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**Nuclear Data Development Work in Support of the
National Bureau of Standards ISNF Project**

February 1976—July 1980

MASTER

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NUCLEAR DATA DEVELOPMENT WORK IN SUPPORT OF THE
NATIONAL BUREAU OF STANDARDS ISNF PROJECT
February 1976-July 1980

by

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ABSTRACT

Work in several areas was completed by the Los Alamos Scientific Laboratory for the National Bureau of Standards in connection with the Intermediate-Energy Standard Neutron Field (ISNF) project during this reporting period. These areas include supplying multigroup cross-section sets from ENDF/B-IV appropriate for ISNF calculations; determining the effects of small changes in calculational parameters, including cross-section changes, in ISNF results; providing additional selected multigroup cross-sections sets from both ENDF/B-IV and ENDF/B-V; and performing comparison ISNF calculations using discrete ordinates and Monte Carlo codes. Plans for future work are briefly mentioned.

I. INTRODUCTION

During the past three and one-half years, the Los Alamos Scientific Laboratory (LASL) has provided neutron multigroup cross sections for and made comparison calculations in support of the National Bureau of Standards (NBS) Intermediate-Energy Standard Neutron Field (ISNF) project.¹ The ISNF is an irradiation facility at NBS designed to produce a strong component of neutrons in the energy range of interest for fast-neutron reaction-rate technology.

LASL support of the ISNF project has generally fallen into four categories, namely:

1. Providing space-dependent multigroup cross sections from ENDF/B-IV in 53 neutron energy groups.
2. Performing a number of calculations to determine the effects of changing several calculational parameters by small amounts.

3. Providing additional 53-group cross sections from ENDF/B-IV and ENDF/B-V.
4. Performing comparison discrete ordinates and Monte Carlo calculations.

II. DESCRIPTION OF ISNF FACILITY

The ISNF facility consists of a spherical cavity of 30.0 cm diameter in the graphite thermal column of the NBS reactor. Eight ^{235}U fission source disks are mounted symmetrically near the inner surface of the cavity. Each disk is made of enriched uranium metal 16 mm in diameter x 0.015 mm thick (93% enrichment, 0.476 or 0.511 g each) and positioned at 1 cm from the surface of the 30-cm diameter cavity. The eight disks are irradiated by thermal neutrons from the graphite column and produce a total source strength of about 6×10^{11} n/s. The spectrum of neutrons from the source disks is modified by a spherical boron-aluminum shell with 14.26 cm outside diameter, placed concentrically within the cavity. Two boron-aluminum shells have been used to date, which have thicknesses of 1.293 cm and 0.638 cm. An access port in the thermal column allows for placement of samples at the center of this experimental arrangement.

Figure 1 shows the one-dimensional model we have used in our calculations for ISNF-1, that is, the ISNF configuration for the 1.293-cm thick B-Al shell. Note that the eight ^{235}U fission disks have been homogenized into a 0.1 cm thick source region located about 1 cm from the cavity surface. Also note that the thermal column was taken to be a graphite spherical shell with a diameter of 130 cm. The central flux we have calculated² for this model is shown in Fig. 2.

III. PRODUCTION OF SPACE-DEPENDENT CROSS SECTIONS FROM ENDF/B-IV

Discrete ordinates (S_n) calculations were made with the ONETRAN code³ using 240-group⁴ cross sections as input. These cross sections had previously been processed⁵ from ENDF/B-IV with the NJOY code.⁶ Total cross sections for ^{12}C , ^{27}Al , and ^{10}B in 240 neutron energy groups are shown in Figs. 3-5, respectively. The initial flux guess required as part of the ONETRAN input was the ^{235}U fission spectrum, supplied by NBS.⁷ Resulting angular fluxes from the ONETRAN problem were then used in the CIX code⁸ as weighting functions to collapse the 240-group cross sections to the 53 groups of the NBS multigroup structure for a number of space regions of the ISNF. The version of CIX used for this collapse was modified specifically for the ISNF project to handle

Fig. 1.
Calculational model for the ISNF-1 configuration.

Fig. 2.
ISNF central spectrum 240-group calculation.

Fig. 3.
Total cross section for ^{12}C in 240 groups.

Fig. 4.
Total cross section for ^{27}Al in 240 groups.

Fig. 5.
Total cross section for ^{10}B in 240 groups.

angle-dependent weighting fluxes.⁹ This modification was necessary because of the strongly coupled energy- and angle-fluctuations in the angular flux in the graphite region at high energies.

Table I gives the neutron-energy boundaries of the NBS multigroup structure. Table II summarizes the 53-group space-dependent cross-section sets that were supplied to NBS.

IV. EFFECTS OF SMALL CHANGES IN ISNF PARAMETERS

The effects of small changes in isotopic concentration, a change in quadrature, and of using inappropriate space-dependent cross sections were studied. ONETRAN problems were run in the basic 240-group multigroup structure in which the boron and aluminum concentrations were separately increased and decreased by 5%. The central fluxes from each of these cases were then compared with the reference case flux shown in Fig. 2.. Results, expressed as percent differences from the reference case, are shown in Figs. 6-9. As is to be expected, the greatest effects are seen in the boron changes in the thermal region in which, however, the flux is very low.

To study the effects of quadrature, a 240-group problem was run at S-4 and compared with the reference problem (Fig. 2), which was run at S-8. Results can be seen in Fig. 10 in which, again, central fluxes are compared. As shown, the effect is less than 2%, except at very high energies.

In order to study the effect of using different cross-section sets, several ONETRAN problems were run using different 53-group cross-section sets shown in Table II. In all problems, set No. 6 was used for ^{10}B and set No. 9 was used for aluminum. Sets 1, 3, and 4 were used for ^{12}C in different problems, however. Central fluxes from these problems were compared with the re-binned reference case flux. Results are shown in Fig. 11, and as can be seen from this figure, the effects are minimal.

V. ADDITIONAL CROSS-SECTION SETS

Additional 240-group cross sections derived from ENDF/B-IV with the NJOY code were collapsed to the 53-group NBS multigroup structure using the CINX code and angular fluxes from a point inside the graphite thermal column as weighting function. Cross-section sets so processed and provided to NBS include data for ^1H , ^2H , ^{16}O , and ^{235}U .

TABLE I

NEUTRON ENERGY BOUNDARIES OF NBS MULTIGROUP STRUCTURE

<u>Group</u>	<u>E-lower</u>	<u>E-upper</u>
1	1.8221E+07	1.9640E+07
2	1.4918E+07	1.8221E+07
3	1.1618E+07	1.4918E+07
4	9.0484E+06	1.1618E+07
5	6.8729E+06	9.0484E+06
6	6.0653E+06	6.8729E+06
7	4.7237E+06	6.0653E+06
8	3.6788E+06	4.7237E+06
9	3.1664E+06	3.6788E+06
10	2.7253E+06	3.1664E+06
11	2.4660E+06	2.7253E+06
12	2.2313E+06	2.4660E+06
13	1.8731E+06	2.2313E+06
14	1.6122E+06	1.8731E+06
15	1.3534E+06	1.6122E+06
16	1.1080E+06	1.3534E+06
17	9.6164E+05	1.1080E+06
18	8.2085E+05	9.6164E+05
19	6.7206E+05	8.2085E+05
20	4.9787E+05	6.7206E+05
21	4.0762E+05	4.9787E+05
22	3.0197E+05	4.0762E+05
23	2.2371E+05	3.0197E+05
24	1.8361E+05	2.2371E+05
25	1.3569E+05	1.8361E+05
26	1.1109E+05	1.3569E+05
27	8.6517E+04	1.1109E+05
28	6.7379E+04	8.6517E+04
29	5.2475E+04	6.7379E+04
30	4.0868E+04	5.2475E+04
31	3.1828E+04	4.0868E+04
32	2.4788E+04	3.1828E+04
33	1.9305E+04	2.4788E+04
34	1.5034E+04	1.9305E+04
35	1.1709E+04	1.5034E+04
36	9.1188E+03	1.1709E+04
37	5.5308E+03	9.1188E+03
38	3.3546E+03	5.5308E+03
39	2.0347E+03	3.3546E+03
40	1.2341E+03	2.0347E+03
41	7.4852E+02	1.2341E+03
42	4.5400E+02	7.4852E+02
43	2.7536E+02	4.5400E+02
44	1.6702E+02	2.7536E+02
45	1.0130E+02	1.6702E+02
46	6.1442E+01	1.0130E+02
47	3.7267E+01	6.1442E+01
48	1.3710E+01	3.7267E+01
49	8.3153E+00	1.3710E+01
50	2.3824E+00	8.3153E+00
51	8.7642E-01	2.3824E+00
52	4.1399E-01	8.7642E-01
53	1.5200E-01	4.1399E-01

TABLE II
SPACE-DEPENDENT CROSS SECTIONS PROVIDED NBS

Set No.	Inner and Outer Radii of Region of Fluxes Used for Collapse	ISNF Constituent
1	14.92 - 30.06 cm	C-12
2	30.00 - 45.00 cm	C-12
3	14.92 - 65.00 cm	C-12
4	45.00 - 65.00 cm	C-12
5	5.838 - 7.131 cm	B-10, B-11, Al
6	5.838 - 6.392 cm	B-10, B-11, Al
7	6.392 - 6.762 cm	B-10, B-11, Al
8	6.762 - 7.131 cm	B-10, B-11, Al
9	7.131 - 7201 cm	Al

We have also provided cross-section sets processed from ENDF/B-V. These were processed directly into the 53-group structure with the NJOY code. Weighting functions supplied by NBS as well as "built-in" weighting functions in the NJOY code were used in the processing. The NBS weighting functions consisted of spectra calculated for 1/4 (NBS-1) and 3/4 (NBS-2) thicknesses of the pressure-vessel-simulation in the ORNL PCA experiment. Several nuclide concentrations (values of σ_0) were specified in the processing. This part of the work is summarized in Table III.

VI. DISCRETE ORDINATE AND MONTE CARLO COMPARISONS

Finally, comparison calculations of the ISNF facility were made using the Monte Carlo code MCNP.¹⁰ Results¹¹ have been reported at an American Nuclear Society meeting; comparisons with NBS experimental results¹² were also made in the course of these investigations. The MCNP calculations consisted of two types, namely, 240-group discrete-reaction cross sections and continuous energy kinematics (DR) and complete continuous energy (CE). A point detector was placed at the center of the ISNF for purposes of tallying the central spectrum. The Monte-Carlo calculations used 300 K ENDF/B-IV data for neutron transport but both ENDF/B-IV and ENDL¹³ data for spectral indexes and other parameters of interest.

Fig. 6.
Five percent decrease in ^{10}B concentration.

Fig. 7.
Five percent increase in ^{10}B concentration.

Fig. 8.
Five percent decrease in aluminum concentration.

Fig. 9.
Five percent increase in aluminum concentration.

Fig. 10.
S-N quadrature changed to S-4.

Fig. 11.
Effects of different carbon sets on the central flux.

TABLE III
CROSS-SECTION SETS PROCESSED FROM END^F/B-V

Table No.	Nuclide	ID	Legendre Order	Weighting Function	Sigma Zero
1	Fe	NBFE1A	P ₀	NBS-1	0.1 b/a
2			P ₁		
3			P ₂		
4		NBFE1B	P ₀		Infinite
5			P ₁		
6			P ₂		
7		NBFE2A	P ₀	NBS-2	0.1 b/a
8			P ₁		
9			P ₂		
10		NBFE2B	P ₀		Infinite
11			P ₁		
12			P ₂		
13	²³⁸ U	NBU28A	P ₀	4	10 b/a
14			P ₁		
15			P ₂		
16		NBU28B	P ₀		50 b/a
17			P ₁		
18			P ₂		
19		NBU28C	P ₀		100 b/a
20			P ₁		
21			P ₂		
22		NBU28D	P ₀		300 b/a
23			P ₁		
24			P ₂		
25		NBU28E	P ₀		1000 b/a
26			P ₁		
27			P ₂		
28		NBU28F	P ₀		10000 b/a
29			P ₁		
30			P ₂		
31		NBU28G	P ₀		Infinite
32			P ₁		
33			P ₂		

*NOTES:

1. Weighting functions NBS-1 and NBS-2 were supplied by NBS. Weighting function number 4 is a "built-in" weighting function in the NJOY code consisting of a thermal Maxwellian + a "1/E" region + a fission spectrum for which break points and nuclear temperatures are specified by the user. For the ²³⁸U problems in the above table, breakpoints were specified at 1 eV and 50 keV; the nuclear temperatures specified were 0.05 eV and 0.7 MeV. The breakpoint and temperature chosen for the thermal region are somewhat arbitrary as this region is unimportant in these problems, but those at the high-energy end were selected on the basis of the 1975 NBS evaluated fission spectrum for ²³⁸U (in 40 groups).
2. All problems were run for a temperature of 300 K.
3. The tables have matrix dimensions of 56x53, i.e., 53 groups plus positions for absorption, $\bar{\nu}\sigma_f$, and total cross sections.

Figure 12 shows the percent difference between the central flux for the ONETRAN and MCNP(CE) calculations. (Since 90% of the neutron spectra is between 8 keV and 3.5 MeV, the graph is somewhat truncated.)

Some calculated and experimental spectral indexes are presented in Table IV. The numbers in parentheses represent the percent relative difference with the NBS experiment in the ISNF-1 configuration. Results indicate a 9 to 13% difference in the $^{238}\text{U}/^{235}\text{U}$ fission cross section and less difference for the $^{239}\text{Pu}/^{235}\text{U}$ fission data.

Additional comparisons are made in Table V. In this table, integral quantities derived from calculations with the NBS evaluated spectrum and the ISNF-1 spectrum are compared. Comparison calculations using the ENDL library are also included in the table. Results from this table as well as from Table IV indicate that there may be discrepancies in the cross-section information used in fast-reactor spectra; therefore, these comparisons should be repeated using ENDF/B-V data. As a matter of fact, these calculations are already underway as part of a continuation of this work for NBS.

TABLE IV
SPECTRAL INDEXES FOR CALCULATED AND EXPERIMENTAL ISNF-1 SPECTRA
 $\sigma(x)/\sigma[^{235}\text{U}(n,f)]$
All Data ENDF/B-IV Unless Noted

Reactions(X)	240-Group	C.E. Monte Carlo ^a	D.R. Monte Carlo ^a	NBS Experiment
$^{239}\text{Pu}(n,f)$	1.117 (-3.3) ^b	1.108 (-4.1)	1.105 (-4.3)	1.155 + 1.8%
$^{238}\text{U}(n,f)$	0.0836 (-9.4)	0.0817 (-11.5)	0.0814 (-11.8)	0.0927 + 1.1%
		0.0840 (-9.0) ^c		
		0.0848 (-8.1) ^d		

- a. Relative error (1σ) for Monte Carlo is approximately 1% for all cases.
b. Number in parenthesis is percent relative differences with NBS experiment.
c. Both ^{235}U and ^{238}U are ENDL data.
d. Only ^{238}U is ENDL data.

Fig. 12.
Percent difference between discrete-ordinate and
continuous-energy Monte Carlo at ISNF-1 Center.

TABLE V

COMPARISON OF CALCULATED INTEGRAL CROSS SECTIONS FOR ^{235}U AND ISNF-1 SPECTRA

	^{235}U Spectra ^a	ISNF-1 Spectra		
	ENDF/B-IV (Multigroup)	ENDF/B-IV (Multigroup)	ENDF/B-IV (Monte Carlo)	ENDL (Monte Carlo)
Flux ^b		1.3850-3	1.4042-3	1.4065-3
$^{235}\text{U}(\text{n},\text{f})$	1.241 (1.705) ^c	1.6313	1.6465	1.6644
$^{238}\text{U}(\text{n},\text{f})$	0.295 (0.310) ^c	0.13632	0.13458	0.13969
$^{239}\text{Pu}(\text{n},\text{f})$	1.781 (1.81) ^c	1.8219	1.8245	1.8247

a. NBS evaluated spectrum

b. Energy-integrated flux at sample

c. NBS experiments, Ref. 12.

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