MUSE-4 BENCHMARK CALCULATIONS USING MCNP-4C AND DIFFERENT NUCLEAR DATA LIBRARIES

Nadia Messaoudi and **Edouard Mbala Malambu**
SCK·CEN
Boeretang 200, B-2400 Mol, Belgium
Email: nmessaou@sckcen.be

Abstract

Current calculation methods and nuclear data are well validated for conventional nuclear reactor systems. However there is a further need for validating the computational tools and the nuclear data for ADS applications. The OECD/NEA, in co-operation with CIEMAT (Spain) and CEA (France), therefore launched a benchmark based on the MUSE-4 experiments being carried out at Cadarache, France, to simulate the neutronics of a source-driven sub-critical system. This paper summarises the calculated results of the MUSE-4 benchmark obtained from the Monte Carlo code MCNP (Version 4Ca) using different nuclear data evaluations, and shows the sensitivity of the requested results with regard to the nuclear data used. All the calculated results will be compared against measured data after the completion of the experiments foreseen for the end of 2003.

Introduction

In ADS systems, a sub-critical multiplying medium is driven by an external spallation source produced by the interaction of proton on a spallation target. The main role of ADS systems would be to burn minor actinides and selected fission-products. Even though current calculation methods and nuclear data are well validated for conventional nuclear reactor systems, there is a further need for validating the computational tools and the nuclear data (different nuclear evaluations) for ADS applications.

For this purpose, the MUSE-4 experiment based benchmark was launched by the OECD/NEA in co-operation with CIEMAT (Spain) and CEA (France). The MUSE-4 experiments (***MU***ltiplication ***S***ource ***E***xterne) are being carried out at Cadarache, France, during 2001-2003, using the MASURCA facility, a reactor dedicated to the neutronics studies of fast reactor lattices. The experiments investigate both critical and sub-critical configurations changing the sub-criticality level. For sub-critical configurations, the deuteron accelerator GENEPI provides an external neutron source.

The MUSE-4 benchmark is divided in three steps, each one concerns a specific configuration. The first two steps concern two critical configurations, i.e. the COSMO and the MUSE-4 critical reference (1 112 cells) configurations, and the third step is to simulate a 976 cells MUSE-4 sub-critical configuration driven by an external neutron source. For each step, main neutronics parameters such as reactivity level, spectral indexes, neutron energy spectra, and delayed neutron fraction, etc. are requested. This paper summarises results focusing on step 3 calculations of the benchmark for the configuration "976 cells MUSE-4" with both evaluations: ENDF/B-VI and JEF-2.2 data. For steps 1 and 2, only criticality level results for the "COSMO" and the "1 112 cells MUSE-4 critical reference" configurations are presented.

Benchmark model

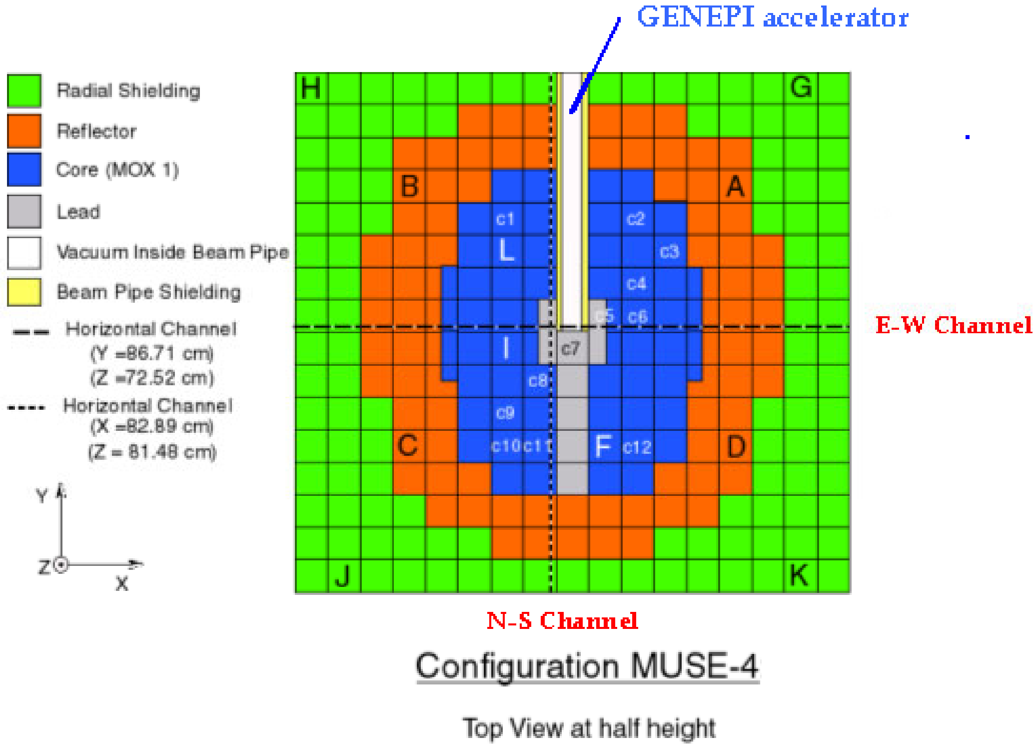
Sub-critical MUSE-4 configuration

The MASURCA facility is a fast spectrum experimental device, with an arrangement of tubes of $10.6\times10.6\times164.16\ \text{cm}^3$ each, building a parallel-piped assembly of 17×16 tubes, with a total dimension of $180.2\times169.6\times164.16\ \text{cm}^3$ in the MUSE-4 configurations. For step 3 of the benchmark, the configuration used inside the MASURCA facility is a 976-cells MUSE-4 configuration with a sub-critical level "SC2" ($K_{eff} \sim 0.97$).

As shown in Figure 1, this configuration consists of 3 regions: (1) sodium cooled MOX fuel zone in the central part of the core, (2) surrounding the core, which is a reflector zone made of sodium and Stainless steel and finally (3) a shielding zone containing Stainless steel at the periphery of the core. The GENEPI accelerator, built in ISN at Grenoble in France, was coupled with the MASURCA facility to provide the external neutron source. For this purpose, at the mid plane level, the core comprises a vacuum region.

In the benchmark, the neutron source is created via the $T(d,n)^4He$ reaction. Tritium is chosen as the target material. The deuteron beam, provided by the GENEPI accelerator, has a time structure of 1µs pulses repeated at 1 kHz. Neutrons are produced in an anisotropic angular distribution with an energy range varying from 15.24 MeV to 13.1 MeV.

Figure 1. **MUSE-4 configuration**



Requested results

The results to be reported were the following: K*eff* and K*source* for the sub-critical configuration, ^{235}U fission rates along vertical and horizontal channels, actinide reaction rates and spectra at the centre of these channels. Some kinetic parameters such as β*eff* and mean neutron lifetime and other time depending parameters were also requested.

A complete description of the benchmark model, including all geometry and material data required to develop the detailed computational model of the 976-cells MUSE-4 configuration, and all the requested results for each step can be found in reference. [1]

Calculation tools

The whole MUSE-4 core was modelled with the Monte Carlo code MCNP (version 4Ca), [2] describing all geometry details. Both KCODE and SOURCE mode calculations have been performed depending on the results required. Self-shielding effects in the unresolved resonance range were taken into account by using a probability-table treatment for some isotopes. An important number of histories were used to get more confident results with good statistics.

Most of the tallies (i.e.,^{235}U fission rate, spectra, etc.) were estimated inside a cube with a volume of 1 cm^3 in which the specified position was the centre. Figures 2 and 3 show the 976-cells sub-critical MUSE-4 configuration as it was modelled by the MCNP code.

With regard to the nuclear data used, mainly two sets of nuclear data evaluations were used: ENDF/B-VI.5 from the MCNP-4C package [2] and a locally generated library based on JEF-2.2. [3,4] The latter was prepared based on the JEF-2.2 with the nuclear data processing code system NJOY-97.99 except for ^{239}Pu cross-sections. For this isotope, the "JEF-CEA-corr. ^{239}Pu" file was used.

Figure 2. **MUSE-4 configuration**

Top view at half height

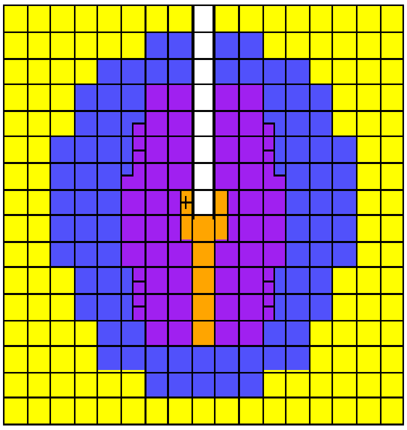
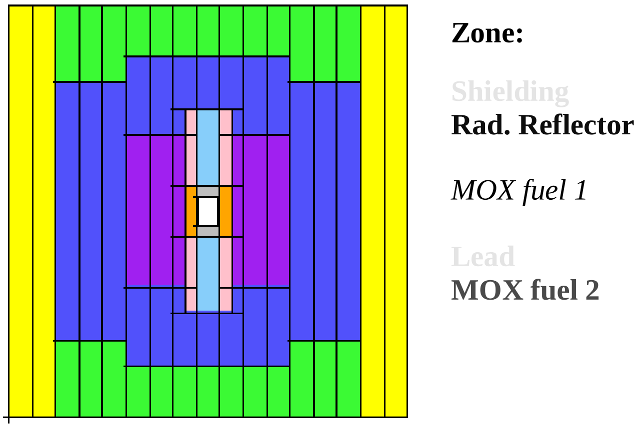


Figure 3. **MUSE-4 configuration**

View at Y=90.1 cm



Results and analysis

1. Steps 1 & 2

For both configurations (the critical “COSMO” and the “1 112 cells MUSE-4” configurations), experimental criticality values are available. These values are given in Table 1 and compared to the calculated values by the MCNP code with both evaluations: ENDF/B-VI and JEF-2.2. Between parentheses, are reported the differences of these values with the experimental value.

Table 1. ***Keff* in COSMO and 1 112 cells MUSE-4 configurations**

K*eff*	**Exp. value**	**ENDF/B-VI**	**JEF-2.2**
COSMO	0.99870	1.00718 (848)	1.00792 (922)
1 112 cells MUSE-4	0.99920	1.00687 (767)	1.00123 (203)

The standard deviation of the calculated K*eff* values are 12 and 8 pcm for COSMO and 1 112 cells configurations respectively and those of the experimental values are about 200 pcm for the COSMO configuration and about 150 pcm for the 1 112 cells MUSE-4 configuration. [5,6]

2. Step 3

Keff and Ksource values

Up to now, it is possible to compare the calculated results between them only for the 976 cells MUSE-4 configuration. After the completion of MUSE-4 experiences in early 2003, a more thorough investigation into calculation methods and nuclear data will be carried out by comparing the calculated results against the experimental data. Without going into detail on all the requested results in the framework of the benchmark, only the most relevant ones at this stage are presented below.

The calculated K*eff and* K*source* with the different nuclear libraries are summarised in Table 2 below. The statistical errors from the MCNP calculations are also reported between parentheses.

Table 2. **Comparison of calculated K*eff* and K*source* values**

	ENDF/B-VI	**JEF-2.2**	**Diff.** (pcm)
K*eff*	0.97456 (± 0.00007)	0.96983 (± 0.00008)	+473
K*source*	0.98747	0.98473	+274
K*source*-K*eff* (pcm)	1291	1490	–
φ* source efficiency	2.06	2.01	–

K*source* is defined as a ratio of neutron production (by fission and (*n,xn*) reactions) and neutron loss (by capture, fission, escape and (*n, xn*) reactions); the formula used is as follows: [1]

$$K_{source} = \frac{(\nu_f \Sigma_f \Phi) + \sum_x (x\Sigma_{(n,xn)}\Phi)}{(\Sigma_c \Phi) + (\Sigma_f \Phi) + \sum_x (\Sigma_{(n,xn)}\Phi) + (\Omega.\nabla\Phi)}$$

As shown in Table 2, JEF-2.2 data produce smaller values for both K*eff* and K*source* compared to ENDF/B-VI data, but the former gives the most closed value to the expected experimental sub-criticality ($K_{eff} \sim 0.97$). Regarding the neutron balance, if we consider the term of neutron loss by capture, ENDF/B-VI based results show +15% difference compared to JEF-2.2 based results.

The source efficiency is a direct coupling factor between the fundamental mode multiplication and the intensity of the external neutron source; it relates the external source neutron multiplication to the multiplication of neutrons from an average fission. [7] The relative source efficiency φ*of the source neutron is defined as

$$\varphi^* = \frac{\frac{1-Keff}{Keff}}{\frac{1-Ks}{Ks}}$$

The calculated relative source efficiency values are given in Table 2 and both ENDF/B-VI and JEF-2.2 produce almost the same values.

Regarding ^{235}U fission rate results, two horizontal channels are chosen: East/West and North/South channels. They represent an interest because they are passing through different material zones in the core, so the data influence on ^{235}U fission rates in these material zones can be seen. ^{235}U fission rate values are normalised, so that the sum is equal to 1 for each channel.

As shown in Figures 1 and 2, for the East/West horizontal channel, results based on JEF-2.2 and ENDF/B-VI data show discrepancies less than ±4.5% for ^{235}U fission rate in the MOX fuel and lead zones, but the discrepancies become larger in the reflector and shielding zones (up to ±10% and ±15% respectively). The main components are Fe and Na in the reflector zone and Fe in the shielding zone.

For the North/South horizontal channel, the maximum discrepancy is ± 2.2% in the reflector zone and this value decreases to ±1% in the fuel zone.

Figure 1. **^{235}U fission rate in channel “East West”**

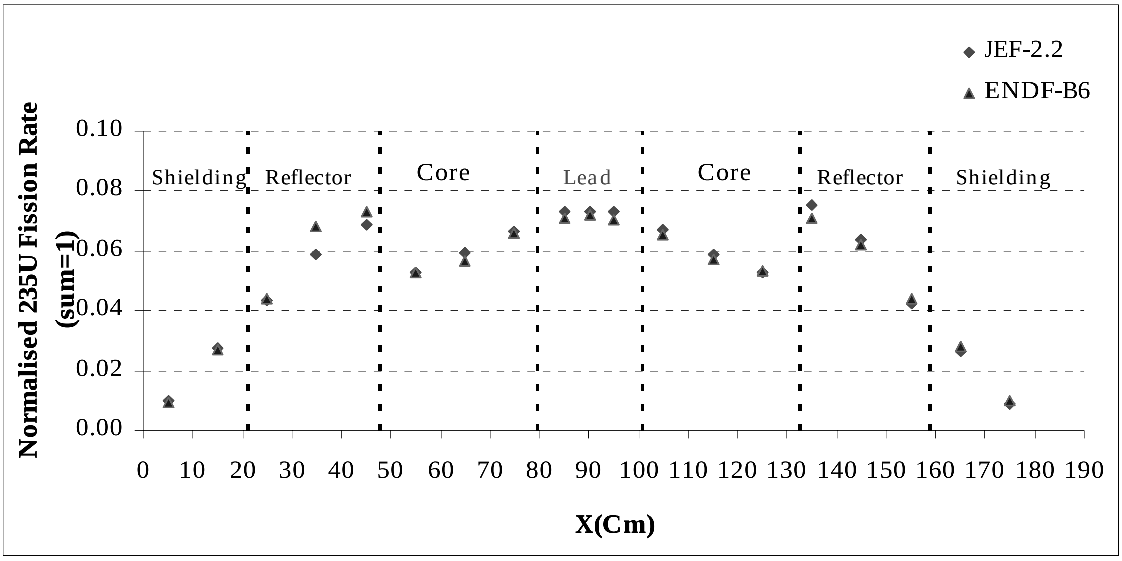
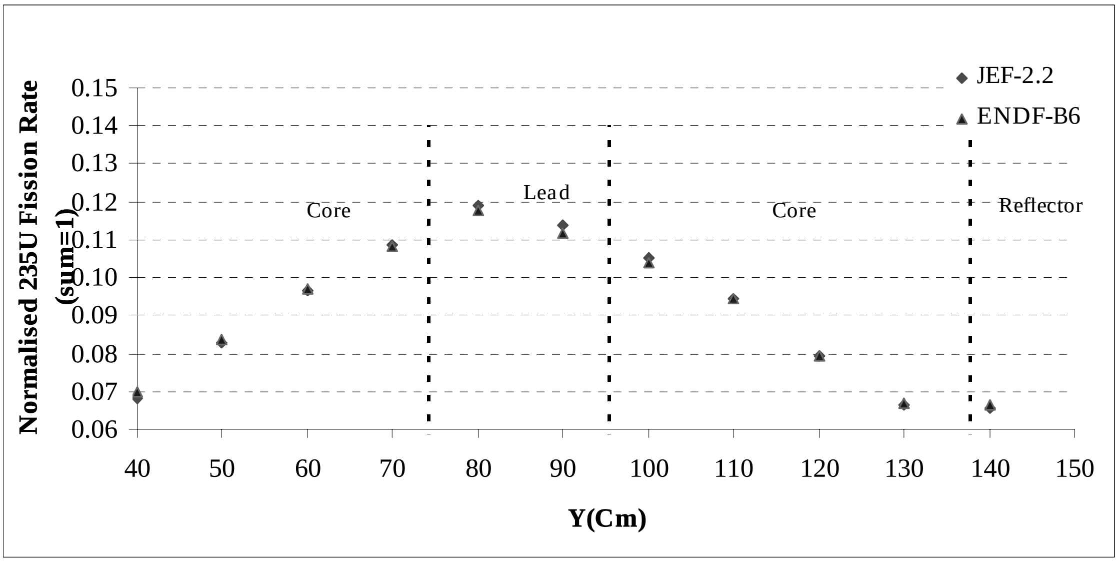


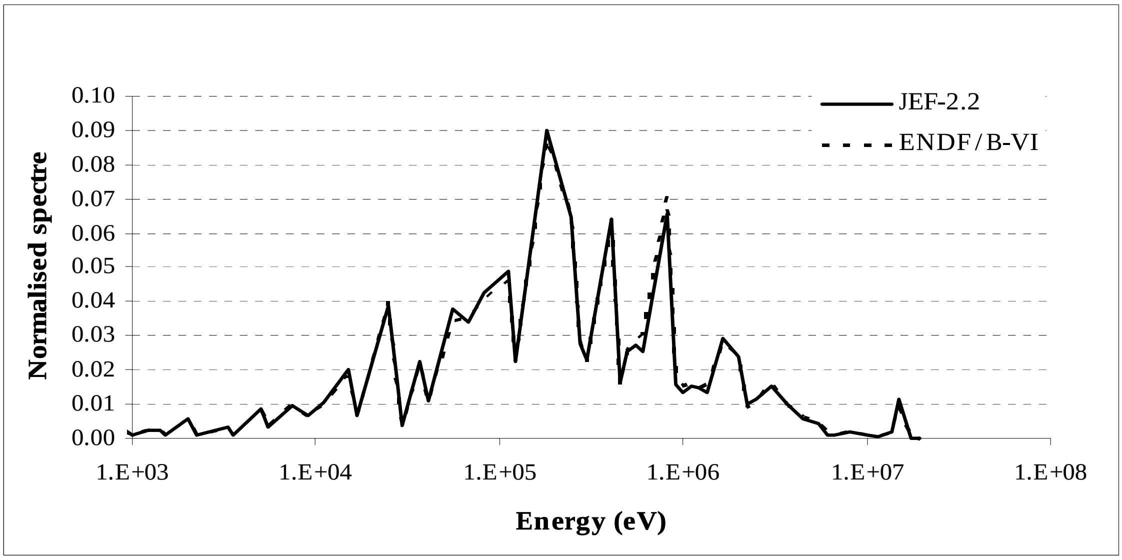
Figure 2. **^{235}U fission rate in channel “North-South”**



In general, for both channels, the ^{235}U fission rates show good agreement in the fuel zone with both ENDF/B-VI and JEF-2.2 evaluations.

The spectra, shown in Figure 3, are normalised so that the total flux is equal to 1. Nuclear data did not show a significant influence on the spectra, although slight differences are observed in some energy ranges (E~100 keV). It is interesting to note that, for both evaluations, the neutron surplus appears in the energy range (E>10MeV) due to the external source (d,T) which generates neutrons with the energy range between 15.24 MeV and 13.1 MeV.

Figure 3. **Neutron spectra in channel “East-West”**



Summarising remarks

In this paper, related to the MUSE-4 benchmark, main results obtained from the MCNP calculations were summarised. The analysis of results was essentially focused on Step 3 calculation results. However, since the experimental data are not available yet for Step 3, only a comparison between calculated results obtained with both ENDF/B-VI and JEF-2.2 was made.

With regard to K*eff* and K*source* values, the differences between ENDF/B-VI and JEF-2.2 based results are less than 500 pcm and 300 pcm, respectively. However, ENDF/B-VI data produce a larger value for the two parameters. As for the source efficiency, both data sets give almost the same values.

Concerning calculated ^{235}U fission rates in the East/West and North/South horizontal channels, the results based on the two data libraries show a good agreement in the fuel zone, but the discrepancies between them become larger in the reflector and the shielding zones.

The measurements of main neutronics parameters in the MUSE-4 sub-critical configuration “SC2” are foreseen for 2003. After the completion of experimental measurements, a more comprehensive analysis and comparison of calculated results against experimentally measured data will be undertaken to understand better the origin of the discrepancies observed.

REFERENCES

[1] D. Villamarín, R. Soule and E. González (2001), *Benchmark on Computer Simulation of MASURCA Critical and Sub-critical Experiments (MUSE-4 Benchmark)*, OECD/NEA document, NEA/SEN/NSC/WPPT(2001)5.

[2] J.F. Briesmeister (2000), Editor, *MCNP – A General Monte Carlo N-Particle Transport Code – Version C*, Los Alamos National Laboratory Report LA-13709-M.

[3] C. Nordborg and M. Salvatores (1994), *Status of the JEF Evaluated Data Library, Proceedings of Int. Conf. on Nuclear Data for Science and Technology*, Gatlinburg, TN, USA, p. 680.

[4] H. Wienke (2001), *Production and Resting of Vitamin-B6 Multi-group Coupled Neutron/photon and MCNP-Compatible Continuous-Energy* Cross-section *Libraries, based upon Various Evaluated Cross-section Data Files*, SCK•CEN report, BLG 889, August.

[5] R. Soule, W. Assal and D. Villamarin (2001), *Geometrical and Physical Data Associated to the MUSE-4 Reference Configuration*, CEA report, NT-SPEx-LPE-01-015.

[6] R. Soule, private communication.

[7] K. Tucek *et al.* (2001), *Source Efficiency in an* Accelerator-driven *System with Burnable Absorbers*, Proceedings of Int. Conf. on Back-end of the Fuel Cycle: From Research to Solutions, Global(2001), September 9-13, Paris, France.