American Journal of Engineering Research (AJER)
e-ISSN: 2320-0847 p-ISSN : 2320-0936
Volume-10, Issue-01, pp-24-30
www.ajer.org
Research Paper Open Access

Generation of WIMSD-5B Multigroup Constants Library Based on JEFF-3.2 Nuclear Data and its Validation through some Benchmark Experiments Analysis and its Comparison with some other Libraries

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ABSTRACT: *This study deals with the benchmark analysis of a cross section library generated from JEFF-3.2 nuclear data for the WIMSD-5B code system by calculating the theoretical results of the integral parameters for TRX and BAPL benchmark lattices of thermal reactor. The nuclear data processing is performed by a new executable NJOY99.0. The integral parameters, such as* $k_{eff,}$, ρ^{28}, δ^{25}, δ^{28} *and* C^* *, of five uranium-fuel thermal assemblies TRX-1, TRX2, BAPL-UO2-1, BAPL-UO2-2, and BAPL-UO3-3 have been investigated using the latest version WIMSD-5B of the reactor lattice transport code WIMS. The calculated results are compared with those of experimental values, the original WIMS library and previously calculated in JENDL-3.3 data library. It was found that the calculated integral parameters are in good agreement with the experimental results as well as with the other previously published values. Hence, it can be said that data library JEFF-3.2 is sufficiently reliable for thermal reactor calculations of TRIGA Mark-II research reactor. The cross-section library, thus obtained, can be used for the neutronic and safety parameter calculations of the thermal reactor in future.*

KEYWORDS: *NJOY99.0, JEFF-3.2, TRX and BAPL Benchmark Lattices, Integral Parameters, and WIMSD-5B.*

Date of Submission: 29-12-2020 Date of acceptance: 10-01-2021

I. INTRODUCTION

WIMS [1] is one of the most widely used general purpose thermal reactor analysis code available on non-commercial basis. One of the most common uses is to generate few group cross section libraries in problem dependent form to interface with neutronic codes. The supporting WIMS cross section library being very old provides a scope for improvement of reactor calculation results by generating WIMS library based on latest release of the evaluated data files, such as; ENDF/B-VII, [2] (The US Evaluated Nuclear Data Library), JEFF-.3.2 (Joint European Fission Fusion), JENDL-3.3 [3] (Japanese Evaluated Nuclear Data library), and JEF-2.2 [4], (Joint European File) etc. First of all without specific applications the quality of the data can't be fully understood. In addition, comprehensive data processing for specific application may incur significant error that may affect the quality of the final results. Furthermore, very few codes are available in the public domain that can handle processing of the new data with dependable accuracy. Cullen's work [5] proved many of the data processing codes to be obsolete. After careful analysis of these facts NJOY99.0 [6] was chosen since it includes sophisticated methods of correct reconstruction using multi-level Breit-Wigner resonance parameters, Doppler broadening by accurate point kernel method, group to group thermal scattering matrices and special thermal law treatment. It also includes the flux weighted fission fraction vectors, and a weighting flux produced by a point solution of the slowing down problem that accurately accounts for broad and intermediate resonance effects. Each of these treatments can play a vital role in WIMS library production. In addition the NJOY99.0 has capability to handle ENDF-6 format [7], which is used in ENDF/B-VII and several other basic data files. NJOY99.0 also provides a sophisticated and wider scope for "THERMR" treatment incorporating S (α,β) data in ENDF/B-VII. Some of these scattering law data is extremely important for TRIGA Reactor calculations.

This makes demand for new data library for TRIGA reactor calculations. The work is also intended to address the performance of the modified WIMSR processing capability and some of the input parameter options provided in the WIMSR. This will provide useful information for the other NJOY users. To validate the generated multi group library TRX 1-2, BAPL1-3 [8] benchmark lattices have been analyzed, for which experimental results, as well as results using improved methods with state-of-the-art data bases have been reported by some advanced laboratories. For these calculations available standard inputs and models have been used with no additional approximation. The TRX and BAPL analysis provided options for further application of the data for the analysis of the TRIGA research reactor. A seven-group library of group constants to support CITATION [9] calculations has been generated using the WIMSD-5B for neutronic analysis of 3 MW TRIGA research reactors. First of all to gain confidence with the new library parametric studies with (TRX1-2 and BAPL1-2-3) relatively simple critical lattices have been applied. The data processing methodology were established by benchmarking the processed group constants with the similarly processed customized data. The generated library has been used for specific practical applications for validation purposes. The integral parameters studies benchmarking TRIGA Mark-II research reactor experimental and operational data will be analyzed.

II. NUCLEAR DATA PROCESSING

The NJOY Nuclear Data Processing System [10-14] is a modular computer code designed to read evaluated nuclear data in ENDF format , transform the data in various ways, and output the results as libraries designed to be used in various applications. The principal advantage of NJOY is its most general-purpose applicability and comprehensive capability to process data in the recent ENDF format. Because, the Evaluated Nuclear Data File (ENDF) format [7] is used all around the world. NJOY takes the basic data from the nuclear data library and converts them into forms needed for applications. The NJOY99.0, [6] latest version of NJOY, was used to process the data library using the modules RECONR, BROADR and ACER of NJOY code. For WIMS library generation, the following modules of NJOY are in sequence as follows: 'NJOY-MODER-RECONR-BROADR-UNRESR-THERMR-GROUPR-WIMSR'. A flow diagram of the processing scheme is shown in Fig. 1

2.1. General remarks on data processing

The selection of some important data processing input parameters defines the range of applicability of a multigroup data library. The demands of the WIMS library in particular are rather high, since it has to cover the requirements for a large variety of lattices, differing in the type of moderator, fuel/ moderator volume ratio, lattice pitch, operating conditions etc. In this work, the input option selection has been made on basic principles, having in mind a typical light water reactor (LWR). However, the applied principles and the assumptions as described below are valid for other reactor types, too.

2.1.1 Averaging spectrum

For averaging the group constants we used the mid-life PWR flux spectrum, one of the in-built input options of the GROUPR module (IWT = 5; EPRI.CELL LWR) of NJOY. For some materials, special treatment (IWT= -5; NJOY flux calculator option) was applied in the resonance range, where appropriate.

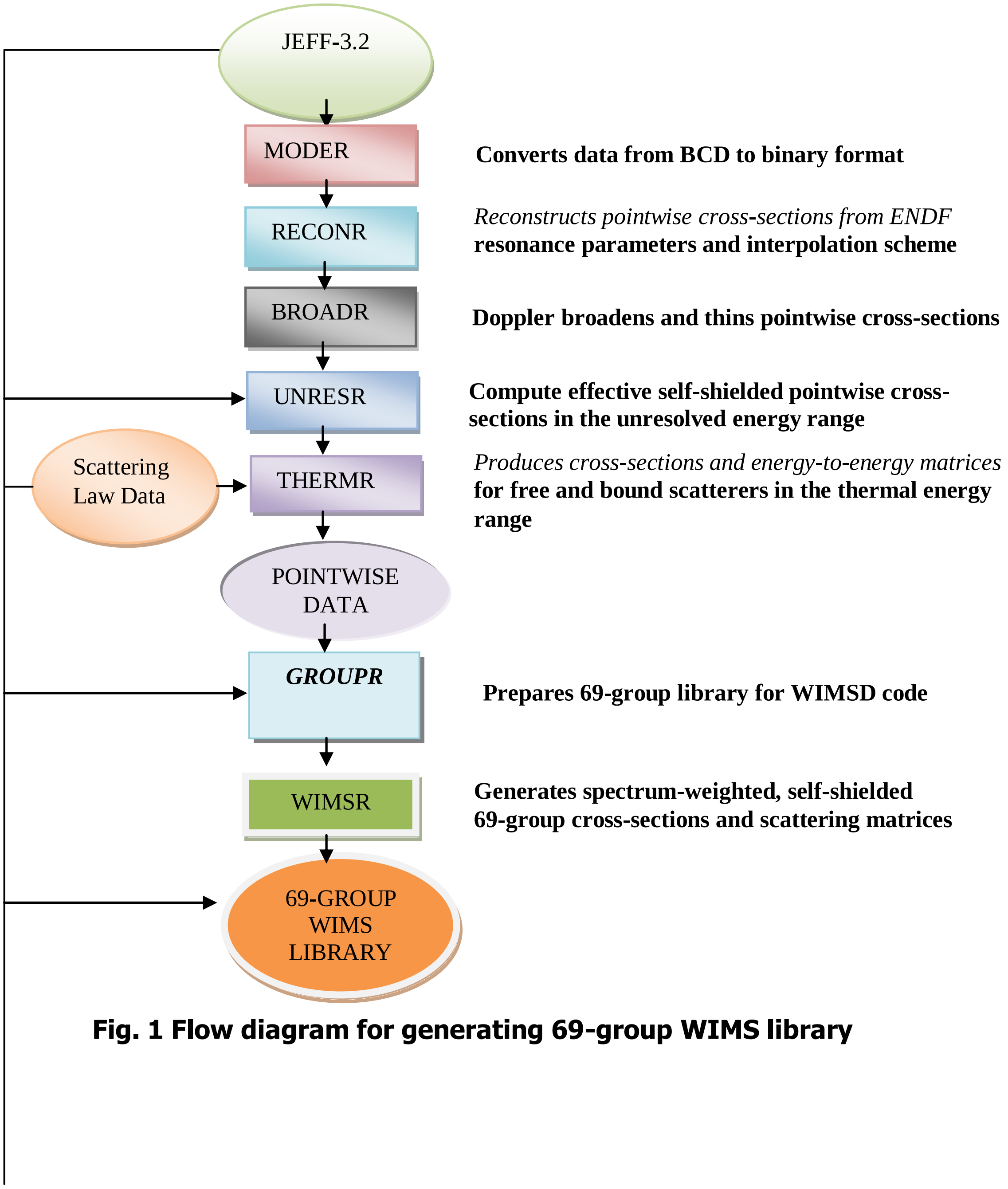

Fig. 1 Flow diagram for generating 69-group WIMS library

III. DESCRIPTION OF THE BENCHMARKS

3.1. The Benchmark Experiments

To study the quality of the nuclear data and the tools for analysis, the calculated integral parameters are often compared to the measured values of the benchmark experiments, which are relatively simple critical lattices that can be modeled without too many approximations.

By comparing the calculated integral parameters to the measured values, the overall performance of the new library can be estimated.

Integral effects

In order to test the integral effects of the new data, a WIMS library was generated, which included the following materials:

- Hydrogen bound in water,
- Oxygen,
- Aluminum,

- Uranium-235,
- Uranium-238.

Such a library is adequate to perform calculations for the benchmark lattices such as TRX-1, TRX-2, BAPL-1, BAPL-2 and BAPL-3, which were defined in WLUP Stage-1.

3.2. Experimental Facility of TRX and BAPL

3.2.1Benchmark Name and Type

For this analysis, two types of benchmark lattices are used

A. TRX-1 and TRX-2, (water) H_2O-moderated uranium lattices and

B BAPL–1 through 3, H_2O moderated uranium oxide critical lattices.

A. System description of TRX

These benchmarks are water moderated uranium critical lattices of slightly enriched (1.3 wt.%) uranium rods with diameters of 0.98297 cm in a triangular pattern . Measured lattice parameters include ρ^{28}, δ^{25}, δ^{28} and C*. These lattices directly test the U-235 resonance fission integral and thermal fission cross section. They also test U-238 shielded resonance capture and the thermal capture cross section. They are sensitive to the U-238 fast fission cross-section, U-238 inelastic scattering and U-235 fission spectrum. The scattering and thermal absorption cross sections of H_2O are very important also.

B. System description of BAPL

These experiments consist of H_2O moderated uranium oxide critical lattices of 1.311 wt.% enriched uranium oxide rods with diameters of 0.9728 cm in a triangular pattern. The measured parameters include ρ^{28},δ^{25}, δ^{28} and B^2. Three lattices with moderator to fuel volume ratios of 1.43, 1.78 and 2.40 are specified.

Physical properties of TRX and BAPL

The physical properties of TRX and BAPL are given in the following TABLE 1 and TABLE 2 respectively.

TABLE 1: Physical properties of TRX

Region	Outer radius in cm	Isotope	Concentration (X10^{24} atoms/cm^3)
Fuel	0.4915	^{235}U	6.2530×10^{-2}
		^{238}U	4.7205×10^{-2}
Void	0.5042	--	--
Clad	0.5753	Al	6.025×10^{-2}
Moderator	*	$^{1-}$H	6.676×10^{-2}
		^{16}O	3.338×10^{-2}

* lattices spacing of 1.8060 and 2.1740 cm respectively in triangular arrays.

TABLE 2: Physical properties of BAPL

Region	Outer radius in cm	Isotope	Concentration (X10^{24} atoms/cm^3)
Fuel	0.4864	^{235}U	3.112×10^{-2}
		^{238}U	$2.3127^2\times10^{-2}$
		O	4.6946×10^{-2}
Void	0.5042	--	--
Clad	0.5753	Al	6.025×10^{-2}
Moderator	*	H	6.676×10^{-2}
		O	3.338×10^{-2}

*Lattices spacing of 1.5578, 1.6523 and 1.8057 cm respectively in triangular arrays.

IV. PARAMETRIC STUDIES

The presently available WIMSD nuclear data library has been empirically adjusted to achieve reasonable agreement between the calculated and experimental integral parameters. The main goal of the present study is to obtain a new multigroup library, which has relatively good performance. To validate the new

multigroup library the parametric study has been performed. TRX-1, TRX-2, BAPL-1, BAPL-2 and BAPL-3 benchmark lattices [8] have been analyzed with WIMS.
4.1 Description of the Integral Parameters to be studied
The integral parameters calculated using the new JEFF-3.2 based WIMS library are as follows:

k_{eff} = Effective Multiplication Factor
ρ^{28} = Ratio of epithermal to thermal ^{238}U captures
= $(\Sigma_c)^{38}{}_{epth}$ / $(\Sigma_c)^{38}{}_{th}$ = $(\Sigma_a\text{-}\Sigma_f)^{38}{}_{epth}$ / $(\Sigma_a\text{-}\Sigma_f)^{38}{}_{th}$
δ^{25} = Ratio of epithermal to thermal ^{135}U fission
= $(\Sigma_f)^{35}{}_{epth}$ / $(\Sigma_f)^{35}{}_{th}$
δ^{28} = Ratio of ^{238}U fissions to ^{235}U fissions= $(\Sigma^t{}_f)^{38}$ / $(\Sigma^t{}_f)^{35}$
C^* = Ratio of ^{238}U captures to ^{235}U fissions
= $(\Sigma^t{}_c)^{38}$ / $(\Sigma^t{}_f)^{35}$ = $(\Sigma^t{}_a\text{-}\Sigma^t{}_f)^{38}$ / $(\Sigma^t{}_f)^{35}$

V. RESULTS AND DISCUSSIONS

The first important task was to investigate the quality of GENDF data generated from JEFF-3.2 basic data. It was observed that the produced GENDF data is very much consistent with LANL processed library data**.** This led to confidence to process these GENDF data into WIMS format using NJOY99.0. The lattices were modeled with WIMSD-5B based on optimized inputs suggested by the WIMS library update project. The integral parameters of the two lattices TRX, and BAPL, demonstrate the performance of the new library. The comparison among the calculated k_{eff} values with the experimental results, the original WIMS library and previously calculated in JENDL-3.3 [3] for TRX and BAPL benchmarks are shown in TABLE 3.

TABLE 3: Comparison of calculated k_{eff} for TRX and BAPL with Experimental, the original WIMS and JENDL- 3.3 library.

ASSEMBLY	JEFF-3.2 (Calculated)	WIMS [15]	Experimental	JENDL-3.3 [16]
TRX-1	0.9875(-1.25) $	1.0023(0.23) $	1.0000(0.30) #	0.9866(-1.33) $
TRX-2	0.9885(-1.15)	0.9966(-0.34)	1.0000(0.10)	0.9882(-1.17)
BAPL-1	0.9960(-0.04)	1.0030(0.30)	1.0000(0.10)	0.9979(-0.20)
BAPL-2	0.9957(-0.43)	1.0006(0.06)	1.0000(0.10)	0.9971(-0.29)
BAPL-3	0.9965(-0.33)	0.9982(-0.18)	1.0000(0.10)	0.9967(-0.33)

Percentage of uncertainty in experimental measurements.

$(Error in %) = [(Calculated value–Experimental value)/ Experimental value] x 100

TABLE-3 indicates that the effective multiplication factor k_{eff} for TRX and BAPL show better performance with the original WIMS library compared to other results as a whole. For TRX-1 and TRX-2 the calculated values of k_{eff} are better than JENDL-3.3 library. For BAPL-1, the calculated result is better than original WIMS and JENDL-3.3 library.

Overall, the values of k_{eff} are in good agreement with experimental value with some uncertainties.

Comparison of the calculated integral parameters values for TRX with experiment, JENDL-3.3 and the original WIMS library, are summarized in TABLE 4.

TABLE 4: Summary of WIMS Results Based on JEFF-3.2 Data for TRX Benchmark Lattices and Comparison with Experiment, JENDL-3.3 and the Original WIMS Library

LATTICE	Library	ρ^{28}	δ^{25}	δ^{28}	C^*
TRX-1	JEFF-3.2 (Calculated)	**1.3341** (1.06) $	**0.0997** (1.01)	**0.0961** (-2.61)	**0.7912** (-0.72)
	JENDL-3.3[16]	1.33225 (0.93)	0.09616 (-2.53)	0.09820 (3.8)	0.79094 (-0.75)
	WIMS[15]	1.2631 (-4.31)$	0.0990(0.31)	0.0965(2.02)	0.7745 (-2.82)
	Expt.	1.320(1.6) #	0.0987(1.0)	0.0946(4.3)	0.797(1.0)
TRX-2	JEFF-3.2 (Calculated)	0.8289 (-1.15)	**0.0590** (-3.84)	**0.0700** (1.08)	**0.6372** (-1.51)

	JENDL-3.3[16]	0.82759 (-1.12)	0.05903(-3.85)	0.07008(1.13)	0.63681 (-1.57)
	WIMS[15]	0.7967 (-4.81)	0.0610(-0.64)	0.0695(0.30)	0.6321 (-2.31)
	Expt.	0.837(1.9)	0.0614(1.3)	0.0693(5.1)	0.647(0.9)

Percentage of uncertainty in experimental measurements.

$(Error in %) = [(Calculated value–Experimental value)/ Experimental value] x 100

TABLE 4 shows that for TRX benchmark lattices the calculated results for ρ^{28} and C^* are better than those of original WIMS. The percent of uncertainty is even less than the experimental uncertainty. For δ^{25},δ^{28} and C^*, the calculated results are better than JENDL-3.3 library. For δ^{25} and δ^{28}, the original WIMS results are better than those of calculated results. As a whole, the values of all integral parameters are in good agreement with experimental values with some uncertainties.

Comparison of the calculated integral parameters values for BAPL with experiment, JENDL-3.3 and the original WIMS library, are summarized in TABLE 5.

TABLE 5: Summary of WIMS Results Based on JEFF-3.2 Data for BAPL Benchmark Lattices and Comparison with Experiment, JENDL-3.3 and the Original WIMS Library

LATTICE	Library	ρ^{28}	δ^{25}	δ^{28}	C^*
BAPL-1	JEFF-3.2 (Calculated)	1.346179598 (-3.15) $	0.08097002 (-3.60)	0.073128201 (-6.24)	0.7900070314
	JENDL-3.3[16]	1.34442(-3.27)	0.80923(-3.66)	0.07591(-2.67)	0.78944
	WIMS[15]	1.3454 (-3.21)	0.8040 (0.05)	0.0755 (-3.23)	0.7960
	Expt.	0.837 (1.9)	0.0614 (1.3)	0.0693 (5.1)	0.647 (0.9)
BAPL-2	JEFF-3.2 (Calculated)	1.093880796 (-2.33)	0.0661594 (-2.70)	0.065601281 (-6.28)	0.7197657445
	JENDL-3.3[16]	1.11297(-0.62)	0.06607(-2.84)	0.06546(-6.48)	0.71902
	WIMS[15]	1.1227 (0.24)	0.0687 (1.0)	0.0652 (-6.8)	0.7282
	Expt.	0.837 (1.9)	0.0614 (1.3)	0.0693 (5.1)	0.647 (0.9)
BAPL-3	JEFF-3.2 (Calculated)	0.868805434 (-4.10)	0.050878827 (-2.15)	0.074987505 (3.15)	0.64320496
	JENDL-3.3[16]	0.86970(-4.00)	0.05084(-2.23)	0.05380(-5.61)	0.64240
	WIMS[15]	0.8849 (-2.32)	0.0529 (1.73)	0.0538 (-5.56)	0.653
	Expt.	0.906 (1.1)	0.0520 (1.9)	0.0570 (5.3)	0.000

Percentage of uncertainty in experimental measurements

$(Error in %) = [(Calculated value–Experimental value)/ Experimental value] x 100

Table 5 shows that for BAPL-1 benchmark lattice, the calculated value of ρ^{28} is better than other libraries and vice-versa for BAPL-2 and BAPL-3. The calculated value of δ^{25} is better than that of JENDL-3.3. For BAPL-2 and BAPL-3 benchmark lattices, the calculated value of δ^{28} is better than other libraries and vice-versa for BAPL-1. Overall**,** the values of all integral parameters are in good agreement with experimental values with some uncertainties.

VI. CONCLUSION

The applied data processing method as shown in Fig. 1 represents state-of-the-art technology to generate WIMS library. The new executable NJOY99.0 with the introduced modifications in the WIMSR module nicely handled the new features in ENDF-6 format and very much consistent with the WIMS library format requirements. These modifications may be considered for inclusion while making an updated version of NJOY.

The present study shows a good consistency among the calculated integral parameters using JEFF-3.2, the experimental results, the original WIMS library and previously calculated JENDL-3.3 for both the benchmark lattices. It is obvious that different evaluated nuclear data library is the cause of the difference between the calculated results and other results. From the study it was concluded that almost all of the calculated integral parameters remained within the uncertainty limit of the measurements. Hence, it may be mentioned that data file library JEFF-3.2 is sufficiently reliable for thermal reactor calculations and also reliable for further advanced calculations of 3 MW TRIGA Mark-II research reactor commissioned at AERE, Saver, Dhaka, Bangladesh.

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Sheikh Md.Tazul Islam, et. al. "Generation of WIMSD-5B Multigroup Constants Library Based on JEFF-3.2 Nuclear Data and its Validation through some Benchmark Experiments Analysis and its Comparison with some other Libraries."*American Journal of Engineering Research (AJER)*, vol. 10(1), 2021, pp. 24-30.