**Analysis of a Neutron Scattering
Integral Experiment on Iron for Neutron
Energies from 1 to 15 MeV**

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MASTER

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ANALYSIS OF A NEUTRON SCATTERING INTEGRAL EXPERIMENT ON
IRON FOR NEUTRON ENERGIES FROM 1 TO 15 MeV

S. N. Cramer and E. M. Oblow

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Abstract

Monte Carlo calculations were made to analyze the results of an integral experiment with an iron sample to determine the adequacy of neutron scattering cross-section data for iron. The experimental results analyzed included energy-dependent NE-213 detector count rates at a scattering angle of 90 deg and pulse-height spectra for scattered neutrons produced in an iron ring pulsed with a 1- to 20-MeV neutron source. The pulse-height data were unfolded to generate secondary neutron spectra at 90 deg as a function of incident neutron energy. Multigroup Monte Carlo calculations using the MORSE code and ENDF/B-IV cross sections were made to analyze all reported results. Discrepancies between calculated and measured responses were found for inelastic scattering reactions in the range from 1 to 4 MeV. These results were related to deficiencies in ENDF/B-IV iron cross-section data.

Acknowledgement

The authors wish to acknowledge the aid of J. D. Drischler in preparing the graphical results. The multigroup cross sections were generated by W. E. Ford as part of the AMPX project of the Computer Sciences Division.

I. Introduction

Calculations of neutron integral count rates and secondary neutron energy spectra were performed for comparison with the results of an integral measurement on iron. The calculations and the experiments^{1,2} were done at Oak Ridge National Laboratory as part of the Defense Nuclear Agency data testing program. This effort was designed to test neutron scattering and gamma-ray production data for several nuclides of interest to DNA for incident neutron energies from 1 to 15 MeV. The calculations, experiments, and comparisons presented here are similar to those already completed for carbon,³ nitrogen,⁴ and oxygen.⁵ The experimental procedures designed specifically for the data testing program are outlined in Ref. 2.

The current experiment consisted of a ring of natural iron pulsed by a collimated beam of neutrons traveling approximately 50 meters from source to sample. An NE-213 detector was used to detect the neutrons scattering from the sample. The data were reduced to neutron counts as a function of time and reported as counts per incident neutron as a function of incident neutron energy by using time-of-flight considerations. Pulse-height information was also recorded as a function of arrival time so that the differential spectrum of neutrons could be obtained by unfolding techniques as a function of incident neutron energy. The experimental data are reported in Ref. 1.

All calculations used to analyze the experiments were made with the MORSE⁶ multigroup Monte Carlo code using multigroup neutron cross-section data from the DNA library⁷ processed by the AMPX⁸ code system. The results of the analysis are presented in the form of comparisons of the experimental and calculated results.

The experimental arrangement is described in Section II and the calculational model in Section III. Experimental and calculated results are presented in Section IV followed by a discussion in Section V and conclusions in Section VI.

II. Experimental Arrangements

The ORNL experimental setup is shown in Fig. 1. The Oak Ridge Electron Linear Accelerator (ORELA) was used to create a white pulsed neutron source (12 nsec burst width) from the $\text{Be}(\gamma, n)$ reaction. These neutrons were collimated into a beam which traveled along a 47.35-meter flight path to the scattering sample forming a uniformly distributed mono-directional source at the sample position. The source and flight path are shown in Fig. 2.

The scattering sample consisted of a stepped iron ring 25.38 cm in outer diameter, 15.30 cm in inner diameter, and 3.72 cm thick. The iron density was 7.826 gm/cm^3 (complete specifications of the sample can be found in Ref. 1). A 4.22 cm x 4.65 cm NE-213 detector was placed at the center of the ring creating a scattering angle of 90 deg with respect to the incident beam direction. The detector was shielded from the incident beam with a lead collimator. Experimental data was obtained in the form of integral count rates and pulse-height spectra as a function of incident neutron energy.

III. Calculational Model

A. Codes and Cross-Section Data

All calculations presented in this report were made with the MORSE⁶ multigroup Monte Carlo code using multigroup neutron cross-section data processed by the AMPX⁸ code system.

The iron cross-section data set used in the calculations was taken from the DNA MAT 4192 data file (equivalent to ENDF/B-IV MAT 1192). The sample was assumed to be pure iron with a density of 0.084402 atoms/barn-cm.

The cross sections for this study were processed using AMPX into a 141 neutron group structure with a P_8 Legendre expansion. A $1/E$ weighting function was used to simulate the incident source spectrum. The cross-section group structure is given in Table 1 along with the detector

Fig. 1. Experimental Setup for the Iron Integral Experiment.

Fig. 2. Neutron Source and Flight Path at ORELA Used for ORNL Integral Experiment.

Table I. Neutron Energy Group Structure and Detector Response

Group No.	Upper Energy (eV)	Detector Response	Group No.	Upper Energy (eV)	Detector Response
1	2.0000E 07	1.5590E-01	51	4.4631E 06	2.6150E-01
2	1.9409E 07	1.5600E-01	52	4.3312E 06	2.6490E-01
3	1.8835E 07	1.5620E-01	53	4.2022E 06	2.6850E-01
4	1.8279E 07	1.5650E-01	54	4.0790E 06	2.7210E-01
5	1.7739E 07	1.5610E-01	55	3.9584E 06	2.7570E-01
6	1.7214E 07	1.5500E-01	56	3.8414E 06	2.7930E-01
7	1.6706E 07	1.5350E-01	57	3.7279E 06	2.8300E-01
8	1.6212E 07	1.5200E-01	58	3.6177E 06	2.8660E-01
9	1.5738E 07	1.5170E-01	59	3.5108E 06	2.9020E-01
10	1.5268E 07	1.5190E-01	60	3.4071E 06	2.9380E-01
11	1.4817E 07	1.5240E-01	61	3.3064E 06	2.9740E-01
12	1.4379E 07	1.5330E-01	62	3.2087E 06	3.0110E-01
13	1.3954E 07	1.5450E-01	63	3.1138E 06	3.0470E-01
14	1.3541E 07	1.5610E-01	64	3.0218E 06	3.0830E-01
15	1.3141E 07	1.5800E-01	65	2.9325E 06	3.1190E-01
16	1.2758E 07	1.6010E-01	66	2.8459E 06	3.1540E-01
17	1.2376E 07	1.6250E-01	67	2.7610E 06	3.1890E-01
18	1.2010E 07	1.6460E-01	68	2.6801E 06	3.2240E-01
19	1.1655E 07	1.6610E-01	69	2.6009E 06	3.2580E-01
20	1.1311E 07	1.6740E-01	70	2.5241E 06	3.2920E-01
21	1.0977E 07	1.6870E-01	71	2.4495E 06	3.3260E-01
22	1.0652E 07	1.6890E-01	72	2.3771E 06	3.3590E-01
23	1.0337E 07	1.7080E-01	73	2.3068E 06	3.3920E-01
24	1.0032E 07	1.7220E-01	74	2.2387E 06	3.4240E-01
25	9.7355E 06	1.7420E-01	75	2.1725E 06	3.4550E-01
26	9.4478E 06	1.7630E-01	76	2.1083E 06	3.4860E-01
27	9.1686E 06	1.7860E-01	77	2.0460E 06	3.5170E-01
28	8.8976E 06	1.8090E-01	78	1.9855E 06	3.5470E-01
29	8.6347E 06	1.8340E-01	79	1.9269E 06	3.5760E-01
30	8.3795E 06	1.8600E-01	80	1.8699E 06	3.6050E-01
31	8.1319E 06	1.8870E-01	81	1.8146E 06	3.6340E-01
32	7.8916E 06	1.9160E-01	82	1.7610E 06	3.6610E-01
33	7.6584E 06	1.9460E-01	83	1.7090E 06	3.6890E-01
34	7.4320E 06	1.9780E-01	84	1.6585E 06	3.7150E-01
35	7.2124E 06	2.0100E-01	85	1.6095E 06	3.7430E-01
36	6.9993E 06	2.0460E-01	86	1.5619E 06	3.7720E-01
37	6.7924E 06	2.0860E-01	87	1.5157E 06	3.8010E-01
38	6.5917E 06	2.1290E-01	88	1.4709E 06	3.8290E-01
39	6.3969E 06	2.1730E-01	89	1.4275E 06	3.8570E-01
40	6.2078E 06	2.2190E-01	90	1.3853E 06	3.8850E-01
41	6.0244E 06	2.2620E-01	91	1.3444E 06	3.9130E-01
42	5.8463E 06	2.3010E-01	92	1.3046E 06	3.9400E-01
43	5.6736E 06	2.3380E-01	93	1.2661E 06	3.9670E-01
44	5.5059E 06	2.3740E-01	94	1.2287E 06	3.9930E-01
45	5.3432E 06	2.4090E-01	95	1.1923E 06	4.0100E-01
46	5.1858E 06	2.4430E-01	96	1.1571E 06	4.0240E-01
47	5.0320E 06	2.4760E-01	97	1.1229E 06	4.0360E-01
48	4.8833E 06	2.5110E-01	98	1.0897E 06	4.0470E-01
49	4.7390E 06	2.5460E-01	99	1.0575E 06	4.0560E-01
50	4.5990E 06	2.5800E-01	100	1.0263E 06	4.0640E-01

Table I (Cont'd.)

Group No.	Upper Energy (eV)	Detector Response
101	9.9594E 05	4.0700E-01
102	9.6650E 05	4.0760E-01
103	9.3794E 05	4.0810E-01
104	9.1022E 05	4.0810E-01
105	8.8332E 05	4.0740E-01
106	8.5722E 05	4.0640E-01
107	8.3189E 05	4.0520E-01
108	8.0730E 05	4.0390E-01
109	7.8345E 05	4.0240E-01
110	7.6029E 05	4.0080E-01
111	7.3782E 05	3.9910E-01
112	7.1602E 05	3.9720E-01
113	6.9486E 05	3.9530E-01
114	6.7432E 05	3.9330E-01
115	6.5440E 05	3.9120E-01
116	6.3506E 05	3.8900E-01
117	6.1629E 05	3.8420E-01
118	5.9808E 05	3.7690E-01
119	5.8040E 05	3.6910E-01
120	5.6325E 05	3.6090E-01
121	5.4660E 05	3.5250E-01
122	5.3045E 05	3.4370E-01
123	5.1478E 05	3.3460E-01
124	4.9956E 05	3.2540E-01
125	4.8480E 05	3.1600E-01
126	4.7047E 05	3.0650E-01
127	4.5657E 05	2.9680E-01
128	4.4308E 05	2.8710E-01
129	4.2998E 05	2.7520E-01
130	4.1727E 05	2.5810E-01
131	4.0494E 05	2.4010E-01
132	3.9298E 05	2.2160E-01
133	3.8136E 05	2.0260E-01
134	3.7009E 05	1.8320E-01
135	3.5916E 05	1.6350E-01
136	3.4854E 05	1.4350E-01
137	3.3824E 05	1.2330E-01
138	3.2825E 05	1.0340E-01
139	3.1854E 05	8.9650E-02
140	3.0913E 05	7.8590E-02
141	3.0000E 05	7.3370E-02

efficiencies. The neutron groups are equally spaced in lethargy between 20 MeV and 300 keV.

B. Calculational Procedure

Neutrons were followed from production to detection as a function of space, angle, and time. Neutron histories were started uniformly per unit lethargy from 20 MeV to the lowest energy with reported experimental data. The initial spatial coordinates of the neutrons were determined by selecting x and y uniformly over the effective cross-sectional area of the neutron beam and placing z at the leading edge of the sample. Neutrons were started straight ahead in the z direction.

Source neutrons in each energy group were given initial times determined by the time-of-flight of a neutron at the midpoint of each energy group to the leading edge of the sample. Relativistic velocities were used throughout the calculations. The initial times were smeared with a Gaussian approximation of the experimentally determined time spread as follows:

$$\Delta t = (R1 - R2) \times T \quad (1)$$

where $R1$ and $R2$ are random numbers and $T = 12$ nsec.

The calculation model for the ORNL experiment is the same as that shown in Fig. 1 except for the fact that the detector was approximated as a point flux detector. This assumption was shown to have negligible effect on the results reported and simplified the calculations considerably.

Count rates were calculated as $\phi \times \epsilon \times A$ where ϕ is the flux at the detector center determined by next flight estimation, ϵ is the detector efficiency given in Table 1, and A is the detector cross-sectional area, 19.6 cm^2 . The count rates were converted to counts per MeV per incident source neutron by multiplying the count rate by the time bin width and by dividing by the corresponding energy group width in MeV. The fraction

of incident neutrons in each energy group is equal (within statistics) since the group boundaries were equally spaced in lethargy and the starting energies were selected uniformly in lethargy.

The detector count rates were reported as functions of the incident neutron energy. The time bins for the calculation were determined from the energy group boundaries, E , as follows:

$$T = \frac{D/c}{\sqrt{1 - \frac{1}{\left(1 - \frac{E'}{2c^2}\right)^2}}} \quad (2)$$

where,

T = flight time in sec from accelerator source to sample face for a neutron energy E at the source,

D = distance in cm from accelerator source to sample face,

$E' = 1.91322 \times 10^{12} \times E$, where E is the energy in MeV,

c = speed of light in cm/sec.

Although the neutron flight times scattering in the sample and traveling to the detector are included in the calculations, they are generally small compared to the flight time of the neutrons from the source to the sample as determined by Eq. (2).

The calculated secondary energy spectra for the experiment included the empirically determined energy resolution of the detector given by R , the full-width at half-maximum value of the resolution function in percent:

$$R = \sqrt{A + B/E} \quad (3)$$

where A was 250, B was 670, and E was an energy in MeV uniformly selected in the energy group of the detected particle. The spectra were obtained by time-dependent calculations with time bins being determined by Eq. (2) where E corresponded to the broad group energy boundaries used in unfolding the experimental pulse-height spectra.

IV. Comparison of Experimental and Calculated Results

The figures which follow summarize the calculations performed for comparison with the experimental data. All calculations were made with the MORSE Monte Carlo code using the ENDF/B-IV iron cross-section set. The integral neutron count rate comparisons at 90 deg are given in Figs. 3, 4, and 5. In all figures the error bars represent one standard deviation of the mean value. Figures 6 through 12 give the secondary neutron energy spectra comparisons. In the multiple energy spectra figures, each set of comparisons is plotted at the mid-point of the appropriate incident neutron energy bin (i.e., the plot at 12 MeV on the slanted energy scale corresponds to the spectrum of secondary neutrons arising from incident neutrons in the 11.0 to 13.0 MeV energy range).

V. Discussion

The lack of a complete set of angular-dependent integral and spectral experimental data (i.e., results at other than 90 deg) make it difficult to draw conclusions about specific problems in the ENDF/B-IV iron data set specifically with regard to elastic scattering cross sections. It should be pointed out that as an integral detector, NE-213 is most responsive to neutrons with energies between 500 keV and 2 MeV. Above and below this energy range the detector efficiencies drop off considerably (see Table I). The integral results therefore tend to be most sensitive to neutrons emerging at low energies from non-elastic scattering events. In addition to this factor, the choice of a 90-deg detector location also favors detection of non-elastically scattered neutrons. For all energies above 1 MeV the angular distribution for elastic scattering is considerably forward peaked and in moving to high incident neutron energies 90-deg elastic scattering becomes decreasingly important compared to small angle scattering events. These two factors make the entire experiment predominantly a non-elastic scattering measurement test which is shown graphically in the spectral results given in Figs. 6 through 12.

What is clear from the integral results shown in Figs. 3, 4, and 5 is that there are significant disagreements between the experimental and calculated results. The largest discrepancies appear in the 10- to 12-MeV incident neutron energy range where the calculations are low by about 30%. In the 3- to 5-MeV range and above 14 MeV smaller disagreements appear with the calculations being high by about 20%. The results below 2.0 MeV and more specifically below 1.0 MeV (see Fig. 5) indicate some larger discrepancies. It appears, however, that these latter disagreements are the result of fine structure effects, in that the experimental data averaged over 100-keV intervals would be in good agreement with the calculated results. The angular-dependent elastic scattering cross-section data (i.e., Legendre coefficients) are simply not evaluated to the resolution of the integral experiment data so the calculations only represent the average scattering behavior.

Turning to the secondary spectral results, it becomes somewhat easier to identify the cause of the observed discrepancies in the integral count rate results. From Figs. 6 through 8 it is clear that the elastic scattering portion of the secondary spectrum (corresponding to the highest energy peak in each curve) is calculated reasonably well for incident neutron energies up to about 4.0 MeV. As the inelastic levels in this energy range begin to contribute to the lower energy portion of the scattered neutron spectrum, large discrepancies begin to show up. In the 1.5 to 1.75 MeV incident energy bin, scattering from the first inelastic level at 0.86 MeV begins to appear as a second peak in the curve at lower energies. The calculation of the secondary spectrum from such inelastic events appears to be overpredicted by as much as a factor of two, however. As each higher energy inelastic level is excited (at energies of 2.0, 2.6, and 3.0 MeV), a similar overprediction of the secondary neutron flux in the spectrum occurs (see Figs. 7 and 8). Moving 1 MeV or more above the threshold of each level, however, seems to result in good agreement between calculated and experimental results. It appears to be the data in the region just above threshold (i.e., 300 keV to 1 MeV above threshold) that seems to be the cause of the discrepancies. These results are reflected in the integral curves which are very

Fig. 3. Comparison of the Integral Count Rate Results for the ORNL Iron Integral Experiment.

Fig. 4. Comparison of the Integral Count Rate Results for the ORNL Iron Integral Experiment.

Fig. 5. Comparison of the Integral Count Rate Results for the ORNL Iron Integral Experiment.

ORNL DWG 75-17892

Fig. 6. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

ORNL DWG 75-17893

Fig. 7. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

Fig. 8. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

sensitive to such inelastic events as evidenced by the overpredictions at about 1.5 MeV, 2.1 MeV and above 2.6 MeV in Fig. 4.

The trend in overpredicting the lowest energy end of the spectrum continues up through incident neutron energies of 7 MeV (see Figs. 9 and 10). The evaluated data, on which the calculations are based, contain discrete level inelastic information up to incident neutron energies of about 4.5 MeV, at which point continuum inelastic data begins in tabulated form so as to retain some discrete level structure. Above 7 MeV the evaluation changes over to a temperature model description of continuum inelastic. At the point of this changeover to the temperature model, the overpredictions just above threshold disappear and the calculated results agree with the experimental results up to about 10 MeV. This behavior would seem to indicate that problems exist in the cross section data for discrete inelastic scattering just above threshold. Less likely is the possibility that there is some anisotropy in inelastic events just above threshold (to check this latter effect data at other detector angles would be needed).

Above an incident neutron energy of about 10 MeV the tail of the secondary spectrum is uniformly undercalculated (see Figs. 11 and 12) except that at the highest energies near 14 MeV the lower portion of the tail is overcalculated. These discrepancies, coupled with the NE-213 efficiency bias toward low energy neutrons, is responsible for the integral discrepancies seen in Figs. 3 through 5. Above 10 MeV several thresholds for scattering are reached, most important of which is the $^{56}\text{Fe}(n,2n)$ reaction threshold at about 11.2 MeV. Since the secondary spectra for continuum scattering reactions is more or less independent of initial energy, the low energy spectral discrepancies in the 1- to 2-MeV range are likely related to these partial cross sections. Although anisotropic effects cannot be ruled out completely, results from the Livermore pulsed sphere program^{11,12} indicate similar secondary spectra behavior for angular integrated iron scattering results, supporting the above conclusion. The discrepancies in the 4- to 8-MeV region of the secondary spectra, on the other hand, are very likely the result of deficiencies in the continuum and discrete inelastic data.

ORNL DWG 75-17895

Fig. 9. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

ORNL DWG 75-17896

Fig. 10. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

ORNL DWG 75-17897

Fig. 11. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

ORNL DWG 75-17898

Fig. 12. Comparisons of the Secondary Neutron Energy Spectra for the ORNL Iron Integral Experiment.

The valley in the secondary energy distribution between 8 to 10 MeV in Fig. 12 showed discrepancies in past evaluations but it appears that the ENDF/B-IV data has remedied the problem. This region is very sensitive to the treatment of data for continuum and discrete inelastic scattering which lead to undercalculation of the spectrum by factors of two and three in previous analyses.^{9,10} As evidenced by the present results, the discrepancies caused by previous iron data files has more or less disappeared (although the statistical errors in the results are fairly large in this region). Recent calculations by Howerton¹² for a similar integral experiment also confirm this conclusion. At lower incident neutron energies in the range from 6 to 10 MeV the valley discrepancy does show up again and the problem here also is probably in the inelastic scattering cross section for discrete levels as handled by the combination of a tabulated data file and a continuum temperature model treatment.

In all the curves above incident neutron energies of 5 MeV there are large discrepancies in comparisons of secondary spectra near the elastic scattering peak. Although these results indicate discrepancies that surely exist in the elastic data, elastic scattering to 90 deg is orders of magnitude lower than small angle scattering in iron at these energies. It appears difficult to get such a small angular-dependent cross section accurately measured and evaluated, but there are few applications where these events will be important. The high energy neutron albedo on an iron first wall in a CTR device might be one of these, however.

VI. Conclusions

Several significant deficiencies in the ENDF/B-IV iron data files still exists as evidenced by the analysis of the ORNL experimental results. In the 1- to 4-MeV incident neutron energy range the cross sections for inelastic scattering to the first three levels in ⁵⁶Fe appear to be too large by from 30-100% just above threshold. At energies above

6 MeV the continuum and tabulated discrete level inelastic data appear to be alternately too high or too low. From 6 to 12 MeV the cross sections for both discrete inelastic and continuum inelastic data are too low and from 13 to 15 MeV it appears that the continuum inelastic data are high and the cross sections for some inelastic levels are still low. Discrepancies appear in the elastic scattering data above incident neutron energies of about 5 MeV. Not too much significance can be placed in these disagreements, however, since the bulk of the scattering is highly forward peaked at these energies. The conclusions drawn about the non-elastic scattering data above 13 MeV are consistent with results reported for iron from the Livermore pulsed sphere integral experiment program.

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