Romanian Reports in Physics, Vol. 64, No. 1, P. 81–93, 2012

COMPARATIVE CALCULATIONS FOR BENCHMARK PROBLEMS IN HEAVY WATER CELLS*

C. AIOANEI

Institute for Nuclear Research Pitesti,
PO.Box-78, 115400-Pitesti, Romania; E-mail: corina.aioanei@nuclear.ro

Received July 7, 2010

Abstract. The paper presents comparative results for main types of lattice cell calculation performed by using WIMS code, WIMSD5B version. The lattice cell calculations main goal is to obtain the optimal input parameters combination that gives closer results to IAEA measurements. The comparison was made for IAEA benchmark problems applied to heavy water lattices with same sets of configurations. IAEA nuclear data libraries updated in WLUP (WIMS Libraries Updates Project) project were used. The input data have been set from test problems description. Comparisons have been performed for following heavy water cell configuration (contains D_2O both as coolant and moderator): (a) Th5-HW-AECL-ZED2: 19 fuel rod clusters (1/6/12) with ThO_2–UO_2 fuel; single pitch 28 cm hexagonal ThO_2 fuel containing 1.5 wt% enriched UO_2 (93.02 at.% U^{235}), fuel rod diameter 1.153 cm, rod centre radius 0.0/1.468/2.837 cm, fuel material density 9.33 g/cm^3, clad material zircaloy 2, sheath material density 6.55 g/cm^3, temperature 294.8K (all components); (b) UO2-HW-AECL-ZED2: 37 fuel rod clusters (1/6/12/18); single pitch 28.58 cm square UO_2 fuel, fuel rod diameter 1.21 cm, rod centre radius 0.0/1.4885/2.8755/4.3305 cm, fuel material density 10.50 g/cm^3, clad material zircaloy 4, sheath material density 6.55 g/cm^3, temperature 294.8K (all components); (c) Th3–HW-BNL-bnl_thd2o1: eight D_2O moderated subcritical lattices of 3% $^{233}UO_2$–97% ThO_2 rods in hexagonal patterns, fuel rod diameter 1.092 cm, fuel material density 8.9618g/cm^3, clad material zircaloy 2, sheath material density 6.8365g/cm^3, temperature 293 K (all components), lattice pitch 2.170 cm. Lattice calculations were done in order to observe which combination gave closer results to IAEA measurements for effective multiplication constant k-eff, average fission and neutron flux spectra corresponding to 69 and 172 energy group libraries.

Key words: HEAVY WATER lattice cell, benchmark problem, WIMS.

1. INTRODUCTION

The paper presents comparative results for the main types of lattice cell calculation performed by using the available versions of WIMS and DRAGON codes: WIMSD5B and DRAGON 3.05. The comparison was made for IAEA heavy water lattice cell benchmark problems with the same configuration sets.

* Paper presented at the Annual Scientific Session of Faculty of Physics, University of Bucharest, June 18, 2010, Bucharest-Măgurele, Romania.

Main objectives of this work were: a) To test the performance of new IAEA libraries generated by WLUP; b) To compare the results obtained with considered libraries from different primary nuclear data; c) To detect the contradictory trend from results for main materials.

In order to perform the calculations following codes and libraries were used:

1) *WIMS (Winfrith Improved Multigrup Scheme)* – a bi-dimensional physics code which is using multigroup transport theory and collision probability methods to obtain flux distribution, reaction rates in projection of given lattice and the multiplication coefficients k-inf and k-eff. In this approach, the following important approximations were taken into consideration: using of the energy groups – cross sections are complicated functions in energy and is necessary their averaging in same modes over the discrete energy ranges, in the case of actual WIMS nuclear data; simplifications of geometric representations – the real situations are tri-dimensional and our models are bi-dimensional or even one-dimensional. The regions model is divided in discrete spatial meshes which permit the numerical calculations of the neutron flux.

2) In *WLUP (WIMS Library Up-date)* AIEA project, there were obtained new cross sections for libraries versions WIMSD-5B which are available in NEA library. The new versions of libraries are public on AIEA site. In addition to these libraries, the input data for a series of benchmark problems inclusive for heavy water cells are available. Using of WLUP libraries in this contract supposes also modifications on WIMS code source because of materials number increasing.

The results were compared with those corresponding to [1], WIMS input data files being taken from [1], without constructed them by taking into account benchmark problems descriptions [2].

For the proposed calculations the following libraries have been used [1]: IAEA (WIMS library on 69 energy groups); IAEAGX (WIMS library on 172 energy groups); ENDFB7 (WIMS library on 69 energy groups, based on ENDF/B-VII.0 evaluated nuclear data library); ENDFB7GX (a library on 172 energy groups, based on ENDF/B-VII.0 evaluated nuclear data library); JEFF31 (library on 69 energy groups, based on JEFF- 3.1 evaluated nuclear data); JEFF31GX (library on 172 energy groups, based on JEFF- 3.1 evaluated nuclear data library); ENDFB6 (WIMS library on 69 energy groups, based on ENDF/B-VI evaluated nuclear data library); ENDFB6GX (WIMS library on 172 energy groups, based on ENDF/B-VI evaluated nuclear data library); JENDL3 (library on 69 energy groups, based on JENDL-3.2 evaluated nuclear data); JENDL3GX (library on 172 energy groups, based on JENDL-3.2 evaluated nuclear data); JEF22 (library on 69 energy groups, based on JEF-2.2 evaluated nuclear data); JEF22GX (library on 172 energy groups, based on JEF- 2.2 evaluated nuclear data).

The energy structure for the two types of libraries used is: a) WIMS libraries on 69 energy groups: 14 fast groups with the energy range from 9.118eV to 10MeV, 13 resonant groups with the energy range from 4eV to 9.118eV, 42 thermal groups with the energy range from 0 to 4eV; b) the libraries on 172 energy groups: 45 fast groups with the energy range from 9.119eV to 19.64MeV, 47 resonant groups with the energy range from 4eV to 9.119eV, 80 thermal groups with the energy range from 0 to 4eV.

3) *DRAGON* is a 3-dimensional physic code which is using an operational model for reactivity insertion of control devices in reactor core. Through the generation of a usual set of incremental network parameters, these are used in reactor core calculations [3].

The comparisons were made on following configurations with heavy water:

a) Th5–HW-AECL-ZED2 case. Fuel material: ThO_2 (98.5 wt %) – UO_2 (1.5 wt %); Enrichment: 93.0 wt% in ^{235}U; Lattice geometry = Hexagonal; Lattice pitch = 28 cm; Coolant, Moderator: D_2O; Number of fuel rods: 19 (1/6/12), Fuel material density = 9.33 g/cm^3; Radius of rod centers: 0.0/1.468/2.837 cm; Sheath material: Zry-2; Fuel rods radius= 0.5765 cm; Sheath material density = 6.55 g/cm^3; Sheath internal radius = 0.5815 cm; Coolant tube density = 2.7 g/cm^3; Coolant tube internal radius = 3.683 cm; Coolant tube thickness = 0.127 cm; Temperature (all components) = 294.8 K (Fig. 1).

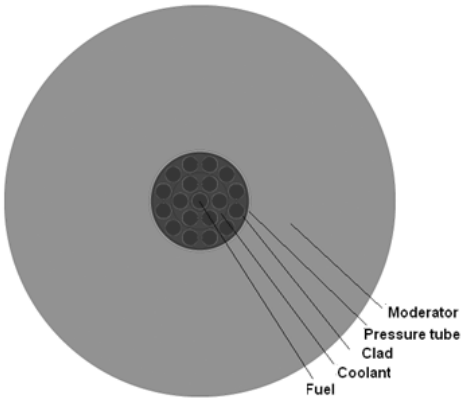


Fig. 1 – Bundle geometry; Th5–HW-AECL-ZED2 problem.

b) UO_2-HW-AECL-ZED2 case. Fuel material: UO2 (nat.); Enrichment: 0.72 wt% in ^{235}U; Lattice geometry = Square; Lattice pitch = 28.58 cm; Coolant, Moderator: D_2O; Number of rods: 37 (1/6/12/18); Fuel material density = 10.50 g/cm^3; Radius of rod centers 0.0/ 1.4885/ 2.8755/ 4.3305 cm; Sheath material Zry-4; Fuel rods radius - central: 0.5965 cm, others: 0.6050 cm; Sheath material density = 6.55 g/cm^3;

Sheath internal radius = 0.61 cm; Pressure and Calandria tubes density= 2.7 g/cm^3; Pressure tube internal radius = 5.195 cm; Calandria tube internal radius = 6.35 cm; Pressure tube thickness = 0.315 cm; Calandria tube thickness = 0.32 cm; Coolant tube thickness = 0.127 cm; Temperature (all components) = 294.8 K (Fig. 2).

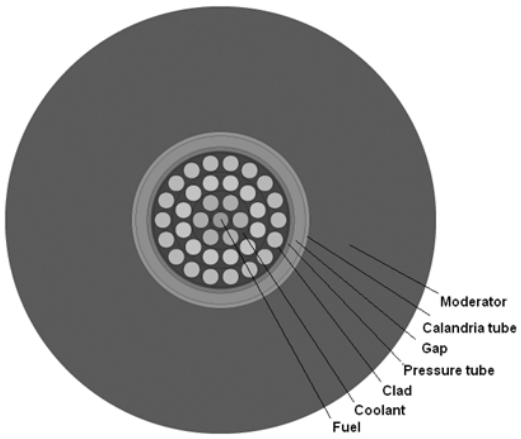


Fig. 2 – Bundle geometry; UO2-HW-AECL-ZED2 problem.

c) Th3-HW-BNL-bnl_thd2o1 case. Fuel material: ThO_2 (97 wt%) – UO_2 (3 wt%); Enrichment: 0 wt% in ^{235}U; Lattice geometry = hexagonal; Lattice pitch = 2.17 cm; Coolant, Moderator: D_2O; Fuel density = 8.9618 g/cm^3; Fuel rods radius = 0.5461 cm; Fuel rod diameter = 1.092 cm; Clad material: Zircaloy 2; Clad density = 6.8365 g/cm^3; Clad outer radius = 0.63373 cm; Clad thickness = 0.08763 cm; Vm/Vf (Moderator Volume/Fuel Volume) in the lattice cell = 3.0047; Temperature (all components) = 293 K (Fig. 3).

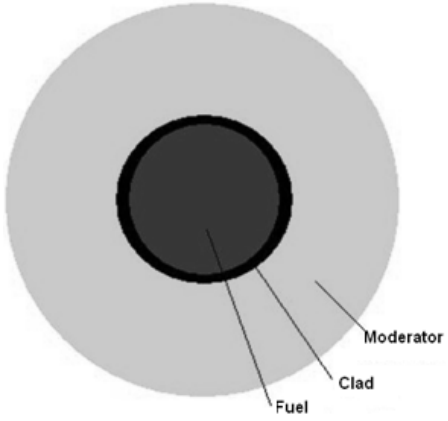


Fig. 3 – Bundle geometry; Th3-HW-BNL-bnl_thd2o1 problem.

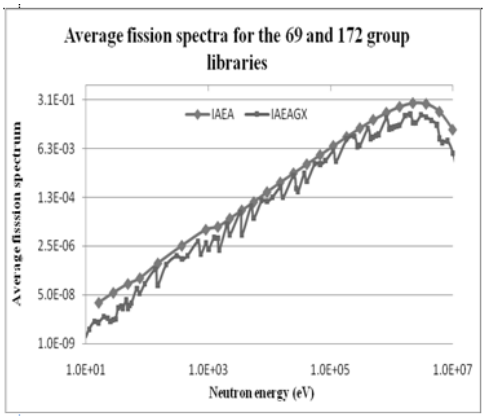
2. THE FISSION SPECTRA

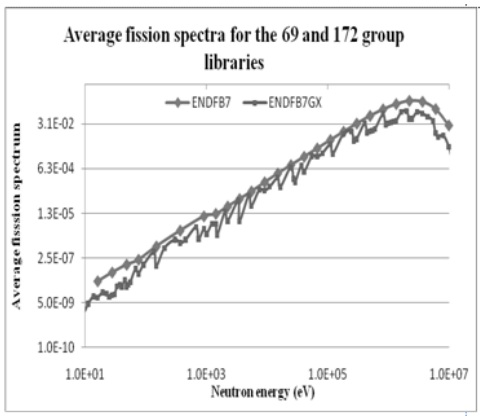
In Figs. 4, 5 and 6 the average fission spectra *versus* the neutron energy for the considered "pairs" of nuclear data libraries (a "pair" is represented by the same library on 69 and 172 energy groups, respectively) are given.

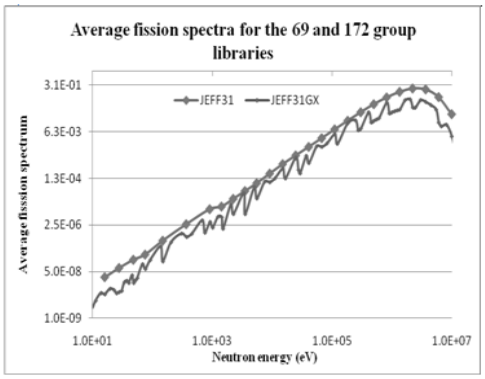
For each case the averaged fission spectra have been compared. Fission spectra characterizing the 172 energy group libraries follow the one characterizing the 69 energy group libraries. From the graphic representations it can be observed that the refinement in 172 energy groups gives to the spectra a shape which is getting closer to the real simulated phenomenon (these oscillations) in opposition with the 69 energy groups case (the spectra is almost flat).

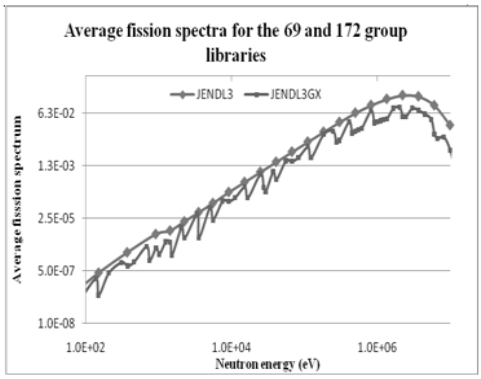
The average fission spectra show a good agreement with those presented in IAEA benchmark problem [1].

a) Th5–HW-AECL-ZED2 case (Fig. 4):









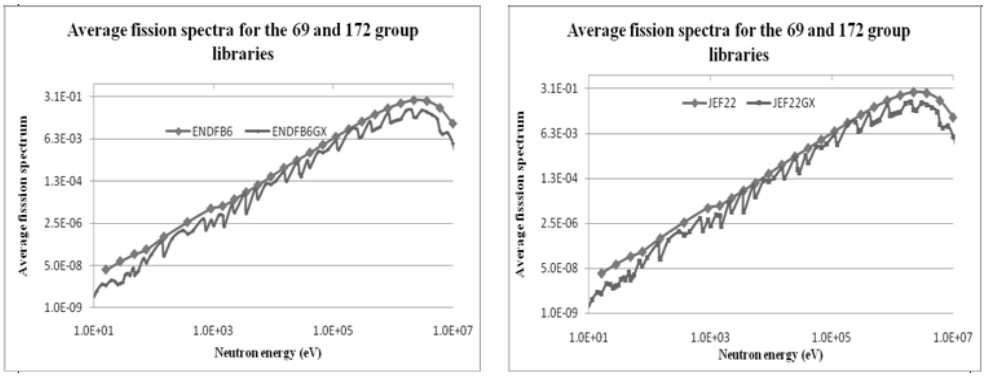
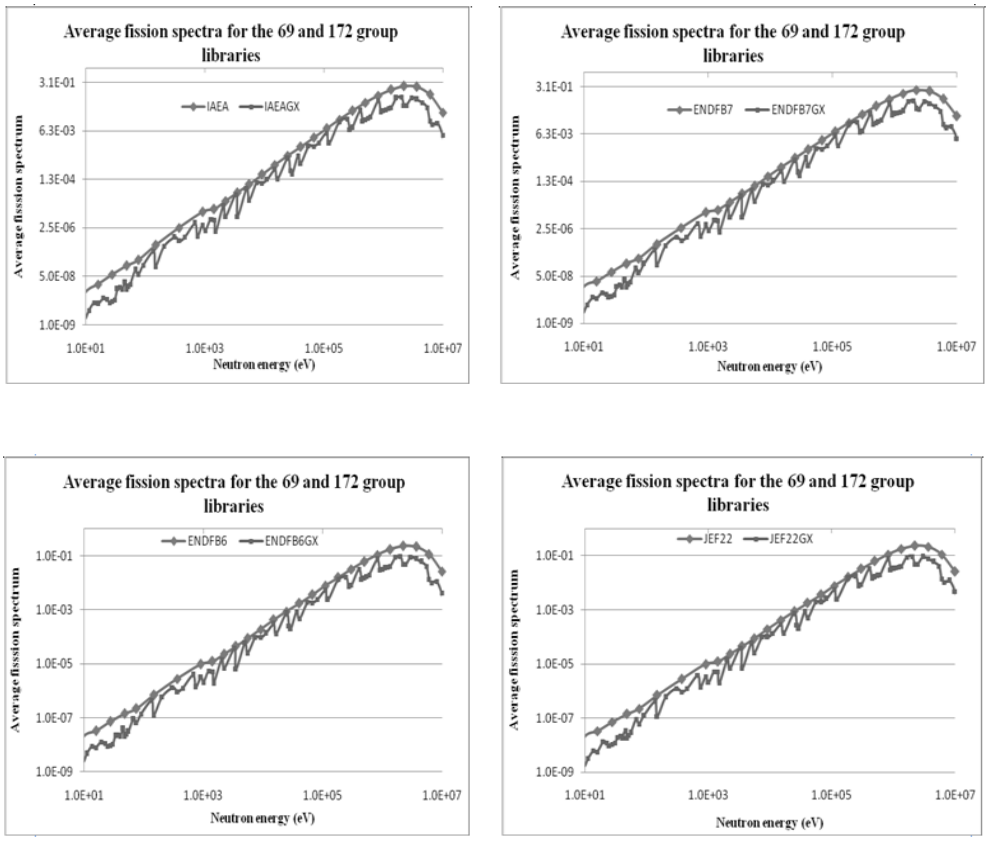


Fig. 4 – Average fission spectra; Th5–HW-AECL-ZED2 case; WLUP considered libraries.

b) UO_2-HW-AECL-ZED2 case (Fig. 5):



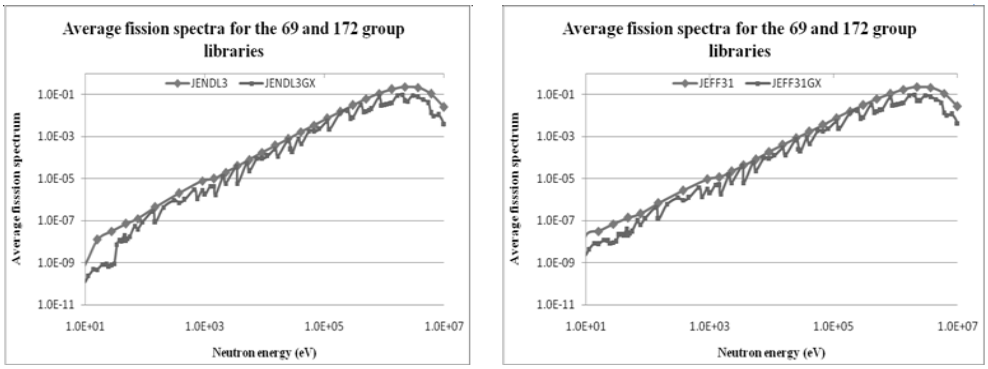
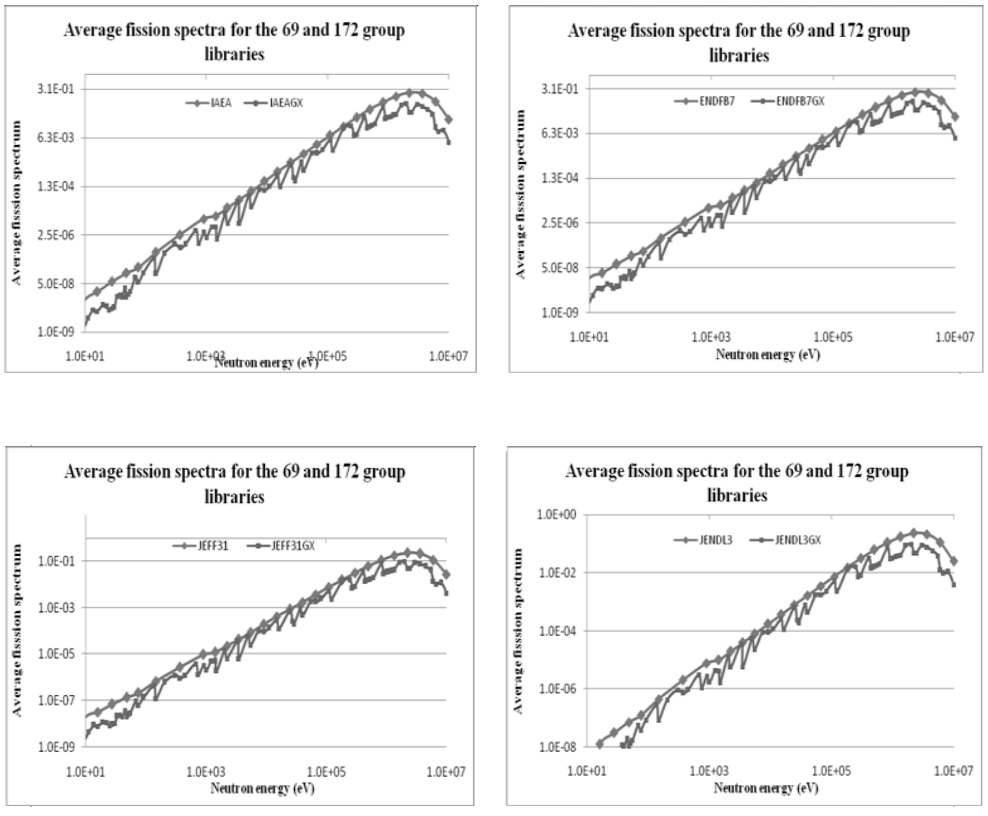


Fig. 5 – Average fission spectra; UO2-HW-AECL-ZED2 case; WLUP considered libraries.

c) Th3-HW-BNL-bnl_thd2o1 case (Fig. 6):



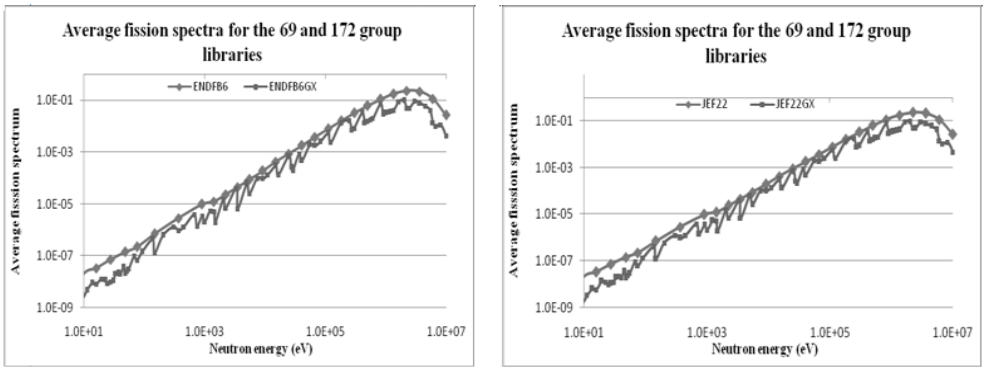


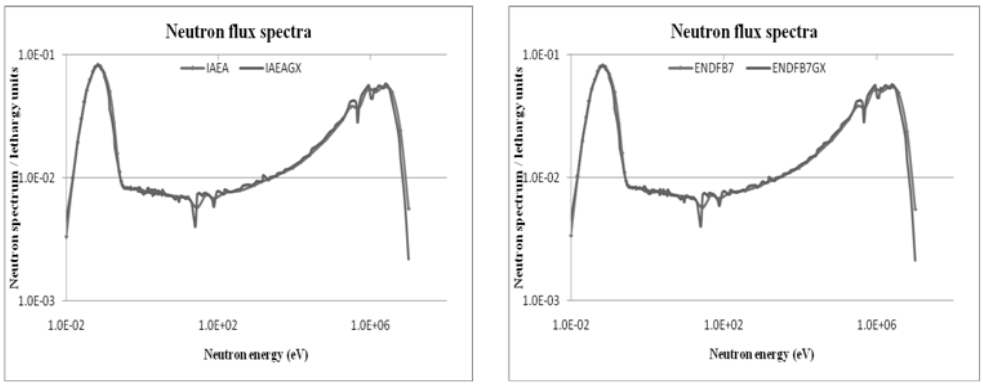
Fig. 6 – Average fission spectra; Th3-HW-BNL-bnl_thd2o1 case; WLUP considered libraries.

3. THE NEUTRON FLUX SPECTRA

In Figs. 7, 8 and 9 the neutron flux spectra for the considered cases are given. Likewise in the case of average fission spectra, in the neutron flux spectra, it can be observed an increasing of irregularities from 69 energy group libraries to the 172 energy group libraries.

These spectra are represented in the considered lattice cells as function of energy and give us the moderating mode of neutrons. Also, this refinement is a qualitative leap for the analysis of interest parameters in diffusion codes, particularly for resonant energy region where a special treatment is requested.

a) Th5–HW-AECL-ZED2 case (Fig. 7):



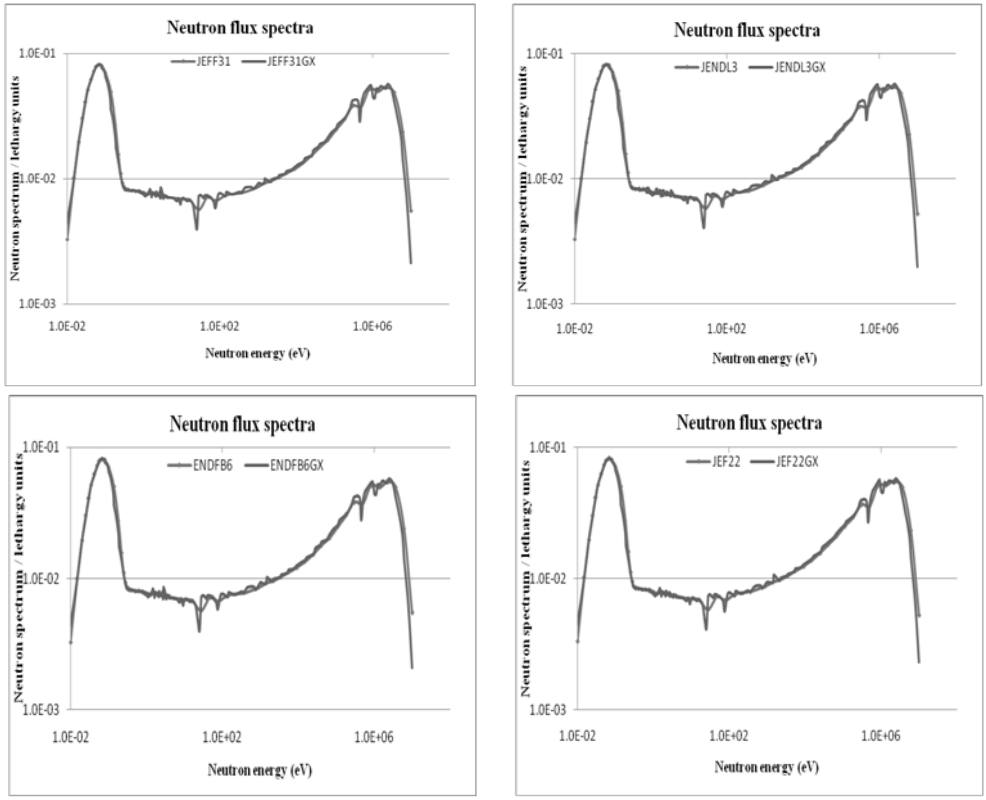
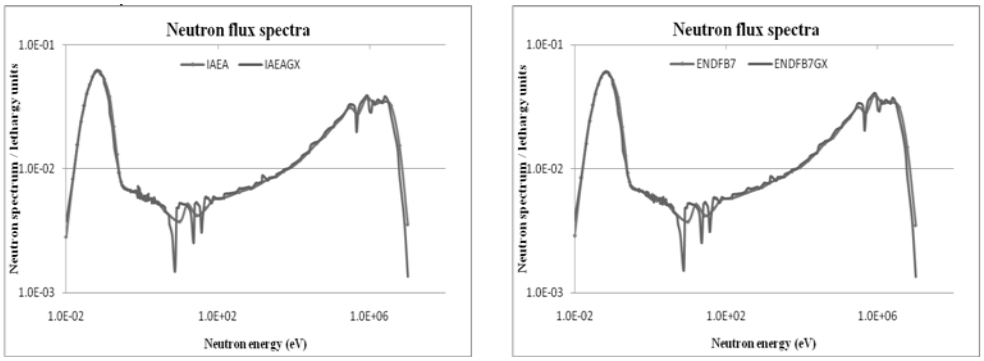


Fig. 7 – Neutron flux spectra; Th5–HW-AECL-ZED2 case; WLUP considered libraries.

b) UO_2-HW-AECL-ZED2 case (Fig. 8):



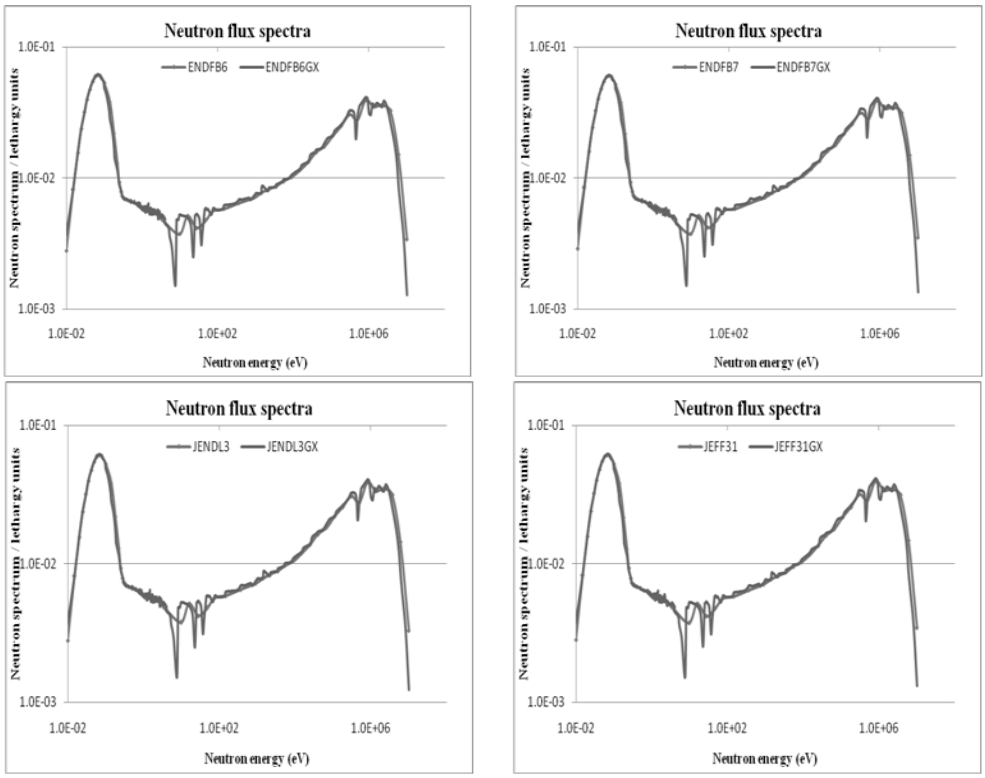
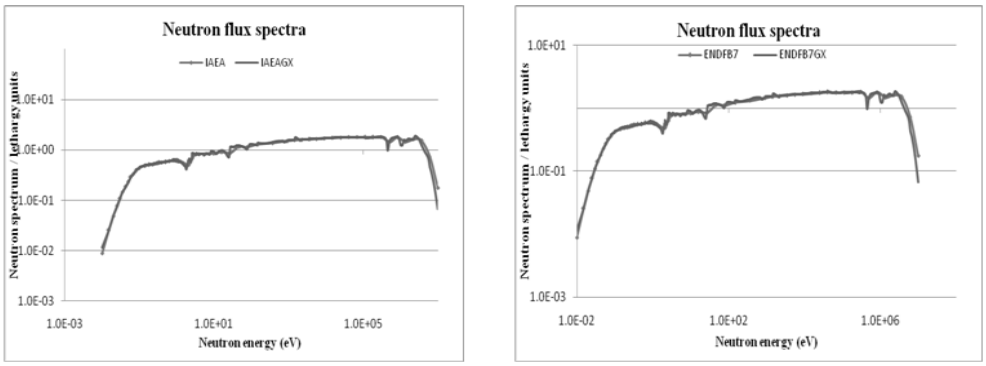


Fig. 8 – Neutron flux spectra; UO2-HW-AECL-ZED2 case; WLUP considered libraries.

c) Th3-HW-BNL-bnl_thd2o1 case (Fig. 9):



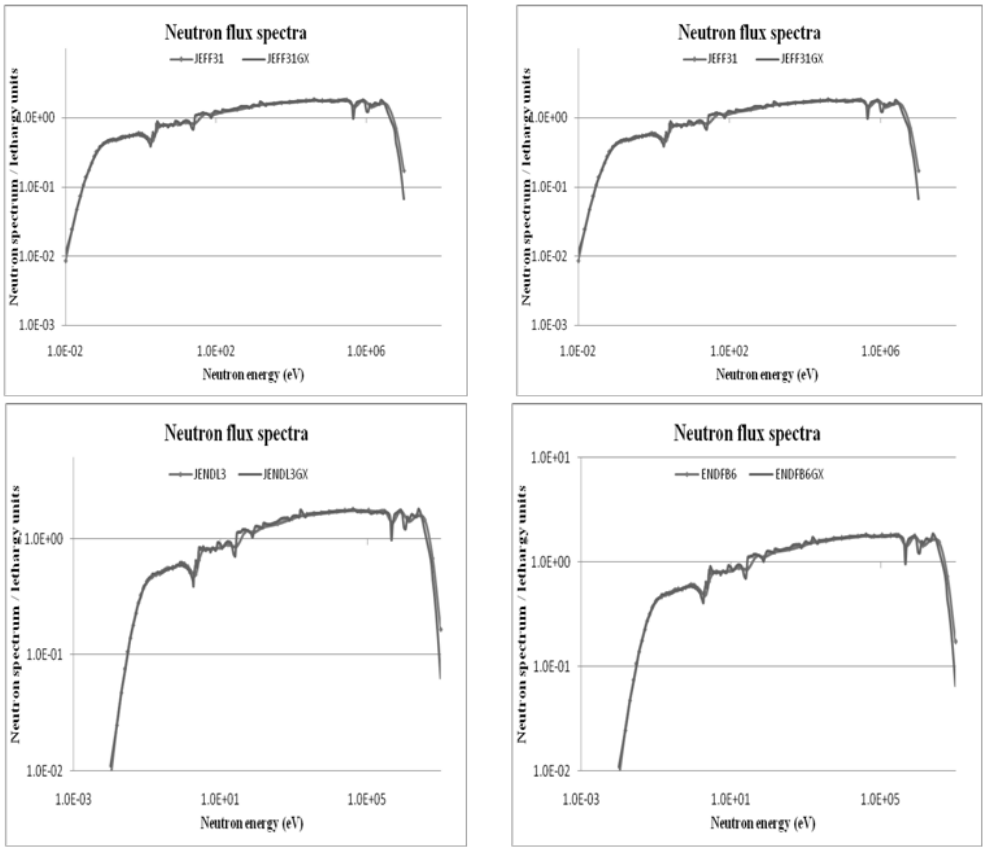


Fig. 9 – Neutron flux spectra; Th3-HW-BNL-bnl_thd2o1 case; WLUP considered libraries.

4. RESULTS AND DISCUSSIONS

There are 2 sequences for benchmark problems: standard and supplementary. The standard sequence of tests includes a set of benchmarks that can be analyzed using codes. A supplementary sequence of benchmarks may require additional processing such as cross-section homogenization, whole core calculations, etc.

The standard sequence of benchmarks is classified in two categories:

– Criticality experimental benchmarks (main parameter compared: k-eff);

– Burn up benchmarks (main parameters compared: isotopic concentrations of actinides and fission products as a function of burn up).

In Tables 1 and 2 the calculated values for k-eff and k-inf, in two of the considered cases, by using WIMS and DRAGON codes calculations, are presented.

A maximum deviation value of Δρ = 0.45052 mk in the multiplication coefficient k-eff corresponding to WIMS calculations and Δρ =2.74125 mk in k-inf between WIMS and DRAGON codes calculations were obtained.

Table 1

k-eff and k-inf results for WIMS and DRAGON calculations; Th5–HW-AECL-ZED2 case

LATTICE	*BENCHMARK*	*WIMS*	Δρ (mK)	*WIMS*	*DRAGON*	Δρ (mK)
	K_{eff}	K_{eff}		K_{inf}	K_{inf}	
IAEA	1.00536	1.00525	0.11082	1.09516	1.09747	1.92528
ENDFB7	1.00684	1.00679	0.04637	1.09606	1.09871	2.19721
JEFF31	1.00472	1.00447	0.24772	1.09374	1.09649	2.29139
JENDL3	1.00298	1.00253	0.44355	1.09193	1.09495	2.52591
ENDFB6	1.00123	1.00116	0.06584	1.09069	1.09315	2.06830
JEF22	1.00515	1.00491	0.24057	1.09368	1.09626	2.14603
IAEAGX	1.00719	1.00716	0.02662	1.09704	1.09848	1.19826
ENDFB7GX	1.00870	1.00863	0.07372	1.09786	1.09980	1.60673
JEFF31GX	1.00660	1.00634	0.26161	1.09556	1.09760	1.69316
JENDL3GX	1.00475	1.00433	0.41720	1.09367	1.09602	1.96466
ENDFB6GX	1.00300	1.00295	0.05169	1.09242	1.09418	1.46657
JEF22GX	1.00706	1.00712	0.05620	1.09591	1.09763	1.42987

Table 2

k-eff and k-inf results for WIMS and DRAGON calculations; UO2-HW-AECL-ZED2 case

LATTICE	*BENCHMARK*	*WIMS*	Δρ (mK)	*WIMS*	*DRAGON*	Δρ (mK)
	K_{eff}	K_{eff}		K_{inf}	K_{inf}	
IAEA	1.00536	1.00525	0.11082	1.09516	1.09747	1.92528
ENDFB7	1.00684	1.00679	0.04637	1.09606	1.09871	2.19721
JEFF31	1.00472	1.00447	0.24772	1.09374	1.09649	2.29139
JENDL3	1.00298	1.00253	0.44355	1.09193	1.09495	2.52591
ENDFB6	1.00123	1.00116	0.06584	1.09069	1.09315	2.06830
JEF22	1.00515	1.00491	0.24057	1.09368	1.09626	2.14603
IAEAGX	1.00719	1.00716	0.02662	1.09704	1.09848	1.19826
ENDFB7GX	1.00870	1.00863	0.07372	1.09786	1.09980	1.60673
JEFF31GX	1.00660	1.00634	0.26161	1.09556	1.09760	1.69316
JENDL3GX	1.00475	1.00433	0.41720	1.09367	1.09602	1.96466
ENDFB6GX	1.00300	1.00295	0.05169	1.09242	1.09418	1.46657
JEF22GX	1.00706	1.00712	0.05620	1.09591	1.09763	1.42987

The results are in good agreement with the reference, taken into consideration that the exact material compositions, heavy water purity and information about spacers are not available for the public.

The differences presented above can be also explained by the absence of Sn nuclear data from our data libraries. The difference smaller than 3mk met in DRAGON code calculations relative to WIMS code calculations is due to the lack of leakage in the code treatment applied for the diffusion.

The good agreement in fission spectra and critical parameters for the considered WLUP libraries confirms the validity of our method of calculation.

REFERENCES

1. *** WIMS Library Update Project (WLUP); http://www-nds.iaea.org.
2. ****WIMS-D LIBRARY UPDATE*, International Atomic Energy Agency, 2007.
3. G. Marleau, A. Hébert, R. Roy, A User Guide for DRAGON3.05c, IGE–174 rev. 6c, Institut de Génie Nucléaire, École Polytechnique de Montréal, 2006.