27
5/7

UCID - 16728

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the laboratory.

LAWRENCE LIVERMORE LABORATORY

University of California/Livermore, California

A COMPARISON OF CALCULATED AND EXPERIMENTAL NEUTRON
SPECTRA FROM THE LLL PULSED SPHERE PROGRAM
USING THE TART MONTE CARLO CODE AND
THE LLL EVALUATED NUCLEAR
DATA LIBRARY

R. J. Howerton

May 1972

MASTER

Prepared for U.S. Atomic Energy Commission under contract no. W-7405-Eng-48

DISTRIBUTION OF THIS DOCUMENT UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

A COMPARISON OF CALCULATED AND EXPERIMENTAL NEUTRON
SPECTRA FROM THE LLL PULSED SPHERE PROGRAM
USING THE TART MONTE CARLO CODE AND
THE LLL EVALUATED NUCLEAR
DATA LIBRARY

R. J. Howerton

May 1972

As part of the continuing program of checking both neutronics codes and evaluated nuclear data, several of the neutron spectra measured in the LLL pulsed sphere program⁽¹⁾ have been calculated using the TART⁽²⁾ Monte Carlo neutronics code and the LLL Evaluated Nuclear Data Library.⁽³⁾

As a check of the TART code, the MCN code⁽⁴⁾ was run at LASL by E.D. Cashwell to calculate some of the same pulsed spheres as those calculated by TART, with both codes using the same LLL Evaluated Nuclear Data Library. Within Monte Carlo statistics the results were essentially identical. Since both the handling of the evaluated data and the method of calculation are different in the two codes, these results either validate both codes or attest to the biggest coincidence ever documented. We assume the former. To be more explicit, the MCN code uses evaluated cross sections in a pointwise mode as presented in the evaluation, while TART averages the pointwise cross sections into 175 pre-selected groups. The most striking difference in the method of calculation of the spectra is that MCN does an

expectation calculation while TART does an analogue calculation. Because of an error in communications, the first MCN calculation was done with an incorrect energy distribution for the n,2n neutrons for iron: the peak of the energy distribution was shifted by 500 keV. The MCN results clearly differed from the TART results. After locating and correcting the error, the calculations agreed. The final conclusions are that the codes are sensitive to the input data, and that the calculations agree when the same input is used.

The attached graphs illustrate the degree of agreement between TART calculations and the experimental neutron spectra for 16 pulsed spheres. For the detector at 30° the experimental values for times greater than 340 nanoseconds are not to be taken seriously, according to J.D. Anderson of E-division. For the detector at 120° the same situation obtains above 420 nanoseconds. Note that 100 nanoseconds must be added to the flight times as labeled on the abscissae of the plots. Thus the values labeled $2.4E+02$ nanoseconds on the 30° plots are at 340 ($3.4E+02$) nanoseconds.

For some of the work done early in the pulsed sphere program, the location of the elastic peak is shifted in time from the calculated value. Note for example the 30° water plot (Fig. 1), which is the extreme example of this apparent disagreement. Similarly, the time resolution is difficult to determine. The full width at half maximum value is input to the calculations and affects the height and width of the elastic peak. For these calculations the values presented in Reference 1 were used. By changing these values within their uncertainty, the elastic peak value can be matched. However, the ground rules established for these calculations preclude making

changes either in the evaluated data or in the method of calculation solely to obtain agreement between experiment and calculation. A more meaningful comparison between calculation and experiment in this region is that of the integral under the elastic peak. For the 30° comparisons, the integrals were obtained from zero to 160 nanoseconds, at which point the measured and calculated spectra have reached a value at least one order of magnitude less, and, for heavy materials, as much as two and one-half orders of magnitude less, than the elastic peak values. The corresponding upper limit for the 120° integrals is 220 nanoseconds. Table I presents these data. Note that the best agreement between experiment and calculation occurs for the neutronically thinnest spheres with disagreement increasing with increasing thickness. This is as it should be. Any error in the evaluation should be magnified as the material becomes thicker.

The work reported here is the result of the efforts of many people. A code, for editing the TART calculation, and magnetic tapes containing the pulsed sphere experimental data, were supplied by John Kammerdiener and Clint Logan. Ernie Plechaty, in addition to his efforts with the TART code, converted the pulsed sphere experimental data to a form convenient for retrieval from the photo-store, modified the edit code for TTY operation, and wrote a code for displaying the combined results of the calculations and the experiments on the TMDS. Heinz Barschall participated on a daily basis in discussing the representation of the physics in the data evaluations, suggesting auxiliary calculations which would check TART usage of the data, and arranging for Ed Cashwell of LASL to make the MCN calculations. John Anderson has made valuable suggestions (for the past many years) with

respect to the physics of the emission spectra used in the evaluations and has also provided advice as to the regions of greatest validity of the pulsed sphere measurements. Steve Grimes calculated emission spectra from nuclear models which were compared with the same quantities estimated from nuclear systematics. Eugene Goldberg provided much of the impetus required to insure that this collaborative effort was carried out. I did the calculations and performed most of the evaluations which were tested by this series of calculations. I must claim the dubious distinction of accepting the responsibility for lack of agreement between calculation and experiment. That is the reason that this report is authored by me and the participation of others delineated in the body of the report. I feel it would be unfair to imply by co-authorship that others should accept the responsibility for any such disagreement.

The pulsed spheres comprise the only set of integral neutron experiments for 14 MeV neutrons that span the mass range of elements from the lightest to the heaviest. There is a gap from iron to lead (from mass ~ 56 to mass ~ 208) which will be filled in during the fall of 1972 by a series of pulsed spheres for elements with intermediate masses. For most elements or isotopes, microscopic neutron emission spectra for incident 14 MeV neutrons have not been measured. Enough emission spectra have been measured, however, so that when they are considered together with the many measurements of neutron emission spectra from charged particle induced reactions, one can infer from systematics a recipe for the emission spectra, especially the non-equilibrium (high energy) portion.

It is possible to fit any or all of the pulsed spheres by a process

of successive approximations, in which the cross sections and spectra are adjusted until the degree of fit is as desired. However, we have chosen instead to use the pulsed sphere calculations as tests of existing evaluated data, and to test the recipes used for the fission spectra and high energy portion of the emission spectra from inelastic scattering; we have chosen not to concentrate on fitting the experimental pulsed sphere spectra by adjusting microscopic cross sections and spectra. The most important use of these comparisons between spectral calculations and measurements is as a diagnostic tool, to direct attention to elements that apparently have poor-quality evaluations. Once we have identified such a material, the evaluation is examined for obvious errors. Experimental microscopic data are checked for new or overlooked data, and changes are made in the evaluation if there is a reason for such a change based on experimental data, reliable theoretical calculations, or an established recipe. If there is no reason to change the data based on one of these three considerations, no change is made.

The degree of fit exemplified by the figures is considered to range from adequate to good for the LLL evaluated library. We have also made calculations using the ENDF/B-III library for iron, lead, aluminum and titanium pulsed spheres. In each case the agreement between calculation and experiment has been significantly worse than the agreement shown here. In the near future calculations will be made for the other pulsed spheres using the ENDF/B-III library. The purpose in doing the comparisons using ENDF/B-III data is to determine whether some of those evaluations should be adopted for the LLL evaluated library. So far the results have been negative.

REFERENCES

1. C. Wong, J.D. Anderson, P. Brown, L.F. Hansen, J.L. Kammerdiener, C. Logan and B. Paul, "Livermore Pulsed Sphere Program Summary through July 1971," UCRL-51144, Rev. 1 (1972).
2. E.F. Plechaty, J.R. Kimlinger, "TART Monte Carlo Neutron-Transport Code," UCIR-522 (1971).
3. R.J. Howerton, R.J. Doyas, T.C. Michels, S.T. Perkins, "Evaluated Nuclear Cross Section Library," UCRL-50400, Vol. 4 (1971).
4. E.D. Cashwell, Private Communication (1972).

Table I. Integrals of the Time Spectra Under the Elastic Peak

Material	Sphere Thickness (mean free paths)	Angle (degrees)	Experimental Integral	Calculated Integral	Calc.-Exp. Exp.
H ₂ O	1.9	30	.309	.274	-.113
H ₂ O	1.9	120	.336	.297	-.116
D ₂ O	2.1	30	.302	.269	-.109
Li ⁶	0.5	30	.815	.799	-.020
Li ⁶	0.5	120	.831	.817	-.017
Li ⁷	0.5	30	.815	.813	-.002
Li ⁷	0.5	120	.835	.831	-.005
Be ⁹	0.8	30	.718	.670	-.067
C	0.5	30	.757	.736	-.027
C	0.5	120	.840	.837	-.003
N	1.1	30	.668	.612	-.084
Mg	0.7	30	.664	.721	+.086
Mg	0.7	120	.742	.794	+.070
Al	0.9	30	.590	.583	-.012
Al	0.9	120	.647	.646	-.002
Ti	1.2	30	.521	.549	+.054
Fe	0.9	30	.615	.615	+.000
Fe	0.9	120	.674	.683	+.013
Fe	4.8	30	.073	.058	-.205
Fe	4.8	120	.078	.070	-.102
Pb	1.4	30	.545	.483	-.114
Pb	1.4	120	.508	.533	+.049
U ²³⁵	0.7	30	.645	.686	+.064
U ²³⁵	0.7	120	.732	.789	+.078

Table I. (contd)

Material	Sphere Thickness (mean free paths)	Angle (degrees)	Experimental Integral	Calculated Integral	Calc.-Exp. Exp.
U^{238}	0.8	30	.643	.653	+.015
U^{238}	0.8	120	.708	.749	+.058
Pu^{239}	0.7	30	.646	.706	+.093
Pu^{239}	0.7	120	.723	.790	+.093

Figure 1.

Figure 2.

Figure 3.

Figure 4.

Figure 5.

Figure 6.

Figure 7.

Figure 8.

Figure 9.

Figure 10.

Figure 11.

Figure 12.

Figure 13.

Figure 14.

Figure 15.

Figure 16.

Figure 17.

Figure 18.

CNTS (TRGT IN) PER NSEC. (TOT CNTS (TRGT OUT))

Figure 19.

Figure 20.

Figure 21.

Figure 22.

Figure 23.

Figure 24.

Figure 25.

Figure 26.

Figure 27.

Figure 28.

DISTRIBUTION

LLL Internal Distribution

TID File

R. J. Howerton, L-71

B. J. Weis, L-375

1 - 5

External Distribution

Randall E. Morton, Nucl. Engr. Dept.
University of Washington, Seattle, Wash.

U. S. Energy Res. & Dev. Admn., TIC,
Oak Ridge, Tennessee

27

NOTICE

"This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research & Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights."