, the $^{235}\text{U}$, the $^{233}\text{U}$, and the $^{239}\text{Pu}$, we previously generated cross-sections using the NJOY code, these cross-sections come from the main evaluations ENDF/B-VII, JEFF-3.1, JENDL-3.3 and JENDL-4.

The Monte Carlo calculation that we carried out consisted in determining the $k_{\text{eff}}$ parameter, the difference between the calculation and the experiment depends mainly on the type of evaluation used as well as the fissile core of the benchmarks considered this difference remains acceptable all the same. So that we can say, that our results are in good agreement with those obtained experimentally.

Author details

Sanae El Ouahdani*1, Hamid Boukhal2, El Mahjoub Chakir3, Ahmed Gaga1, Houda Elyaakoubi2, Mustapha Makhloul2, Abdelayaz Ahmed4, Abdessamad Didi5 and Mohamed Bencheikh6

1 Polydisciplinary Faculty, LRPSI Laboratory, Physics Department, Sultan Moulay Slimane University, Beni Mellal, Morocco

2 Faculty of Sciences, ERSN, Abdelmalek Essaadi University, Tetouan, Morocco

3 Faculty of Sciences, LHESIR, Ibn Tofail University, Kenitra, Morocco

4 Faculty of Lawder, Physics Department, University of Abyan, Abyan, Yemen

5 National Center for Energy Sciences and Nuclear Techniques, Rabat, Morocco

6 Faculty of Sciences and Technologies, Physics Department, Mohammedia Hassan II University of Casablanca, Mohammedia, Morocco

*Address all correspondence to: selouahdani@gmail.com

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