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Effect of updated WIMSD libraries on neutron energy spectrum at irradiation site of Pakistan Research Reactor-1 using 3D modeling

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Abstract

International Atomic Energy Agency (IAEA) has recently released new WIMSD libraries based on current cross-section evaluations. Using these libraries the effect of different evaluated data sets on effective multiplication factor and neutron energy spectrum was studied with the help of 3D reactor simulation code CITATION. Simulation methodology adopted in this work was validated by analyzing IAEA 10 MW benchmark reactor.

The k_{eff} values obtained using all newly released libraries are within 0.45% to the experimental value, while the old library released in 1981 resulted in calculated value 1.05% larger than experimental. The flux spectrum obtained for standard fuel element using 3D modeling is smaller in fast energy range and higher in thermal energy range than is calculated using the 1D model for the standard cell. In the flux trap, differences of about −4% to 13% were found in thermal flux using the newly released libraries as compared to that obtained using 1981 WIMSD library. The major differences in the flux spectra between newly available libraries and the 1981 WIMSD library in thermal energy range are due to the differences in cross-sections of hydrogen bound-in-water. The use of only newly available cross-sections of hydrogen bound-in-water with 1981 WIMSD library resulted in significant improvement in value of k_{eff} as well as in the flux spectrum. Moreover the differences among new libraries in the thermal

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energy range are also due to these cross-sections. Difference in fission spectra from different libraries is responsible for differences of flux spectra in the fast energy range. These differences in flux are reduced significantly in the fast energy range by only replacement of fission spectra.

1. Introduction

The nuclear reaction cross-section data is one of the most important parameters required for theoretical simulations in the field of reactor physics and nuclear engineering and design. Since there does not exist any simple relationship for these cross-sections, so huge efforts are required to obtain estimates for cross-section data of various materials. For safe operation of research and power reactors this data has to be obtained and validated integrally by experiments and theoretical calculations. The work on upgradation of cross-section data have been continuously carried out by several centers in USA, UK, Japan, Russia and China etc. and the data files are upgraded in standard ENDF-6 formats. The recent evaluated nuclear data files include Evaluated Nuclear Data File ENDFB-VI Release 8, Japanese Evaluated Nuclear Data Library JENDL-3.2 (Nakagawa et al., 1995), Joint Evaluated File JEF-2.2 (IAEA, 1993), USSR Evaluated Nuclear Data Library BROND (Manokhin, 1989) and Chinese Evaluated Nuclear Data Library CENDL-2 (IAEA, 1997) etc. The effects of data from different sources have also been analyzed using different codes and standard benchmark problems. The most frequently used data files for benchmark calculations are different versions of ENDFB, JENDL and JEF data files. Usually Monte Carlo simulation codes have been used for simulations of these benchmarks (Kahler, 2003; Ravnik and Jeraj, 2003; Okumura and Mori, 2003; Elam and Rearden, 2003; Santos et al., 2001). Although accurate reference solutions for specific reactor physics problem can be obtained using stochastic techniques employed in Monte Carlo methods, they are still very computation intensive to provide a full range of solutions for reactor performance or transient analysis where variations in many parameters such as temperatures, densities and pressure must be considered. There is still a central role in these types of analyses for deterministic methods.

Winfrith Improved Multigroup Scheme version-D (WIMS-D) is one of the widely used deterministic computation tools for basic reactor physics computations including burnup calculations in a wide variety of reactor types. It is a general purpose 1D multigroup neutron transport theory code used to simulate the lattice cell of variety of geometries. It calculates cell averaged group constants, such as diffusion coefficients, absorption and fission cross-sections, and scattering matrix for a given number of energy groups. The infinite multiplication factor is computed for the cell, and if buckling is provided calculation of effective multiplication factor is also done. In its calculations WIMS-D uses a library which provides the knowledge of the various relevant neutron–nuclear reaction cross-sections in the form of multigroup library. It contains information about number of fast, resonance and thermal groups, their

energy boundaries, fission spectrum, burnup data for each nuclide in the library, microscopic cross-sections, resonance tabulation and P_1 scattering for principal moderators like hydrogen, graphite etc. Using this library, the code first computes cell averaged parameters with simplified geometric representation for all library groups, and then using these cell averaged parameters condensed cross-sections for specified number of groups are computed with detailed geometry. The code also performs two group calculations (fast and thermal energy groups) of all above mentioned parameters. The D4 version of the code was released initially in 1981 with its 69 group UK origin library having 14 fast, 13 resonance and 42 thermal groups. Due to its availability and versatility WIMS-D4 has been used widely by laboratories worldwide for research, analysis and design of various types of research and power reactors, especially in developing countries. The code has also been frequently used for analysis of Pakistan Research Reactor-1 (PARR-1). The past analyses include core neutronics, conversion from HEU to LEU fuel, thermal hydraulics, transient analysis, and determination of the neutron energy spectrum (Aslam and Ahmad, 2002; Malkawi and Ahmad, 2001). The available cross-section library released initially with WIMS-D4 from UK was used in these calculations. Since the cross-section data in this library was based on very old evaluations, so there was a need to prepare a library which contains recent cross-section data to enable scientists and reactor designers to make use of the most recent evaluated nuclear data files for research and power reactor calculations. Since WIMS-D4 requires this data in its typical library format, different laboratories have developed the WIMS-D4 library in upgraded forms, or new libraries were established for special purposes (Schwerer and Lemmel, 2002; Jasiulevicius, 2003; Mufiz-ur-Rahman and Takano, 2001), but none of these libraries is available easily or free of cost. International Atomic Energy Agency (IAEA) has conducted a project "WIMSD Library Update Project (WLUP)" for processing of basic nuclear data files in WIMS-D4 multigroup library format, and its integral validation by analyzing several selected benchmark reactors. As a result of this coordinated project a number of WIMSD libraries (WLUP, 2001) are made available freely via WLUP web page in ASCII form. Utility code for conversion from ASCII to binary format is also available via same web page. These libraries were developed by processing data from different newly released basic evaluated cross-section data files, mainly ENDF/B-VI.8, JENDL-3.2 and JEF-2.2, CENDL-3.2 and Russian Evaluated Data Library FOND-2.2 (Koscheev et al., 2001). Some other reaction data, e.g., dosimetry data for different materials was taken from evaluated nuclear data file JENDL/D-99, with missing information from point-wise version of ENDF/B-VI.7. Not only the cross-sections updated in previous version of the library, but several new materials are also added into these libraries. Table 1 gives sources of IAEA library data for some important materials from different neutron data files in development of IAEA libraries. The fission spectrum for IAEA library was computed by averaging out isotope spectra of ^{235}U, ^{238}U and ^{239}Pu with weights 54%, 8% and 38%, respectively (Leszczynski et al., 2003).

After release of different WIMSD libraries by IAEA based on recent cross-section data, it is necessary to study the effect of new cross-sections on different reactor physics parameters of the operating reactors. We have already studied the effect of these

Table 1
The number of materials used in development of WIMSD IAEA libraries from different source files

Source data file	Material
ENDFB/VI.8	H bound in H_2 O, O, Si, Al, C and ^{235}U
CENDL-2.1	^{238}U
FOND-2.2	^{239}Pu

libraries on the multiplication factor and energy spectrum of a typical material test reactor by performing only 1D lattice calculations from WIMS-D4 code directly (Ahmad et al., 2004). There are several limitations in 1D modeling, due to which we can only calculate core average parameters. Moreover, 1D calculation ignores the presence of excess water and structural materials present in the core as these also affects the flux spectrum. More accurate model is needed to determine the flux pattern at certain location in the core, e.g., at irradiation sites.

Validation studies based on the analysis of discrepancies between calculated and measured reactor properties play a central role in the process leading to the improvement of reactor physics codes and their associated nuclear data libraries, as well as to the assessment of the accuracy of calculations. The nuclear data libraries can be adjusted to reduce the discrepancies. However, for the adjustments to be generally valid it is important to demonstrate that the numerical methods and physics models used in the codes provide an accurate treatment of all the complexities of the model. For this purpose either the computations are done using various codes based on different mathematical treatments, or by comparing results with the experimental data.

This paper deals with the evaluation of reactor parameters such as multiplication factors and neutron energy spectrum at irradiation sites of PARR-1 using 3D modeling of the reactor core and improved cross-sections available in different newly released WIMSD libraries. An inter comparison of multiplication factor and flux pattern is made between different libraries, as well as improvements in the results were analyzed as compared to previously employed 1981 WIMSD library by comparing with the available experimental data.

2. Reactor description

Pakistan Research Reactor-1 is a typical pool type material test research reactor (MTR). It was originally designed to operate at 5 MW power with 93% high enriched uranium (HEU) fuel and was made critical in 1965. PARR-1 was converted to operate on low enriched uranium (LEU) fuel with less than 20% enriched in ^{235}U. Some general data of low enriched PARR-1 core is given in Table 2. For in-core irradiation, the core has been provided with flux traps generated by rearranging the fuel elements so that there is space of one or more element locations in the core. The details of standard fuel element, control fuel elements and irradiation facilities can bee seen elsewhere (Aslam and Ahmad, 2002; Ahmad et al., 2004; Khan et al., 1992).

Table 2
Data for low enriched uranium cores of IAEA 10 MW benchmark reactor (IAEA, 1992a) and Pakistan Research Reactor-1 (Khan et al., 1992) used for analysis

	IAEA benchmark reactor	Pakistan Research Reactor-1
Coolant, moderator	Water	Water
Reflector	Water, graphite	Water, graphite
Clad material	Aluminium	Aluminium
Control rod type	Fork type	Oval shape
Fuel material	U_3Si_2–Al	U_3Si_2–Al
Fuel enrichment (w%)	19.75	19.99
Uranium density (g/cm^3)	4.5	3.8
Fuel element dimensions (mm^3)	$76.00 \times 80.00 \times 600.00$	$79.63 \times 75.92 \times 600.00$
Lattice pitch(mm)	81.0×77.0	81.0×77.1
Shape of fuel plates	Flat	Flat
Coolant channel thickness (mm)	2.19	2.10
Weight of ^{235}U (g)		
Standard fuel element	390.0	290.0
Control fuel element	288.0	163.9
Number of fuel plates		
Standard fuel element	23	23
Control fuel element	17	13
Number of dummy plates in CFE	4	2
Fuel plate dimensions (mm)		
Width	66.40	66.92
Thickness (inner plates)	1.27	1.27
Thickness (outer plates)	1.50	1.50
Thickness of clad (mm)		
Inner plates	0.380	0.380
Outer plates	0.495	0.495
Fuel meat dimensions (mm)		
Length	600.00	600.00
Width	63.00	62.75
Thickness	0.51	0.51
Side plates dimensions (mm)		
Thickness	4.80	4.50
Width	80.00	79.63

3. Analysis procedure

3.1. Simulation methodology

Core calculations were performed in three dimensions using reactor simulation code CITATION. Fueled and non-fueled portions of each standard and control fuel element were modeled separately assuming all control rods withdrawn. CITATION was used to calculate flux spectra in different locations of the core. The CITATION code needs macroscopic absorption and ν-fission cross-sections, diffusion coefficient (D) and scattering matrix for all groups. WIMS-D4 code was used for computation

of these group constants for different regions of the core. Plate type fuel cell was used with the SLAB geometry option of WIMS-D4. Since the cross-section data in the WIMS-D4 output is very large and difficult to rearrange in the format which is required in CITATION input, especially in case of 69 energy groups outputs, therefore a preprocessing program XSECL was developed using Turbo C to extract these group constants along with fission spectrum in the input format of CITATION code from WIMS-D4 output. All the libraries were used one-by-one to generate group constants using WIMS-D4 code. Same 3D modeling of the core with these different sets of cross-sections was used to obtain results.

When using only 1D modeling of the whole core, the cell used was modeled into 1D unit by using literally only the fuelled width of the element. This fuel cell represents 23rd part of a fuel element. The details of this cell can be seen elsewhere (Ahmad et al., 2004).

The number densities in fuel regions are calculated using the following correlation for the porosity in the fuel meat (Snelgrove et al., 1987):

$$V_P = 0.072V_F - 0.275V_F^2 + 1.32V_F^3, \quad (1)$$

where, V_P and V_F are the volume fractions of porosity and U_3Si_2 dispersant in the fuel meat, respectively.

3.2. Validation of calculation methodology

We have already validated the procedure for 1D modeling by using WIMS-D4 code and AECL benchmark reactor (Ahmad et al., 2004). The current procedure of computation (using 3D modeling) was verified using IAEA 10 MW benchmark MTR reactor (IAEA, 1980), with core configuration shown Fig. 1. As PARR-1 utilizes silicide fuel so the reference results of the benchmark problem were taken for the same fuel. Some details of the benchmark reactor are given in Table 2. To provide a comparison of the two reactors, data of PARR-1 is also tabulated in the same table. The control fuel elements have different shape than that of PARR-1. The cross-sectional view of CFE is shown in Fig. 2. Other details can be seen in the references (IAEA, 1980, 1992a,b). The 3D calculations for the core were performed using CITATION code. The macroscopic cross-sections were generated using WIMS-D4 code with five broad energy groups given in Table 3. The calculations were done using all the 69 energy group libraries available for WIMS-D4.

3.2.1. Modeling of SFE and CFE in xy-plane

The planner models for standard and control fuel elements (SFE and CFE) are shown in Fig. 3. To model SFE in three dimensions, the standard element (including associated water in spacing between elements) was divided into three separate regions in *xy*-plane; one region representing the fueled portion of the fuel element with one dimension equal to fuel meat width (63.00 mm) and the second dimension equal to one side of the element (81.00 mm), and the other two identical regions on both sides of this fueled region, composed of non-fueled portions of the fuel element having dimensions 7.00 mm × 81.00 mm. To obtain macroscopic cross-sections of

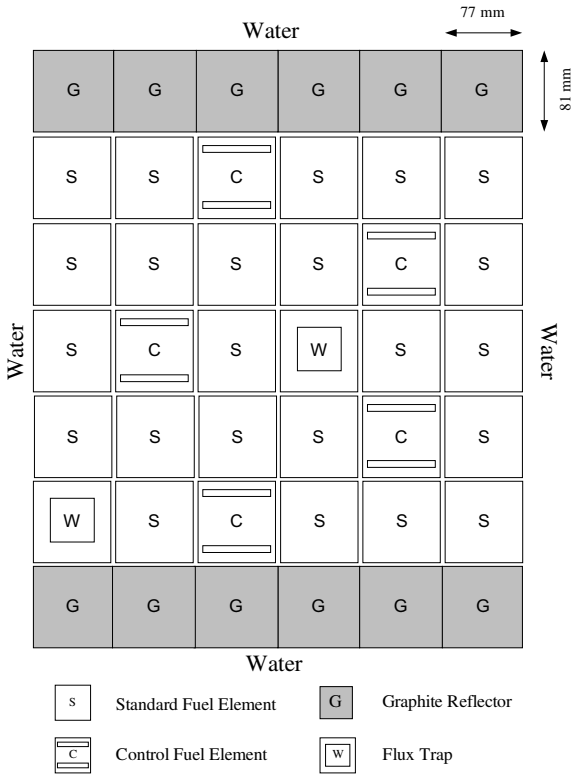

Fig. 1. IAEA 10MW benchmark reactor configuration as defined in IAEA-TECDOC-233 (IAEA, 1980).

central fueled region of SFE, WIMS-D4 was used with cell consisting of four regions, namely: uranium silicide fuel, aluminum cladding, light water moderator and an extra region containing mixture of aluminum and water. The extra region contains extra aluminum in end plates (since these plates have greater clad thickness 4.95 mm instead of 3.8 mm) and the excess water facing these end plates. This four region cell is given in Fig. 4. The two side regions (7.00 mm × 81.00 mm) containing aluminum of side plates and ends of fuel plates (greater than 63.00 mm where there is no fuel meat), the water in between side plates of two fuel elements and between fuel plates ends (greater than 63.00 mm) were modeled separately.

Since calculations were performed with all absorber rods out, the control fuel element (including associated water in spacing between elements) was modeled in five regions. Two identical non-fuel regions are modeled similar to that of fuel element, while the central portion was divided into three regions, one region representing the fuelled portion (with 17 fuel plates) having dimensions 63.00 mm × 58.82 mm and two identical regions on both sides of this fueled region with dimensions 63.00 mm × 11.09 mm representing the aluminum guide plates and the their associated water channels. To obtain macroscopic cross-sections of central (fueled) region of

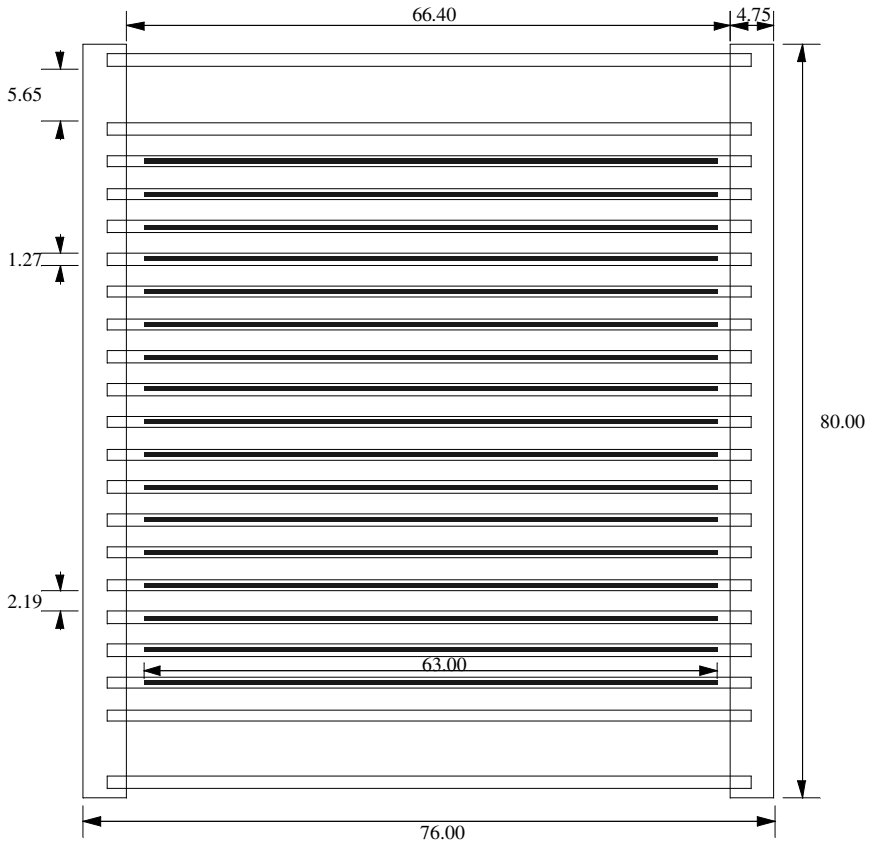

Fig. 2. The cross-sectional view of a control fuel element of IAEA benchmark reactor (all dimensions are in mm) (IAEA, 1980).

Table 3
Group structure used for cross-section generation in WIMS-D4 for calculation of multiplication factor

Group no.	Groups of library	Energy bound (eV)	
		Upper	Lower
1	1–5	1.0×10^7	8.21×10^5
2	6–15	8.21×10^5	9.118×10^3
3	16–27	9.118×10^3	4.0
4	27–45	4.0	0.625
5	46–69	0.625	0.0

CFE the cell model is same as that employed for fueled region of SFE, except there is no extra region in this case. For two identical follower regions in CFE, each with 11.09 mm thickness, cell consists of three regions including half coolant width (1.45 mm) of average of coolant channels on both sides of guide plates, aluminum

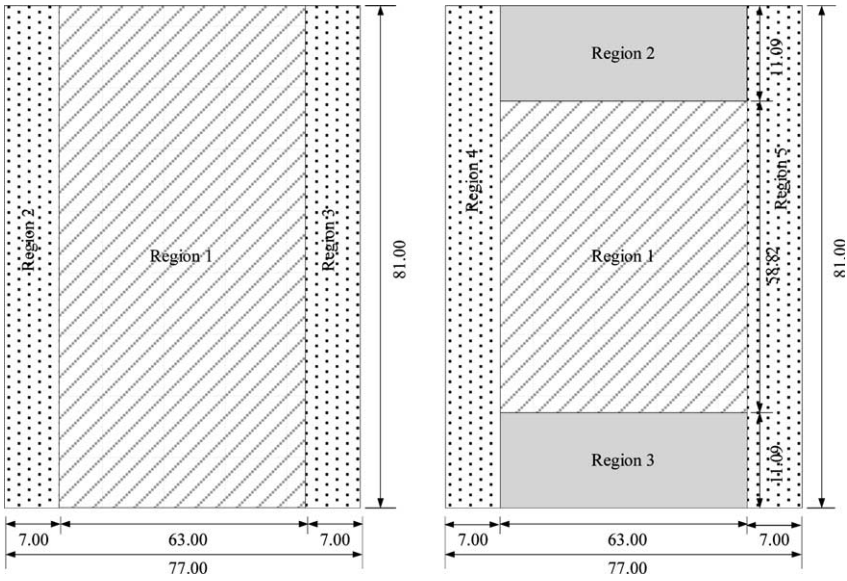

Fig. 3. Planar models of standard and control fuel elements of IAEA benchmark reactor used in CITATION (all dimensions are in mm, not to scale).

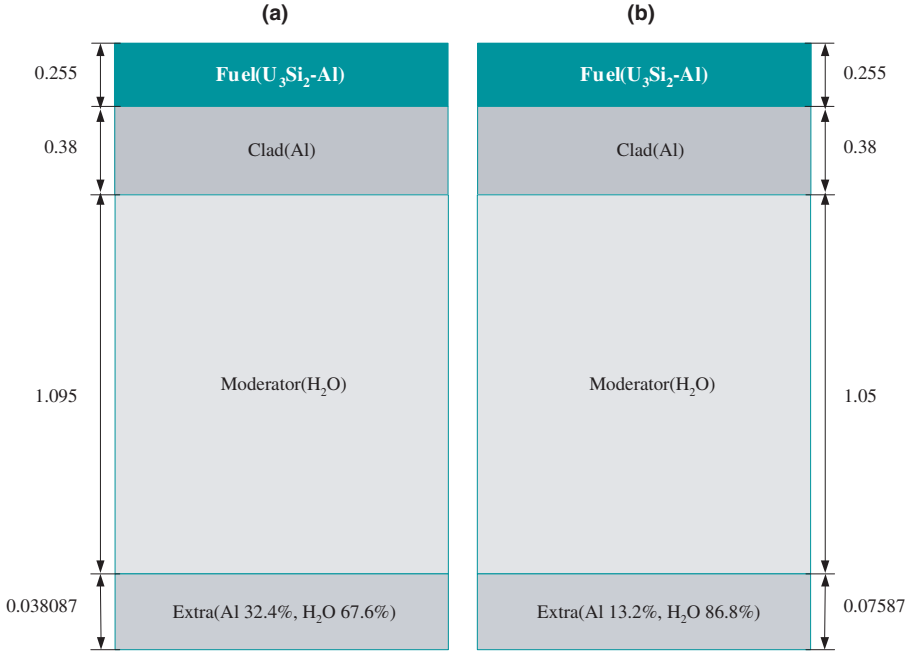

Fig. 4. Unit-cell used in WIMS-D4 input for fuel region of standard fuel element of: (a) IAEA benchmark reactor, (b) PARR-1 (all dimensions are in mm not to scale).

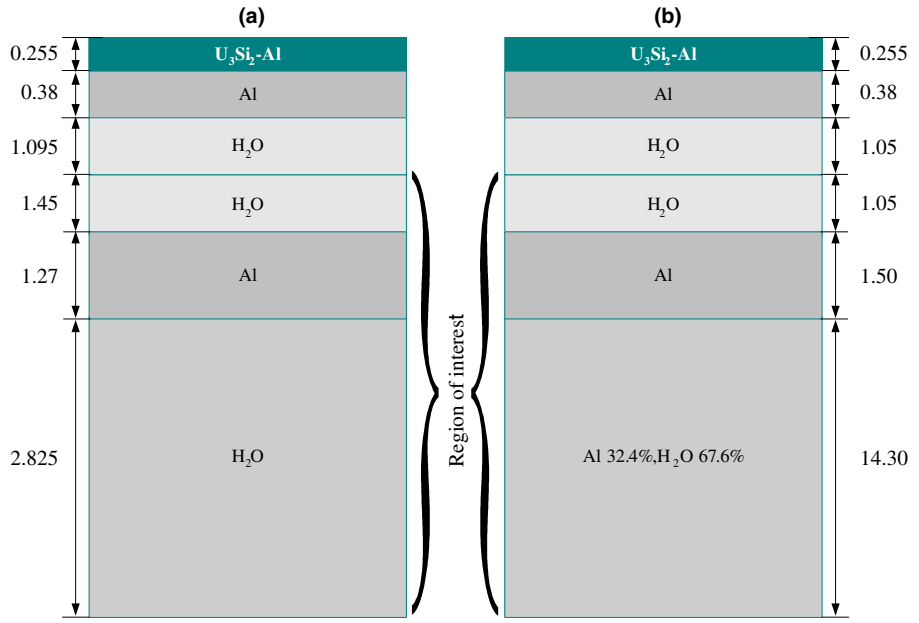

Fig. 5. Unit-cell used in WIMS-D4 input for follower region of control fuel element of: (a) IAEA benchmark reactor, (b) PARR-1 (all dimensions are in mm not to scale).

guide plate (1.5 mm) and half water thickness (2.825 mm) of the follower in between two aluminum guide plates. To provide flux spectrum for group constants computation, uranium silicide fuel followed by aluminum cladding and light water moderator were used. The REGION card in WIMSD input was used to extract the required cross-sections for follower region. The cell model for to generate group constants for follower region is shown in Fig. 5(a), with bracketed regions representing the follower region. It may be noted that the model for CFE presented in the article (IAEA, 1992a) is incorrectly shown in figures. The follower region dimensions are specified 1.075 cm instead of 1.109 cm. This discrepancy was probably introduced by reproducing figures by authors from their other article (IAEA, 1992b) for the same benchmark problem with coolant channel thickness of 0.223 cm.

The thickness of water reflector was taken equal to three times the dimension of a fuel element in respective direction, 23.1 cm facing side plates of elements and 24.3 cm behind the graphite reflector.

3.2.2. Modeling of core in axial direction

A 15.0 cm reflector region containing a homogenized mixture of 25% Al and 75% H_2O is added above and below the core to compensate the non-fuel length of fuel plates, side plates and the grid plate support structure for the elements. A 20.0 cm thick water layer was also added outside this layer. The axial modeling of the core is represented in Fig. 6(a).

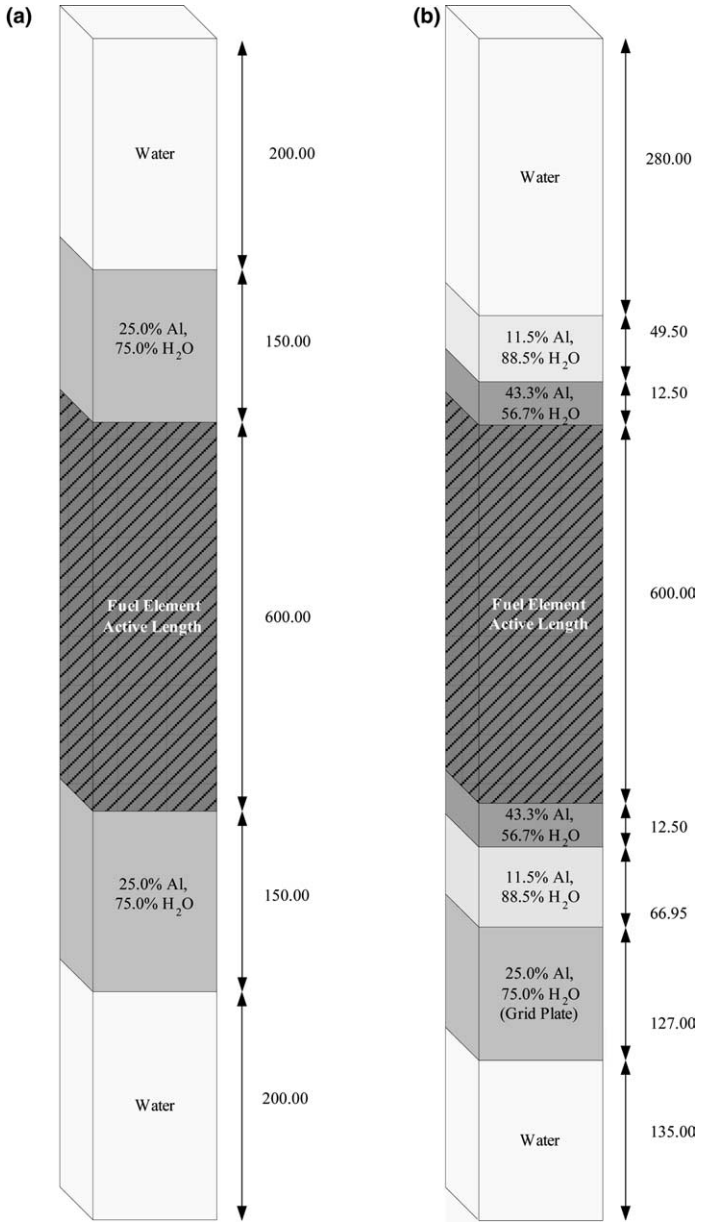

Fig. 6. Axial models of: (a) IAEA 10 MW benchmark reactor, (b) Pakistan Research Reactor-1 (all dimensions are in mm, not to scale).

3.2.3. Results

Number densities used in cell average group constants calculations for different materials in different regions of benchmark problem are tabulated in Tables 4 and

Table 4
Number densities of different materials in the cell for IAEA 10 MW benchmark reactor

Region	Slab thickness (cm)	Temperature (K)	Material	Number density ($\times 10^{24}$) cm^{-3}
Fuel	0.0255	293.0	^{235}U	0.002228
			^{238}U	0.009054
			^{27}Al	0.032519
			^{29}Si	0.007521
Clad	0.038	293.0	^{27}Al	0.060221
Moderator	0.1095	293.0	^{1}H	0.066873
			^{16}O	0.033437
Extra	0.003087	293.0	^{1}H	0.059046
			^{16}O	0.029023
			^{27}Al	0.007949

Table 5
Number densities of different materials in the cell for IAEA 10 MW benchmark reactor for regions containing only aluminum and water

Region	Dimensions (mm^2)	Material	Number density ($\times 10^{24}$) cm^{-3}
Side plates region	7.00×81.00	^{27}Al	0.046058
		^{1}H	0.015727
		^{16}O	0.007863
Follower region	63.00×11.09	^{27}Al	0.013793
		^{1}H	0.051557
		^{16}O	0.025778

Table 6
Comparison of calculated and reported results for benchmark problem

Method of computation	Library name	Calculated k_{eff}	% Difference with reference[a] k_{eff}
WIMS-D4 and CITATION	IAEA	1.186376	−0.33
	ENDFB	1.183001	−0.61
	JENDL	1.189985	−0.03
	JEF	1.193346	0.26
	WIMSD 1981	1.191452	0.10

[a] Reference value of k_{eff} is 1.1903 (IAEA, 1992a).

5. Table 6 gives a comparison with the reference value of k_{eff} calculated using 3D static diffusion theory code DIF3D (IAEA, 1992a) with cross-section data from ENDF/B-IV using EPRI-CELL code. It can be seen from this table that the values calculated using all libraries are close to the reported values, with a difference of −0.61% to 0.26%. The minor differences between all libraries and with DIF3D are due to differences in the cross-section files used.

4. Analysis of Pakistan Research Reactor-1

4.1. Three Dimensional modeling of the core

The core used in this analysis is first high power core of PARR-1 and its configuration is shown in Fig. 7, containing 17 standard fuel elements (marked as S1 through S17 in the figure) and five control fuel elements (marked as C1 through C5 in the figure) arranged in 6×4 matrix. The active core dimensions are $32.4 \times 46.26 \times 60.0\ \text{cm}^3$. There are two irradiation water boxes (flux traps) at one side of the core created by replacing two fuel elements (marked as W1 and W2 in the figure). The core is surrounded by unit density light water from all six sides. The whole core and the reflectors are modeled in x-direction using 22 regions, three region per fuel element and two region for each of both side reflectors, in y-direction using 16 regions, three region per fuel element and two region for each of both side reflectors, and in z-direction eight regions were used. The detail description of different regions of the core is stated below.

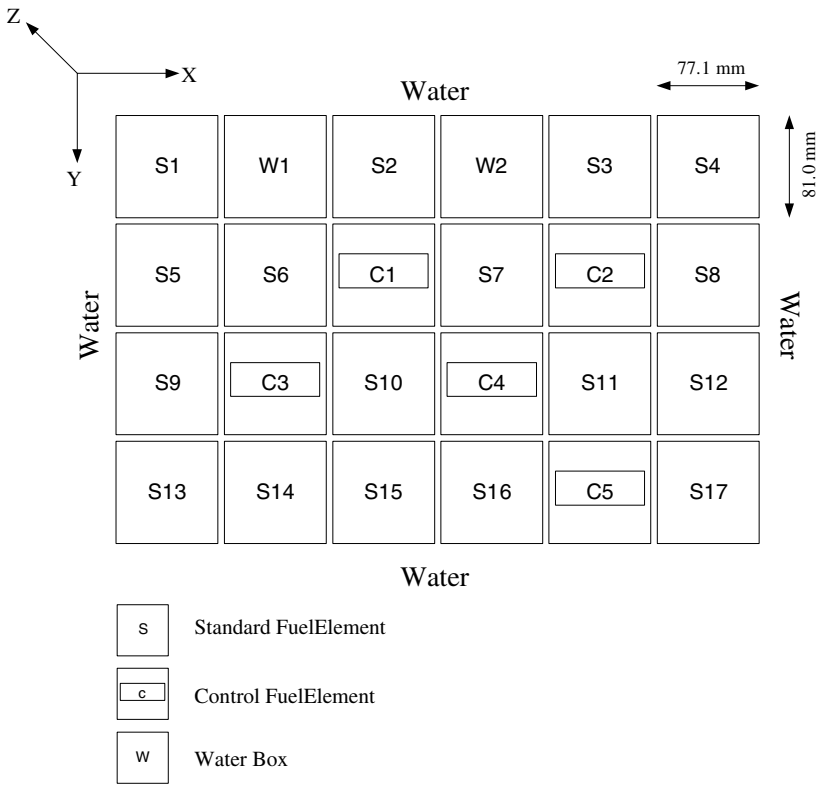

Fig. 7. The planar configuration of the core of the Pakistan Research Reactor-1.

4.1.1. Modeling of fuel elements in xy-plane

The standard fuel element was modeled in three regions, one with dimensions 62.75 mm × 81.00 mm, and two side regions with dimensions 7.18 mm × 81.00 mm. The procedure is similar as discussed in benchmark reactor. The planar models of SFE and CFE are shown in Fig. 8. The 1D cell model for fueled portion of SFE is illustrated in Fig. 4(b), and corresponding number densities for first three regions can be seen elsewhere (Ahmad et al., 2004), while for extra region these are given in Table 7. Since the control fuel element is different in shape from that in benchmark reactor,

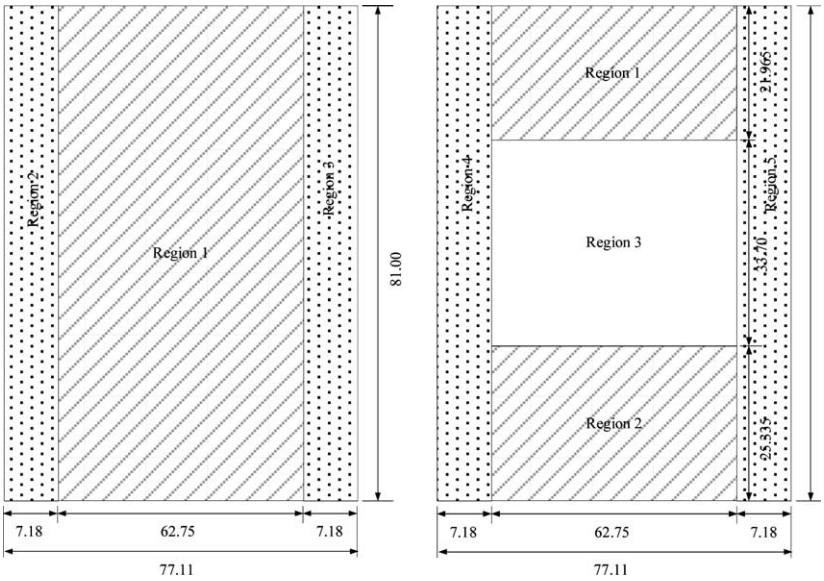

Fig. 8. Planar models for standard and control fuel elements of PARR-1 used in CITATION (all dimensions are in mm, not to scale).

Table 7
Number densities in extra regions for cells for fuelled portions of standard fuel element and control fuel element of PARR-1

Cell	Slab thickness (cm)	Temperature (K)	Material	Number density ($\times 10^{24}$) cm^{-3}
Fuel element	0.007587	293.0	^{27}Al	0.000964
			^{1}H	0.065803
			^{16}O	0.032902
Control element region with six fuel plates	0.014542	293.0	^{27}Al	0.044275
			^{1}H	0.001771
			^{16}O	0.000885
Control element region with seven fuel plates	0.012464	293.0	^{27}Al	0.044281
			^{1}H	0.001770
			^{16}O	0.000885

Table 8
Number densities in different regions of SFE and CFE containing homogenous mixture of aluminium and water

Region	Dimensions (mm^2)	Material	Number density ($\times 10^{24}$) cm^{-3}
Standard fuel element side plates	7.175×81.00	^{27}Al	0.043540
		^{1}H	0.018524
		^{16}O	0.009262
Control fuel element side plates	7.175×81.00	^{27}Al	0.049683
		^{1}H	0.011703
		^{16}O	0.005851
Central region of follower	62.75×28.60	^{27}Al	0.000960
		^{1}H	0.065808
		^{16}O	0.032904

the five regions in this case include: two regions representing the fueled portions with seven fuel plates and six fuel plates having dimensions 62.75 mm × 25.335 mm and 62.75 mm × 21.965 mm, respectively. The third central region 62.75 mm × 33.70 mm, representing the control rod guide region contains only aluminum and water. For the two regions of CFE containing fuel plates the difference with the fuel cell is only in extra region thickness and number densities. The specifications for these regions are tabulated along with number densities in extra regions of fuel cells in Table 7. The cross-sections of middle follower region of the CFE and regions containing side plates of fuel elements were calculated using WIMS-D4 with REGION card input option. Fig. 5(b) represents the model of the cell used to generate cross-sections for the middle non-fueled follower region of CFE. The number densities for the regions modeled as homogenous mixture of water and aluminum are given in Table 8. Similar procedure was also used for computation of reflector cross-sections and for the water in water boxes.

4.1.2. Modeling of core in axial direction

The core of PARR-1 in axial direction has fueled portion, and non-fueled portions containing non-fueled portions of fuel elements and the supporting structure. The core was modeled axially in six regions. One region 600.00 mm of the active fuel element height, a 12.50 mm reflector region containing a homogenized mixture of 43.3% Al and 56.7% H_2O is added above and below the active core height to compensate the un-fueled length of fuel plates. Outside this layer, 49.50 mm reflector region above and 66.95 mm reflector region below were added for representation of the extra length of side plates, thus having a homogeneous mixture of 11.5% Al and 88.5% H_2O. Again a 127.00 mm region was added below for representation of the grid plate support structure for the elements. The axial modeling of PARR-1 core is shown in Fig. 6(b). To reduce the time of computation in case of calculation of flux spectra using 69 energy groups the model was simplified by assuming axial symmetry. Since in this case we are only presenting inter comparison of spectra for different libraries so small change (0.1%) in multiplication factor is ignorable. Lower half portion of the model as presented in Fig. 6(b) is taken in this case.

4.2. Results

Five libraries including 1981 WIMSD library and four newly released libraries IAEA, ENDFB/VI, JENDL and JEF were used to generate group constants for different regions of the core. The discrete ordinate method with default order 4 was used for the solution with the convergence criterion 0.00001 using TOLERANCE card in input to WIMS-D4. These group constants were then used, one by one in CITATION input for 3D calculations, to see the effect of newly available cross-sections on the criticality and the flux distribution.

4.2.1. The comparison of flux spectra from 1D and 3D codes

The neutron energy spectrum obtained from 1D model using WIMS-D4 code alone for PARR-1 core is compared with that obtained from 3D modeling using WIMS-D4 and CITATION. The flux from WIMS-D4 was computed for the buckling value to get same k_{eff} as got using 3D modeling and same library. The plot of both flux spectra is shown in Fig. 9, where the spectrum from WIMS-D4 was compared with that from CITATION for the standard fuel element S10. Both flux spectra follow the same pattern. 3D modeling gives the thermal flux greater in magnitude than that obtained directly from 1D code WIMS-D4, while the fast flux is less in case of 3D modeling. WIMS-D4 models the core assuming an infinite array of the representative cells of the fuel element without taking into account the excess water and structural materials present in the core. Since water is a strong moderator and plays its roles to shift neutrons from high energies to low energies, so in case of CITATION modeling the greater thermal flux is due to the water reflectors on six sides

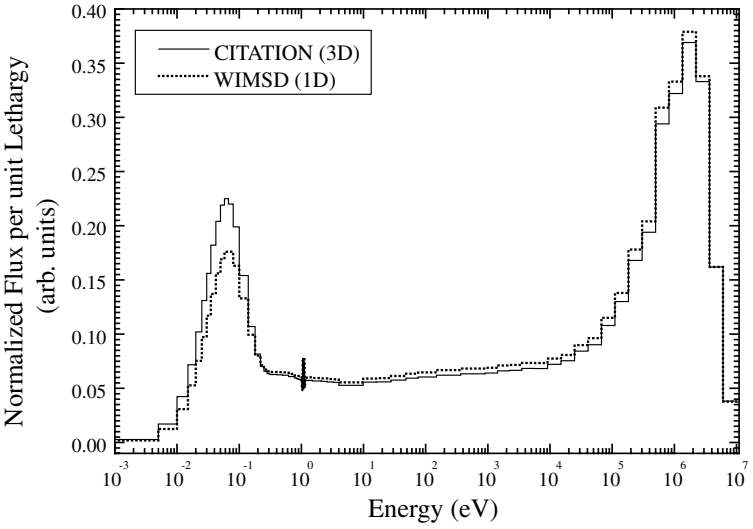

Fig. 9. Comparison of fluxes obtained for standard fuel element (S10) of PARR-1 core using 1D modeling (WIMS-D4) and 3D modeling (WIMS-D4 and CITATION).

Table 9
Multiplication factors for Pakistan Research Reactor-1 using different libraries

Library	Calculated k_{eff}	% Difference with experimental value
ENDFB	1.041381	−0.45
IAEA	1.043185	−0.28
JENDL	1.047463	+0.13
JEF	1.050520	+0.42
1981 WIMSD	1.057127	+1.05

The values of k_{eff} are rounded to six decimal places.
The experimental value of k_{eff} is 1.046135.

of the core, two water boxes in the core, and the excess water in control fuel elements.

4.2.2. Comparison of multiplication factors

For computation of the effective multiplication factor, computations were performed using all available libraries with five energy groups. The effective multiplication factors obtained are given in Table 9 for comparison, along with measured value (Ansari et al., 1994). The k_{eff} values for all libraries are within ±0.45% with experimental value except 1981 WIMSD library for which is 1.05% larger than experimental value. The closest matches exist for IAEA and JENDL libraries from experimental value for which the differences are −0.28% and 0.13%, respectively. The ENDFB library gives lower value than IAEA library. The difference in multiplication factors observed using libraries from different origins is mainly due to difference in sources of data. The effective multiplication factor from available 1981 WIMSD library is higher than all the new libraries.

4.2.3. Comparison of energy spectrum

The neutron energy spectra in water box W2 were obtained using CITATION code with group constants generated by WIMS-D4 and all the libraries with all available 69 groups. The flux obtained using 69 energy groups, using 1981 WIMSD library along with the spectra obtained by using 69 energy group WLUP libraries is illustrated in Fig. 10. From this plot it can be seen that all the spectra follow the same pattern, with some differences. In fast energy range these differences are seen among all libraries, whereas in thermal energy range all newly released libraries have fluxes very close to each other having significant differences with 1981 WIMSD library. To clearly see the differences among the fluxes obtained from new libraries the ratios of group fluxes from newly released ENDFB, JENDL and JEF libraries to group fluxes obtained using IAEA library are plotted in Fig. 11. It can be seen that the flux spectra from ENDFB library and IAEA library have very close match. Less than 0.3% difference is encountered below 2 MeV, while maximum difference of about 3.5% is seen in first group (highest energy group in library). The JENDL library has also very close results with IAEA library, and below 2 MeV the flux spectrum from this library agrees within 1% with that obtained using IAEA library, and maximum difference of 4.5% is

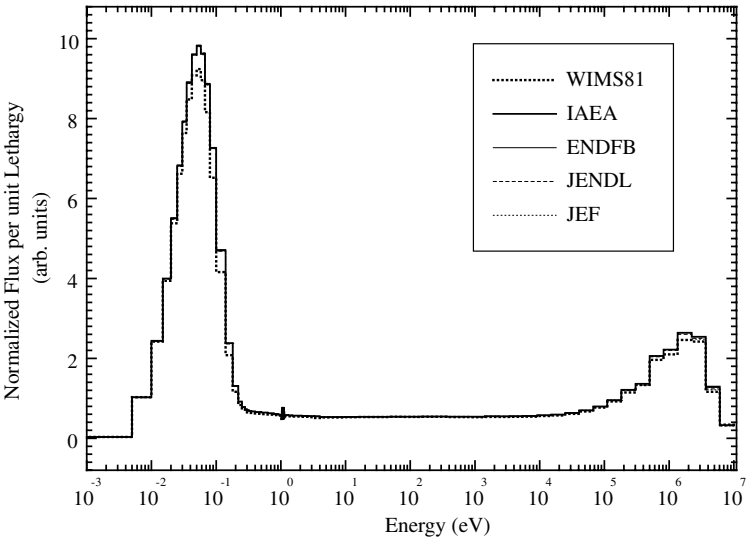

Fig. 10. Flux spectra in water box (W2) of PARR-1 core obtained using various WIMSD libraries with 3D modeling of the core.

observed at 4 MeV. JEF library gives deviation in maximum range of energy among all WLUP libraries with IAEA library, although the maximum difference is less than 3.5% in first energy group (of the library). The differences in thermal range and epithermal range arise from the basic differences in the data libraries themselves. The near results of IAEA library from ENDFB library is due to the fact that in development of IAEA library, most of the data related to MTRs is taken from ENDFB library as can be seen from Table 1.

To clearly analyze the difference in flux using different libraries to the flux obtained from the 1981 WIMSD library the ratio of fluxes obtained by the WLUP libraries to that obtained from the 1981 WIMSD library are plotted in Fig. 12. Valuable differences are encountered in thermal energy range in comparison of results from newly available libraries with the 1981 WIMSD library results, as well as in fast energy range above 4 MeV. The deviations in the flux obtained using newly available libraries from that obtained using the 1981 WIMSD library is maximum at 0.2 eV in the thermal region, and at highest energies in the fast energy region. In the lowest energy group the ratio of the flux obtained from new libraries to that obtained from 1981 WIMSD library is about 0.98 for all libraries except JEF for which the ratio is 0.96. This ratio gradually increases with increase in energy and has maximum value of 1.14 at 0.2 eV (except for JEF library for which this value is 1.12). Another peak is also observed at around 4 eV where ratio is 1.09 for all libraries except JEF library for which this ratio is 1.07. In fast energy range the maximum difference is observed in first energy group (of library) where this flux ratio 0.88 to 0.95, different for all libraries. The plot of flux ratio has similar trend in all cases.

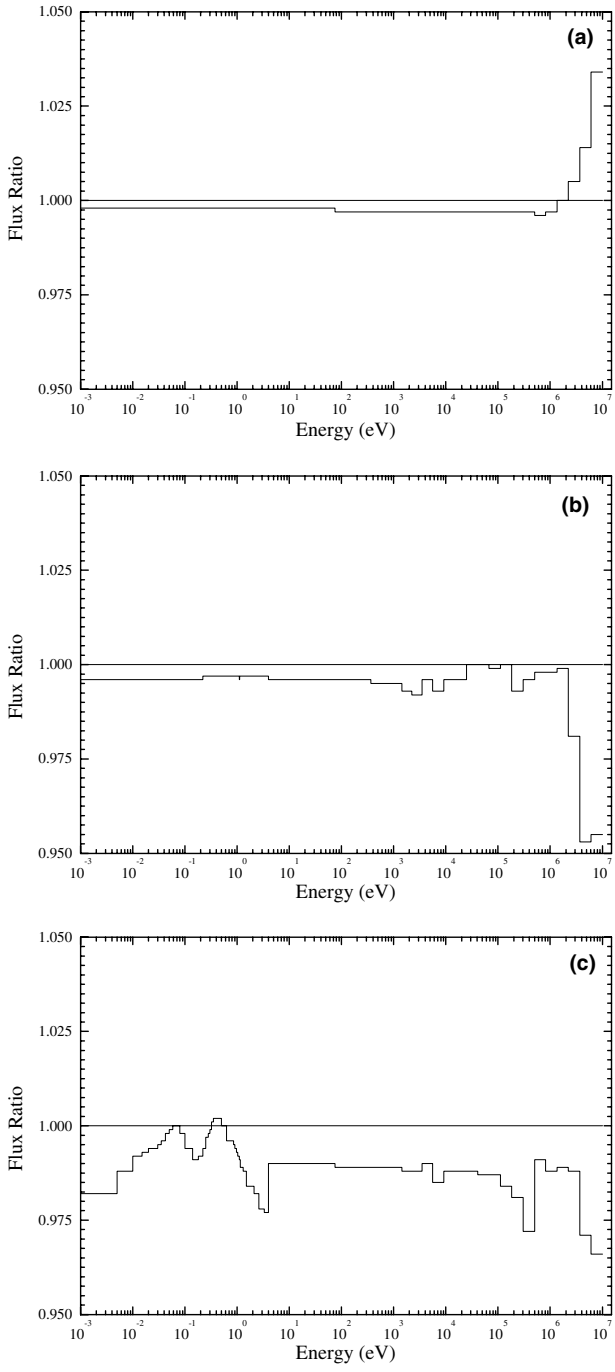

Fig. 11. Ratio of group fluxes obtained using: (a) ENDFB, (b) JENDL and (c) JEF libraries to the group fluxes obtained using newly released IAEA library.

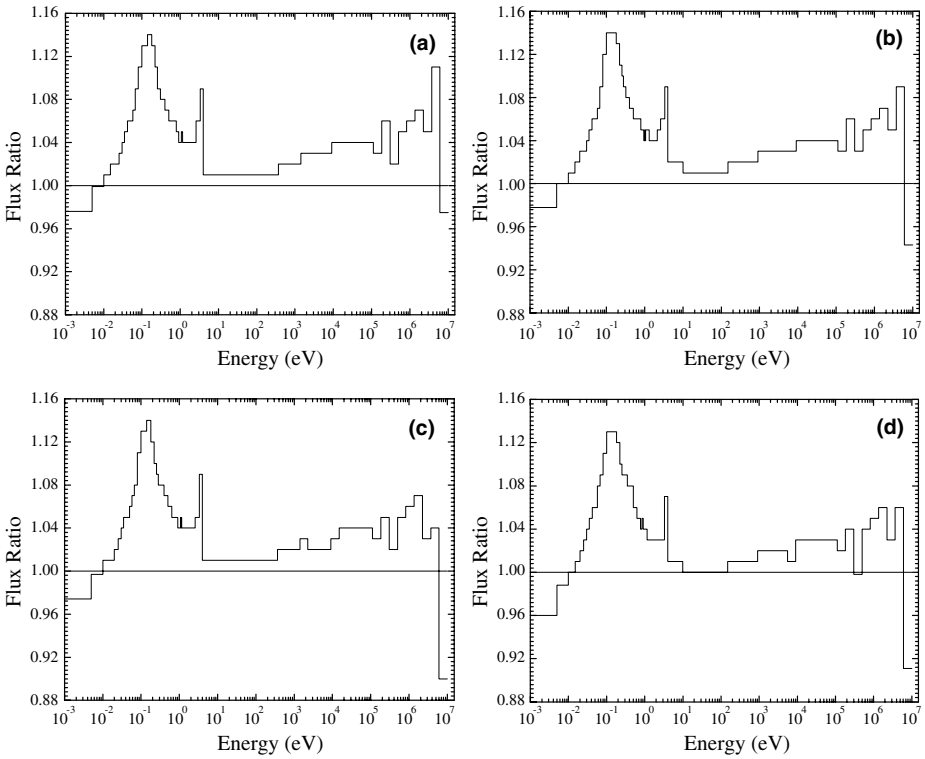

Fig. 12. Ratio of group fluxes obtained using: (a) IAEA, (b) ENDFB, (c) JENDL and (d) JEF libraries to the group fluxes obtained using 1981 WIMSD library.

4.2.4. Effects of cross-sections of hydrogen bound-in-water

It was observed that the differences in thermal energy spectrum obtained using WLUP libraries arise due to difference in cross-sections of hydrogen bound-in-water. As absorption cross-sections of hydrogen bound-in-water are almost the same among all WLUP libraries, so the transport cross-sections are responsible for these differences. These transport cross-sections are same in ENDFB and IAEA libraries, while different among all other libraries.

We have analyzed the effect of hydrogen cross-sections differences among the libraries, by replacing these cross-sections in JENDL and JEF libraries with that from IAEA library. For WLUP libraries the change is illustrated by plotting new ratios in Fig. 13. It can be seen from this figure that after replacement, the flux spectra in thermal energy range became in good agreement. The plot of ratio of transport cross-section of hydrogen bound-in-water of JENDL and JEF libraries with that of IAEA library is shown in Fig. 14. The difference of these cross-sections of IAEA library with JENDL library exist above 60 eV (fast and epithermal regions), while the with JEF library below 4 eV (in thermal region). Since JEF library has more difference in these cross-sections with IAEA library as compared to the difference between

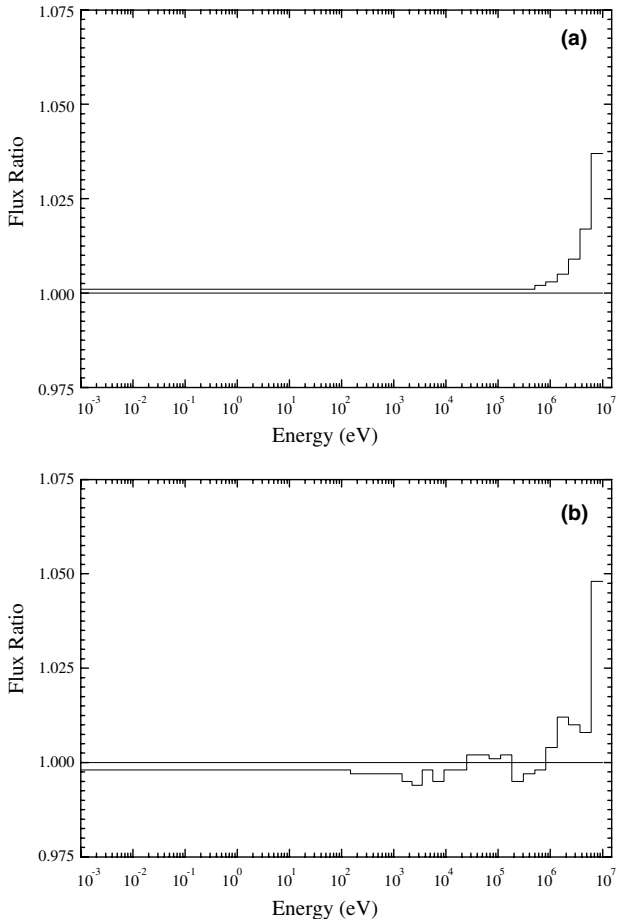

Fig. 13. Ratio of fluxes obtained using cross-sections of hydrogen bound-in-water from IAEA library with all other data from: (a) JENDL and (b) JEF libraries to that obtained using IAEA library.

JENDL and IAEA cross-sections, the difference in flux spectrum with IAEA library is also greater in case of JEF library as compared to JENDL library.

For 1981 WIMSD library we have also analyzed the effect of cross-sections of hydrogen bound-in-water by replacing cross-sections of hydrogen (bound-in-water) in 1981 WIMSD library with these cross-sections from Hydrogen (bound-in-water) from new libraries. The multiplication factors and flux spectra were computed for all four cases, and were compared with the results of corresponding new libraries. The ratios of fluxes from new libraries to that obtained from cross-section replaced 1981 WIMD libraries are shown in Fig. 15. The spectra obtained for all the cases have shown same trend. It can be seen from the figure that both the flux spectra agree within 0.5% below 0.1 MeV for first three libraries, while the flux from JEF library has an agreement within 1% mostly below 0.1 MeV. The effective multiplication

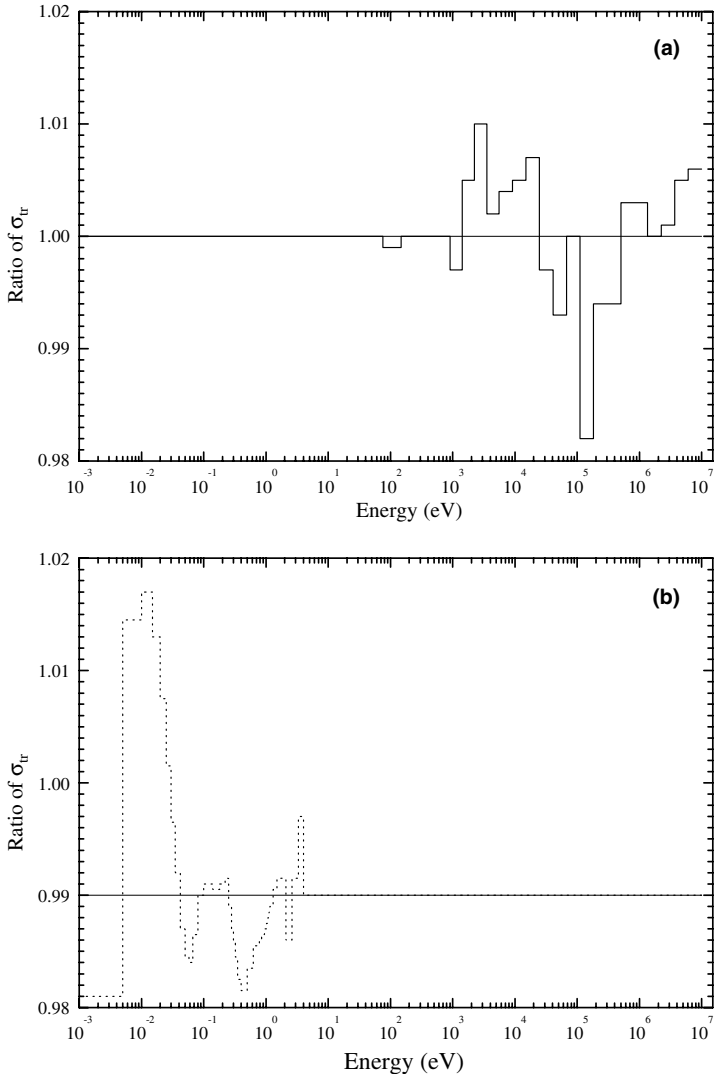

Fig. 14. Ratio of transport cross-sections of hydrogen bound-in-water from: (a) JENDL and (b) JEF libraries to these cross-sections from IAEA library.

factor obtained from the hydrogen replaced WIMSD libraries are given in Table 10. For comparison, the differences with effective multiplication factors from new libraries as well as with experimental value are also tabulated here. Since the cross-section data for hydrogen bound-in-water in IAEA library was taken from ENDFB, so the result is same for these WIMSD libraries. It can be seen that replacement of only the cross-sections of hydrogen bound-in-water in 1981 WIMSD library, the differences in k_{eff} between the 1981 WIMSD library and new libraries is reduced to less

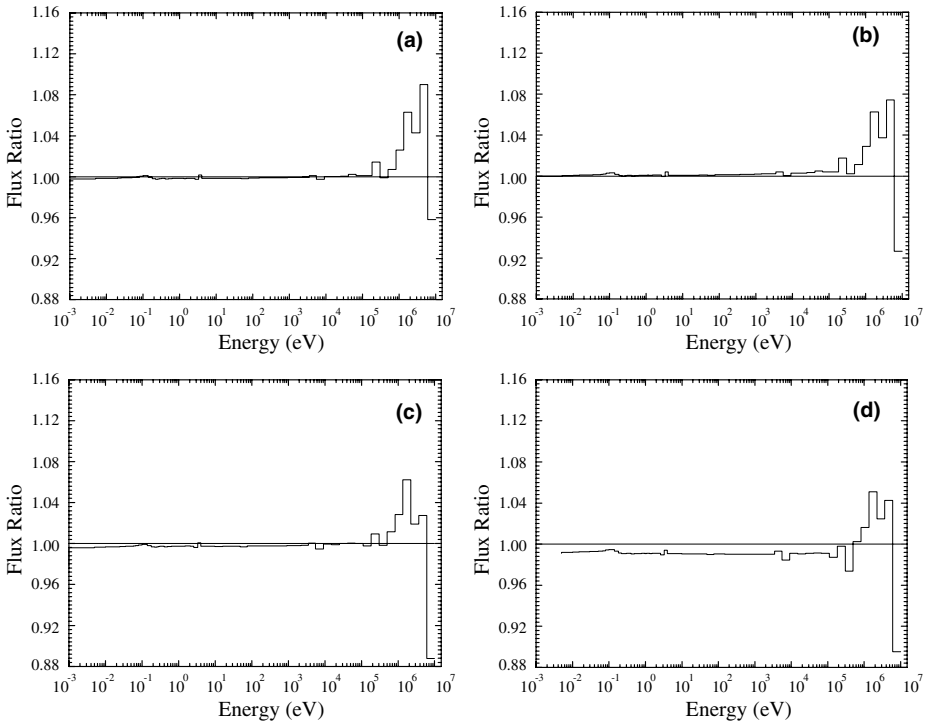

Fig. 15. Ratio of fluxes obtained from 1981 WIMSD libraries after replacing cross-sections of hydrogen bound-in-water from new libraries to that obtained directly from new libraries: (a) IAEA, (b) ENDFB, (c) JENDL and (d) JEF libraries.

Table 10
Comparison of effective multiplication factors obtained by using cross-sections of hydrogen bound-in-water from new libraries along with all other cross-sections from 1981 WIMSD library

Library used for hydrogen cross-sections	k_{eff} (1981 WIMSD library cross-sections replaced)	% Difference with multiplication factor	
		1981 WIMSD (1.057127)	Experimental value (1.046135)
ENDFB	1.041806	−1.45	−0.41
IAEA	1.041806	−1.45	−0.41
JENDL	1.042126	−1.42	−0.38
JEF	1.041599	−1.47	−0.43

than 0.85%. The difference with the experimental value also reduced to −0.38% to −0.43%.

4.2.5. Effects of fission spectrum

In fast energy range the differences arise due to fission spectrum which is very important in case of fast neutrons specially. There are differences of 0.4–0.5% in

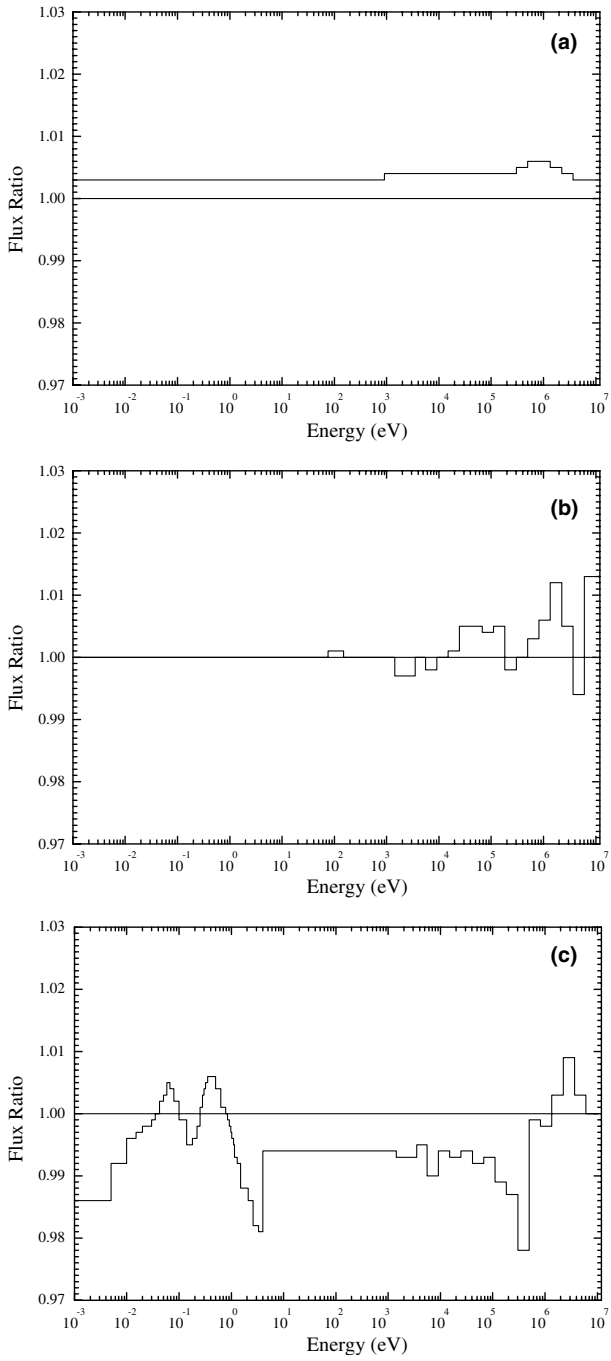

Fig. 16. Ratio of fluxes obtained using fission spectrum from IAEA library with all other data from: (a) ENDFB, (b) JENDL and (c) JEF libraries to fluxes obtained using IAEA library.

the fission spectra of different newly released WIMSD libraries at high energies. In Fig. 16, we have given ratios of the group fluxes after replacement of fission spectra of ENDFB, JENDL ad JEF libraries with fission spectrum from IAEA library. It

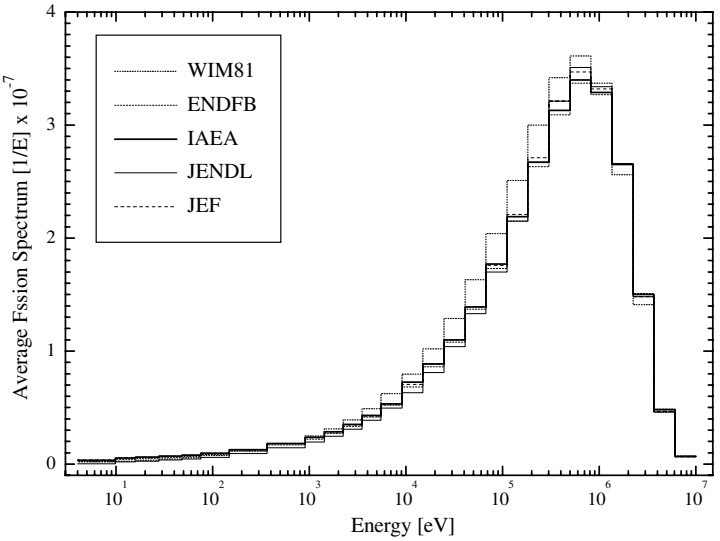

Fig. 17. Fission spectra from newly released libraries along with fission spectrum from 1981 WIMSD library.

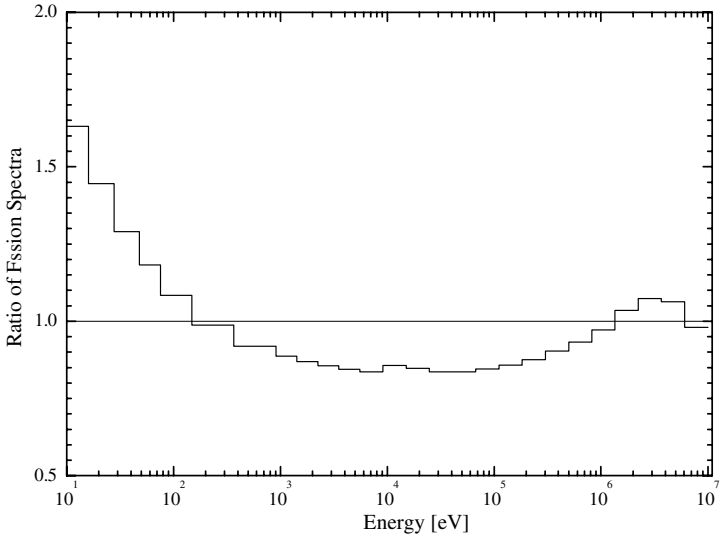

Fig. 18. Ratio of fission spectrum from IAEA library to that from WIMSD 1981 library.

can be seen that the flux spectra of all the libraries agree in the fast region within 1.3% after this replacement.

The fission spectra from 1981 WIMSD library and new libraries are plotted together in Fig. 17. The ratio of fission spectrum from 1981 WIMSD library to fission spectrum from IAEA library is also given in Fig. 18. Although the ratio is very high in the thermal region, the fission spectrum is very small. At high energies the ratio is small but due to very large number of fission neutrons produced at these energies makes this ratio very significant. To clearly analyze the effect of replacement of fission spectrum in 1981 WIMSD library with fission spectra from newly released libraries, the ratio of fluxes obtained by the WLUP libraries to that obtained from the fission spectrum replaced 1981 WIMSD libraries with replaced hydrogen data are plotted in Fig. 19. It can be seen that by replacement of fission spectrum, the differences in fluxes at high energies reduced significantly. The difference for IAEA library reduced from 9% to 7%, for ENDFB library 8% to 3%, for JENDL library 11% to 3% and for JEF library 10% to 4%.

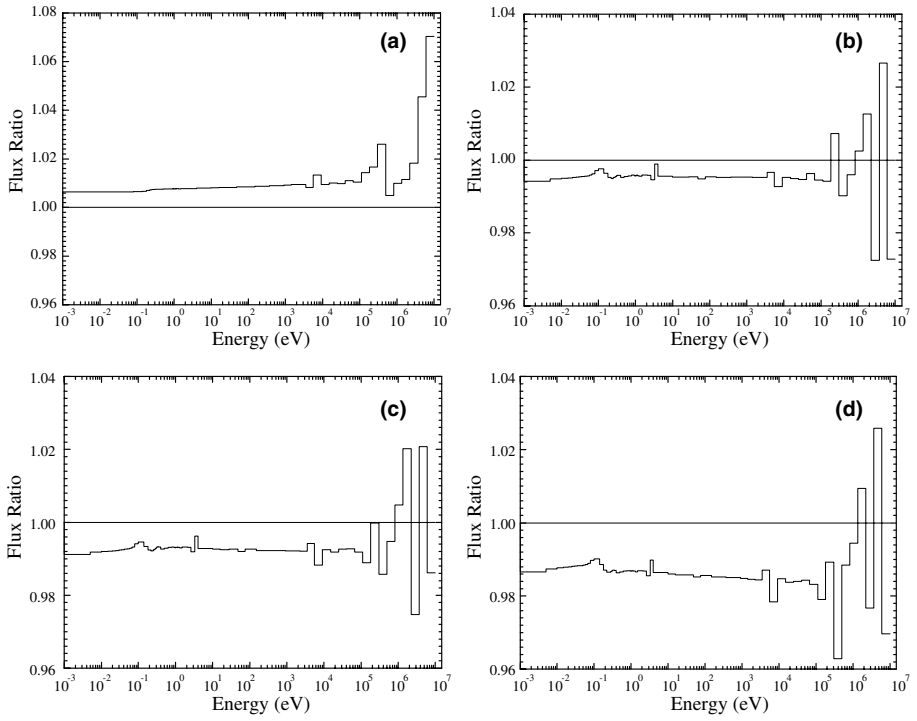

Fig. 19. Ratio of fluxes obtained using fission spectrum and hydrogen from: (a) IAEA, (b) ENDFB, (c) JENDL and (d) JEF libraries in WIMSD 1981 library to the fluxes obtained using respective libraries from which data was taken.

5. Conclusions

Based on our analysis it may be concluded that:

- The flux spectrum obtained using 1D modeling is higher in fast energy range and smaller in thermal energy range, due to neglect of excess water and structural materials in the core in 1D modeling.
- The major differences in the flux spectra between newly available libraries and the 1981 WIMSD library in thermal energy range are due to the cross-sections of hydrogen bound-in-water. The use of only newly available cross-sections of hydrogen bound-in-water results in major improvement in value of k_{eff} as well flux spectra. The minor differences among all new libraries in the thermal energy range are also due to these cross-sections.
- The differences in flux among libraries in the fast energy range are due to differences in fission spectra. The replacement of fission spectra reduced these differences significantly in the fast energy range.

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