

Comparison of JEFF-3.1.2 and JENDL-4.0u for TRIGA MARK-II Calculation Through the Benchmarking of Integral Parameter of TRX and BAPL Lattices of Thermal Reactor

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Abstract: The objective of this paper is to select an inimitable nuclear data library from JEFF-3.1.2 & JENDL-4.0u which are valid for theoretical safety analysis of TRIGA MARK-II research reactor. In this work the integral parameter (such as k_{eff} , ρ^{28} , δ^{25} , δ^{28} , C^*) of TRX and BAPL benchmark lattices of thermal reactors are compared with the experimental result by Cross Section Evaluation Working Group (CSEWG), USA. The nuclear data processing code NJOY99.0 is used to generate 69-group cross-section library from the basic evaluated nuclear data files JEFF-3.1.2 & JENDL-4.0u. TRX and BAPL benchmark lattices are modeled with optimized inputs, which are suggested in the final report of the WIMS Library Update Project Stage-I (WLUP). The integral parameters of five uranium-fuel thermal assemblies: TRX-1 and TRX-2 and BAPL-UO₂-1, BAPL-UO₂-2 & BAPL-UO₂-3 are calculated with the help of reactor lattice code WIMSD-5B based on the generated 69-group cross-section library. Form the comparison of the integral parameters with the experimental values it is found that the obtained results between the two libraries is nearly alike with some uncertainties. But the degrees of uncertainties for the values of integral parameters of JEFF-3.1.2 library are comparatively less. JEFF-3.1.2 is the better library and could be selected for the neutronic calculation of TRIGA Mark-II research reactor at AERE, Savar, Dhaka, Bangladesh.

Keywords: BAPL, JEFF-3.1.2, JENDL-4.0u, NJOY99.0, TRIGA MARK-II, TRX and WIMSD-5B

1. Introduction

A 3 MW TRIGA Mark-II research reactor has been operating in Bangladesh since 1986 at the Atomic Energy Research Establishment (AERE), Savar, Dhaka. The TRIGA Mark-II research reactor of Bangladesh Atomic Energy Commission (BAEC) is the first nuclear reactor in this country, which has been designed and constructed by the General Atomic of USA [1]. The installation of the reactor was started at the end of 1980 under a non-turnkey project, where local participation was about 50%. The reactor achieved its first criticality in the morning of 14 September 1986. This may be identified as a major event in the scientific

annals of the country. The reactor was tested and commissioned fully at the end of the October 1986. Since its commissioning, the reactor has been used in various fields of research and utilization; such as, neutron activation analysis (NAA), neutron radiography, neutron scattering, production of radioisotopes, training of manpower, academic research etc [2]. Through these activities the reactor meets the need of the people of Bangladesh to some extent. To determine the neutron flux and the value of the effective multiplication factor (k_{eff}) for a reactor, one has to solve the neutron transport equation. Considering the rates at which neutrons of different energies moving in different directions enter and leave a small volume element derives this equation. The ENDF-6 library is the latest recommended evaluated nuclear

data file for use in nuclear science and technology applications. These advances focus on neutron cross sections, fission product yields, decay data and represent work by the USA Cross Section Evaluation Working Group in nuclear data evaluation that utilizes developments in nuclear theory, modeling, simulation and experiment [3, 4]. To study the neutronic parameters including effective multiplication factor, neutron fluxes, power distributions, power peaking factors, excess reactivity and control rod worth calculation by using evaluated nuclear data library, it is very important to select the appropriate data library [5]. The available data libraries are Japanese evaluated nuclear data library (JENDL) [6], Joint Evaluated Fission and Fusion Data Library (JEFF) in Europe [7], ENDF/B-VI in USA [8], China evaluated nuclear data library (CENDL) [9] and BROND in Russia [10]. JEFF is high quality evaluated nuclear data library for accessible and prospective nuclear energy systems and this library involves evaluation efforts that cover the main nuclear data needs in the fields of fission and fusion applications [11]. Now JEFF-3.1.2 is available which is modified edition of JEFF-3.1.1 [12]. JENDL-4.0 was released in 2010 which contains neutron-induced reaction data for 406 nuclides. JENDL-4.0 is last updated at January, 2016 named JENDL-4.0u. A recent study provide the validation of the data files of JEFF-3.1.2 & JENDL-4.0u for the theoretical study of TRIGA Mark-II research reactor [13, 14]. The aim of this study is to choice a more efficient library for TRIGA calculation among the two valid libraries through the comparison of integral parameter of benchmark lattices TRX and BAPL by using two computer programs NJOY99.0 [15] and WIMSD-5B [16, 17].

2. Methods

The two computer program; NJOY99.0 and WIMSD-5B are used to compare the evaluated data files JEFF-3.1.2 and JENDL-4.0u through benchmarking TRX and BAPL benchmark lattices.

2.1. Computer Code NJOY99.0

The updated version NJOY99.0 of NJOY has the capability to process data in ENDF-6 format [18], which is used in JEFF-3.1.2 and JENDL-4.0u. The chain of NJOY99.0 modules [19] used to generate the 69-group cross section library from the basic data files of JEFF-3.1.2 & JENDL-4.0u is shown schematically in figure 1. NJOY directs the flow of data through the other modules and contains a library of common functions and subroutines used by the other modules. RECONR reconstructs point-wise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes. BROADR adds temperature dependence to the point-wise cross sections generated by the RECONR module. UNRESR computes effective self-shielded point-wise cross sections in the unresolved energy range. THERMR produces cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range. GROUPE generates self-shielded

multi-group cross sections, group-to-group scattering matrices, photon-production matrices and charged-particle cross sections from point-wise input. ERRORR computes multi-group covariance matrices from ENDF uncertainties. MODER converts ENDF "tapes" back and forth between ASCII format and special NJOY blocked-binary format. WIMSR prepares libraries for the thermal reactor assembly codes WIMSD.

Table 1. Corresponding energy of 69 groups.

| Fast Groups | | Thermal Groups | |
|------------------------|-----------------------------|----------------|-----------------------|
| Group | E _{max} (eV) | Group | E _{max} (eV) |
| 1 | 1.00000E+07 | 28 | 4.00000E+0 |
| 2 | 6.06550E+06 | 29 | 3.30000E+0 |
| 3 | 3.67900E+06 | 30 | 2.60000E+0 |
| 4 | 2.23100E+06 | 31 | 2.10000E+0 |
| 5 | 1.35300E+06 | 32 | 1.50000E+0 |
| 6 | 8.21000E+05 | 33 | 1.30000E+0 |
| 7 | 5.00000E+05 | 34 | 1.15000E+0 |
| 8 | 3.02500E+05 | 35 | 1.12300E+0 |
| 9 | 1.83000E+05 | 36 | 1.09700E+0 |
| 10 | 1.11000E+05 | 37 | 1.07100E+0 |
| 11 | 6.73400E+04 | 38 | 1.04500E+0 |
| 12 | 4.08500E+04 | 39 | 1.02000E+0 |
| 13 | 2.47800E+04 | 40 | 9.96000E-01 |
| 14 | 1.50300E+04 | 41 | 9.72000E-01 |
| Resonant Groups | | 42 | 9.50000E-01 |
| Group | E_{max} (eV) | 43 | 9.50000E-01 |
| 15 | 9.11800E+03 | 44 | 9.10000E-01 |
| 16 | 5.53000E+03 | 45 | 8.50000E-01 |
| 17 | 3.51910E+03 | 46 | 7.80000E-01 |
| 18 | 2.23945E+03 | 47 | 6.25000E-01 |
| 19 | 1.42510E+03 | 48 | 5.00000E-01 |
| 20 | 9.06899E+02 | 49 | 4.00000E-01 |
| 21 | 3.67263E+02 | 50 | 3.50000E-01 |
| 22 | 1.48729E+02 | 51 | 3.20000E-01 |
| 23 | 7.55014E+01 | 52 | 3.00000E-01 |
| 24 | 4.80520E+01 | 53 | 2.80000E-01 |
| 25 | 2.77000E+01 | 54 | 2.50000E-01 |
| 26 | 1.59680E+01 | 55 | 2.20000E-01 |
| 27 | 9.87700E+00 | 56 | 1.80000E-01 |
| | | 57 | 1.40000E-01 |
| | | 58 | 1.00000E-01 |
| | | 59 | 8.00000E-02 |
| | | 60 | 6.70000E-02 |
| | | 61 | 5.80000E-02 |
| | | 62 | 5.00000E-02 |
| | | 63 | 4.20000E-02 |
| | | 64 | 3.50000E-02 |
| | | 65 | 3.00000E-02 |
| | | 66 | 2.50000E-02 |
| | | 67 | 2.00000E-02 |
| | | 68 | 1.50000E-02 |
| | | 68 | |

Table 2. *k_{eff}* assessment of TRX benchmark lattices.

| Lattices | JEFF-3.1.2 | JENDL-4.0u | Experiment (CSEWG, 1986) |
|----------|-------------------|------------------|--------------------------|
| TRX-1 | 0.9853975 (1.46%) | 0.978300 (2.17%) | 1.0000 |
| TRX-2 | 0.9826511 (1.73%) | 0.98149 (1.85%) | 1.0000 |

2.2. Reactor Code WIMSD-5B

The new version code WIMSD-D, formally to be identified as WIMSD-5B, developed on the basis of the old WIMSD version of Atomic Energy Authority (AEA) Technology; was implemented on operating system with Lahey F7713 FORTRAN compiler. In this version, additional possibilities proposed by the code users have been included. The unique WIMSD structure is used with 69 energy group; i.e. 14 fast group, 13 resonance group and 42 thermal groups [20]. The associated energy of 69 groups is presented in table 1. Reaction of U-235 and U-238 has been taken to calculate the integral parameters of TRX and BAPL lattices by using WIMSD-5B code. The cross-section data sets in thermal region have been processed using WIMS library utility code WILLIE for U-235 and U-238 isotopes and compared as well.

2.3. Benchmark Lattices

Two types of benchmark lattices H₂O- moderated uranium lattices and H₂O-moderated uranium oxide critical lattices are used to benchmarking the calculated evaluated nuclear data files. TRX-1 & TRX-2 [21] are the H₂O- moderated uranium lattices as well as BAPL-UO₂-1, BAPL-UO₂-2 and BAPL-UO₂-3 are H₂O-moderated uranium oxide critical lattices. The material and dimensional properties of benchmark lattices are listed in table 3 [22] and table 4 [23] respectively. The interaction of U-235 and U-238 isotopes at 300K are used to calculate the integral parameter of TRX and BAPL lattices using the lattice code WIMSD-5B for the two nuclear data libraries. The absorption cross-section, fission cross-section and capture cross-section of U-235 and U-238 in the thermal and epithermal range for each TRX and BAPL lattices have been determined using WIMSD-5B.

2.4. Calculation Techniques

The isotopes listed in the table 5 are linked with the TRIGA Mark-II at AERE, Dhaka, Bangladesh [24]. These isotopes are processed using NJOY99.0, which can touch the new attribute of the database, in RECONR- BROADR- UNRESR- THERMR- GROUPT- WIMSR cycle by Pentium-IV PC in DOS command mode at the department of Physics, Jahangirnagar University, Bangladesh [25]. Using the WILLIE and WIMSD-5B code two 69-group cross-section libraries are generated from the processed isotope of JEFF-3.1.2 & JENDL-4.0u. For TRX-1, TRX-2, BAPL-UO₂-1, BAPL-UO₂-2 and BAPL-UO₂-3 lattices; the fission cross-section, absorption cross-section, captured cross-section of U-235 and U-238 are computed through the two generated 69-group cross-section libraries by using WIMSD-5B. The effective multiplication factor k_{eff} defined by equation 1 [26] and the other integral parameters (k_{eff} , ρ^{28} , δ^{25} , δ^{28} , C^*) of TRX and BAPL lattices listed [27] in table 2 are calculated and compared with the experimental values by CSEWG [28]. The library provides integral value of TRX and BAPL lattices in minimum deviation from the standard values will be the expected library.

Table 3. Properties of TRX benchmark lattice.

| Segment | External radius in cm | Nuclei | Concentration (E 24 atoms/cm ³) |
|-----------|-----------------------|------------------|---|
| Fuel | 0.4915 | ²³⁵ U | 6.2530E-04 |
| | | ²³⁸ U | 4.7205E-02 |
| Void | 0.5042 | ----- | ----- |
| Clad | 0.5753 | Al | 6.025E-02 |
| Moderator | * | ¹ H | 6.676E-02 |
| | | ¹⁶ O | 3.338E-02 |

*Lattices spacing of 1.8060 cm, 2.1740 cm respectively in triangular arrays

Table 4. Properties of BAPL benchmark lattice.

| Segment | External radius in cm | Nuclei | Concentration (E 24 atoms/cm ³) |
|-----------|-----------------------|------------------|---|
| Fuel | 0.4864 | ²³⁵ U | 3.1120E-04 |
| | | ²³⁸ U | 2.3127E-02 |
| Void | 0.5042 | ----- | ----- |
| Clad | 0.5753 | Al | 6.025E-02 |
| Moderator | ** | ¹ H | 6.676E-02 |
| | | ¹⁶ O | 3.338E-02 |

**Lattices spacing of 1.5578, 1.6523 and 1.8057 cm respectively

Table 5. Concern isotope of TRIGA with the respective material ID.

| SL. NO. | Isotope | Material ID. |
|---------|-----------|--------------|
| 01 | 1-H-1 | 125 |
| 02 | 5-B-10 | 525 |
| 03 | 6-C-12 | 625 |
| 04 | 7-N-14 | 725 |
| 05 | 8-O-16 | 825 |
| 06 | 13-Al-27 | 1325 |
| 07 | 14-Si-28 | 1425 |
| 08 | 24-Cr-52 | 2431 |
| 09 | 25-Mn-55 | 2525 |
| 10 | 26-Fe-56 | 2631 |
| 11 | 28-Ni-58 | 2825 |
| 12 | 40-Zr-91 | 4028 |
| 13 | 68-Er-166 | 6837 |
| 14 | 68-Er-167 | 6840 |
| 15 | 82-Pb-207 | 8234 |
| 16 | 92-U-235 | 9228 |
| 17 | 92-U-238 | 9237 |

$$k_{eff} = \frac{\text{(neutrons production from fission in one generation)}}{\text{(neutron absorption in the preceding generation + neutron leakage in the preceding generation)}} \quad (1)$$

$$\rho^{28} = \text{Ratio of epithermal to thermal neutron captures cross-section of } ^{238}\text{U}$$

$$= \frac{(\Sigma c)^{38}_{epth}}{(\Sigma c)^{38}_{th}} = \frac{(\Sigma a - \Sigma f)^{38}_{epth}}{(\Sigma a - \Sigma f)^{38}_{th}} \quad (2)$$

$$\delta^{25} = \text{Ratio of epithermal to thermal neutron fission cross}$$

section of ^{235}U

$$= (\Sigma_f^{35})_{\text{epth}} / (\Sigma_f^{35})_{\text{th}} \quad (3)$$

δ^{28} = Ratio of ^{238}U fission to ^{235}U fission

$$= (\Sigma_f^t)^{38} / (\Sigma_f^t)^{35} \quad (4)$$

C^* = Ratio of ^{238}U captures to ^{235}U fissions

$$= (\Sigma_c^t)^{38} / (\Sigma_f^t)^{35} = (\Sigma_a^t - \Sigma_f^t)^{38} / (\Sigma_f^t)^{35} \quad (5)$$

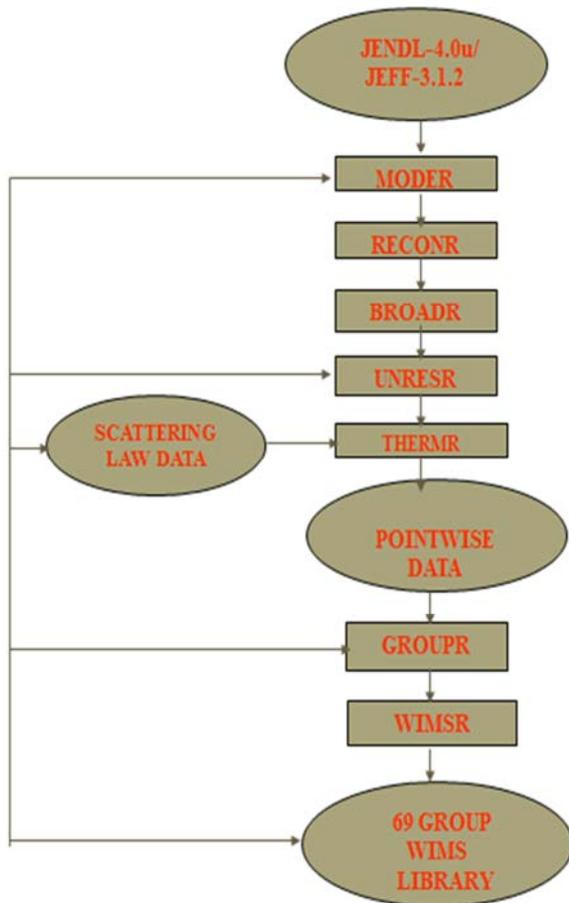


Figure 1. Flow chart of nuclear data processing code NJOY99.0.

3. Results & Discussions

3.1. Cross-Section Comparison

The calculated neutron cross-section of ^{235}U for TRX-1, TRX-2, BAPL- UO_2 -1, BAPL- UO_2 -2 and BAPL- UO_2 -3 benchmark lattices for JENDL-4.0u and JEFF-3.1.2 are plotted in figure 2 to figure 6 (Ep.A= epithermal absorption cross section, Th.A= thermal absorption cross section, T. A= total absorption cross section, Ep.F= epithermal fission cross section, Th.F= thermal fission cross section, T.Cp= total capture cross section and T.F= total fission cross section). The neutron cross-section of ^{235}U for JENDL-4.0u and JEFF-3.1.2 for each benchmark lattices are plotted in figure 7 to figure 11. It is observed that the cross-sections of ^{235}U are identical for both JENDL-4.0u and JEFF-3.1.2 in each

benchmark lattice. For ^{238}U the cross-sections are almost similar for each lattice of both library but total captured cross-section in BAPL lattice is slightly larger and total fission cross-section is smaller in JEFF-3.1.2 data library.

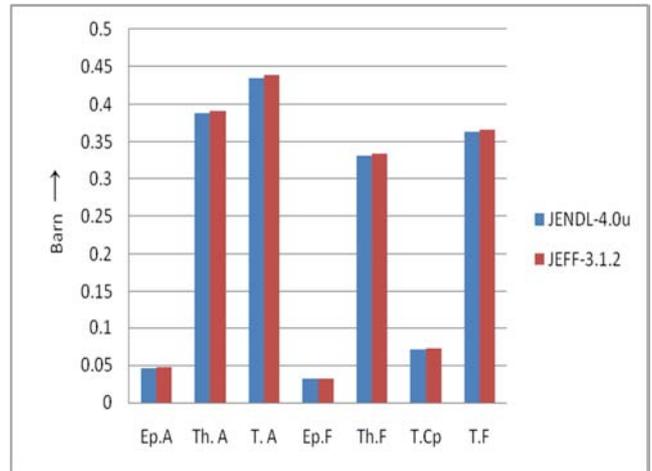


Figure 2. Cross-section comparison of U-235 for TRX-1 lattice.

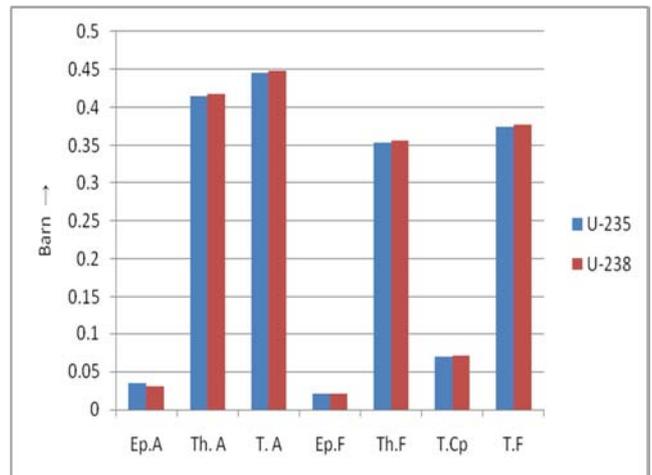


Figure 3. Cross-section comparison of U-235 for TRX-2 lattice.

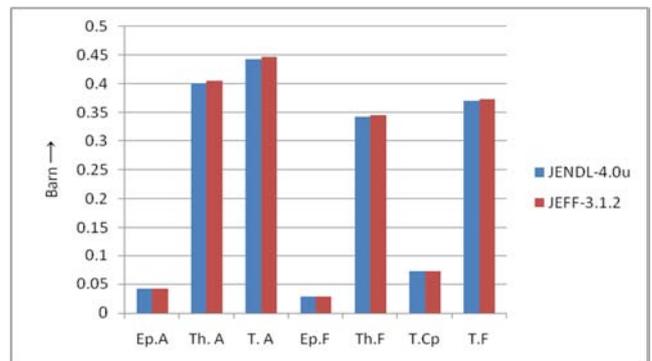


Figure 4. Cross-section comparison of U-235 for BAPL-1 lattice.

3.2. K_{eff} Comparison

The evaluated value the effective multiplication factor for JENDL-4.0u and JEFF-3.1.2 library for TRX benchmark lattice are listed in Table 2. Table 6 represents the evaluated

value of k_{eff} for BAPL benchmark lattice of both nuclear data library. The value enclosed in first parenthesis indicates the percentage of variation of the evaluated value from the corresponding standard value. It is observed that the values of k_{eff} in TRX-1 & TRX-2 lattices are closer to the standard values for JEFF-3.1.2 than the JENDL-4.0u library. The value of k_{eff} is equal in BAPL-2 lattice of both library but deviation of k_{eff} is larger in BAPL-1 & BAPL3 lattice for JENDL-4.0u.

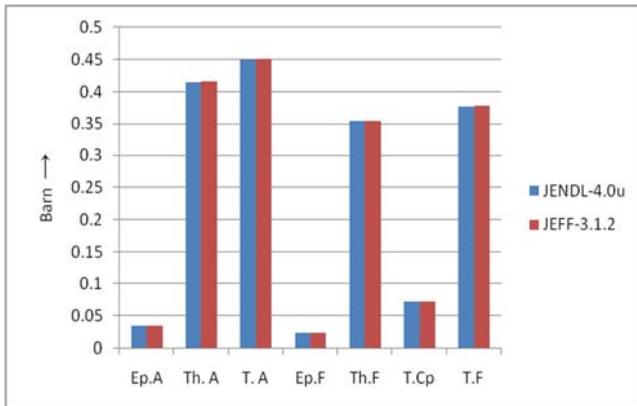


Figure 5. Cross-section comparison of U-235 for BAPL-2 lattice.

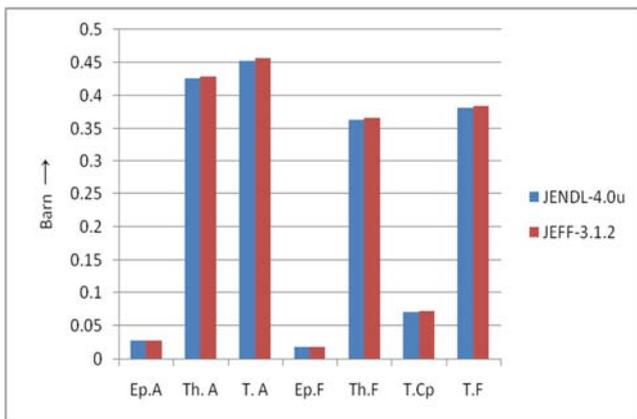


Figure 6. Cross-section comparison of U-235 for BAPL-3 lattice.

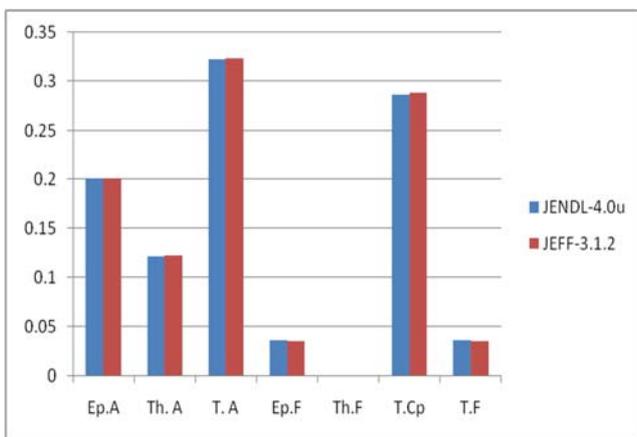


Figure 7. Cross-section comparison of U-238 for TRX-1 lattice.

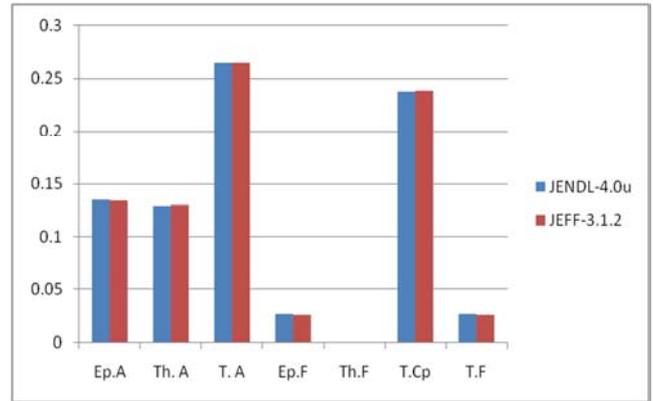


Figure 8. Cross-section comparison of U-238 for TRX-2 lattice.

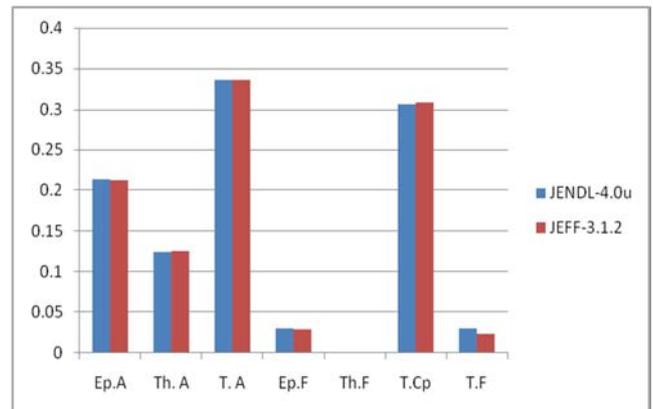


Figure 9. Cross-section comparison of U-238 for BAPL-1 lattice.

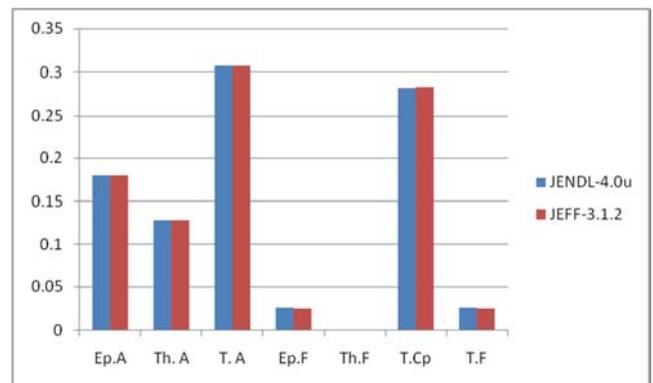


Figure 10. Cross-section comparison of U-238 for BAPL-2 lattice.

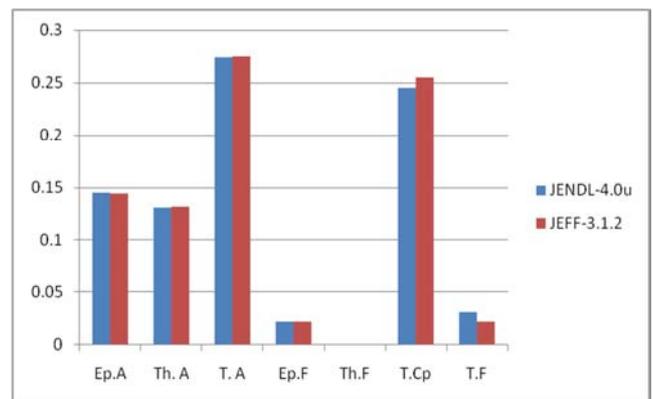


Figure 11. Cross-section comparison of U-238 for BAPL-3 lattice.

3.3. Comparison of ρ^{28} , δ^{25} , δ^{28} , C^*

ρ^{28} , δ^{25} , δ^{28} and C^* are the integral parameter of benchmark lattice. The values of the integral parameter of TRX & BAPL benchmark lattices for two libraries are listed in table 7 & table 8 respectively. The values of δ^{25} are equal in TRX-2 lattice. The values of C^* are slightly closer to the experimental values by CSEWG in TRX-1, TRX-2 lattices for JENDL-4.0u than JEFF-3.1.2 data library. The values of ρ^{28} , δ^{25} , δ^{28} are found closer to the experimental values by CSEWG for TRX-1 and TRX-2 lattices. The percent of error are more for the values of ρ^{28} , δ^{25} in BAPL-3 lattice but the other values of BAPL-1, BAPL-2 and BAPL-3 more closely for JEFF-3.1.2 than JENDL-4.0u. The maximum deviation of the values of all integral parameters from the experimental values is found for JENDL-4.0u is 9% for ρ^{28} in BAPL-2 lattice. Therefore, almost the integral parameters are closer to the standard values for JEFF-3.1.2 than JENDL-4.0u.

4. Conclusion

This analysis deals with comparison of neutron cross-section of U-235& U-238 and integral parameters of TRX & BAPL benchmark lattices with the experimental values by CSEWG for evaluated nuclear data libraries JENDL-4.0u & JEFF-3.1.2 by using nuclear data processing code NJOY99.0 as well as reactor lattice code WIMSD-5B. From the comparison of cross-section of U-235& U-238 for five benchmark lattices it is found that there are no remarkable variations observed in the two libraries JENDL-4.0u & JEFF-3.1.2. The value of the effective multiplication factor (k_{eff}) plays an important role to control the reactor directly and $K_{eff}=1$ provides the reactor is in critical condition. For both libraries the k_{eff} is less than 1 indicates reactor is in subcritical stage. The deviation of value of k_{eff} form critical condition is same only for one lattice for both library and deviation is minor for four benchmark lattices for JEFF-3.1.2 than JENDL-4.0u. This implies the values of k_{eff} for JEFF-3.1.2 are very closer to the critical condition i.e. closer to the experimental values by CSEWG. The Comparison of the values of ρ^{28} , δ^{25} , δ^{28} and C^* provide that the deviation of that calculated value for TRX & BAPL lattices are smaller in JEFF-3.1.2 than JENDL-4.0u library. The overall observations reflect that almost values of integral parameters are comparatively closer to the standard values for the evaluated nuclear data library- JEFF-3.1.2. Therefore it could be concluded that JEFF-3.1.2 is to be chosen for theoretical safety analysis of TRIGA reactor at AERE, Dhaka, Bangladesh for better performance.

Table 6. k_{eff} assessment of BAPL benchmark lattices.

| Lattices | JEFF-3.1.2 | JENDL-4.0u | Experiment (CSEWG, 1986) |
|----------|------------------|-----------------|--------------------------|
| BAPL-1 | 0.9828444 (1.7%) | 0.97743 (2.2%) | 1.0000 |
| BAPL-2 | 0.9849318 (1.5%) | 0.98481 (1.5%) | 1.0000 |
| BAPL-3 | 0.987897 (1.21%) | 0.98277 (1.72%) | 1.0000 |

Table 7. Integral parameter assessment of BAPL benchmark lattices.

| Lattices | Integral Parameter | JEFF-3.1.2 | JENDL-4.0u | Experiment (CSEWG, 1986) |
|----------|--------------------|-----------------|----------------|--------------------------|
| TRX-1 | ρ^{28} | 1.3466 (2.0%) | 1.3517 (2.4%) | 1.3200 |
| | δ^{25} | 0.0958 (2.9%) | 0.09573 (3.0%) | 0.0987 |
| | δ^{28} | 0.0949 (0.31%) | 0.09958 (5.2%) | 0.0946 |
| | C^* | 0.78848 (1.06%) | 0.79023 (0.8%) | 0.7970 |
| TRX-2 | ρ^{28} | 0.832 (0.59%) | 0.8353 (1.32%) | 0.8370 |
| | δ^{25} | 0.05868 (4.4%) | 0.05867 (4.4%) | 0.0614 |
| | δ^{28} | 0.0685 (1.1%) | 0.0708 (2.16%) | 0.0693 |
| | C^* | 0.6322 (2.2%) | 0.63327 (2.1%) | 0.6470 |

Table 8. Integral parameter assessment of BAPL benchmark lattices.

| Lattices | Integral parameters | JEFF-3.1.2 | JENDL-4.0u | Expt. (CSEWG, 1986) |
|----------|---------------------|---------------|----------------|---------------------|
| BAPL-1 | ρ^{28} | 1.4767 (6.0%) | 1.48610 (6.4%) | 1.3900 |
| | δ^{25} | 0.0821 (2.2%) | 0.08143 (3.0%) | 0.08400 |
| | δ^{28} | 0.0774 (0.8%) | 0.0772 (1.0%) | 0.0780 |
| | C^* | 0.8250 | 0.82811 | |
| BAPL-2 | ρ^{28} | 1.2101 (8.5%) | 1.22360 (9.0%) | 1.1200 |
| | δ^{25} | 0.0661 (2.7%) | 0.06601 (3.0%) | 0.0680 |
| | δ^{28} | 0.0679 (3.0%) | 0.06721 (3.9%) | 0.0700 |
| | C^* | 0.7460 | 0.74501 | |
| BAPL-3 | ρ^{28} | 0.9440 (1.7%) | 0.95002 (1.1%) | 0.9606 |
| | δ^{25} | 0.0507 (2.3%) | 0.05090 (2.1%) | 0.0520 |
| | δ^{28} | 0.0553 (2.9%) | 0.05487 (3.7%) | 0.0570 |
| | C^* | 0.6616 | 0.66349 | ... |

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