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Customization of ENDF/B-VI and JENDL3.2 Basic Data for MCNP Calculation and Measurements of Neutron Cross Section at INST, AERE, SAVAR

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The NJOY94.10+, a version of NJOY, has been installed in a VAX computer under Open VMS operating system. ENDF/B-VI, latest release of ENDF data, has been also implemented in the same system. A data library has been processed using the modules RECONR, BROADR and ACER of NJOY code. MCNP4B2 computer code has been used to validate the prepared data library for some benchmark experiments. The results obtained have been found to be in good agreement with the experimental results. Excitation function have been measured for $^{81}\text{Br}(n,\alpha)^{78}\text{As}$, $^{79}\text{Br}(n,\alpha)^{76}\text{As}$, $^{73}\text{Ge}(n,p)^{73}\text{Ga}$, $^{72}\text{Ge}(n,p)^{72}\text{Ga}$, $^{64}\text{Zn}(n,p)^{64}\text{Cu}$, $^{68}\text{Zn}(n,\alpha)^{65}\text{Ni}$, and $^{70}\text{Zn}(n,2n)^{69m}\text{Zn}$ reactions in the neutron energy range, 13.57-14.71 MeV via Activation technique.

1. Introduction

The NJOY [1] nuclear data processing system is a comprehensive computer code for producing pointwise and multigroup nuclear cross sections and related quantities from evaluated nuclear data in the ENDF format. The latest version, ENDF/B-VI [2], of the release 3 has been used to generate cross section for some benchmark problems and TRIGA reactor calculations.

2. Generation of Cross Section Library for MCNP4B2

For the MCNP continuous-energy neutron-photon Monte Carlo code, the ACER module prepares libraries in ACE (a compact ENDF) format. One of the design goals for MCNP has been to use the most detailed presentation of the physics of a problem that is practical. Therefore, the ACE format has evolved to include all the details of the ENDF representations for neutron and photon data. However, for sake of efficiency, the representation of data in ACE format is quite different from that in ENDF.

The following benchmarks demonstrate and test the preparation of ACE-format libraries for the MCNP code. The materials selected for processing were H-1, O-16, AL-27, U-234, U-235, U-238, Pu-239, Pu-240, Er-166, Er-167.

3. Comparison with benchmark problems

This study was undertaken to benchmark the generated continuous energy neutron cross sections for the Monte Carlo code MCNP4B2 against a set of critical experiments performed at room temperature to establish the basic data processing capability developed at INST, AERE, Savar. To determine the validity of the generated neutron cross section from ENDF/B-VI and JENDL3.2 for MCNP4B2 (latest version of MCNP) five experimental critical assemblies were analyzed. Each system was modeled and the simulation results were compared with the experimental data.
(i) **GODIVA**: The specifications used to define a bare uranium sphere were taken from the data of G.E. Hansen and H.C. Paxton [3] which was originally generated at Los Alamos National Laboratory, USA and then revised there in 1969. Lady GODIVA, as the setup was called, is an example of a fast neutron critical system. It was a simple geometry, consisting of a 52.42kg sphere of U (93.71)-93.71% $^{235}$U enriched. The density of the system was measured and found to be 18.74 gm/cc. These data correspond to a sphere of radius equal to 8.741 cm.

(ii) **JEZEBEL at 95.5% $^{239}$Pu Enrichment**: Jezebel was similar to the Godiva experiment and was reevaluated by G.E. Hansen and H.C. Paxton [3] at LANL in 1969. This system consisted of a bare plutonium sphere. Two different isotopic combinations of $^{240}$Pu and $^{239}$Pu were analyzed - a $^{239}$Pu composition of 95.5% and one of 80%. In both instances, the remaining material was $^{240}$Pu. These are "fast" critical assemblies with a relatively hard spectrum. The 95.5% $^{239}$Pu system was a 17.02 kg sphere with a density of 15.61 gm/cc and a radius of 6.385 cm.

(iii) **JEZEBEL at 80% $^{239}$Pu Enrichment**: The 80% enriched system had a critical mass of 19.46 kg, a density of 15.73 gm/cc and a radius of 6.660 cm.

(iv) - (v) **TRX-1 and TRX-2 Experiments**: This pair of experiments [4] are parts of the CSEWG thermal benchmarks and consisted of cylindrical aluminum clad metallic fuel rods in water. The pitch was triangular and the system was modeled as an infinite medium. Published leakage factors were then [5] used to obtain the effective multiplication factor as well as other integral quantities. The experiments were conducted at room temperature. The pitches for TRX-1 and TRX-2 are 1.806 cm and 2.174 cm respectively. The parameters of the experiments are as follows.

<table>
<thead>
<tr>
<th>Material</th>
<th>Outer radius (cm)</th>
<th>Isotope</th>
<th>Atom/Density (atom/barn-cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>0.4915</td>
<td>U-235</td>
<td>6.2530e-4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>U-238</td>
<td>4.7205e-2</td>
</tr>
<tr>
<td>Void</td>
<td>0.5042</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>Clad</td>
<td>0.5753</td>
<td>Al-27</td>
<td>6.0250e-2</td>
</tr>
<tr>
<td>Moderator</td>
<td>----</td>
<td>H-1</td>
<td>6.6706e-2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-16</td>
<td>63.3380e-2</td>
</tr>
</tbody>
</table>

4. Monte Carlo Simulation and Results

All MCNP simulations were performed on a 133 MHz Pentium PC under Windows95 operating system. The required cross section sets used as the various temperatures were generated in our laboratory at Institute of Nuclear Science & Technology (INST) from both the ENDF/B-VI and JENDL3.2 data using the NJOY94.10 cross section generation code which constructs, broadens and formats the data into the appropriate form for MCNP. Another two cross section sets were also used which were derived from ENDF/B-VI data processed at Los Alamos National Laboratory, USA and JENDL3.2 data processed at Japan Atomic Energy Research Institute (JAERI), Japan, in order to compare our processed data with those processed in advanced laboratories in the world. Full S(α,β) treatment [6] was used for thermal scattering of hydrogen in the water and this was obtained from the standard set that accompanied the MCNP4B2 code. The computation for all the cases were run using 500 cycles containing 3000 particles each, with 100 settle cycles to give a total of 1,200,000 histories. However, for TRX-1 & 2, 150 cycles were run containing 3000 particles each with 25 settle cycles to give a total of 375,000 histories. The code generates $k_{eff}$ information using
the track length, collision and absorption estimators, as well as various combinations of these, to give a total of eleven estimates for the $k_{\text{eff}}$ value. The combined average of the absorption/collision/track-length estimator is quoted as the $k_{\text{eff}}$ value in MCNP. In addition to the eigenvalue comparisons, local integral quantities like fission density comparisons were included for some of the experiments. The experimental uncertainty in the eigenvalues for TRX 1-2 experiments have been reported as about 0.2%. A relative error of 0.003 was assumed to be an acceptable fluctuation in the MCNP tally. The results from the GODIVA and JEZEBEL simulations are presented in Table I and for TRX-1 and TRX-2 in Table II.

**Table I. Results from the simulation of the GODIVA and JEZEBEL experiment**

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Experimental result with (relative error)</th>
<th>$k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>MCNP4B2 result with (relative error)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>LANL</td>
</tr>
<tr>
<td>GODIVA</td>
<td>1.00000 (0.00300)</td>
<td>0.99546 (0.00053)</td>
</tr>
<tr>
<td>JEZEBEL</td>
<td>1.00000 (0.00300)</td>
<td>1.00194 (0.00051)</td>
</tr>
<tr>
<td>(95.5%)</td>
<td></td>
<td>1.00847 (0.00053)</td>
</tr>
<tr>
<td>JEZEBEL</td>
<td>1.00000 (0.00300)</td>
<td>1.00847 (0.00053)</td>
</tr>
<tr>
<td>(80%)</td>
<td></td>
<td>1.00847 (0.00053)</td>
</tr>
</tbody>
</table>

**Table II. Result from the simulation of the TRX-1 and TRX-2 experiment**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Experiment Studied</th>
<th>Experimental result with (relative error)</th>
<th>MCNP4B2 result with (relative error)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>ENDF/B-VI</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>LANL</td>
</tr>
<tr>
<td>$k_{\text{inf}}$</td>
<td>TRX-1</td>
<td>1.17932 (0.00200)</td>
<td>1.17777 (0.00067)</td>
</tr>
<tr>
<td></td>
<td>TRX-2</td>
<td>1.16645 (0.00200)</td>
<td>1.16441 (0.00063)</td>
</tr>
<tr>
<td>$k_{\text{eff}}$</td>
<td>TRX-1</td>
<td>1.00000 (0.00200)</td>
<td>0.99863 (0.00067)</td>
</tr>
<tr>
<td></td>
<td>TRX-2</td>
<td>1.00000 (0.00200)</td>
<td>0.99625 (0.00063)</td>
</tr>
<tr>
<td>$\delta^{28}$</td>
<td>TRX-1</td>
<td>0.09460 (0.00410)</td>
<td>0.09885 (0.00195)</td>
</tr>
<tr>
<td></td>
<td>TRX-2</td>
<td>0.06988 (0.00350)</td>
<td>0.06988 (0.00185)</td>
</tr>
</tbody>
</table>
The eigenvalue estimates of MCNP using our processed data from ENDF/B-VI and JENDL3.2, as shown in Table I, compare very well with the GODIVA and JEZEBEL experiments and the relative errors are also much lower than the acceptable limit for MCNP. In some instances MCNP calculation using our processed data shows relatively better agreement than those with processed data of LANL and JAERI laboratories and this is due to the fact that we used less fractional tolerance the neutron cross section using the NJOY data processing code.

In case of the TRX-1 & 2 experiments, in addition to the $k_{\text{eff}}$ and $k_{\text{inf}}$ values, the $^{238}\text{U}$ to $^{235}\text{U}$ total fission reaction ratio, $\delta^{28}$, has also been studied. This factor is used to convert infinite medium simulation results to the actual finite critical experiment results. Table II shows that the eigenvalue predicted by MCNP using our processed data from ENDF/B-VI and JENDL3.2 is found to be in excellent agreement with experimental results and the relative error is also very much within the acceptance limit.

5. Conclusion

The set of critical experiments studied in this report have different fuel types, temperatures and fuel-to-moderator ratios. Thus a study of these experiments provides a rigorous test of the performance of any processed cross section for MCNP code. The results for different critical experiments obtained with our processed data are found to be in very good agreement with the experimental values. The deviation from the mean is well within the acceptance limit for MCNP. In some instances MCNP calculation using our processed data shows relatively better agreement than those obtained with data processed in LANL and JAERI laboratories, as because we used less fractional tolerance to generate the neutron cross section using the NJOY data processing code. It is also clear that the MCNP code coupled with the processed cross section from ENDF/B-VI and JENDL3.2 data is accurate enough to serve as a benchmark to compare with the experimental results. This study has also provided an independent validation of the ENDF/B-VI and JENDL3.2 data and the NJOY cross section processing code for reactor criticality calculations at different temperatures. The results demonstrates that the data processed at INST can be used with confidence for our reactor calculations. Therefore, the Er-166 and Er-167 cross sections processed in INST were used to support MCNP calculations for our TRIGA reactor which yielded very good agreement with experimental results.

6. 14 MeV Neutron Nuclear Data Measurements

6.1 Introduction

Extensive measurements of fast neutron induced reactions cross sections on structural materials of fission and fusion reactors have been carried out during the last decades at several laboratories over the neutron energy range from threshold upto 15.0 MeV. Excitation function of some reactions on the isotopes of Zn, Ge and Br in the neutron energy range 13.74 to 14.71 MeV have been measured. The measured cross section data together with nuclear model calculations using statistical code EXIFON are reported here in some cases.

6.2 Experimental

High purity target materials of Zinc, Germanium and Bromine pellets each sandwiched between aluminium foils were irradiated at $0^\circ$, $30^\circ$, $40^\circ$, $60^\circ$, $70^\circ$, $80^\circ$, $90^\circ$, $110^\circ$, $120^\circ$ and $166^\circ$ in a ring geometry arrangement over a period of 1-3 hours. Neutrons were produced at J-25
neutron generator via dt reaction with 110 keV deuterons and 300 μA beam. The effective neutron energy at each angular position was determined by measuring the ratio of the $^{89}$Zr to $^{92m}$Nb specific activities induced in Zr and Nb foils by (n,2n) reactions [7]. $^{27}$Al(n,α)$^{24}$Na served as monitor reaction. Cross section data for this reaction was taken from Vonach [8]. The radioactivity of the reaction products was measured by using a high resolution HPGe detector. The detector was calibrated with a set of standard gamma ray sources. Canberra S-100 MCA master board package based personal computer system was used for the data acquisition. Gamma software GANAAS has been used for the analysis of gamma ray spectra. The count rates were corrected for dead time loss, coincidence effect, detector efficiency and gamma transition intensities.

6.3 Results and Discussions

This work literature data [9-24] and values obtained via nuclear model calculations with the statistical code EXIFON [25], based on model of statistical multistep direct and multistep compound reactions, are shown in figs. 1-6 as a function of neutron energy. The uncertainty in the cross section values represents both systematic and statistical errors.

Acknowledgement

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References

Figure 1: Excitation function of \( ^{75}\text{Br}(n,p)^{79}\text{As} \) reaction in 13 - 15 MeV neutron energy region.

Figure 2: Excitation function of \( ^{73}\text{Ge}(n,p)^{73}\text{Ga} \) reaction in 13 - 15 MeV neutron energy region.

Figure 3: Excitation Function of \( ^{73}\text{Ge}(n,p)^{73}\text{Ga} \) reaction.

Figure 4: Excitation Function of \( ^{64}\text{Zn}(n,p)^{64}\text{Cu} \) reaction.

Figure 5: Excitation Function of \( ^{64}\text{Zn}(n,p)^{64}\text{Ni} \) reaction.

Figure 6: Excitation Function of \( ^{70}\text{Zn}(n,p)^{69}\text{Zn} \) reaction.

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