VERIFICATION OFENDF/B-VII.0, ENDF/B-VII.1 AND JENDL-4.0 NUCLEAR DATA LIBRARIES FOR CRITICALITY CALCULATIONS USING NEA/NSC BENCHMARKS

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1. Introduction

Increased installation of thermal neutron energy systems (PWR, LWR, BWR) could lead to possible depletion of uranium resources and not negligibly, it produces tonnes of radioactive spent fuel.A key to solve this issue could be the operation of fast neutron reactors. Reliable calculation tools are very important in terms of design and development of experimental reactors for new generation of nuclear reactors. The possibility to perform correct calculations is always connected to the quality of available nuclear data libraries. In order to create a gas-cooled fast reactor (GFR) model using MCNP code, precise from the reactor physics view, we had to at first verify the calculation code installation at our computer system and also to verify nuclear data libraries selected for our calculation. We chose the up-to-date data libraries from Brookhaven National Laboratories: ENDF/B-VII[1],[2] and from Japanese Nuclear Data Committee: JENDL-4.0[3].

2. Calculation code

In the calculation, the MCNP5[4]version 1.60 was used. MCNP5 is a general-purpose Monte Carlo radiation transport code for modelling the interaction of particles (neutrons) with matter. Its greatest advantage is the ability to model three-dimensionally the core and the reactor structures. Further it uses continuous neutron energy spectra in the neutron transport calculation. For reaction calculations, established evaluated data files (continuous energy neutron cross-section libraries) are used. This code enables calculations of neutron flux per surface or volume element in criticality or fix source mode.

3. Nuclear data libraries

Nuclear data represents measured (or evaluated) probabilities of various physical interactions involving the nuclei of atoms. It is used to understand the nature of such interactions by providing the fundamental input to many models and simulations, such as fission and fusion reactor calculations, shielding and radiation protection calculations, criticality safety, nuclear physics research et al.It groups all experimental data relevant for nuclear physics and nuclear applications. It includes a large number of physical quantities, like reaction cross sections (which are generally functions of energy and angle), nuclear structure and nuclear decay parameters, etc. It can involve neutrons, protons, deuterons, alpha particles, and most of the nuclear isotopes which can be handled in a laboratory. There are three major reasons to need high-quality nuclear data: nuclear safety, theoretical model development of nuclear physics, and applications involving radiation and nuclear power.

With regard to fast reactors, nuclear data are necessary for understanding the physical processes underlying the operation of nuclear power plants (NPP), performing the calculations in optimizing the parameters of reactors and NPPs as a whole, solving external fuel cycle problems, and deciding on alternative lines of development of nuclear engineering. Nuclear data with the required accuracy are needed, since errors lead to indeterminacy in predicting the reactor parameters. Broad indeterminacies, in turn, lead to large and expensive allowance margins in planning. The data accuracy must be improved still further.

The following should be noted to understand the transition from the accuracy of estimated nuclear data to experimental arrangement requirements. In order to satisfy the requirements imposed on nuclear data, it is necessary to improve the accuracy of individual experiments by analyzing and eliminating errors to the maximum extent possible and also develop new experimental methods. The fact is that systematic errors are revealed only by comparing results obtained by means of different methods[5].

ENDF/B-VII.0

The Evaluated Nuclear Data Files (ENDF) libraries are a collection of documented data evaluations stored in a defined computer-readable format that can be used as the main input to nuclear data processing programs. ENDF/B-VII.0 was released by the U.S. Cross Section Evaluation Working Group (CSWEG) in December 2006. It contains data primarily for reactions with incident neutrons, protons, and photons on almost 400 isotopes, based on experimental data and theory predictions.

The principal advances over the previous ENDF/B-VI library are the following: (1) New cross sections for U, Pu, Th, Np and Am actinide isotopes, with improved performance in integral validation criticality and neutron transmission benchmark tests; (2) More precise standard cross sections for neutron reactions on H, ^{6}Li, ^{10}B, Au and for ^{235,238}U fission, developed by a collaboration with the IAEA and the OECD/NEA Working Party on Evaluation Cooperation (WPEC); (3) Improved thermal neutron scattering; (4) An extensive set of neutron cross sections on fission products developed through a WPEC collaboration; (5) New methods for uncertainties and covariances, together with covariance evaluations for some sample cases; etc.[1].

ENDF/B-VII.1

The ENDF/B-VII.1 library is the latest recommended evaluated nuclear data file for use in nuclear science and technology applications, and incorporates advances made in the five years since the release of ENDF/B-VII.0. These advances focus on neutron cross sections, covariances, fission product yields and decay data, and represent work by the US CSEWG in nuclear data evaluation that utilizes developments in nuclear theory, modeling, simulation, and experiment.

The principal advances in the new library are: (1) An increase in the breadth of neutron reaction cross section coverage, extending from 393 nuclides to 423 nuclides; (2) Covariance uncertainty data for 190 of the most important nuclides, as documented in companion papers in this edition; (3) R-matrix analyses of neutron reactions on light nuclei, including isotopes of He, Li, and Be; (4) Modifications to thermal neutron reactions on fission products (isotopes of Mo, Tc, Rh, Ag, Cs, Nd, Sm, Eu) and neutron absorber materials (Cd, Gd); (5) Improved minor actinide evaluations for isotopes of U, Np, Pu, and Am and an adoption of JENDL-4.0 evaluations for isotopes of Cm, Bk, Cf, Es, Fm, and some other minor actinides; (6) Fission product yield advances for fission-spectrum neutrons and 14 MeV neutrons incident on ^{239}Pu; etc.

Integral validation testing of the ENDF/B-VII.1 library is provided for a variety of quantities: For nuclear criticality, the VII.1 library maintains the generally-good performance seen for VII.0 for a wide range of MCNP simulations of criticality benchmarks, with improved performance coming from new structural material evaluations, especially for Ti, Mn, Cr, Zr and W. For Be we see some improvements although the fast assembly data appear to be mutually inconsistent. Actinide cross section updates are also assessed through comparisons of fission and capture reaction rate measurements in critical assemblies and fast reactors, and improvements are evident[2].

JENDL-4.0

The fourth version of the Japanese Evaluated Nuclear Data Library has been produced in cooperation with the Japanese Nuclear Data Committee. In the new library, much emphasis is placed on the improvements of fission product and minor actinide data. Two nuclear model codes were developed in order to evaluate the cross sections of fission products and minor actinides. Coupled-channel optical model parameters, which can be applied to wide mass and energy regions, were obtained for nuclear model calculations. Thermal cross sections of actinides were carefully examined by considering experimental data or by the systematics of neighboring nuclei. Most of the fission cross sections were derived from experimental data. A simultaneous evaluation was performed for the fission cross sections of important uranium and plutonium isotopes above 10keV. New evaluations were performed for the thirty fission-product nuclides that had not been contained in the previous library JENDL-3.3. The data for light elements and structural materials were partly reevaluated. Moreover, covariances were estimated mainly for actinides. The new library was released as JENDL-4.0, and the data can be retrieved from the Web site of the JAEA Nuclear Data Center[3].

4. Selected benchmarks

In many cases, it is entirely necessary to use integral experiments, since the required accuracy of microscopic data may exceed the accuracy attainable in measuring them, and further refinement could entail appreciably greater measurement expenditures. Various benchmarks from the Nuclear Energy Agency (NEA) database [6],[7] are available in order to verify the data libraries. In this paper, two packages of benchmarks were selected: benchmarks for thermal neutron fission and, very important for the development of fast reactors, benchmarks for fast neutron fission.

For calculational analysis of such experiments, special files of cross section data must be prepared that account for Doppler broadening of the resonances in the fuel material and temperature dependence of the thermal scattering law. Cross-section libraries were prepared using NJOY 2012[8].

The first package includes 4 different benchmarks with identification numbers:

- *IEU-COMP-THERM-002* is a benchmark for water-moderated U(17%)O_2 annular rods without absorber and with gadolinium or cadmium absorbers in 6.8-cm-pitch hexagonal lattices at different temperatures.It includes 6 various cases which differ mainly by the use of absorbers, by the number of fuel rods and by the fuel temperature[6].
- *LEU-COMP-THERM-019* is a benchmark for water-moderated hexagonally pitched lattices of U(5%)O_2 stainless steel clad fuel rods. It includes 3 various cases with different critical configuration (pitch value, critical number of fuel rods). Temperature is set to 300K[6].
- *LEU-COMP-THERM-021* is a benchmark for hexagonally pitched partially flooded lattices of U(5%)O_2 zirconium clad fuel rods moderated by water with boric acid. It includes 6 cases with different critical configuration (boric acid concentration, hexagonal pitch, critical height of water and critical number of fuel rods).Temperature is set to 300K[6].

- *LEU-COMP-THERM-026* is a benchmark for water-moderated U(4.92)O_2 fuel rods in 1.29, 1.09, and 1.01 pitch hexagonal lattices at different temperatures. 6 cases in this benchmark have different critical configuration (lattice pitch, number of fuel rods). Temperatures 300 K and 500 K were adopted for the fuel temperatures in the cold and in the hot benchmark models, respectively[6].

  The second package includes 8 integral experiments under handbook names:
- *PU-MET-FAST-006* – Plutonium sphere reflected by normal uranium using FLATTOP[6].
- *PU-MET-FAST-001* – Polyethylene-reflected plutonium metal sphere subcritical noise measurements(17.02 kg, 1.02 wt.% Ga)[6].
- *PU-MET-FAST-002* – ^{240}Pu JEZEBEL: Bare sphere of plutonium-239 metal (20.1 at.%^{240}Pu, 1.01 wt.% Ga)[6].
- *ZPPR-LMFR-EXP-002* – ZPPR-9 (Zero Power Physics Reactor) experiment: A 650 MWe-class sodium-cooled MOX-fueled FBR core mock-up critical experiment with clean core of two homogenous zones[7].
- *ZPPR-LMFR-EXP-002-step3* – ZPPR-9 (Zero Power Physics Reactor) experiment: A 650 MWe-class sodium-cooled MOX-fueled FBR core mock-up critical experiment with clean core of two homogenous zones[9].Step 3 is a central void case in the core where neutron non-leakage term is dominant for the reactivity change by sodium voiding
- *JOYO-LMFR-RESR-001* – Japan's experimental fast reactor JOYO MK-Icore: sodium-cooled uranium=plutonium mixed oxide fueled fast core surrounded by UO_2 blanket[7].
- *ZPR-LMFR-EXP-001* – ZPR-6 assembly 7: A cylindrical assembly with mixed (Pu, U)-oxide fuel and sodium with a thick depleted-uranium reflector[7].ZPR-6/7 was designed to test fast reactor physics data and methods, so configurations in the Assembly 7 program were as simple as possible in terms of geometry and composition.
- *ZPR-LMFR-EXP-002* – ZPR-6 assembly 7 with high Pu-240: A fast reactor core with mixed (Pu, U)-oxide fuel and sodium and high Pu-240 zone[7].

5. Results

MCNP calculations were performed in criticality mode using the k code card to define number of neutrons per cycle, number of active cycles and expected k_{eff} value (see Tab. 1).

Benchmark	Neutrons per cycle	Experimentalk_{eff}	Discarded cycles	Active cycles
IEU-COMP-THERM-002	2000	-	10	510
LEU-COMP-THERM-019	1000	-	50	500
LEU-COMP-THERM-021	1000	-	50	500
LEU-COMP-THERM-026	10000	-	10	1010
PU-MET-FAST-006	1500	1.0000	25	225
PU-MET-FAST-001	5000	1.0000	15	65
PU-MET-FAST-002	2000	1.0000	10	110
ZPPR-LMFR-EXP-002	250000	1.0011	100	1100
ZPPR-LMFR-EXP-002-step3	50000	1.0000	200	4200
JOYO-LMFR-RESR-001	25000	1.0011	100	500
ZPR-LMFR-EXP-001	20000	1.0005	100	600
ZPR-LMFR-EXP-002	20000	1.0008	100	600

Tab. 1*Parameters of benchmark calculations.*

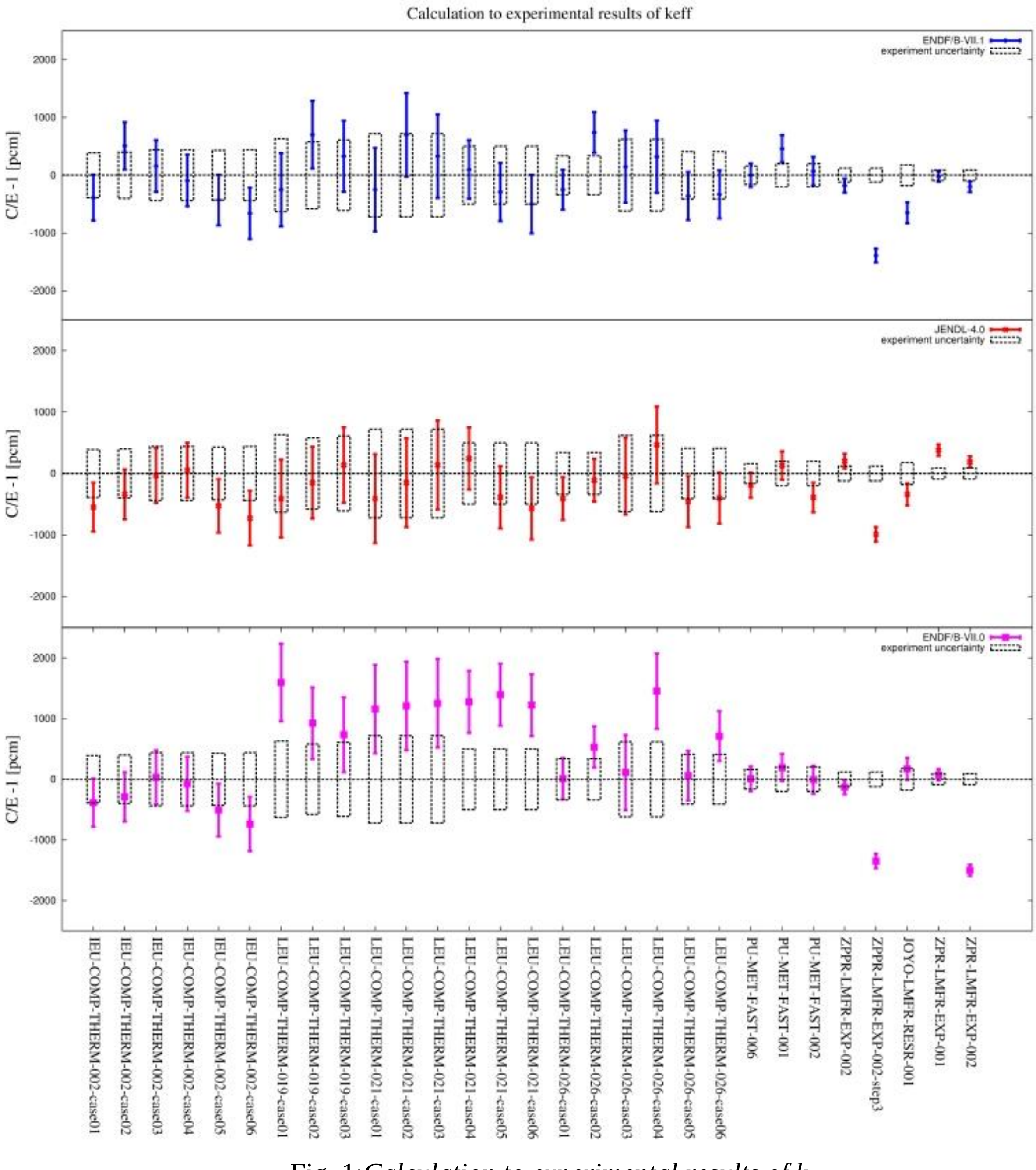

Fig. 1:*Calculation to experimental results of k_{eff}.*

Good agreement of the calculated results with experiment can be found in most of the tasks (see Fig. 1). In particular, the thermal neutron energy benchmarks show positive results (within 1000 pcm). However, two benchmarks (LEU-COMP-THERM-019, LEU-COMP-THERM-021) calculated using ENDF-B/VII.0 data libraries show higher values than expected in all cases, which indicates an error in the calculation. This phenomenon will be further investigated.

The first benchmark IEU-COMP-THERM-002 shows similar course of calculation to experimental results ratio for JEDNL-4.0 and ENDF-B/VII.0, whereas for ENDF-B/VII.1 the results are generally higher and slightly more accurate.

For fast neutron energy benchmarks, the only task which was out of the uncertainty range for all data libraries is ZPPR-LMFR-EXP-002-step3. This could be possibly due to simplifications in the modelling. Results were also quite inconclusive for the ZPR-LMFR-EXP-002(ZPR-6 assembly 7 with high ^{240}Pu content). However, this was still within the uncertainty for the most up-to-date data libraries used – ENDF/B-VII.1 and JENDL-4.0.

6. Conclusions

The paper presents verification of selected nuclear data libraries with the aim to apply them to fast reactor calculations. More precise results were achieved for thermal neutrons calculations. This corresponds with the demand for more precise nuclear data for fast reactors. However, fast neutron calculations show some consistency, in particular between ENDF-B/VII.1 and JENDL-4.0 nuclear data libraries. The results support the idea to prefer using newer ENDF-B/VII.1 instead of the previous version ENDF-B/VII.0. Certainly, there are still some issues to be addressed and there is potential to gain more conclusive results. Although, application of ENDF-B/VII.1 and JENDL-4.0 is expected for further calculations.

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