THE EVALUATION OF MINIMA IN TOTAL NEUTRON CROSS-SECTION BY TRANSMISSION OF FISSION SPECTRA THROUGH THICK SAMPLES

by 6791

WILLIAM HOWARD MILLER

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Approved by:

Major Professor

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1.0 INTRODUCTION

Total neutron cross-section data is available from many sources and reasonable agreement is found between independently determined cross-section tables. However, small discrepancies in the minima of integral cross-section data lead to large errors in transport calculations involving deep penetration. An error of a few percent in the cross-section data can approach an order of magnitude error in transmitted spectrum through a thick sample (ten or more mean free paths). To determine the reliability of literature data the neutron cross-section has been experimentally evaluated by measuring the uncollided neutron spectra transmitted through thick samples. Experimental data were compared to a calculated transmitted spectrum determined as a function of the spectrum, the resolution of the detector, and the particular cross-section data being tested. Since thick samples (three or more mean free paths) were used, the experimental versus calculated analysis is very sensitive to minima in the cross-section.

In this work, total neutron cross-sections were evaluated for iron, lead, liquid oxygen, solid sodium and liquid sodium. The incident neutron spectra for these measurements were obtained from the fast (northeast) beam port of the K.S.U. Triga Mark II reactor and the transmitted neutron spectra were detected with an NE-213 fast neutron spectrometer system. Data were collected with a TMC 4096 Multiparameter Analyzer and the results were unfolded with a suitable computer code.

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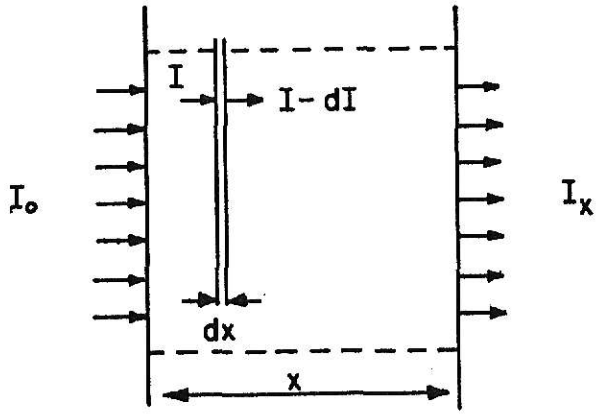
2.0 THEORY

The theoretical basis for this experiment is similar to that applied in the transmission method[9] of cross-section determination. A collimated beam of neutrons striking, perpendicularly, a specified area of a material of thickness x will be attenuated. Considering a thin layer of thickness dx parallel to the surface and recalling the definition of cross-section, it follows that $\Sigma_t dx$ is the fraction of neutrons that will interact with the material. This fraction may be set equal to -dI/I which is the fractional decrease in the neutron beam as the result of passing through thickness dx.



Thus,

$$-\frac{dI}{I} = \Sigma_t dx \qquad (1)$$

Integration over the thickness x of the material gives,

$$I_x = I_o \exp(-\Sigma_t x) \qquad (2)$$

where I_o = number of incident neutrons/cm^2

I_x = number of neutrons/cm^2 left at thickness x

Σ_t = total neutron cross-section

Recalling that this experiment dealt with neutron fluxes as a function of energy, equation 2 can be rewritten as:

$$\phi_{trans}(E) = \phi_I(E)\exp[-\Sigma_t(E)\,t] \tag{3}$$

where ϕ_I = incident flux($n/cm^2 \cdot min \cdot MeV$)

ϕ_{trans} = transmitted flux($n/cm^2 \cdot min \cdot MeV$)

Σ_t = total cross-section

The quantities ϕ and Σ_t are now functions of energy.

In this experiment very large thicknesses (three or more mean free paths) were used causing the argument of the expoential term in equation 3 to be large. Any variation in the total cross-section, Σ_t, would produce an exponential variation in the transmitted flux. This becomes especially apparent for minima in the cross-section. For a given material of thickness t and some mean cross-section $\overline{\Sigma}_t$, equation 3 becomes:

$$\phi_{trans}/\phi_I = \exp(-\overline{\Sigma}_t t) \tag{4}$$

Now, if there is a minima in the cross-section at some energy such that the cross-section is reduced by some fraction k (k<1) of the mean value, then:

$$[\phi_{trans}/\phi_I]_{minima} = \exp[-(1-k)\overline{\Sigma}_t t] \tag{5}$$

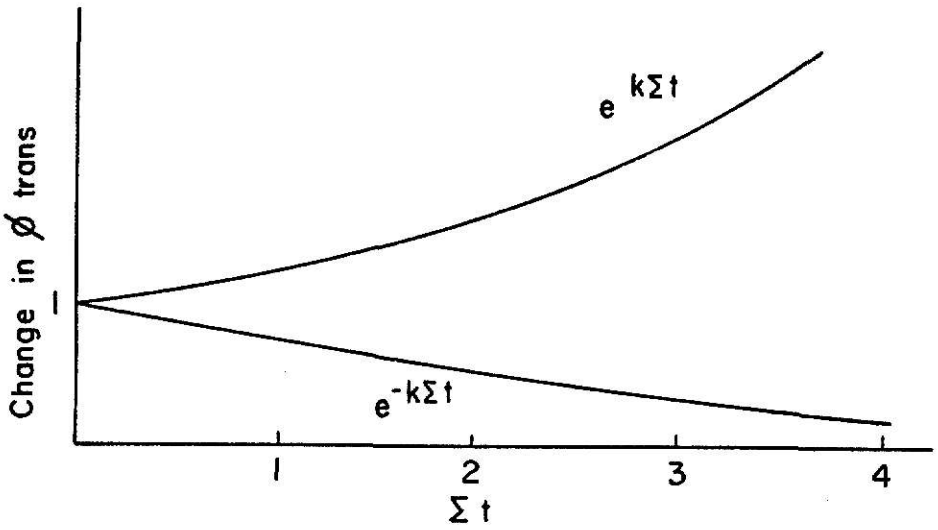
Likewise, for a maxima in the cross-section resulting in an increase in the cross-section by the same fraction k of the mean value, then:

$$[\phi_{trans}/\phi_I]_{maxima} = \exp[-(1+k)\overline{\Sigma}_t t] \tag{6}$$

The fractional change in the transmitted flux, obtained by dividing equation 5 and equation 6 by equation 4, is given by:

$$\text{fractional change for minima} = \exp(k\bar{\Sigma}_t t)$$
$$\text{fractional change for maxima} = \exp(-k\bar{\Sigma}_t t) \tag{7}$$

These two functions are plotted in Fig. 2 and, as can be seen, the resultant change in the transmitted flux at a minima increases greatly for large thicknesses whereas the corresponding change in the transmitted flux at a maxima is small. Therefore, by using large thicknesses in the experiment, the sensitivity to minima becomes great. When the experimental results are compared to the corresponding calculated results, large errors in the transmitted spectrum will appear for small errors in the minima of total cross-section.



If a detection system with infinite resolution was used, the experimentally measured transmitted spectrum could be directly compared to the transmitted spectrum calculated by equation 3. However, the actual resolution of the spectrometer system must be included to "smooth" the calculated spectrum as the experimentally measured spectrum is "smoothed" by the measuring system. The transmitted spectrum can be calculated as:

$$\phi_{trans}(E) = \int_0^\infty \phi_I(E')\exp[-\Sigma_t(E')t]R(E,E')dE' \tag{8}$$

where $\phi_I(E')$ = incident flux at energy E'

Σ_t = total neutron cross-section at E'

R(E,E') = probability of a neutron of energy E' being detected at energy E.

Based upon the unfolded responses of the detection system to mono-energetic neutrons, it can be seen that the resolution function R(E,E') is of the form of a gaussian:

$$R(E,E') = y_o(E) \exp[-\frac{(E-E')^2}{b_o(E)}] \qquad (9)$$

where $y_o = \frac{1}{\sqrt{b_o \pi}}$, which normalizes the function R(E,E') such that $\int R(E,E')\, dE' = 1$

E = neutron energy detected

E' = actual neutron energy

$b_o = (FWHM)^2/4 \cdot \ln(2)$, where FWHM is the full width at half maximum of the gaussian.

Experimental measurements[1,23] have been made to determine R(E,E') at several energies E. These measurements actually give the probability of neutrons of energy E being detected at E', but since the detection system cannot discriminate between neutrons of energy E and E' (within the probability given by this function) it is assumed that neutrons of E' have an equal probability of being detected at E.

If it is assumed that $\phi_I(E')$ and $\Sigma_t(E')$ have values at discrete energy points E_i, then the integral of equation 8 can be integrated piecewise from E_i to E_{i+1}, from E_{i+1} to E_{i+2}, etc. If it is also assumed that the log (ϕ_I) is linear between energy points and that $\Sigma_t(E')$ is linear between energy points, then equation 8 can be integrated into the exact form:

$$\phi_{trans}(E) = \sum_{i=1}^{\infty} \left\{ \left\{ \frac{1}{2} \exp\left| \frac{b_o}{4} \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right)^2 + \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right) (E_i - E) - \Sigma_i \right| \right\} \cdot \right.$$

$$\left\{ \phi_I^i [\mathrm{erf}(y_{i+1}) - \mathrm{erf}(y_i)] + [\mathrm{erf}(z_{i+1}) - \mathrm{erf}(z_i)] \exp\left| \left(\frac{\ln\phi_I^{i+1} - \ln\phi_I^i}{E_{i+1} - E_i} \right) \right. \right.$$

$$\left. \left. \left(E - E_i - \frac{b_o}{2} \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right) \right) - \frac{b_o}{4} \left(\frac{\ln\phi_I^{i+1} - \ln\phi_I^i}{E_{i+1} - E_i} \right)^2 \right| \right\} \right\} \qquad (10)$$

where ϕ_I^i = the incident flux at E_i

Σ_i = cross-section at E_i

$$y_i = \frac{1}{\sqrt{b_o}} \left| E_i - E + \frac{b_o}{2} \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right) \right|$$

$$z_i = \frac{1}{\sqrt{b_o}} \left| E_i - E + \frac{b_o}{2} \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right) - \frac{b_o}{2} \left(\frac{\ln\phi_I^{i+1} - \ln\phi_I^i}{E_{i+1} - E_i} \right) \right|$$

The experiment was performed using several different experimental geometries. For the first condition the detector was placed as far from the beam port as possible (approximately 128 inches). In this case it was assumed that any interaction of a neutron with the sample would either result in absorption or in scattering at an angle larger than the solid angle subtended by the detector. If this assumption is true, only those neutrons that are uncollided will be detected resulting in a true measure of the total cross-section. However, two phenomenon can occur which will cause an error in this measurement. If there is a large probability for forward scattering in the sample, it is possible that neutrons scattering at small angles will reach the detector. To reduce this error a collimator was used directly in front of the detector to reduce its effective area. Thus, those neutrons scattered at shallow angles (solid angles greater than 7.5×10^{-4} steradians) were removed by the collimator. Neutrons scattered

at 0° to the solid angle subtended between sample and detector could be present. Finally, there is a probability that neutrons will be scattered several times in a thick sample and some of these will be scattered back into the solid angle subtended by the detector. In this case, the end of the sample nearest the detector will be fully "illuminated" with neutrons, some of which will be scattered toward the detector. To study this effect, the collimator was placed against the sample, with the detector in the same position as before. With this latter geometry the area of the end of the sample viewed by the detector was smaller than that viewed with the collimator positioned next to the detector and thus a smaller number of multiple scattered neutrons would be expected to be detected.

3.0 EXPERIMENTAL FACILITIES AND EQUIPMENT

3.1 Neutron Source

The northeast fast beam port ("C") of the 250 kW K.S.U. Triga Mark II reactor was used as the source of fast neutrons. This radial beam port is aligned with a cylindrical void in the core reflector graphite as shown in Fig. 3, and is nominally 8 inches in diameter at the reactor face. It is fitted with a lead and borated paraffin 1-1/4 inch square collimator (Fig. 4). The neutron beam from this beam port diverges slightly to approximately five inches by five inches at the reactor bay wall 146 inches from the face of the beam port and is well defined even at this distance.[16] Since there is little material in the path of neutrons coming from the core, the spectrum is essentially a fission spectrum with sufficient neutrons for experimental measurement up to 12 MeV. A 2 inch long bismuth plug inserted in the end of the collimator reduces the gamma background while leaving the neutron spectrum essentially unaffected.

3.2 Neutron Detection System

Neutrons were detected with a proton recoil NE-213 liquid scintillator spectrometer. Fast neutrons produce both neutron-hydrogen and neutron-carbon interactions which are subsequently detected and amplified by a photomultiplier tube. Unfortunately NE-213 responses are not limited to neutron interactions; gamma rays produce electrons in the scintillator which are also detected and amplified. It is possible, however, to electronically distinquish between pulses caused by neutron and gamma ray interactions.

The K.S.U. NE-213 detector and tube base Forte gamma ray discrimination circuit[23] are shown in Fig. 5. The pulse shape discrimination (PSD) output from the Forte circuit is a timing pulse which makes it possible to eliminate the gamma ray pulses. After additional pulse shaping this pulse

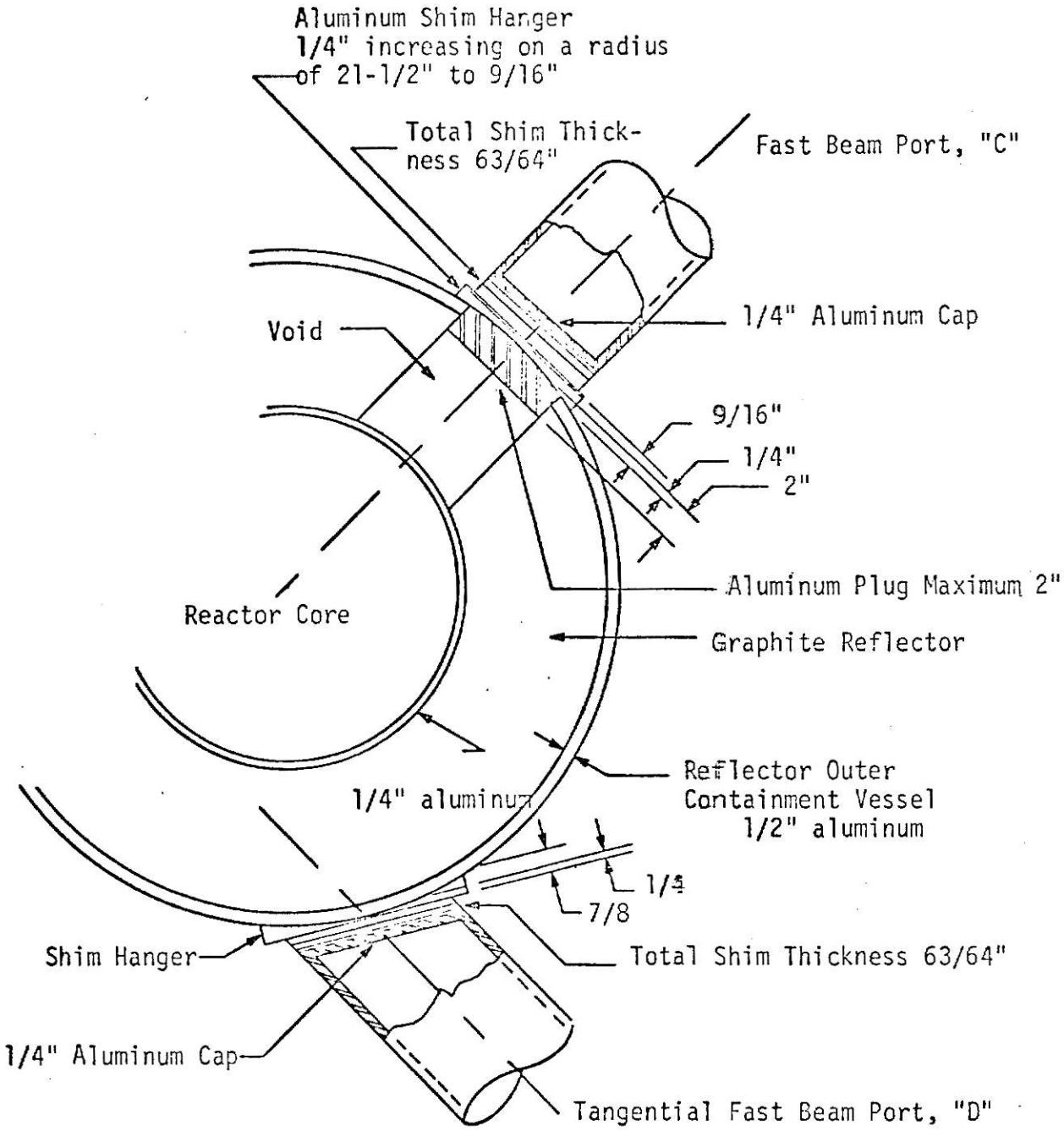


Figure 3 KSU TRIGA reactor core, reflector and beam port assembly.

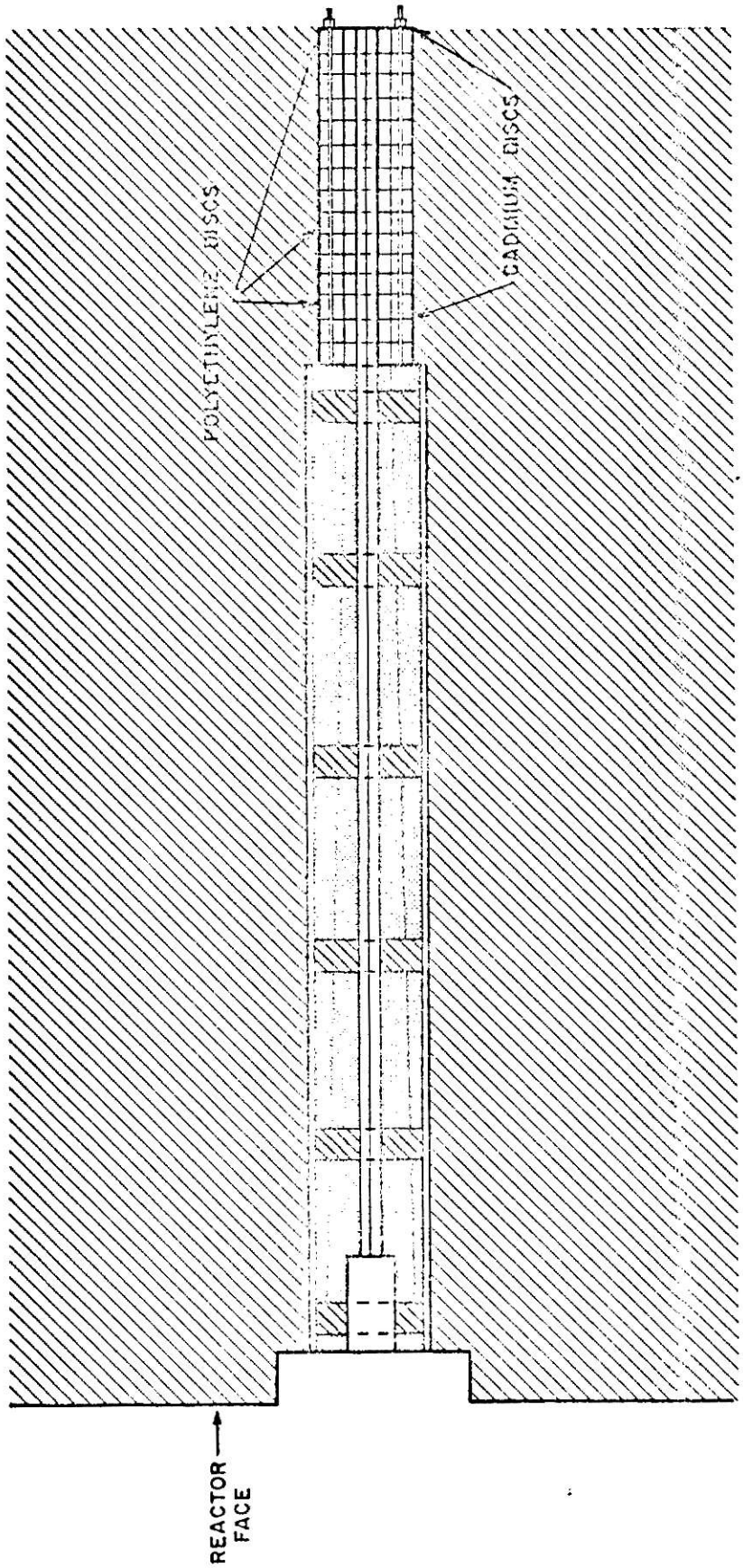


Figure 4 Internal construction of KSU TRIGA beam port collimator.

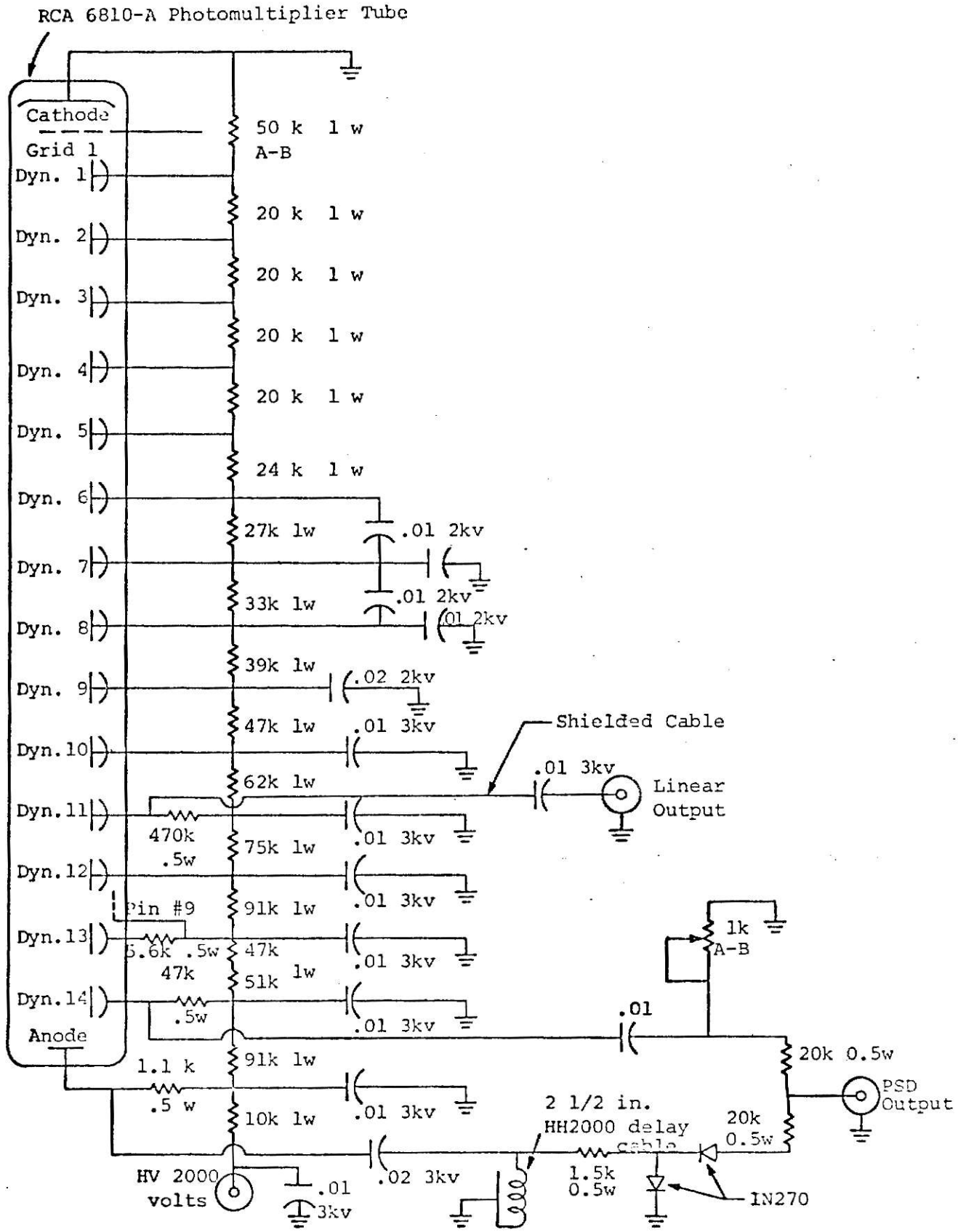


Figure 5 KSU Gamma Ray Pulse Shape Discrimination Circuit

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is used in coincidence with the linear signal as shown in a block diagram of the NE-213 fast neutron spectrometer electronics in Fig. 6. (A description of the design and operating characteristics of the K.S.U. NE-213 fast neutron spectrometer system can be found in a report by Meyer, "Intercalibration of the K.S.U. Fast-Neutron Spectrometer System."[16])

The resolution of the K.S.U. NE-213 system has been measured by Simons.[23] Verbinski made similar measurements on another NE-213 detection system at ORNL.[1] Both of these measurements were analyzed by unfolding the measured monoenergetic neutron response functions with the ORNL FERDOR code. The width of the approximately gaussian peak in the unfolded spectrum gave a measure of the resolution for that particular energy. This resolution was actually the resolution of the combined detection and unfolding processes at that energy.

3.3 Multiparameter Analyzer

A TMC-4096 Multiparameter Analyzer was used to measure the signals coming from the detection system with the resultant data stored in the memory. Readout options included paper tape, magnetic tape and omnigraphic plotter. The magnetic tape was converted directly to cards at the K.S.U. IBM 360-50 facility.

3.4 Sample Containers

For the experimental measurements involving liquid oxygen and sodium, special sample containers were fabricated in K.S.U. shops. The aluminum liquid oxygen container is shown in Fig. 7. It was of double-walled construction with the space between the inner and outer boxes filled with vermiculite insulation. Vermiculite is known for its inert, as well as insulating, properties. During an experiment the container was filled from the top to replace oxygen lost by evaporation.

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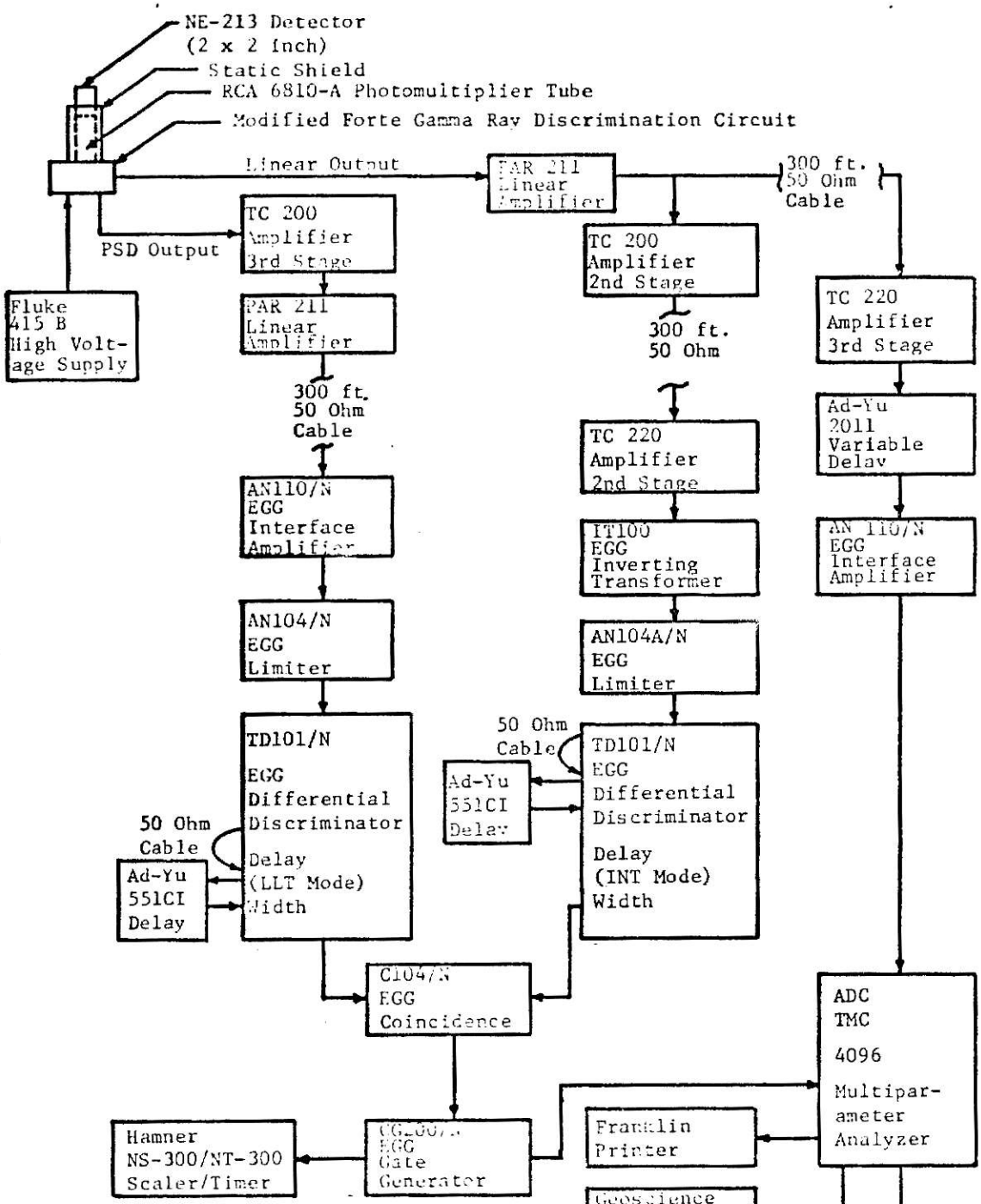


Ad-Yu: Ad-Yu Electronics, Passaic, N.J.
Fluke: John Fluke Mfg., Seattle, Washington
TC: Tennelec, Oak Ridge, Tennessee
Tally: Tally, Seattle, Washington
Omnigraphic: Houston Omnigraphic Corp., Bellaire, Tx.
TMC: Technical Measurements, Corp., North Haven, Ct.
EGG: EG & G Inc., Salem, Massachusetts
Hamner: Hamner Electronics, Princeton, N.J.
Geoscience Nuclear: Geoscience Instruments Corp., Hamden, Conn.

Figure 6 Block Diagram of the KSU NE-213 Fast-Neutron Spectrometer System

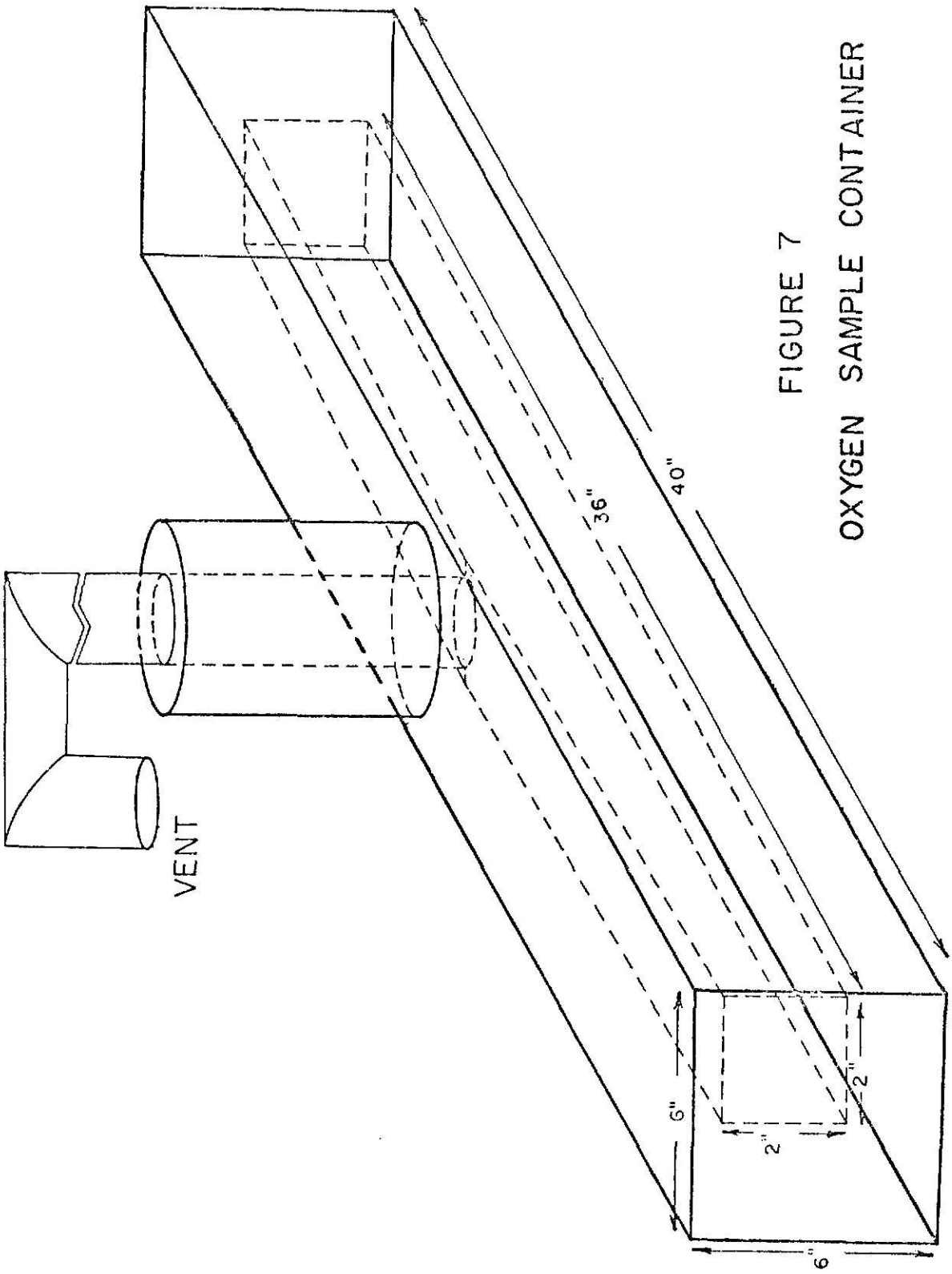


FIGURE 7

OXYGEN SAMPLE CONTAINER

The container for solid sodium was fabricated from stainless steel. The sodium was cast into this container under an inert atmosphere and then the container was sealed. After sealing there was no problem in handling the sodium. The liquid sodium container (Fig. 8) like the oxygen container was also double walled but in this case fabricated from stainless steel. The inner box was wrapped with resistance heating wire to permit heating the sodium sample above the melting point during an experiment. Thermocouples were welded to the container wall to monitor the sodium temperature. Vermiculite was again used as insulation. The inner box was vented into the outer container to allow for the expansion of the sodium during heating. When heated, an inert gas (nitrogen) was constantly passed through the container to reduce oxidation at the sodium-air interface.

3.5 Collimator and Shadow Shield

The neutron collimator was made of methyl methacralate and was 3 inches by 3 inches by 24 inches long with a .318 inch square hole lengthwise through the center. By placing this collimator directly in front of the detector, the effective area of the detector was reduced to .101 square inches. This particularly sized collimator was used to duplicate the geometry used by Straker in a similar experiment at ORNL.[26] By using the collimator the solid angle subtended by the effective detector area was the same as the solid angle subtended by Straker's detector which was placed 50 feet from the sample.

When the collimator was not used directly in front of the detector, a shadow shield was used for background measurements. This shield is an aluminum cylinder approximately 2.5 inches I.D. and 24 inches long and is filled with water. For background measurements in experiments where the collimator was used, the ends were sealed and the void was filled with water.

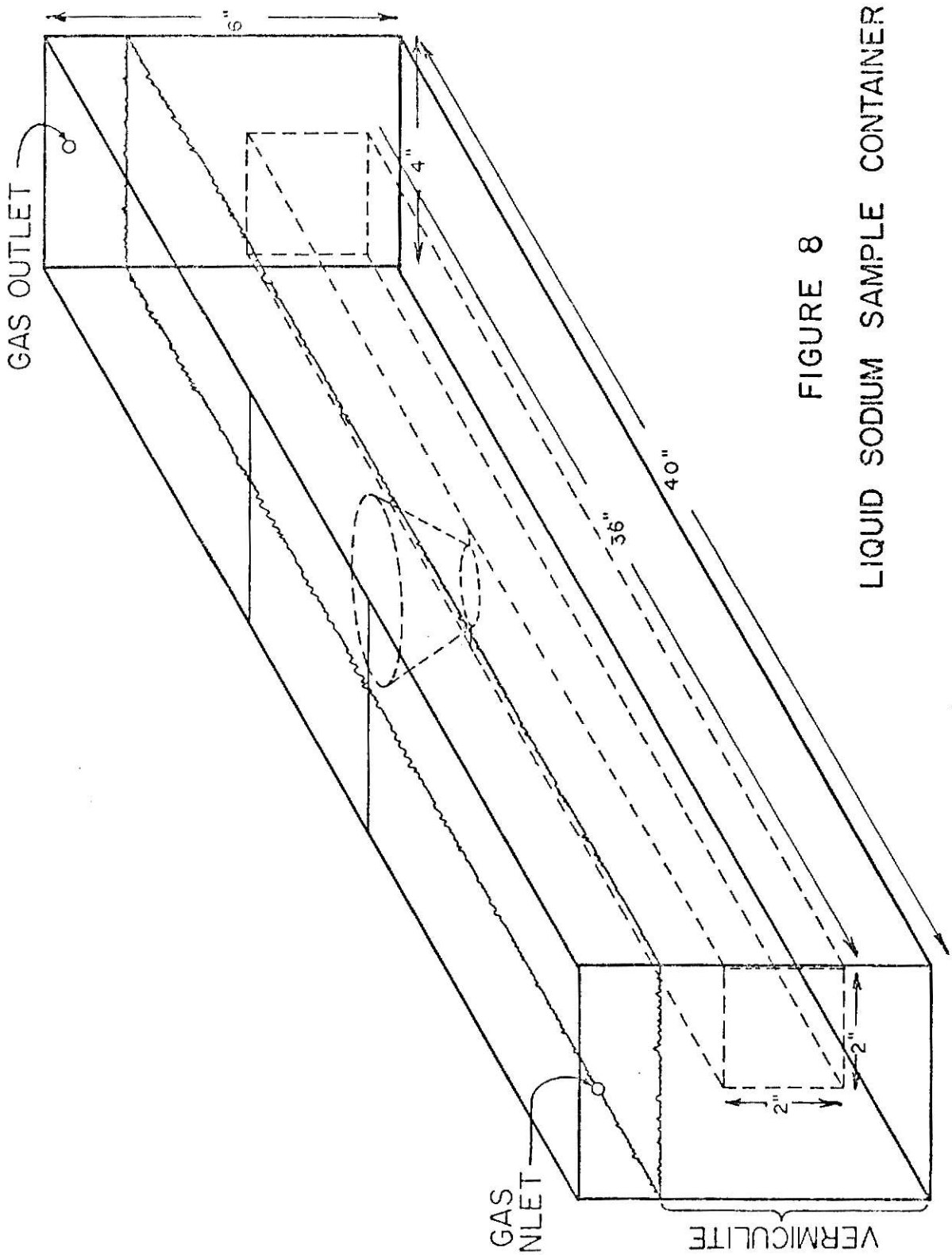


FIGURE 8

LIQUID SODIUM SAMPLE CONTAINER

4.0 EXPERIMENTAL PROCEDURE

4.1 Equipment Calibration

The basic procedure for obtaining a neutron spectrum was the same for all experimental runs. This basic procedure established the detection system parameters, the maximum reactor power and the integrated reactor flux.

4.1.1 Calibration of the detection system - After a twelve hour warm-up period for the NE-213 system, several parameters were checked and adjusted to insure proper response. First, a ^{60}Co gamma-ray spectrum was taken and the extrapolated Compton tail was used to set the energy gain. The gamma rejection ratio was set at >150:1 using the ^{60}Co source; that is, less than one gamma-ray in 150 was counted. The efficiency of the system was also checked using the ^{60}Co source. A one hour PuBe spectrum was measured with the gamma rejection circuit operative. This test spectrum was compared to a standard complex PuBe spectrum to insure that the system was working properly. A ^{60}Co spectrum was again taken immediately before or after each experimental spectrum to reestablish the gain and gamma rejection ratio.

4.1.2 Maximum total flux at the detector. - Due to the sensitivity of the Forte circuit and photomultiplier tube to radiation, the total radiation at the detector was kept below 3 mrem/hr. When the detection system is operative in the anticoincidence mode a 10% dead time on the TMC 4096 corresponds roughly to 3 mrem/hr at the detector. Thus, the 10% dead time was used to establish the maximum reactor power for all experimental runs.

4.1.3 Integrated flux monitor - Nickel foils were activated in the central thimble of the Triga to monitor the integrated flux during an experimental run. Nickel-neutron interactions produce ^{58}Co which decays,

emitting gamma-rays:

$$Ni + n \longrightarrow p + {}^{58}Co$$

$${}^{58}Co \xrightarrow{72\ day} \gamma + \beta^{+} + {}^{58}Fe$$

The total number of counts in the 0.811 MeV photoelectric peak of the ^{58}Co is directly proportional to the integrated flux. (It should be noted that one set of data reported in this work used sulfur as a flux monitor. However, all other experiments used nickel since it has proven to be a more accurate monitor.)

4.2 Neutron Spectrum Measurements

For all spectral measurements the detector, sample, shadow shield and collimator were placed on the centerline of the neutron beam. The detector was placed as far from the reactor as possible, or approximately 136 inches from the face of the beam port. All samples were placed so that the leading edge was flush with the beam port face except for the Pb sample which, because of its shape, could be placed inside the lip of the beam port collimator. When the shadow shield or collimator was used, it was placed as close to the detector as possible.

The experimental arrangement for collecting data without the collimator is shown in Fig. 9. To measure incident spectra the sample was removed or the empty sample container was placed in the beam. The background measurement for an incident spectrum measurement was obtained by placing the shadow shield directly in front of the detector. Foreground and background penetration (transmitted) spectra were collected in a manner similar to that described above except the sample was in place.

Figure 10 shows the geometry of the experimental measurements involving the use of the collimator at the detector. A surveyor's transit was used to insure proper alignment of the collimator and detector with the neutron

FIGURE 9
Experimental Geometry
No Collimator

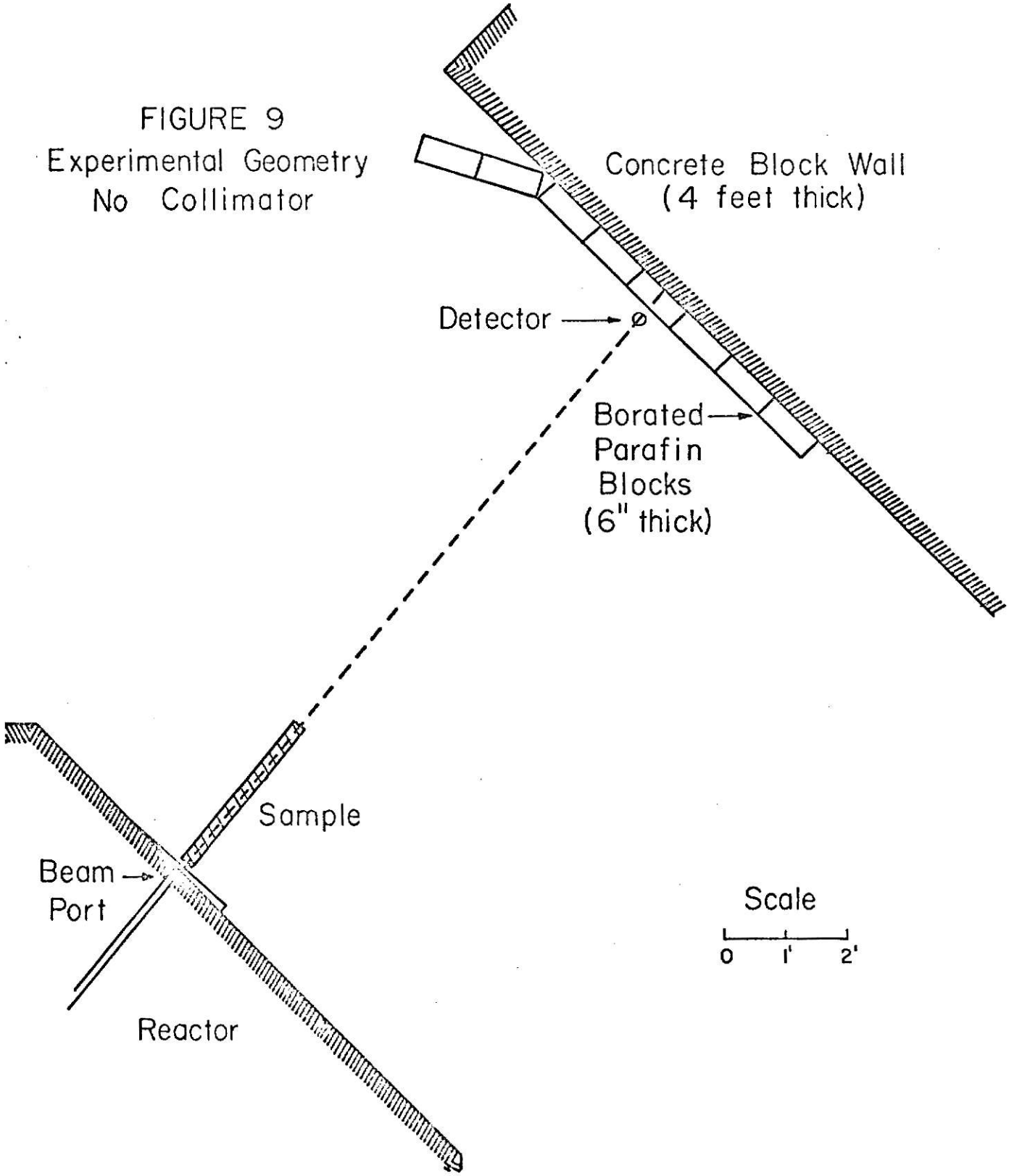
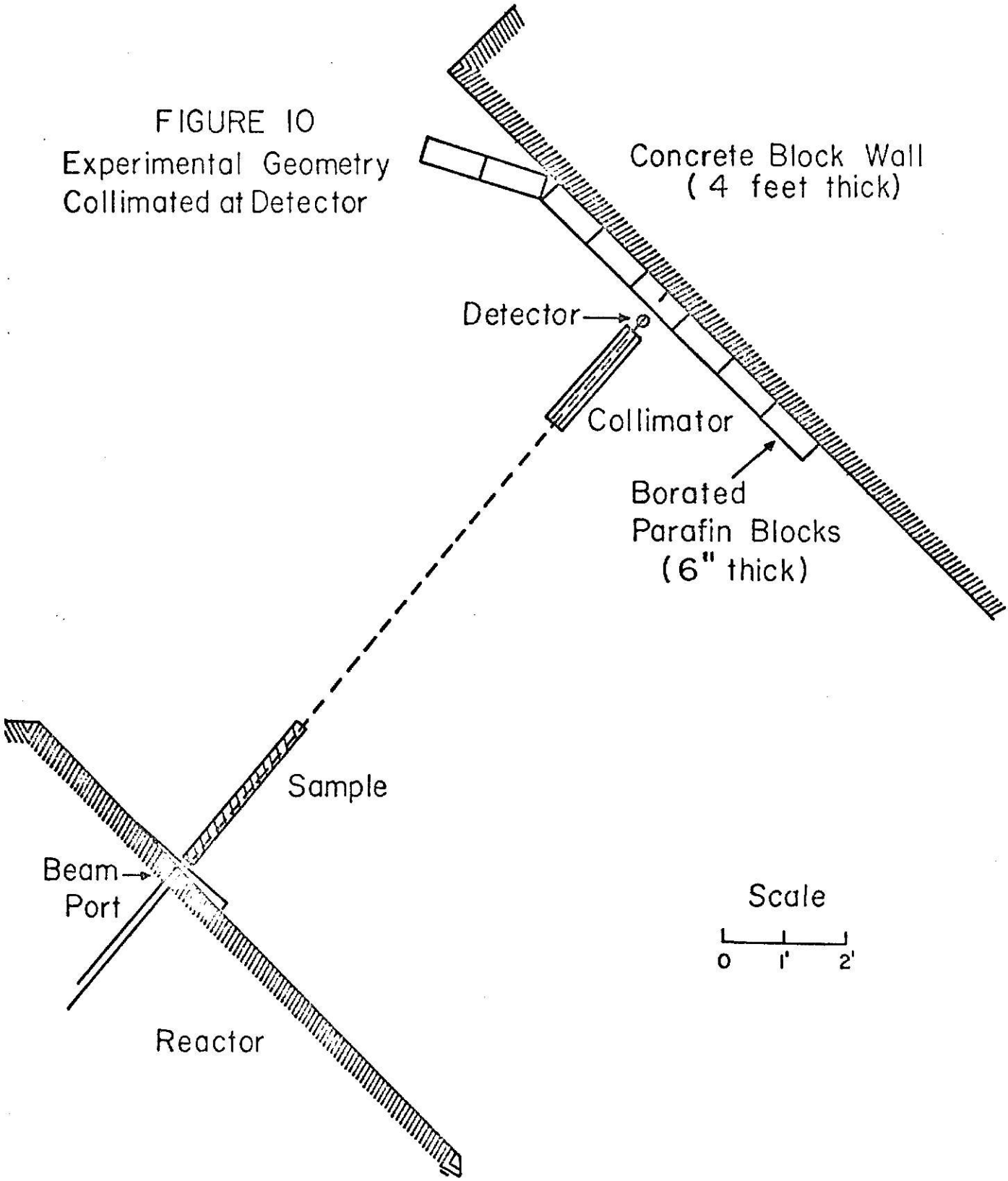


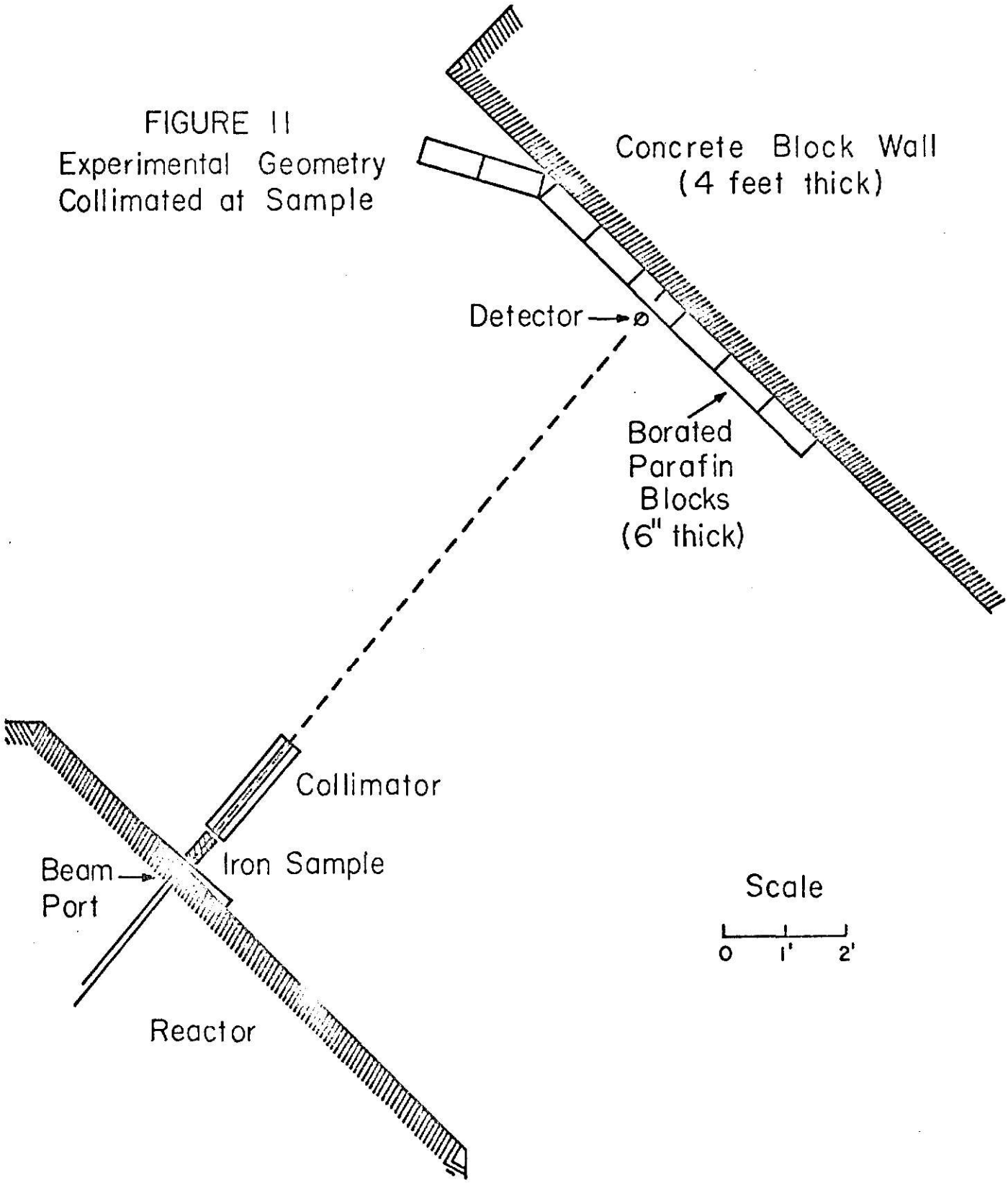
FIGURE 10
Experimental Geometry
Collimated at Detector



beam. Again both foreground and background measurements were made for both incident and penetration spectra, the background being obtained by sealing the end of the collimator and filling the collimator void with water.

One additional measurement was taken with the collimator next to the sample as shown in Fig. 11. The shadow shield was again used in front of the detector for background measurements.

FIGURE 11
Experimental Geometry
Collimated at Sample



5.0 DATA ANALYSIS

5.1 Data Handling

After several spectra were measured, the raw data in the memory of the TMC 4096 were read onto magnetic tape; the tape was subsequently processed to obtain punched cards. A computer code, NUDASBIN, compiled this raw data using the ^{60}Co spectrum, the Ni foil data, and the foreground and background measurements. NUDASBIN treated the raw data using the ^{60}Co data to normalize the raw data with respect to energy. Background subtraction was performed after an integrated flux normalization of the background to the foreground using the Ni foil measurement. The resultant complex spectrum was binned for use by the unfolding code. For this work, the complex spectrum was unfolded with the ORNL code FERDOR.

5.2 Calculated Transmitted Spectra

A computer code, CALFLUX, was written to calculate the transmitted spectra using the measured incident spectra, cross-section data and the resolution of the detector as given in equation 8. Input to the code included the normalization factor between the incident and transmitted measurements based on the Ni data.

5.3 System Resolution Analysis

As stated earlier, the resolution of the detector system had been previously measured by two separate experimenters. To use this data in equation 8, the unfolded results of the mono-energetic neutron spectrum measurements of Verbinski were fitted to a gaussian curve by a KSU computer code, NE213RES. The NE213RES results gave the full width at one-half the maximum (FWHM) for each experimental energy. Simons' data had previously been analysed by a similar procedure. Both sets of resolution data were

then fitted to an nth order polynomial by another computer code, POLYFIT. This formulation gave resolution (FWHM) versus energy (MeV) for the entire system (which included both the detector and unfolding resolution).

6.0 RESULTS

The plots of resolution versus energy for the NE-213 spectrometer system are shown in Fig. 12, along with the polynomial fit for this data. Simons' data set is fitted to a 6th order polynomial and Verbinski's data set is fitted to a 7th order polynomial.

All neutron spectra taken for this work are shown in table 1. Table 2 lists some of the sample constants used.

Figure 13 demonstrates the effect of the resolution function on the transmitted spectra. The "unsmoothed" spectrum was calculated at discrete energies by Equation 3 and the "smoothed" spectrum was calculated at the same energies by Equation 8. The data set used was that for an oxygen penetration run. Figure 14 shows a comparison between two different resolution functions for the same oxygen data. In one case Verbinski's data set is used as the resolution function, and in the other case Verbinski's resolution is increased by 25%. The modified resolution function (the one with FWHM decreased by 25%) shows better agreement with the experimental measurements and was therefore used for all subsequent calculations.

A plot of all the incident spectra taken is shown in Fig. 15. Figures 16 and 17 show the comparison between experimental and calculated transmitted (penetration) spectra for Fe and O_2 measured without the collimator present. Figures 18, 19, 20, and 21 show experimental and calculated results for Fe, Pb, O_2 and Na, respectively, measured with the collimator. For the Fe measurement the collimator was placed next to the sample while for all other measurements the collimator was placed next to the detector. Finally, Fig. 22 shows a comparison between the collimated and uncollimated experimental Fe penetration spectra.

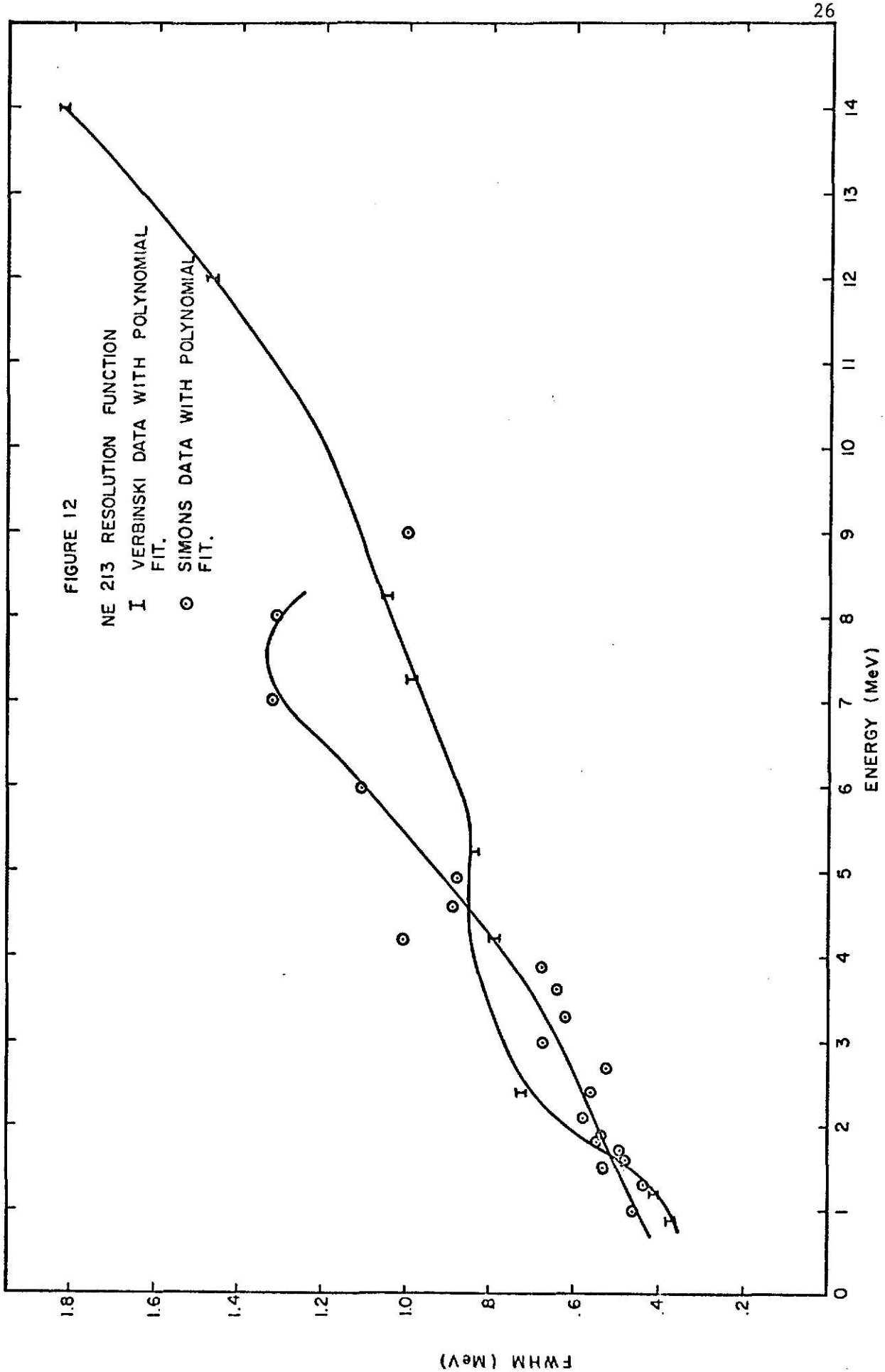


FIGURE 12
NE 213 RESOLUTION FUNCTION
I VERBINSKI DATA WITH POLYNOMIAL FIT.
⊙ SIMONS DATA WITH POLYNOMIAL FIT.
FWHM (MeV)
ENERGY (MeV)
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
.2
.4
.6
.8
1.0
1.2
1.4
1.6
1.8

Table 1

EXPERIMENTAL NEUTRON SPECTRA

Run Number	Description	Geometry Used	Nominal Reactor Power		Fluence (Ni Foil Data)
9-30-70- 4	O_2 Incident	Uncollimated	40	W	52.914 (Sulfur Data)
10-14-71- 4	Fe Incident	Uncollimated	50	W	-
10-23-70- 4	O_2 Penetration #1	Uncollimated	1	kW	1728.8 (Sulfur Data)
10-23-70- 8	O_2 Penetration #2	Uncollimated	1	kW	1412.1 (Sulfur Data)
1-18-71- 4	Incident	Collimator at Detector	135	W	$.1528 \times 10^5$
1-27-71- 6	Pb Pene	Collimated at Detector	50	kW	$.616326 \times 10^7$
2-19-71- 7	O_2 Incident	"	750	W	$.94199 \times 10^5$
2-22-71- 4	Na (Solid) Incident	"	750	W	$.2563 \times 10^5$
2-23-71- 4	O_2 Pene	"	20	kW	$.242035 \times 10^7$
3-16-71- 4	Fe Incident	Collimator at Sample	500	W	$.55465 \times 10^5$
3-16-71- 6	Na (liquid) Incident	Collimator at Detector	1.25	kW	$.16989 \times 10^6$
3-16-71- 9	Fe Pene	Collimator at Sample	16	kW	$.22089 \times 10^7$
3-23-71-13	Fe Pene	Uncollimated	2	kW	$.25849 \times 10^6$
3-24-71- 4	Na (liquid) Pene	Collimated at Detector	30	kW	$.37835 \times 10^7$
3-24-71- 8	Na (solid) Incident	"	30	kW	$.40028 \times 10^7$
3-30-71- 4	Na (solid) Incident	"	1.2	kW	$.1707 \times 10^6$

Table 2

Sample Descriptions

Sample	Nominal Size (inches)	Thickness (cm)	N (atom density) (atoms/cm^3)
Oxygen	2 1/4 x 2 1/4 x 36	91.28	.0403 x 10^{24} *
Fe	2 x 2 x 6	15.24	.0849 x 10^{24}
Pb	3 1/2 dia x 9 1/4	23.49	.033 x 10^{24}
Na (solid)	2 1/2 x 2 1/2 x 36	91.60	.02541 x 10^{24}
Na (liquid)	2 1/2 x 2 1/2 x 36	91.60	.02389 x 10^{24} **

*Corrected to account for void space caused by boiling

**At 165°C (taken from Smithalls[25])

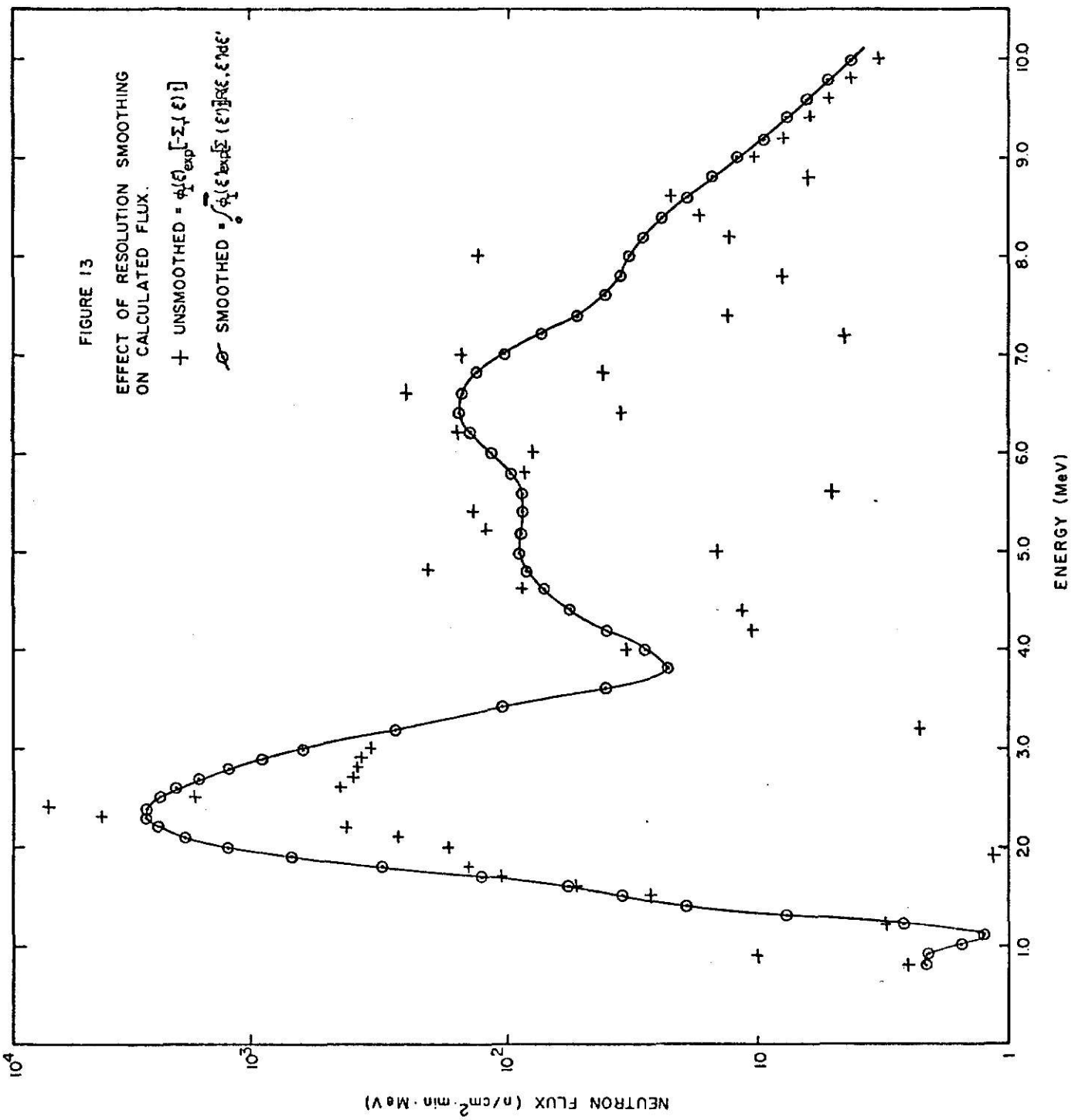


FIGURE 13
EFFECT OF RESOLUTION SMOOTHING ON CALCULATED FLUX.
+ UNSMOOTHED = $\phi_1(E)_{exp}[-\Sigma_1(E)t]$
SMOOTHED = $\int_0^\infty \phi_1(E')_{exp}[\Sigma_1(E')]R(E,E')dE'$
NEUTRON FLUX (n/cm^2·min·MeV)
ENERGY (MeV)
10^4
10^3
10^2
10
1
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0

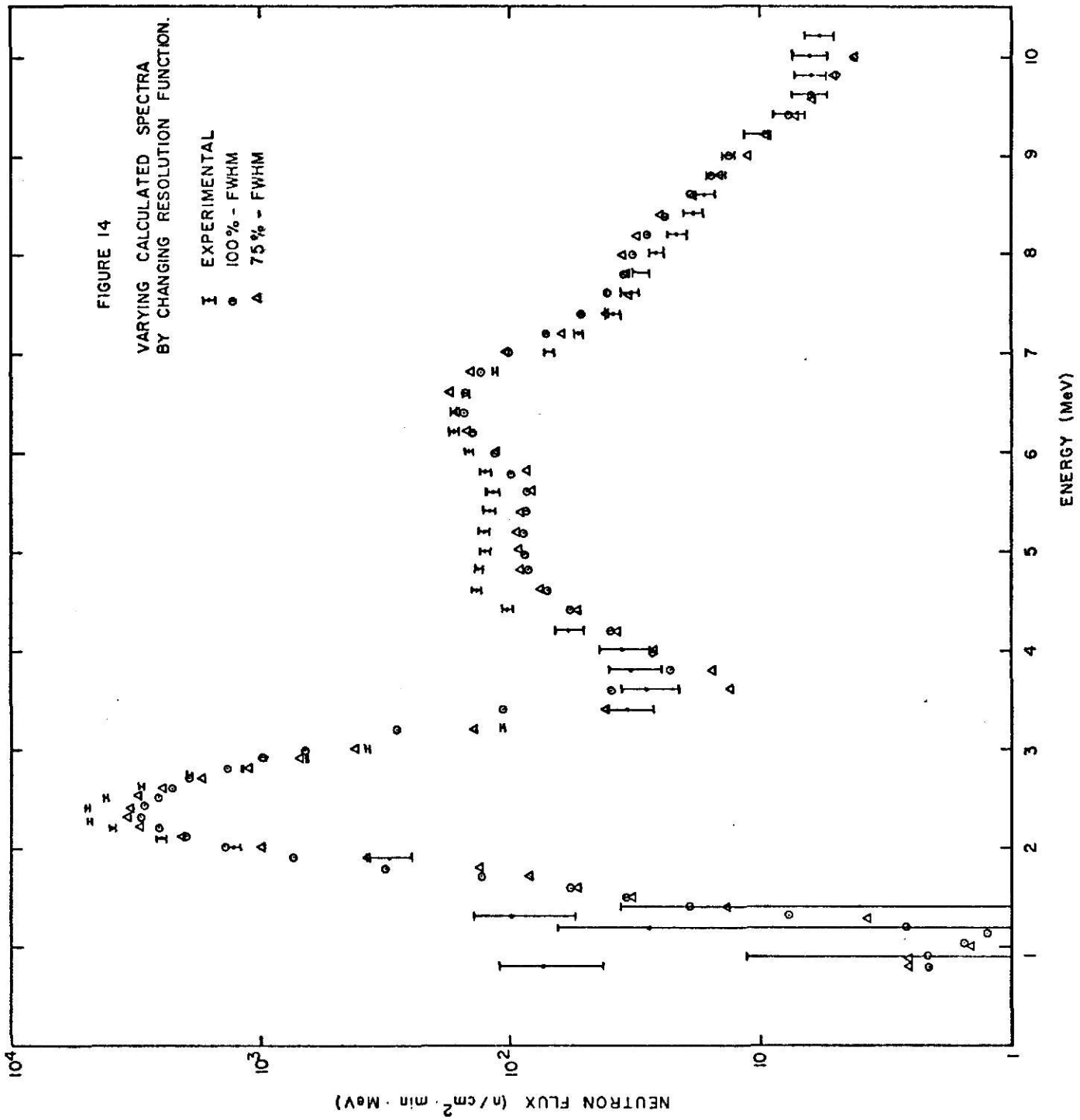


FIGURE 14
VARYING CALCULATED SPECTRA
BY CHANGING RESOLUTION FUNCTION.
I EXPERIMENTAL
100% - FWHM
75% - FWHM
NEUTRON FLUX (n/cm² · min · MeV)
ENERGY (MeV)

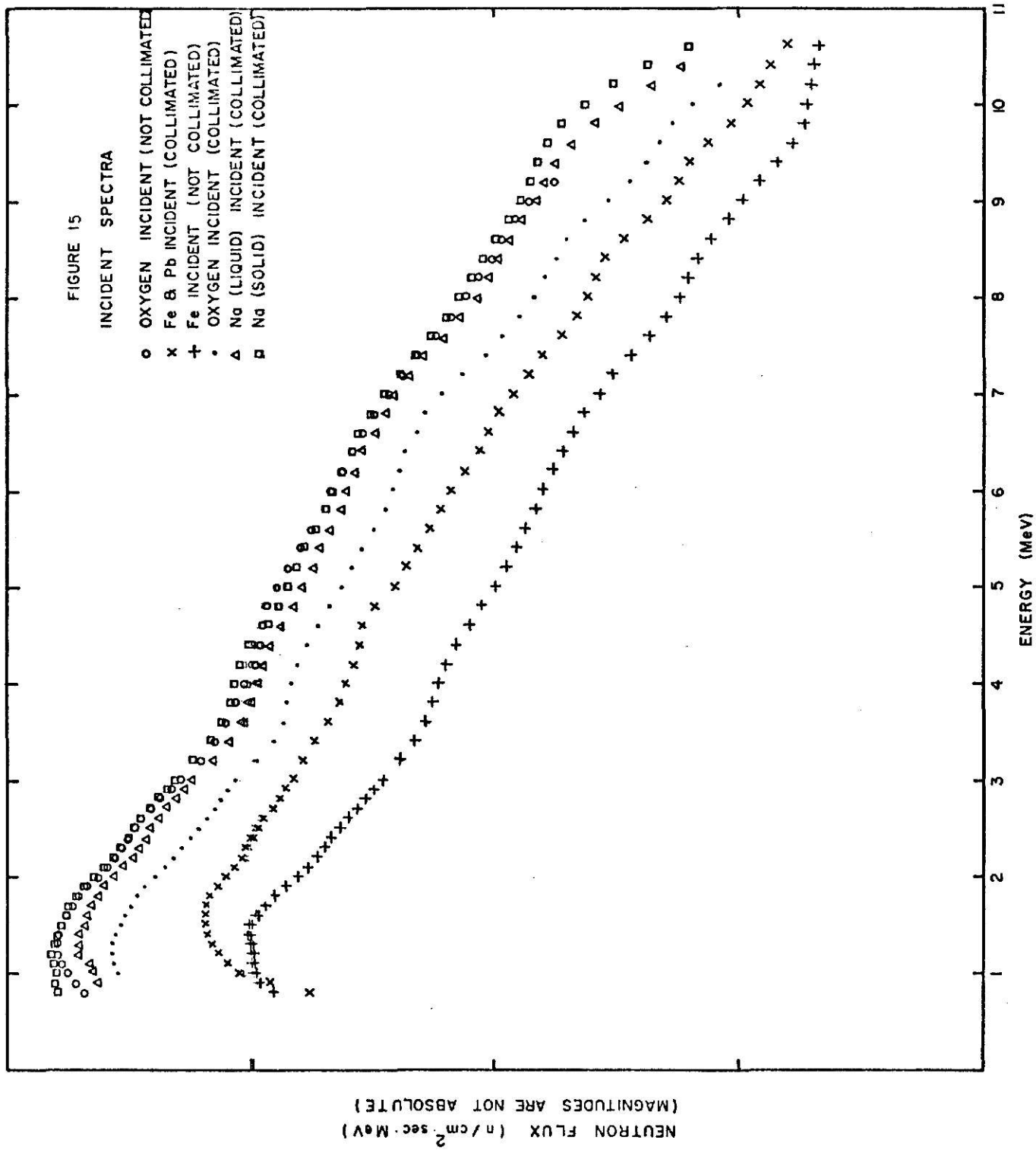


FIGURE 15
INCIDENT SPECTRA
o OXYGEN INCIDENT (NOT COLLIMATED)
× Fe & Pb INCIDENT (COLLIMATED)
+ Fe INCIDENT (NOT COLLIMATED)
• OXYGEN INCIDENT (COLLIMATED)
△ Na (LIQUID) INCIDENT (COLLIMATED)
□ Na (SOLID) INCIDENT (COLLIMATED)
NEUTRON FLUX (n/cm² sec·MeV)
(MAGNITUDES ARE NOT ABSOLUTE)
ENERGY (MeV)
1
2
3
4
5
6
7
8
9
10
11

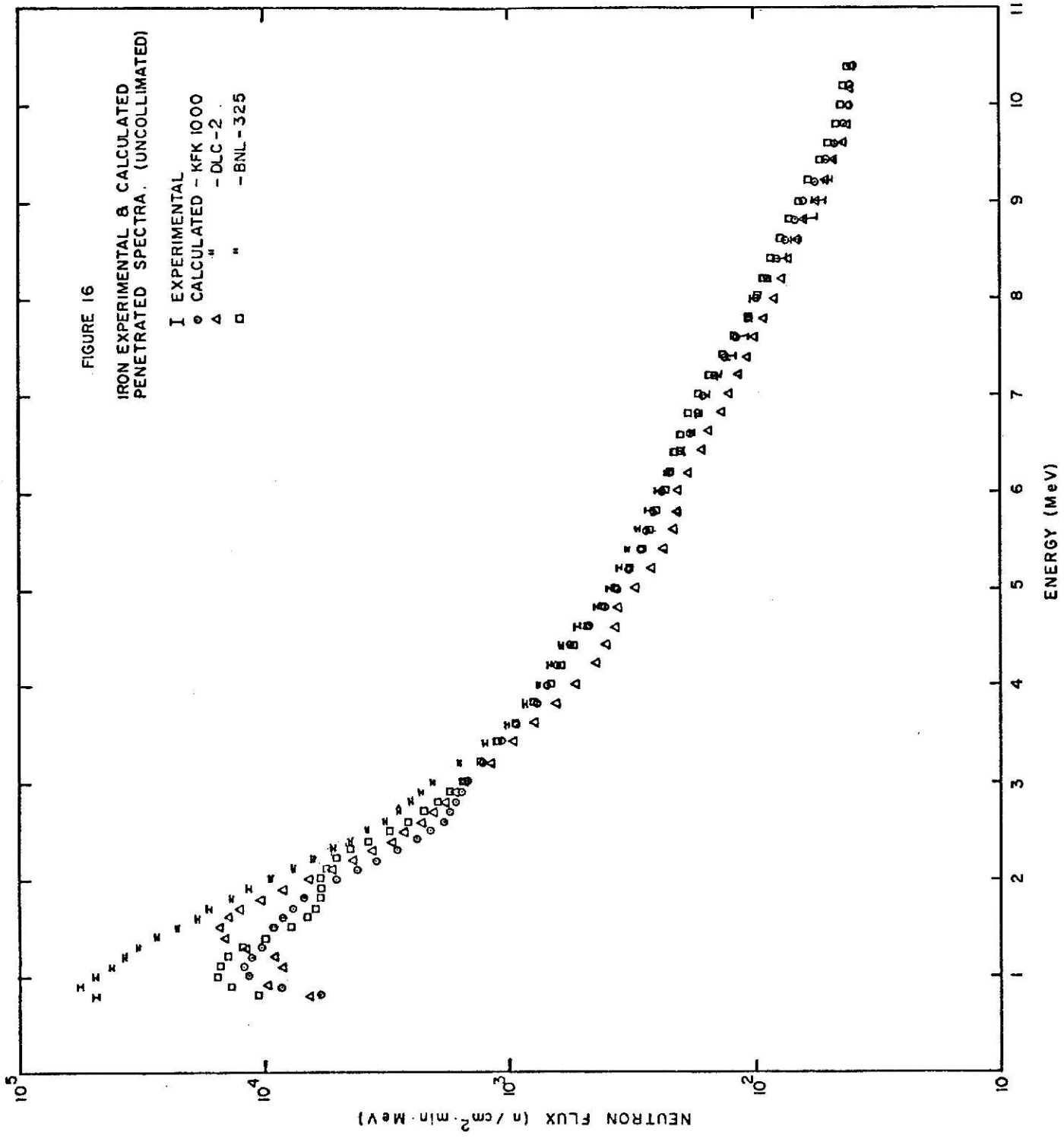


FIGURE 16
IRON EXPERIMENTAL & CALCULATED
PENETRATED SPECTRA. (UNCOLLIMATED)
I EXPERIMENTAL
CALCULATED - KFK 1000
" - DLC-2
" - BNL-325
NEUTRON FLUX (n / cm² · min · MeV)
ENERGY (MeV)

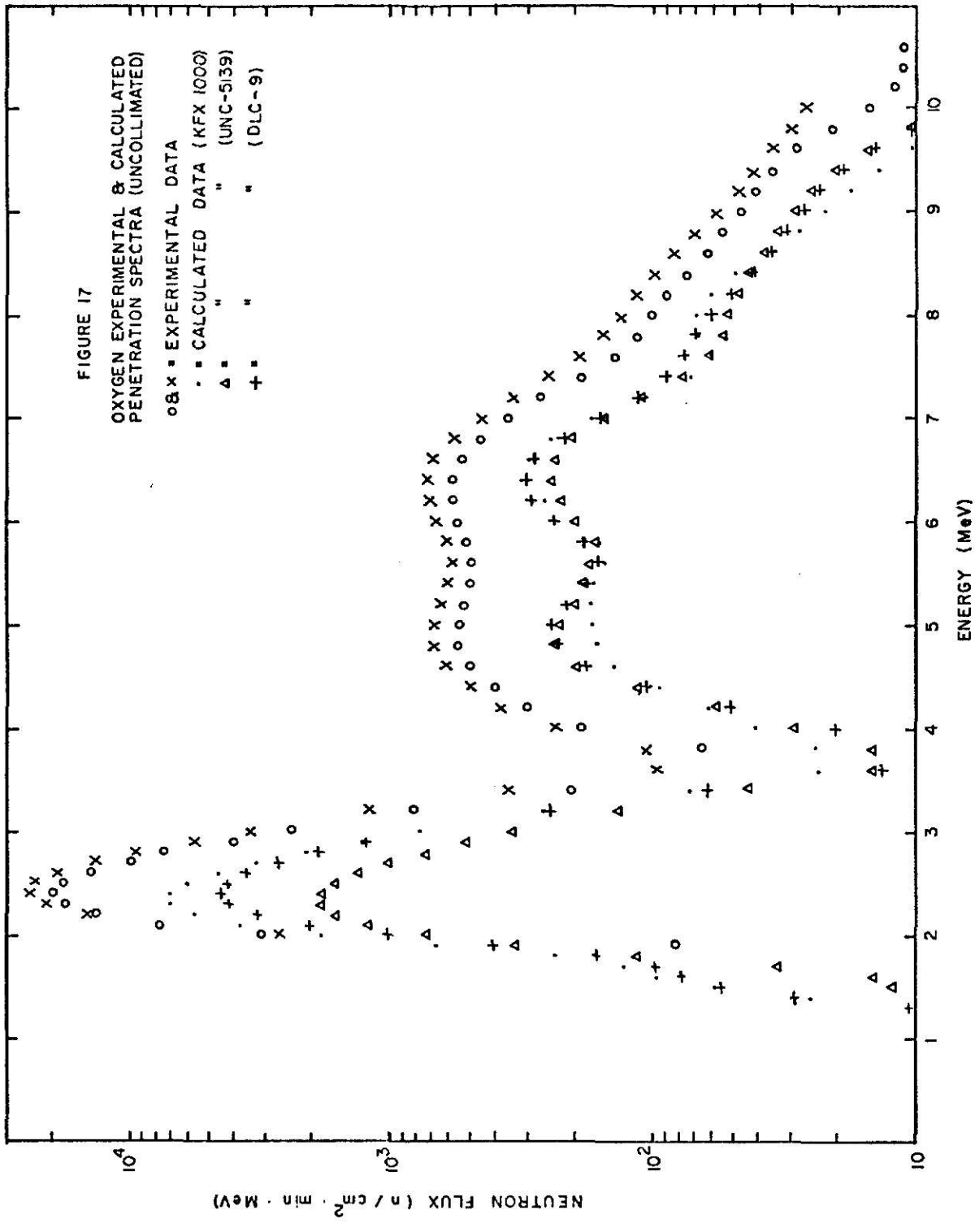


FIGURE 17
OXYGEN EXPERIMENTAL & CALCULATED
PENETRATION SPECTRA (UNCOLLIMATED)
o & x = EXPERIMENTAL DATA
· = CALCULATED DATA (KFX 1000)
Δ = " " (UNC-5139)
+ = " " (DLC-9)
NEUTRON FLUX (n / cm² · min · MeV)
ENERGY (MeV)

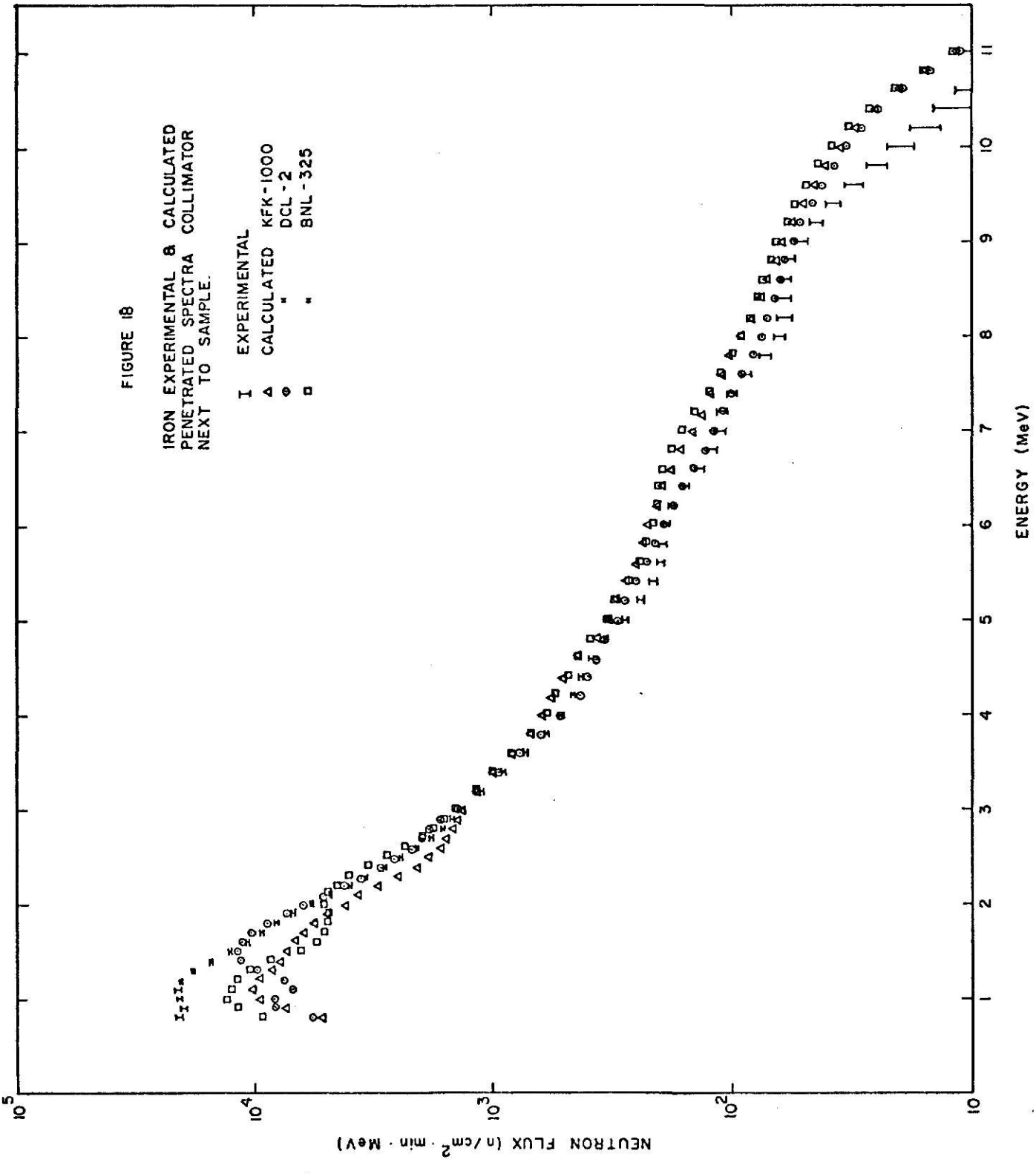


FIGURE 18
IRON EXPERIMENTAL & CALCULATED
PENETRATED SPECTRA COLLIMATOR
NEXT TO SAMPLE.
I EXPERIMENTAL
Δ CALCULATED KFK-1000
● " DCL-2
□ " BNL-325
NEUTRON FLUX (n/cm² · min · MeV)
ENERGY (MeV)
10⁵
10⁴
10³
10²
10
1
2
3
4
5
6
7
8
9
10
11

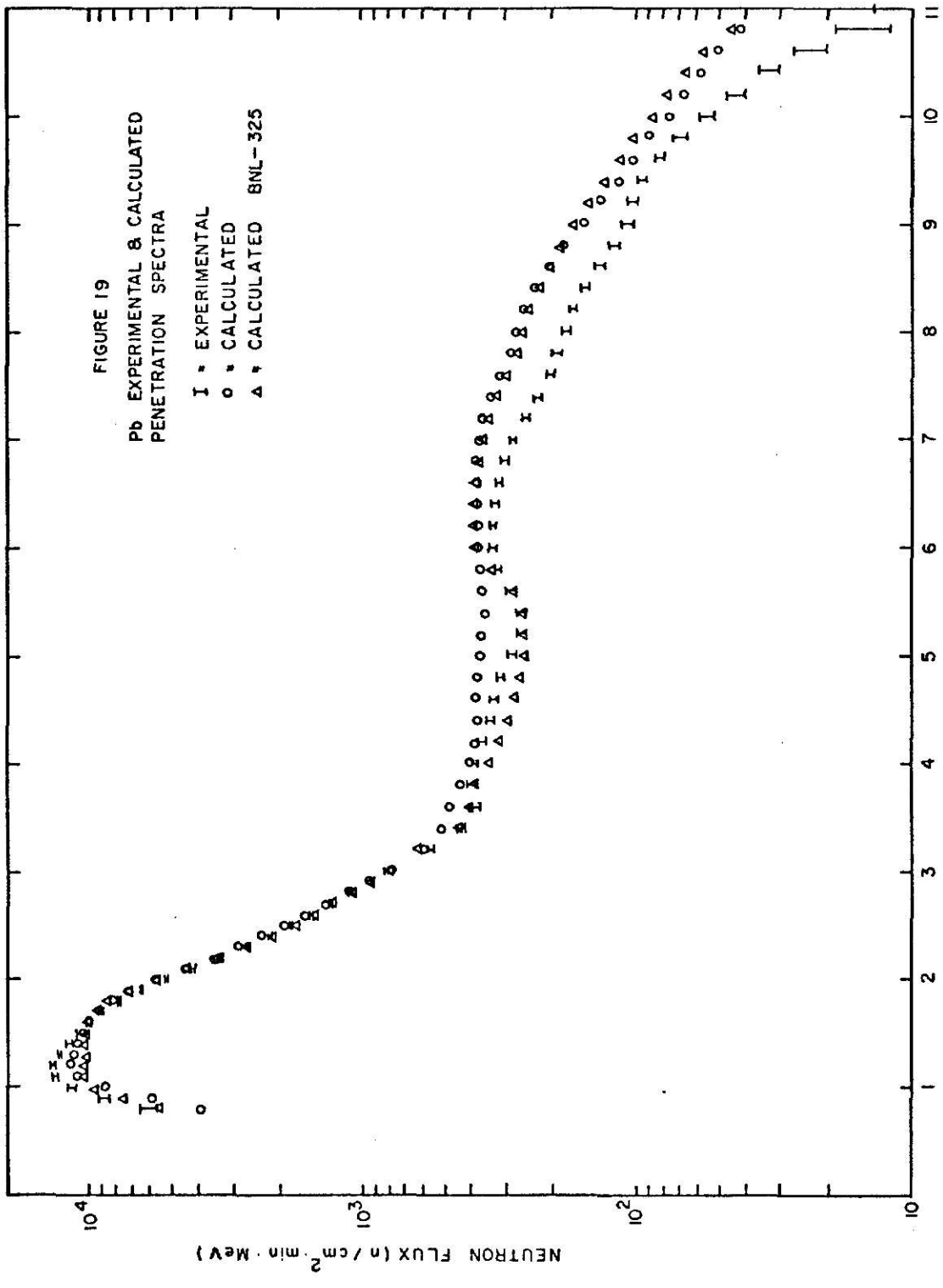


FIGURE 19
Pb EXPERIMENTAL & CALCULATED
PENETRATION SPECTRA
I = EXPERIMENTAL
o = CALCULATED
Δ = CALCULATED BNL-325
NEUTRON FLUX (n / cm² · min · MeV)
ENERGY (MeV)
10⁴
10³
10²
10
1
2
3
4
5
6
7
8
9
10
11

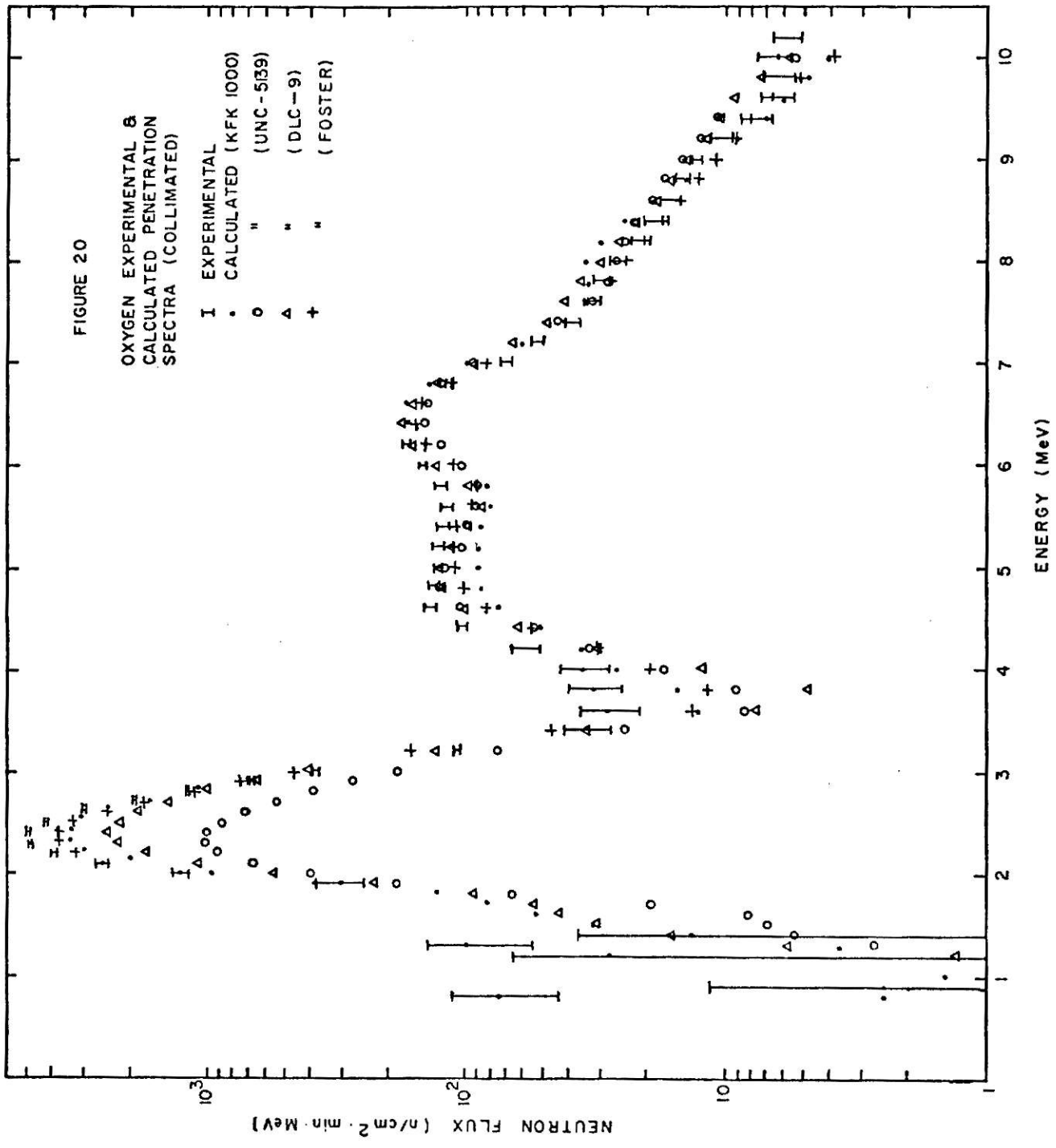


FIGURE 20
OXYGEN EXPERIMENTAL & CALCULATED PENETRATION SPECTRA (COLLIMATED)
I EXPERIMENTAL
• CALCULATED (KFK 1000)
o " (UNC-5139)
Δ " (DLC-9)
+ " (FOSTER)
NEUTRON FLUX (n/cm² · min · MeV)
ENERGY (MeV)

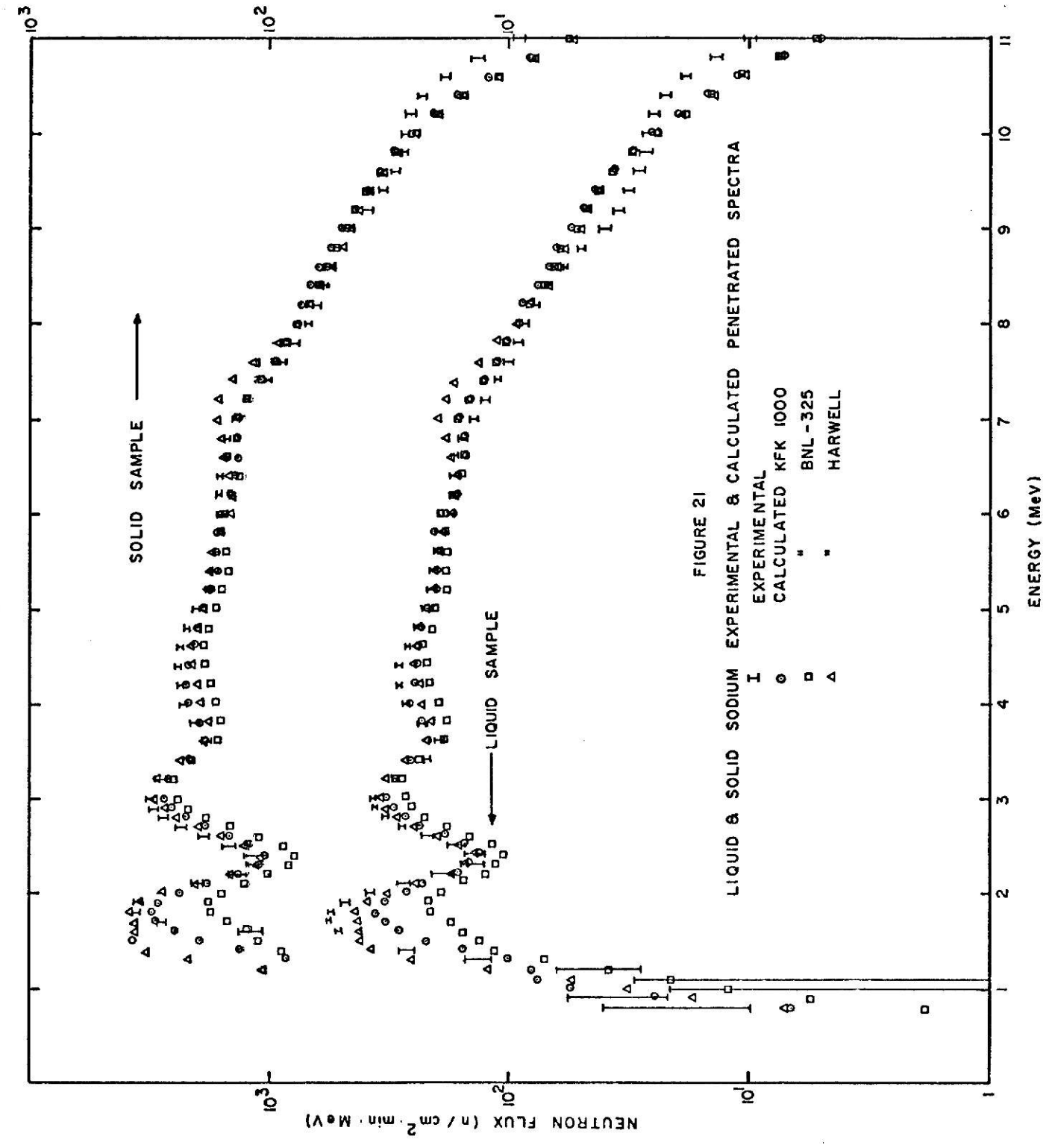

LIQUID & SOLID SODIUM EXPERIMENTAL & CALCULATED PENETRATED SPECTRA
I EXPERIMENTAL
⊙ CALCULATED KFK 1000
□ " BNL-325
△ " HARWELL
SOLID SAMPLE
LIQUID SAMPLE
NEUTRON FLUX (n / cm² · min · MeV)
ENERGY (MeV)
10³
10²
10¹
1
2
3
4
5
6
7
8
9
10
11

FIGURE 21

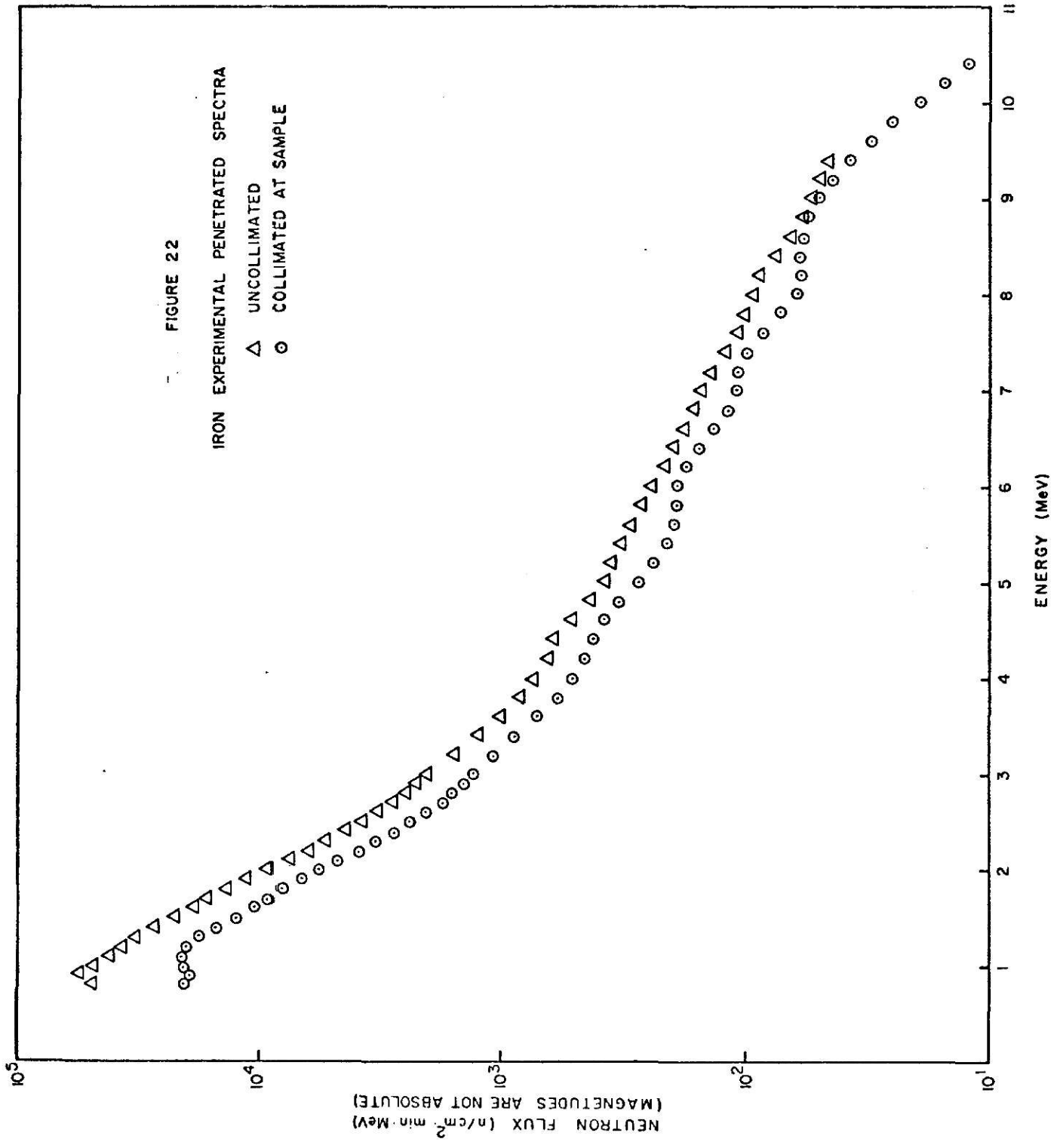


FIGURE 22
IRON EXPERIMENTAL PENETRATED SPECTRA
△ UNCOLLIMATED
⊙ COLLIMATED AT SAMPLE
NEUTRON FLUX (n/cm² min·MeV)
(MAGNETUDES ARE NOT ABSOLUTE)
ENERGY (MeV)

7.0 CONCLUSIONS

7.1 Detector Resolution

As can be seen from Fig. 12, there is reasonable agreement between the two experimental resolution data. Simons' data set shows an unusual effect in that the resolution begins to decrease at approximately 7.5 MeV. This is considered to be an error in his data since there would seem to be no physical phenomenon which would produce this effect. Verbinski's data set does not show this effect in this region and is probably more representative of the actual resolution of the NE-213 detector. However, there is an inflection point in Verbinski's data at 3 MeV which is questionable. The point at 2.3 MeV seems to be in error, causing the resolution in this region to be poorer than that reported by Simons.

In order to check the resolution of the detector system, oxygen was chosen for a penetration measurement. The large minima in the cross-section at 2.35 MeV produces an almost mono-energetic peak at this energy. Therefore, the width of this peak is a good measure of the resolution of the detector. Figure 14 shows a comparison between the experimentally measured and the calculated transmitted spectra for oxygen using the KFK-1000[2] cross-section data (since this data set seems to best predict the transmitted spectrum in the 2.35 MeV region as shown in Fig. 20) and the Verbinski resolution data. Figure 14 also shows the comparison between the two spectra when the Verbinski resolution was improved by 25% (multiplying the FWHM by 75%). This latter calculation was used for the following reasons:

1) Verbinski's resolution data were taken on another NE-213 detector system at ORNL which does not necessarily have the same resolution as the KSU NE-213 detector, but should have a similar shape as a function of energy.

2) Simons' data show a better resolution in the 2.35 MeV region although the resolution at higher energies is in question.

3) Measurements of Na^{22} and Co^{60} spectra taken at ORNL and Kansas State University show that the KSU system appears to have at least as good, if not better, resolution.

4) The use of Verbinski's resolution data (unchanged) in the calculated transmitted spectrum shows poorer resolution in the 2.35 MeV region than does the experimental measurement. Furthermore, by improving the resolution by 25%, good agreement is found between the experimental and calculated results.

It was concluded that, although the calculated transmitted spectrum is not extremely sensitive to the resolution, improving Verbinski's resolution by 25% best describes the KSU NE-213 system resolution for this calculation and was therefore used on all subsequent calculations. The comparison between the calculated and experimental transmitted spectra for the other materials used in this experiment supports this assumption.

7.2 Energy Calibration

The 2.35 MeV peak in the transmitted oxygen spectrum also provides a check on the energy calibration. As can be seen, all of the calculated and experimental peaks fall between 2.35 and 2.40 MeV indicating that the energy calibration of the system is very accurate.

7.3 Consistancy of Experimental Results

Figure 17 shows two experimentally determined transmitted spectra for oxygen. These runs were made to test the consistancy of the experimental results, except for a normalization error, the two runs are identical. The normalization error occurred on this run because sulfur was used as a flux monitor. All subsequent runs used the more reliable nickel foils.

7.4 Forward Scattering Assumptions

As was stated in the theory, the first geometry condition (uncollimated) assumed that any forward scattering at shallow angles would miss the solid

angle subtended by the detector. Figure 17 shows such a run for oxygen. Even though there was a small normalization problem, there was a large discrepancy between the experimental and calculated results throughout the energy range. This discrepancy indicates that the experimental measured cross-section was much less than the published data. This result indicates that many neutrons scattered at shallow angles were reaching the detector. This would cause an increase in the experimental result, as shown, and would therefore make the actual cross-section appear too large. Figure 20 shows the same comparison between experimental and calculated results using the second geometry condition (with the collimator placed in front of the detector). The forward scattering problem was virtually eliminated and good agreement was found between the experimental and calculated results.

The total neutron cross-section predicted by the uncollimated case was about 25% lower than the published data. This error is due to forward scattered neutrons which were reaching the detector, but this forward scattering contribution seems very large. Therefore, a mathematical model was used to predict this discrepancy. DLC-2[4] angular dependent cross-section data set was used with the following assumptions:

1: Any neutron that was scattered at an angle less than the solid angle subtended by the detector was assumed to be unscattered, and therefore, part of the original beam.

2: Any neutron that was scattered at an angle larger than the solid angle subtended by the detector was assumed to be lost from the beam and would not be scattered back into the detector.

3: The probability of neutrons scattering into the solid angle of the detector was equal to the probability of zero angle scattering integrated over the detector solid angle.

Neither of the first two assumptions were entirely valid. Neutrons that were scattered at small angles could be scattered again and miss the detector.

Also, neutrons scattered at large angles could be scattered again back into the solid angle of the detector. However, the discrepancies in these two assumptions tend to cancel each other. Thus, it is possible to predict the transmitted spectrum by:

$$\phi_{trans} = \phi_I \exp[-(\Sigma_t - \Sigma_{fs})t] \tag{11}$$

where Σ_{fs} is the correction in the total neutron cross-section from forward scattered neutrons which reach the detector. Σ_{fs} was calculated using the DLC-2 data and the solid angle of the detector, and the results are shown in Fig. 23. This calculation did not even start to describe the experimentally measured forward scattering contribution. The calculation gave a Σ_t correction of about .01% (see Fig. 23) compared to 25% in the experiment. It is realized that the assumptions made were not completely accurate; however, several orders of magnitude difference between the experimentally measured deviation and the calculated correction are involved. It appears unlikely that refinement of the assumptions would lead to significant improvement of the calculation. Therefore one is led to the conclusion that significant errors may exist in the DLC-2 shallow angle scattering data.

The DLC-2 cross-section data set was first checked against a theoretical minimum cross-section based on the optical model. The Wick's Limit[27] gives the minimum zero angle scattering probability by the following equation:

$$\left.\frac{d\sigma}{d(\cos\phi)}\right|_{0^\circ} \geq \frac{k^2}{8\pi}\,\sigma_{TOT}{}^2 \tag{12}$$

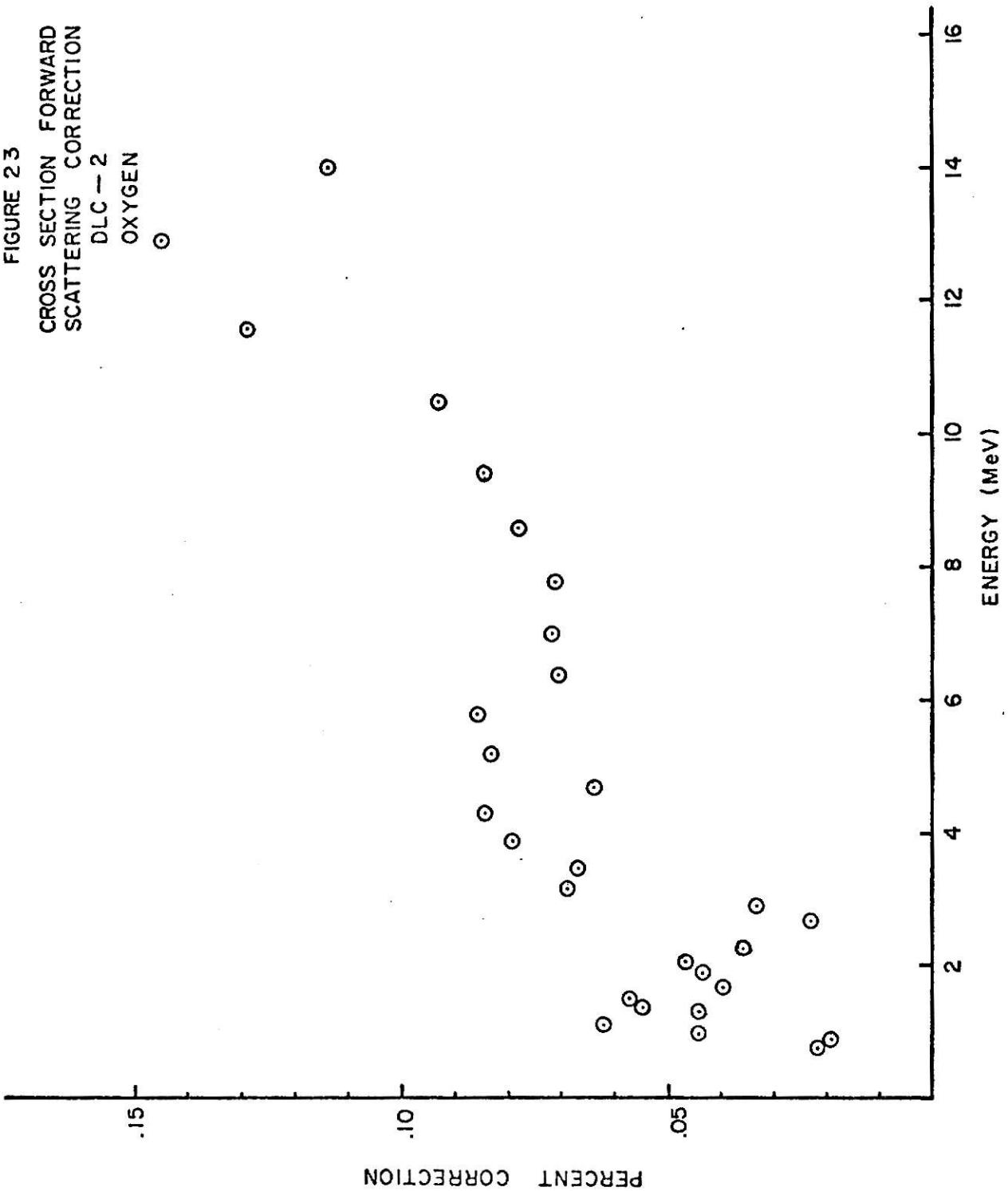
where $k^2 = \frac{2\mu E}{h^2}$

θ = scattering angle in center of mass system

and $\mu = \frac{m \cdot M}{m + M}$

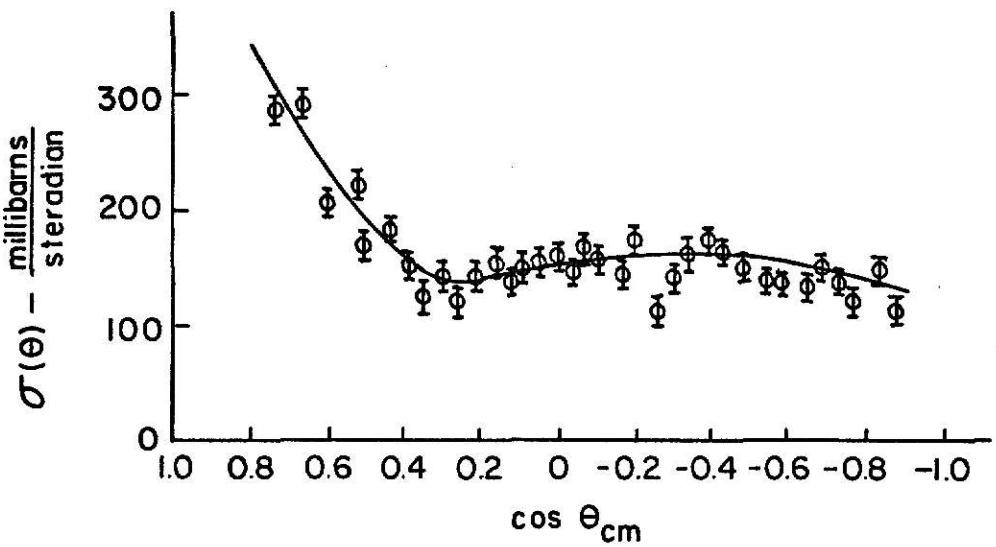
and m,M = masses of the neutron and oxygen atom

FIGURE 23
CROSS SECTION FORWARD SCATTERING CORRECTION
DLC – 2
OXYGEN



This equation was used to check the DLC-2 data at several energies, and the data do indeed satisfy the theoretical minimum. However, this does not indicate that the actual forward scattering probability is not much greater than indicated by the Wick's minimum limit.

If it is assumed that the data taken in this experiment are correct, then there must be an explanation for the large errors in published forward scattering data. It is noted in looking at published data that the differential angular cross-section as a function on angle is not reported between 0° and approximately 30°. For example, the following figure shows such a plot for oxygen at 3.91 MeV taken from BNL-400.[10]



Experimental cross section data can not be taken any closer to the zero angle than 30° because of interference between the neutrons scattered at small angles and the uncollided, transmitted flux. Therefore, the zero angle forward scattering probability is determined by expoential extrapolation of the data from 30° back to 0°. The measurements made in this report indicate that the actual forward scattering probability approaches a δ function, i.e., it is very sharply peaked at the zero angle. The error found in published data

is due to a lack of experimental data in this region. Forward scattering probability at small angles is rarely measured. For many materials the error between the extrapolated zero angle scattering probability and the actual may be small, but for oxygen it appears that the extropolated data are in serious error.

7.5 Multiple Scattering Assumptions

Figure 22 shows a comparison between two iron penetration spectra, one uncollimated and one collimated at the sample. In this example, the effect of multiple scattered neutrons on the penetration data can be seen. A fraction of the incident neutrons were apparently scattered several times in the sample and emerged from the sample in a direction that would intercept the detector. This effect can be seen by the smoothing of the data and in the buildup in the low energy end for the uncollimated case (see Fig. 22). However, the magnitude of the discrepancy caused by multiple scattering of neutrons is much less than that caused by shallow angle scattering of neutrons as can be seen by comparison of Figs. 16 and 18. The uncollimated data points were slightly above the calculated and the collimated were slightly below, but the difference is small. Again, if a true measure of the total neutron cross-section was to be made, the collimator would be used.

7.6 Evaluation of Published Data

The cross section data sets used to obtain the calculated transmitted spectra to be compared with the measurements came from a variety of sources and methods. The KFK-1000[2] data and the data of Foster[7] and Langsford[14] were taken using an accelerator and time light measurements. The BNL-325[11] data set is a compilation of data from many sources and the best line is drawn through all of the combined data. The UNC-5139[20] data set is a

combination of experimental data and theoretical calculations. The DLC[5] data set is grouped cross-section data from the ENDF/B[6] file compiled with the ORNL code SUPERTOG[29] using 1/E spectrum weighting.

7.6.1 Iron (Fig. 18) - All data show good agreement except for energies at about 1.7 MeV or below. Errors in the cross-section compared to the measurements range from approximately 10% to 15% at 1.3 MeV. The DLC-2 data set shows the best agreement with the experimental result (except in the low energy region), although the errors are small for all three data sets. The error above 9.5 MeV is probably due to poor statistics in the experimental spectrum.

7.6.2 Lead (Fig. 19) - Good agreement is found with both data sets. The largest error at 5.7 MeV is only about 4% which is probably within the statistics of the experiment. The BNL data set seems to be best up to 6 MeV, after which both data sets differ from the experimental.

7.6.3 Oxygen (Fig. 20) - In general, much of the data do not adequately describe the depth of the minima at 2.35 MeV. At this point, the calculation based on the Foster data is within 8% of the experimentally measured cross-section data while UNC-5139 is in error by 40%. There is also some problem with most of the data at 4.7 MeV. The best data set over the entire spectrum is the DLC-9 data, except in the 2.35 MeV region. The discrepancy in this region would be expected since the cross-section has been averaged over some energy width and therefore underestimates the depth of the minima.

7.6.4 Sodium (Fig. 21) - Good agreement is found for most of the data for both samples. The experimental data points for the liquid sample tend to be slightly above the calculated as compared to the solid sample. However, the two experimental spectra agree within 3% and the error is probably due to an error in the density calculation for the liquid sample. The comparison

between these two sets of data shows that the experiment is sensitive to density changes as should be noted. The change in the density from the solid to the liquid sample was 6.4% which resulted in an increase in the calculated transmitted flux by approximately 45% at 3 MeV. As can be seen in Fig. 21 this change in the calculated transmitted spectrum due to the density change in the sample was also measured in the experimental transmitted flux since the experimental and calculated results show good agreement.

The BNL data sets show large errors from 5 MeV down, with a cross-section error of 10% at 1.8 MeV. Langsford shows a discrepancy at 7.3 MeV which does not appear in other data nor in the experimental result. An unfolding problem occured with the solid sample below about 1.6 MeV and the data below this point are in error. The fluctuations in the experimental results in the higher energy region are probably statistical in nature and should be disregarded.

8.0 SUGGESTIONS FOR FURTHER STUDY

Now that the experimental procedure has been established, the evaluation of total neutron cross-sections for many materials can be quickly and accurately completed. Possibly the most accurate results would be obtained by using two collimators; one at the sample and one at the detector. This would eliminate both multiple and shallow angle scatters. However, it would be difficult to align both collimators with the equipment now available and single collimation at the detector or at the sample does give adequate results.

In order to study the forward scattering vs. multiple scattering phenomenon several penetration spectra could be taken with varying sample thicknesses and without collimation. If the measured result produced the same error in the total cross-section for all thicknesses, then it could be concluded that forward scattering was contributing a great deal to the measured transmitted spectra. However, if the total cross-section error increased with increasing thicknesses it could be concluded that multiple scattering was contributing to the measured spectra. In this experiment the contribution from forward scattered neutrons would always be present, however, it would be constant for all thicknesses. The contribution from multiple scattering, on the other hand, would increase with increasing thickness. The larger thicknesses would have a greater probability for multiple scattering and some of these neutrons would reach the detector. For small thicknesses (approximately 1 mean free path) the probability of multiple scattering is small, and any contribution to the uncollided flux would be from forward scattering only.

If the experiment outlined in the previous paragraph proves conclusively that there is a large contribution to the uncollided flux from

forward scattering neutrons in the uncollimated geometry, as has been indicated by the data taken at this time, then additional measurements of the actual forward scattering probability should be made. First, a more exact formulation of the actual contribution to the uncollided flux from shallow angle scattering near 0° should be derived based on available angular dependent cross section data. This would be a more precise analysis than was used in deriving equation 11, and would take into account the effects of multiple shallow angle scatters in thicker samples, the physical size of the sample, etc. Measurements could then be made, possibly using several different sized collimators. The use of several collimators would make it possible to check the reliability of the experiment and to gain knowledge of the variation in differential scattering probability with angle for angles very close to the 0° angle. As the solid angle subtended by the detector is increased, the number of neutrons detected is a measure of the forward scattering probability over that particular solid angle. The resultant total cross-section discrepancies would be due to forward scattering and could be used to calculate the differential scattering probability near the 0° angle using the formulation derived.

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10.0 REFERENCES

1. Burris, W. R., "Status of FERDOR Neutron Unscrambling with NE-213 Response Matrix," Intra Laboratory Correspondence, Oak Ridge National Laboratory, Oak Ridge, Tennessee (November 2, 1967).

2. Cierjacks, S., P. Forti, D. Kopsch, L. Kropp, J. Nebe, and H. Unseld, "High Resolution Total Neutron Cross-Sections Between 0.5 - 0.30 MeV," KFK-1000, Institut fur Angewandte Kernphysik, Karlsruhe (June, 1968).

3. Clifford, C. E., E. A. Straker, et al., "Measurements of the Spectra of Uncollided Fission Neutrons Transmitted Through Thick Samples of Nitrogen, Oxygen, Carbon, and Lead: Investigation of the Minimum Total Cross Section," Nucl. Sci. Eng., 27, 299 (1967).

4. DLC-2B, Code Name: Neutron--99 Group Cross-Section, Radiation Shielding Institute Center (July 1, 1969).

5. DLC-9, Code Name: FARS Data 122 Group (104 Neutron, 18 Gamma), Radiation Shielding Institute Center (June 11, 1969).

6. Evaluated Nuclear Data File of the National Neutron Cross Section Center, Brookhaven National Laboratory.

7. Foster, D. G., Oxygen Total Neutron Cross-Section Data, Battelle Northwest (May, 1967).

8. Foster, D. G., and D. W. Glasgow, "Method for Measuring Total Cross-Sections with Neutrons Having Energies from 2.5 to 15 MeV," Nuclear Instruments and Methods, Vol. 36 (January, 1965).

9. Glastone, Samuel, and Alexander Sesonske, Nuclear Reactor Engineering, D. Van Nostrand Co., Inc., Princeton, N. J. (1967).

10. Goldberg, Murrey D., Victoria M. May and John R. Stehn, "Angular Distributions in Neutron-Induced Reactions," BNL 400 (Physics-TID-4500), Brookhaven National Laboratory, National Bureau of Standards, Springfield, Virginia (February 1963).

11. Goldberg, Murrey D., Said F. Mughabghab, et al., "Neutron Cross-Sections," BNL-325, Supplement No. 2 (Physics-TID-4500), Brookhaven National Laboratory, National Bureau of Standards, Springfield, Virginia (February 1967).

12. Handling Metallic Sodium on a Plant Scale, U. S. Industrial Chemicals Co., New York (1959).

13. Jackson, Carey B., Ed., Liquid Metals Handbook, Sodium (NaK) Supplement, U. S. Government Printing Office, Washington D. C. (1955).

14. Langsford, "International Conference on the Study of Nuclear Structure with Neutron Antwerp," (July, 1965).

15. Meyer, Walter, and C. Michael Estes, Private Communication - Unpublished data (April, 1971).

16. Meyer, W., J. W. Thiesing, and C. M. Estes, "Intercalibration of the KSU NE-213 Fast-Neutron Spectrometer System," Technical Progress Report to Division of Research USAEC (AEC Contract No. AT(11-1) 2049), COO-2049-3 Nuclear Engineering, Kansas State University (December 1970).

17. Neal, M. A. and A. E. Miller, Liquid Metals Engineering Center, Canoga Park, California, USAEC, Personal Letter (July 1970).

18. Noffke, Harold of Air Products and Chemicals, Inc., Kansas City, Missouri, Personal Interview (May 8, 1970).

19. "Operation Procedure, Wichita No. 2050-103: Liquid Oxygen," Boeing Company Manual, Wichita, Kansas (April 23, 1968).

20. Ray, J. H., G. Grochowski and E. S. Troubetzkoy, "Neutron Cross Sections of Nitrogen, Oxygen, Aluminum, Silicon, Iron, Deuterium, and Beryllium," UNC-5139, United Nuclear Corporation, Elmsfor, New York (1965).

21. "Safety-Gram, No. 54-c: Liquid Oxygen," Air Products and Chemicals, Inc., Kansas City, Missouri (January 31, 1967).

22. Schwartz, R. B., National Bureau of Standards, Private Communication - Unpublished data (July 1970).

23. Simons, G. G., "Development, Calibration and Utilization of the KSU Fast Neutron Spectrometer System," a Ph.D. Dissertation, Kansas State University (1968).

24. Sitting, Marshall, Sodium--Its Manufacture, Properties, and Uses, Reinhold Publishing Corp., New York, N. Y. (1956).

25. Smithalls, Metals Reference Book, Butterworths, London, England (1967).

26. Straker, E. A., "Experimental Evaluation of Minima in Total Neutron Cross Sections of Several Shielding Materials," ORNL TM-2242, Oak Ridge National Laboratory, Oak Ridge, Tennessee (June 6, 1968).

27. Wick, G. C., Atti Acad. d'Ital., 13, 1203 (1943).

28. Wilk, I. J., "Dangers due to Increased Flammability of Materials in Oxygen-Enriched Atmospheres," Journal of Chemical Education (July 1968).

29. Wright, R. Q., J. L. Lucius, N. M. Greene, and C. W. Craven, "SUPERTOG: A Program to Generate Fine Group Constants and P Scattering Matrices Form ENDF/B," ORNL-TM-2679 (1969).

APPENDIX A

COMPUTER PROGRAMS

CALFLUX

NE213RES

POLYFIT

APPENDIX A

COMPUTER PROGRAMS

CALFLUX

This program calculates the transmitted neutron spectrum through samples and smooths the results with the NE-213 resolution function as given by Equation 10 on page 6. After reading all of the input data, the program establishes a cross-section data point or incident spectrum data point for each energy that appears in either the cross-section or incident spectrum library by calling subroutine ENGRID. The program then begins to calculate the transmitted flux at given energies starting with 0.8 MeV in 0.1 MeV intervals to 3.0 MeV, and then in 0.2 MeV intervals (same energy intervals as the FERDOR output). For each energy the FWHM of the resolution function is calculated, and the actual integration is carried out over some energy width calculated by multiplying constant (PFWHM) times the FWHM. (The contribution to the area under a gaussian curve is small past approximately two times the FWHM from the center of the peak.) The contribution to the transmitted flux from each energy interval over the width of the integration is calculated and summed. The energy intervals are for each E_i to E_{i+1} as established by the subroutine ENGRID.

Only one problem was encountered with this procedure. When large positive slopes were present in the cross-section data, the arguments of Equation 10 became such that the value of the error function (erf) was very close to 1.0. Thus, when the difference between two error functions were taken, the result was set equal to zero by the computer. At the same time, the constants that were being multiplied by this difference became very large; however, the product calculated by the computer was always zero. To overcome this problem, the program tests the value of the difference term,

and if it becomes very small the program calls the subroutine ROMBRG which numerically finds the value of the integral between these two energy points.

Output from CALFLUX includes the physical constants for the sample used and a plot of the input cross-section library and incident spectrum library. The resultant calculated flux is listed and also plotted along with the experimentally measured transmitted flux.

INPUT

Card	Format		
1	8F10.4	1) T	= Sample thickness (cm)
		2) RHO	= Molecular Density (atom/cc) $\times 10^{24}$
2	8F10.4	1) WIDTH	= A multiplication constant times the FWHM at which the resolution gaussian will be truncated
3	8F10.4	1) XNORM	= normalization factor between the incident and penetration integrated flux
4	8F10.4	1) PFWHM	= the percentage of calculated FWHM used for the resolution function
5	8F10.4	1) EMAX	= Maximum energy to which the program will calculate the transmitted spectrum
6	I3	1) NXSECT	= number of points in the cross-section library
7 (Deck)	8F10.4	1) EX(I)	= energy of the ith cross-section data point (MeV)
		2) XSECT(I)	= the ith cross-section (barns)
		3) EX(I+1)	= energy...
		⋮	
		8) XSECT(I+3)	= cross-section...

Card	Format		
8	I3	1)NA	= number of incident spectrum library points
9 (Deck)	(FERDOR output Format)	1) ES(I)	= energy of the ith incident spectrum data point (eV)
		2) SPCT(I)	= the ith incident spectrum point ($n/cm^2 \cdot min \cdot MeV$)
10	I3	1) NE	= number of penetration spectrum library points
11 (Deck)	(FERDOR output Format)	1) EE(I)	= energy of the ith penetration spectrum data point (eV)
		2) SPCTE(I)	= the ith penetration spectrum point ($n/cm^2 \cdot min \cdot MeV$)

NOTE:

1) The library cross-section must extend from .01 to 15 MeV and must exceed the incident spectrum library at both lower and upper energies.

2) The maximum energy in the incident and penetration spectrum library must exceed EMAX.

CALFLUX Listing

```
FORTRAN IV G LEVEL  18                  MAIN                DATE = 71109          22/14/21

              C      THIS PROGRAM CALCULATES TRANSMITTED NEUTRON SPECTRUM
              C      THROUGH SAMPLES AND SMOOTHES THE RESULTS WITH THE
              C      NE 213 RESOLUTION FUNCTION
              C
              C
              C      THE LIBRARY CROSS-SECTION MUST EXTEND FROM .01 TO 15 MEV
              C      AND MUST EXCEED THE SPECTRUM LIBRARY AT BOTH LOWER AND UPPER ENERGIES
              C
              C
              C      T = THICKNESS OF SAMPLE (CM)
              C      RHO = MOLECULAR DENSITY (ATOMS/CC) X 10**24
              C      XNORM = NORMALIZATION FACTOR BETWEEN REACTOR POWER LEVELS FOR
              C              INCIDENT AND TRANSMITTED SPECTRA MEASUREMENTS
              C      NSECT = NUMBER OF ENTRIES IN LIBRARY CROSS-SECTION
              C      EX(I),XS(I) = ENERGY AND CORRESPONDING CROSS-SECTION IN
              C                    CROSS-SECTION LIBRARY (MEV,BARNS)
              C      WIDTH = A MULTIPLICATION CONSTANT TIMES THE FWHM AT WHICH THE
              C              RESOLUTION GAUSSIAN WILL BE TRUNCATED
              C      PFWHM = THE PERCENTAGE OF CALCULATED FWHM USED FOR RESOLUTION FUNCTION
              C      WE(I),WSECT(I) = ENERGY AND CORRESPONDING INCIDENT SPECTRUM FROM
              C                       FROM FERDOR CODE AND MUST EXCEED EMAX
              C      WEE(I),WSPECTE(I) = ENERGY AND CORRESPONDING EXPERIMENTAL
              C                          SPECTRUM FROM FERDOR CODE AND MUST EXCEED EMAX
              C      EMAX = MAXIMUM ENERGY TO WHICH THE PROGRAM WILL CALCULATE THE
              C             TRANSMITTED FLUX
              C
0001                  IMPLICIT REAL*8 (A-H,O-V,X-Z)
0002                  DOUBLE PRECISION DLOG,DEXP,DERF,DABS
0003                  EXTERNAL FCN
0004                  DIMENSION SPCT(75),EE(75),SPCTE(75),X(150),P(150),ENE(75),FL(75)
0005                  COMMON /HOLD1/ EX(100),XS(100),ES(75),SPECTL(75)
0006                  COMMON /HOLD2/ E(150),XSECT(150),FLUL(150)
0007                  COMMON /HOLD3/ ENERGY,BO,NLO
0008                  CALL ERRSET (208,50,1,C,0,0)
0009                900 FORMAT (I3)
0010                901 FORMAT (8F10.4)
0011                902 FORMAT (8X,E10.3,3X,E10.3)
0012                910 FORMAT (1H1,'THIS PROGRAM CALCULATES A SMOOTHED TRANSMITTED SPECTR
                       1UM FROM TABULATED DATA USING THE RESOLUTION FUNCTION OF THE NE 213
                       1',/,40X,'USING THE FOLLOWING PARAMETERS:',////)
0013                911 FORMAT ('0  THE RESOLUTION HAS BEEN TRUNCATED AT',F6.3,'TIMES THE
                       1FWHM OF THE GAUSSIAN')
0014                913 FORMAT('0  THE SAMPLE THICKNESS IS T = ',F10.3,' CM, AND THE MOLEC
                       1ULAR DENSITY IS RHO = ',D10.3,' X 10**24 MOLECULES/CC',//,'   THE
                       2NORMALIZATION FACTOR IS XNORM = ',F10.3)
0015                914 FORMAT ('1','THE CALCULATED, SMOOTHED TRANSMITTED SPECTRA IS: ',//
                       1,5X,'ENERGY',7X,'FLUX TRANSMITTED')
0016                915 FORMAT (5X,F5.1,10X,D12.5)
0017                916 FORMAT (5X,F5.1,10X,D12.5,' POSSIBLE ERROR BECAUSE GAUSSIAN RESOLU
                       1TION CURVE IS BEING TRUNCATED AT .01 MEV')
0018                917 FORMAT ('  PROGRAM HAS BEEN TERMINATED BECAUSE UPPER LIMIT OF INTE
                       1GRATION EXCEEDS CROSS-SECTION LIBRARY')
0019                919 FORMAT ('1   PLOT OF LOG(FLUX) VS ENERGY',//,'    ENERGY    CAL. F
                       1LUX    EXP. FLUX     + = CALCULATED    * = EXPERIMENTAL')
0020                920 FORMAT ('1  THE INPUT CROSS-SECTION LIBRARY IS AS FOLLOWS:',/,6X,'
                       1ENERGY',3X,'CROSS-SECTION')
0021                921 FORMAT ('1   THE INPUT SPECTRUM IS AS FOLLOWS:',/,6X,'ENERGY',3X,'L
                       1OG(SPECTRUM)')
```

```
FORTRAN IV G LEVEL  18                  MAIN               DATE = 71109          22/14/21

0022          922 FORMAT ('0   THE FWHM HAS BEEN MULTIPLIED BY ',F6.3)
0023              PI = 3.141592653
0024              READ 901,T,RHO
0025              READ 901,WIDTH
0026              READ 901,XNORM
0027              READ 901,PFWHM
0028              READ 901,EMAX
0029              READ 900,NXSECT
0030              DO 1 I=1,NXSECT,4
0031            1 READ 901,EX(I),XS(I),EX(I+1),XS(I+1),EX(I+2),XS(I+2),EX(I+3),XS(I+
                 13)
0032              READ 900,NA
0033              DO 20 I=1,NA
0034              READ 902,ES(I), SPCT(I)
0035              ES(I) = ES(I)*0.1D-05
0036           20 SPECTL(I) = DLOG(SPCT(I))
0037              READ  900,NE
0038              DO 42 I=1,NE
0039           42 READ 902, EE(I), SPCTE(I)
0040              DO 44 I=1,NE
0041              IF (SPCTE(I) .LE. 0.000) SPCTE(I) = SPCTE(NE)
0042           44 SPCTE(I) = DLOG(SPCTE(I))
0043              PRINT 910
0044              PRINT 913,T,RHO,XNORM
0045              PRINT 911,WIDTH
0046              PRINT 922,PFWHM
0047              CALL ENGRID (NXSECT,NA,NG)
0048              DO 2 I=1,NG
0049            2 XSECT(I) = XSECT(I)*T*RHO
0050              PRINT 920
0051              CALL PLAT2 (EX,XS,NXSECT)
0052              PRINT 921
0053              CALL PLAT2 (ES,SPECTL,NA)
0054              PRINT 914
0055              NGM1 = NG-1
0056              DO 30 I=1,NGM1
0057              DE = E(I+1)-E(I)
0058              X(I) = (XSECT(I+1)-XSECT(I))/DE
0059           30 P(I) = (FLUL(I+1)-FLUL(I))/DE
0060              WMAX = (EMAX-.3D01)/.2D00 + .2301D02
0061              MAXE = IFIX(WMAX)
0062              DO 3 I=1,MAXE
0063              FLUX = 0.0D00
0064              NNN = 0
0065              IF (I.GT.22)  GO TO 5
0066            4 ENERGY = .7+.1*I
0067              GO TO 6
0068            5 ENERGY = 3.0+.2*(I-23)
0069            6 FWHM = .88525078200-.14836271200I*ENERGY+.13999231900I*ENERGY**2-
                 1.52543823D00*ENERGY**3+.99524939D0-01*ENERGY**4-.10031713D0-01*ENE
                 2RGY**5+.51266417 5D-03*ENERGY**6-.10426077 2D-04*ENERGY**7
0070              FWHM = FWHM*PFWHM
0071              BO = FWHM*FWHM/(0.4D1*0.6931472D0)
0072              AL = BO**.5
0073              ELO = ENERGY-FWHM*WIDTH
0074              IF (ELO-0.01) 7,7,8
0075            7 ELO = 0.01
0076            8 EUP = ENERGY+FWHM*WIDTH
```

```
FORTRAN IV G LEVEL  18                  MAIN              DATE = 71109          22/14/21

0077              IF (EUP-E(NG)) 9,9,10
0078            9 CONTINUE
0079              DO 22 J=1,NG
0080              IF (ELO .LT. E(J)) GO TO 23
0081           22 CONTINUE
0082           23 K = 0
0083              AB = E(J-1)
0084              E(J-1) = ELO
0085           24 K = K+1
0086              K1 = K-1
0087              NLO = J-1+K1
0088              NUP = J+K1
0089           28 IF(E(NUP)  .LT. EUP) GO TO 27
0090              ABC = E(NUP)
0091              E(NUP) = EUP
0092              NNN = 1
0093           27 YLO = (E(NLO)-ENERGY+0.5D0*X(NLO)*B0)/AL
0094              DYLO = DERF(YLO)
0095              YUP = (E(NUP)-ENERGY+0.5D0*X(NLO)*B0)/AL
0096              DYUP = DERF(YUP)
0097              ZLO = YLO-P(NLO)*AL/0.2D01
0098              DZLO = DERF(ZLO)
0099              ZUP = YUP-P(NUP)*AL/0.2D01
0100              DZUP = DERF(ZUP)
0101              CONST = X(NLO)*(E(NLO)-ENERGY)-XSECT(NLO)+0.25*X(NLO)**2*B0
0102              DDY = DYUP-DYLO
0103              IF (DABS(DDY) .LE. 0.1D-13) GO TO 40
0104              FLUX1 = DEXP(FLUL(NLO)+CONST)*DDY
0105              DDZ = DZUP-DZLO
0106              IF (DABS(DDZ) .LE. 0.1D-13) GO TO 40
0107              FLUX2 = DEXP(CONST+P(NLO)*(ENERGY-E(NLO))-X(NLO)*P(NLO)*B0/0.2D01-
                 1P(NLO)*P(NLO)*B0/0.4D01)*DDZ
0108              GO TO 52
0109           40 FLUX1 = 0.0D00
0110              E11 = E(NLO)
0111              E22 = E(NLO+1)
0112              EPS = .1D-01
0113              MRON = 5
0114              NRON = 0
0115              FLUX2 = .2D01*ROMBRG(E11,E22,EPS,MRON,NRON,FCN)/((B0*PI)**.5)
0116           52 FLUX = FLUX+0.5D00*(FLUX1+FLUX2)
0117              IF(K .EQ. 1) E(NLO) = AB
0118              IF (NNN .EQ. 1) GO TO 31
0119              GO TO 24
0120           31 E(NUP) = ABC
0121              FLUX = FLUX *XNORM
0122              ENE(I) = ENERGY
0123              FL(I) = DLOG(FLUX)
0124              IF(ELO .EQ..01) GO TO 12
0125              PRINT 915,ENERGY,FLUX
0126              GO TO 3
0127           12 PRINT 916,ENERGY,FLUX
0128            3 CONTINUE
0129              PRINT 919
0130              CALL PLAT3 (ENE,FL,SPCTE,MAXE)
0131              GO TO 11
0132           10 PRINT 917
0133           11 STOP
```

```
FORTRAN IV G LEVEL  18                  ENGRID              DATE = 71109          22/14/21

0001                SUBROUTINE ENGRID (NXSECT,NA,NG)
0002                IMPLICIT REAL*8 (A-H,O-Z)
0003                 DOUBLE PRECISION DLOG,DEXP,DABS
0004                COMMON /HOLD1/ EX(100),XS(100),ES(75),SPECTL(75)
0005                COMMON /HOLD2/ E(150),XSECT(150),FLUL(150)
0006                FLUL(1) = DLOG(DEXP(SPECTL(1))/0.2001)
0007                E(1) = EX(1)
0008                XSECT(1) = XS(1)
0009                I=1
0010                K = 1
0011                J = 1
0012                I1 = 1
0013                J1 = 0
0014              1 I = I+I1
0015                J = J+J1
0016                K = K+1
0017                IF ((EX(I)-0.1D-05) .GT. ES(J)) GO TO 10
0018                IF (DABS(EX(I)-ES(J)) .LT. 0.1D-05) GO TO 11
0019                E(K) = EX(I)
0020                J1 = 0
0021                I1 = 1
0022                XSECT(K) = XS(I)
0023                FLUL(K) =((SPECTL(J)-FLUL(K-1))*(E(K)-E(K-1))/(ES(J)-E(K-1)))+FLUL
                   1(K-1)
0024                GO TO 12
0025             10 E(K) = ES(J)
0026                J1 = 1
0027                I1 = 0
0028                FLUL(K) = SPECTL(J)
0029                XSECT(K) =((XS(I)-XSECT(K-1))*(E(K)-E(K-1))/(EX(I)-E(K-1)))+XSECT(
                   1K-1)
0030                GO TO 12
0031             11 E(K) = ES(J)
0032                J1 = 1
0033                I1 = 1
0034                FLUL(K) = SPECTL(J)
0035                XSECT(K) = XS(I)
0036             12 CONTINUE
0037                IF (J .GE. NA) GO TO 13
0038                GO TO 1
0039             13 K = K+1
0040                I = I+I1
0041                E(K) = EX(I)
0042                XSECT(K) = XS(I)
0043                FLUL(K) = SPECTL(NA)
0044                I1 = 1
0045                IF (I .GE. NXSECT) GO TO 15
0046                GO TO 13
0047             15 NG = K
0048                RETURN
0049                END
```

```
FORTRAN IV G LEVEL  18                  ROMBRG              DATE = 71109          22/14/21

0001              FUNCTION ROMBRG (A,B,EPS,M,N,FCN)
0002              IMPLICIT REAL*8(A-H,O-Z)
                C ROMBERG INTEGRATION                                              D1530001
0003              DIMENSION P(20)                                                  D1530005
0004              IF(N.LT.0)GO TO 200
0005              IF(N.GT.3)GO TO 200
0006              IF(M-20)99,99,98                                                 D1530007
0007           98 M=20                                                             D1530008
0008           99 X=A                                                              D1530009
0009              MM=M
0010              NN=N+1
0011              EP=FCN(X)                                                        D1530010
0012              X=FCN(B)
0013         2001 SUM=(X+EP)*0.5D0
0014              M=2
0015         2007 AEP=DABS(EP)
0016         2008 AX=DABS(X)
0017         2009 ASUM=(AEP+AX)*0.5D0
0018              FMAX=AEP
0019              IF(FMAX.GE.AX)GO TO 100
0020              FMAX=AX
0021          100 I=1
0022              NC=1
0023              H=B-A
0024              S1=H*SUM
0025              P(1)=S1
0026              AS1=H*ASUM
0027         2002 X=A-H*0.5D0                                                     D1530018
0028              DO 102 J=1,NC
0029              X=X+H                                                          D1530021
0030              M=M+1
0031              EP=FCN(X)
0032         2010 AEP=DABS(EP)
0033              IF(FMAX.GE.AEP)GO TO 101
0034              FMAX=AEP
0035          101 SUM=SUM+EP
0036          102 ASUM=ASUM+AEP
0037         2003 S2=H*SUM*0.5D0                                                  D1530023
0038         2011 AS2=H*ASUM*0.5D0
0039              K=1                                                            D1530025
0040              GO TO 105                                                      D1530026
0041         2012 EP=DABS(S2-S1)
0042         2013 AX=DABS(S2)
0043              GO TO (110,2004,111,112),NN
0044          110 DEP=AX
0045              GO TO 113
0046         2004 DEP=1.000
0047              GO TO 113
0048          111 DEP=AS2
0049              GO TO 113
0050          112 DEP=FMAX
0051          113 T=EP-EPS*DEP
0052              IF(T)107,107,103                                               D1530029
0053          103 IF(I-MM)2005,108,2005
0054         2005 H=H*0.5D0                                                       D1530031
0055              S1=S2                                                          D1530033
0056              AS1=AS2
0057              P(K)=S2                                                        D1530034
```

```
FORTRAN IV G LEVEL  18                  ROMBRG              DATE = 71109          22/14/21

0058                I=I+1                                                          01530045
0059                NC=2*NC
0060                GO TO 2002                                                     01530037
0061              105 IF(K.GT.I)GO TO 2012
0062                J=2*K
0063                D=2**J                                                         01530040
0064                T=S2                                                           01530041
0065             2006 S2=(D*S2-P(K))/(D-1.0D0)                                     01530042
0066                P(K)=T                                                         01530044
0067                K=K+1                                                          01530045
0068                GO TO 105                                                      01530046
0069             108    PRINT 1,I                                                 01530047
0070             1      FORMAT(' M EXCEEDED I= ',I2)                              01530048
0071             107    ROMBRG=S2                                                 01530049
0072                EPS=EP/DEP
0073                GO TO 120
0074              200 PRINT 2,N
0075                2 FORMAT(' ERROR RETURN N= ',I2)
0076              120 RETURN
0077                END
```

```
FORTRAN IV G LEVEL  18                  FCN                 DATE = 71109          22/14/21

0001                FUNCTION FCN(X)
0002                IMPLICIT REAL*8 (A-H,O-Z)
0003                DOUBLE PRECISION  DEXP
0004                COMMON /HOLD2/ E(150),XSECT(150),FLUL(150)
0005                COMMON /HOLD3/ ENERGY,BO,NLO
0006                FLUXL = FLUL(NLO)+((FLUL(NLO+1)-FLUL(NLO))*(X-E(NLO)))/(E(NLO+1)-E
                   1(NLO))
0007                XS = XSECT(NLO)+((XSECT(NLO+1)-XSECT(NLO))*(X-E(NLO)))/ (E(NLO+1)-
                   1E(NLO))
0008                FCN = DEXP(FLUXL-XS)*DEXP(-(ENERGY-X)**2/BO)
0009                RETURN
0010                END
```

```
FORTRAN IV G LEVEL  18                  PLAT2              DATE = 71109          22/14/21

0001                  SUBROUTINE PLAT2(Z,Y,N)
                C
                C      PLOTTING SUBROUTINE PLAT2
0002                  IMPLICIT REAL*8 (A-H,O-W,Y-Z)
0003                  INTEGER XX
0004                  DIMENSION XX(120),Z(N),Y(N),NN(2)
0005                  DATA NN/1H ,1H*/
0006                  YMAX = -1.E50
0007                  YMIN = 1.E50
0008                  DO 3 I=1,N
0009                  IF(Y(I) - YMAX) 5,5,4
0010                4 YMAX = Y(I)
0011                5 IF (YMIN - Y(I)) 3,3,6
0012                6 YMIN = Y(I)
0013                3 CONTINUE
0014                  RANGE = YMAX - YMIN
0015                  DIV = RANGE/100.
0016                  PRINT 30,DIV
0017               30 FORMAT(1H ,25X,' THE SCALE OF THIS GRAPH IS 1 DIVISION =',D12.5,'U
                     1NITS'//,29X,'12345678901234567890123456789012345678901234567890123
                     2456789012345678901234567890123456789012345678901234567890')
0018                  DO 1 J=1,120
0019                1 XX(J) = NN(1)
0020                  IX = 1
0021                  DO 2 I=1,N
0022                  XX(IX) = NN(1)
0023                  X = 1.0+(99./RANGE)*(Y(I)-YMIN)
0024                  IX = IFIX(X)
0025                  XX(IX) = NN(2)
0026                  IF (I .EQ. 1) GO TO 8
0027                  IF((Z(I)-Z(I-1)) .GT. .15D00) GO TO 7
0028                8 PRINT 20,Z(I),Y(I),(XX(J),J=1,101)
0029               20 FORMAT (1H ,2D12.4,'----',101A1)
0030                  GO TO 2
0031                7 IF(Z(I)-Z(I-1) .GT. .25) GO TO 9
0032                  PRINT 10,Z(I),Y(I),(XX(J),J=1,101)
0033               10 FORMAT (1H0,2D12.4,'----',101A1)
0034                  GO TO 2
0035                9 PRINT 40,Z(I),Y(I),(XX(J),J=1,101)
0036               40 FORMAT (1H-,2D12.4,'----',101A1)
0037                2 CONTINUE
0038                  RETURN
0039                  END
```

```
FORTRAN IV G LEVEL  18                  PLAT3              DATE = 71109          22/14/21

 0C01                 SUBROUTINE PLAT3(Z,Y,W,N)
                C
                C      PLOTTING SUBROUTINE PLAT3
                C
                C      THIS SUBROUTINE PLOTS ON THE ORDINATE TWO VARIABLES (Y & W)
                C      VERSES THE VARIBLE Z ON THE ABSISSA.
                C
 0C02                 IMPLICIT REAL*8 (A-H,O-W,Y-Z)
 0C03                 DOUBLE PRECISION DEXP
 0C04                 INTEGER XX,XX2
 0C05                 DIMENSION XX(120),XX2(120),Z(N),Y(N),W(N),NN(3)
 0C06                 DATA NN/1H ,1H+,1H*/
 0C07                 YMAX = -1.E50
 0C08                 YMIN = 1.E50
 0C09                 DO 3 I=1,N
 0010                 IF(Y(I) - YMAX) 5,5,4
 0C11               4 YMAX = Y(I)
 0012               5 IF (YMIN - Y(I)) 3,3,6
 0013               6 YMIN = Y(I)
 0C14               3 CONTINUE
 0C15                 DO 14 I=1,N
 0C16                 IF(W(I)-YMAX) 12,12,13
 0C17              13 YMAX = W(I)
 0C18              12 IF(YMIN-W(I)) 14,14,15
 0C19              15 YMIN = W(I)
 0C20              14 CONTINUE
 0C21                 RANGE = YMAX - YMIN
 0022                 DIV = RANGE/100.
 0023                 PRINT 30,DIV
 0C24              30 FORMAT(1H ,25X,' THE SCALE OF THIS GRAPH IS 1 DIVISION =',E12.5,'U
                     1NITS'//,31X,'12345678901234567890123456789012345678901234567890123
                     2456789012345678901234567890123456789012345678901234567890')
 0C25                 DO 1 J=1,120
 0C26               1 XX(J) = NN(1)
 0027                 IX = 1
 0C28                 IX2 = 1
 0C29                 DO 2 I=1,N
 0030                 XX(IX) = NN(1)
 0C31                 XX(IX2) = NN(1)
 0C32                 X = 1.D+(99./RANGE)*(Y(I)-YMIN)
 0033                 X2  = 1.D+(99./RANGE)*(W(I)-YMIN)
 0034                 IX = IFIX(X)
 0C35                 IX2 = IFIX(X2)
 0036                 XX(IX) = NN(2)
 0037                 IF (IX .NE. IX2) XX(IX2) = NN(3)
 0C38                 Y(I) = DEXP(Y(I))
 0C39                 W(I) = DEXP(W(I))
 0C40                 IF (I .EQ. 1) GO TO 8
 0041                 IF((Z(I)-Z(I-1)) .GE. .1500) GO TO 9
 0C42               8 PRINT 20,Z(I),Y(I),W(I),(XX(J),J=1,101)
 0043              20 FORMAT (1H ,3E9.2,'---',101A1)
 0044              21 FORMAT (1H+,30X,101A1)
 0C45                 GO TO 2
 0C46               9 PRINT 10,Z(I),Y(I),W(I),(XX(J),J=1,101)
 0047              10 FORMAT (1H0,3E9.2,'---',101A1)
 0C48               2 CONTINUE
 0C49                 RETURN
 0C50                 END
```

Sample Input Data - CALFLUX

```
     15.24      .08497
       1.5
     30.826
      0.75
      11.0
40
      0.01        5.00        0.40        5.00        0.50        4.00        0.63        2.50
      0.80        4.00        0.90        2.80        1.00        2.40        1.10        2.80
      1.20        2.50        1.30        3.40        1.38        2.50        1.44        3.70
      1.50        2.00        1.56        3.80        1.60        3.00        2.00        3.00
      2.10        3.50        2.20        3.20        2.40        3.40        2.55        4.20
      2.65        3.40        3.00        3.30        3.20        3.70        3.30        3.10
      3.50        3.60        3.60        3.50        4.10        3.70        4.20        3.20
      4.30        3.70        4.40        3.40        4.50        3.80        5.00        3.70
      7.00        3.60        8.20        3.30        8.30        3.50        8.70        3.20
      8.80        3.30        12.0        2.80        14.0        2.60        15.0        2.50
65
 1    0.800E 06    0.701E 04
 2    0.900E 06    0.785E 04
 3    0.100E 07    0.802E 04
 4    0.110E 07    0.833E 04
 5    0.120E 07    0.848E 04
 6    0.130E 07    0.838E 04
 7    0.140E 07    0.812E 04
 8    0.150E 07    0.781E 04
 9    0.160E 07    0.743E 04
10    0.170E 07    0.714E 04
11    0.180E 07    0.669E 04
12    0.190E 07    0.618E 04
13    0.200E 07    0.566E 04
14    0.210E 07    0.518E 04
15    0.220E 07    0.476E 04
16    0.230E 07    0.443E 04
17    0.240E 07    0.413E 04
18    0.250E 07    0.387E 04
19    0.260E 07    0.360E 04
20    0.270E 07    0.334E 04
21    0.280E 07    0.307E 04
22    0.290E 07    0.283E 04
23    0.300E 07    0.261E 04
24    0.310E 07    0.239E 04
25    0.320E 07    0.191E 04
26    0.330E 07    0.168E 04
27    0.340E 07    0.156E 04
28    0.400E 07    0.148E 04
29    0.420E 07    0.141E 04
30    0.440E 07    0.130E 04
31    0.460E 07    0.110E 04
```

33	0.480E 07	0.105E 04
34	0.500E 07	0.925E 03
35	0.520E 07	0.835E 03
36	0.540E 07	0.773E 03
37	0.560E 07	0.707E 03
38	0.580E 07	0.641E 03
39	0.600E 07	0.600E 03
40	0.620E 07	0.572E 03
41	0.640E 07	0.528E 03
42	0.660E 07	0.468E 03
43	0.680E 07	0.408E 03
44	0.700E 07	0.352E 03
45	0.720E 07	0.302E 03
46	0.740E 07	0.257E 03
47	0.760E 07	0.219E 03
48	0.780E 07	0.189E 03
49	0.800E 07	0.165E 03
50	0.820E 07	0.149E 03
51	0.840E 07	0.137E 03
52	0.860E 07	0.124E 03
53	0.880E 07	0.110E 03
54	0.900E 07	0.961E 02
55	0.920E 07	0.836E 02
56	0.940E 07	0.726E 02
57	0.960E 07	0.628E 02
58	0.980E 07	0.539E 02
59	0.100E 08	0.453E 02
60	0.102E 08	0.366E 02
61	0.104E 08	0.276E 02
62	0.106E 08	0.192E 02
63	0.108E 08	0.124E 02
64	0.110E 08	0.804E 01
65	0.112E 08	0.585E 01
66	0.114E 08	0.506E 01

65

1	0.800E 06	0.208E 05
2	0.900E 06	0.198E 05
3	0.100E 07	0.205E 05
4	0.110E 07	0.215E 05
5	0.120E 07	0.205E 05
6	0.130E 07	0.180E 05
7	0.140E 07	0.152E 05
8	0.150E 07	0.127E 05
9	0.160E 07	0.107E 05
10	0.170E 07	0.932E 04
11	0.180E 07	0.811E 04
12	0.190E 07	0.691E 04
13	0.200E 07	0.576E 04
14	0.210E 07	0.476E 04

15	0.320E 07	0.307E 04
16	0.330E 07	0.236E 04
17	0.340E 07	0.284E 04
18	0.350E 07	0.241E 04
19	0.360E 07	0.207E 04
20	0.370E 07	0.182E 04
21	0.380E 07	0.163E 04
22	0.390E 07	0.148E 04
23	0.400E 07	0.134E 04
24	0.410E 07	0.111E 04
25	0.420E 07	0.897E 03
26	0.430E 07	0.722E 03
27	0.440E 07	0.587E 03
28	0.450E 07	0.515E 03
29	0.460E 07	0.465E 03
30	0.470E 07	0.428E 03
31	0.480E 07	0.389E 03
32	0.490E 07	0.338E 03
33	0.500E 07	0.285E 03
34	0.510E 07	0.243E 03
35	0.520E 07	0.216E 03
36	0.530E 07	0.203E 03
37	0.540E 07	0.196E 03
38	0.550E 07	0.190E 03
39	0.560E 07	0.178E 03
40	0.570E 07	0.158E 03
41	0.580E 07	0.135E 03
42	0.590E 07	0.120E 03
43	0.600E 07	0.114E 03
44	0.610E 07	0.109E 03
45	0.620E 07	0.100E 03
46	0.630E 07	0.867E 02
47	0.640E 07	0.735E 02
48	0.650E 07	0.645E 02
49	0.660E 07	0.612E 02
50	0.670E 07	0.611E 02
51	0.680E 07	0.606E 02
52	0.690E 07	0.575E 02
53	0.700E 07	0.529E 02
54	0.710E 07	0.452E 02
55	0.720E 07	0.381E 02
56	0.730E 07	0.312E 02
57	0.740E 07	0.251E 02
58	0.750E 08	0.200E 02
59	0.760E 08	0.158E 02
60	0.770E 08	0.123E 02
61	0.780E 08	0.929E 01
62	0.790E 08	0.694E 01
63	0.800E 08	0.532E 01
64	0.810E 08	0.442E 01
65	0.820E 08	0.408E 01

THIS PROGRAM CALCULATES A SMOOTHED TRANSMITTED SPECTRUM FROM TABULATED DATA USING THE RESOLUTION FUNCTION OF THE NE 2.3
USING THE FOLLOWING PARAMETERS:

THE SAMPLE THICKNESS IS T = 91.280 CM, AND THE MOLECULAR DENSITY IS RHO = 0.403D-01 X 10**24 MOLECULES/CC

THE NORMALIZATION FACTOR IS XNORM = 25.694

THE RESOLUTION HAS BEEN TRUNCATED AT 1.500TIMES THE FWHM OF THE GAUSSIAN

THE FWHM HAS BEEN MULTIPLIED BY 0.750

THE INPUT CROSS-SECTION LIBRARY IS AS FOLLOWS:

ENERGY	CROSS-SECTION
0.10000-01	0.90000 01
0.50000 00	0.50000 01
0.70000 00	0.10000 01
0.80000 00	0.22000 01
0.90000 00	0.25000 01
0.10000 01	0.50000 01
0.12000 01	0.48000 01
0.13000 01	0.50000 01
0.15000 01	0.22000 01
0.16000 01	0.20000 01
0.17000 01	0.18000 01
0.18000 01	0.17000 01
0.19000 01	0.13000 01
0.20000 01	0.16000 01
0.22000 01	0.13000 01
0.23000 01	0.65000 00
0.23500 01	0.15000 00
0.24000 01	0.50000 00
0.26000 01	0.12000 01
0.28000 01	0.12000 01
0.30000 01	0.12000 01
0.33000 01	0.32000 01
0.36000 01	0.31000 01
0.38000 01	0.35000 01
0.39000 01	0.23000 01
0.40000 01	0.17000 01
0.41000 01	0.13000 01
0.42000 01	0.20000 01
0.43000 01	0.24000 01
0.45000 01	0.15000 01
0.48000 01	0.11000 01
0.50000 01	0.18000 01
0.52000 01	0.12000 01
0.55000 01	0.11000 01
0.56000 01	0.23000 01
0.58000 01	0.12000 01
0.60000 01	0.12000 01
0.63000 01	0.90000 00
0.64000 01	0.14000 01
0.65000 01	0.65000 00
0.68000 01	0.13000 01
0.69000 01	0.80000 00
0.70000 01	0.90000 00
0.72000 01	0.18000 01
0.76000 01	0.11000 01
0.78000 01	0.15000 01
0.80000 01	0.70000 00
0.82000 01	0.13000 01
0.86000 01	0.11000 01
0.88000 01	0.16000 01
0.90000 01	0.12000 01
0.10000 02	0.13000 01
0.10500 02	0.12000 01

THE SCALE OF THIS GRAPH IS 1 DIVISION = 0.[illegible]E-[illegible]

1234567890123456789012345678901234567890123456789012345678901234567890 12345678...

[0] PAPER SPECTRUM IS AS FOLLOWS:
ENERGY LOG(SPECTRUM)
THE SCALE OF THIS GRAPH IS 1 DIVISION = 0.772930-05CTS.

0.80000 00 0.83450 01----
0.90000 00 0.82690 01----
0.10000 01 0.81850 01----
0.11000 01 0.81030 01----
0.12000 01 0.81970 01----
0.13000 01 0.81970 01----
0.14000 01 0.81780 01----
0.15000 01 0.81490 01----
0.16000 01 0.81060 01----
0.17000 01 0.80520 01----
0.18000 01 0.79930 01----
0.19000 01 0.79180 01----
0.20000 01 0.78240 01----
0.21000 01 0.77320 01----
0.22000 01 0.76500 01----
0.23000 01 0.75760 01----
0.24000 01 0.74900 01----
0.25000 01 0.74090 01----
0.26000 01 0.73260 01----
0.27000 01 0.72580 01----
0.28000 01 0.71930 01----
0.29000 01 0.71390 01----
0.30000 01 0.70650 01----

0.32000 01 0.68810 01----

0.34000 01 0.67230 01----

0.36000 01 0.66370 01----

0.38000 01 0.65830 01----

0.40000 01 0.65350 01----

0.42000 01 0.64720 01----

0.44000 01 0.63870 01----

0.46000 01 0.62770 01----

0.48000 01 0.61630 01----

0.50000 01 0.60660 01----

0.52000 01 0.59760 01----

0.54000 01 0.59660 01----

0.56000 01 0.57460 01----

0.58000 01 0.56380 01----

0.60000 01 0.55650 01----

0.62000 01 0.55170 01----

0.64000 01 0.54640 01----

0.66000 01 0.53840 01----

0.68000 01 0.52730 01----

0.70000 01 0.51120 01----

0.72000 01 0.48980 01----

0.74000 01 0.46910 01----

0.76000 01 0.45140 01----

0.78000 01 0.43690 01----

0.80000 01 0.42360 01----

0.82000 01 0.41160 01----

0.84000 01 0.40220 01----

0.86000 01 0.39180 01----

0.88000 01 0.37590 01----

0.90000 01 0.35410 01----

0.92000 01 0.33250 01----

0.94000 01 0.31650 01----

0.96000 01 0.30390 01----

0.98000 01 0.29340 01----

0.10000 02 0.27470 01----

0.10200 02 0.24850 01----

0.10400 02 0.21190 01----

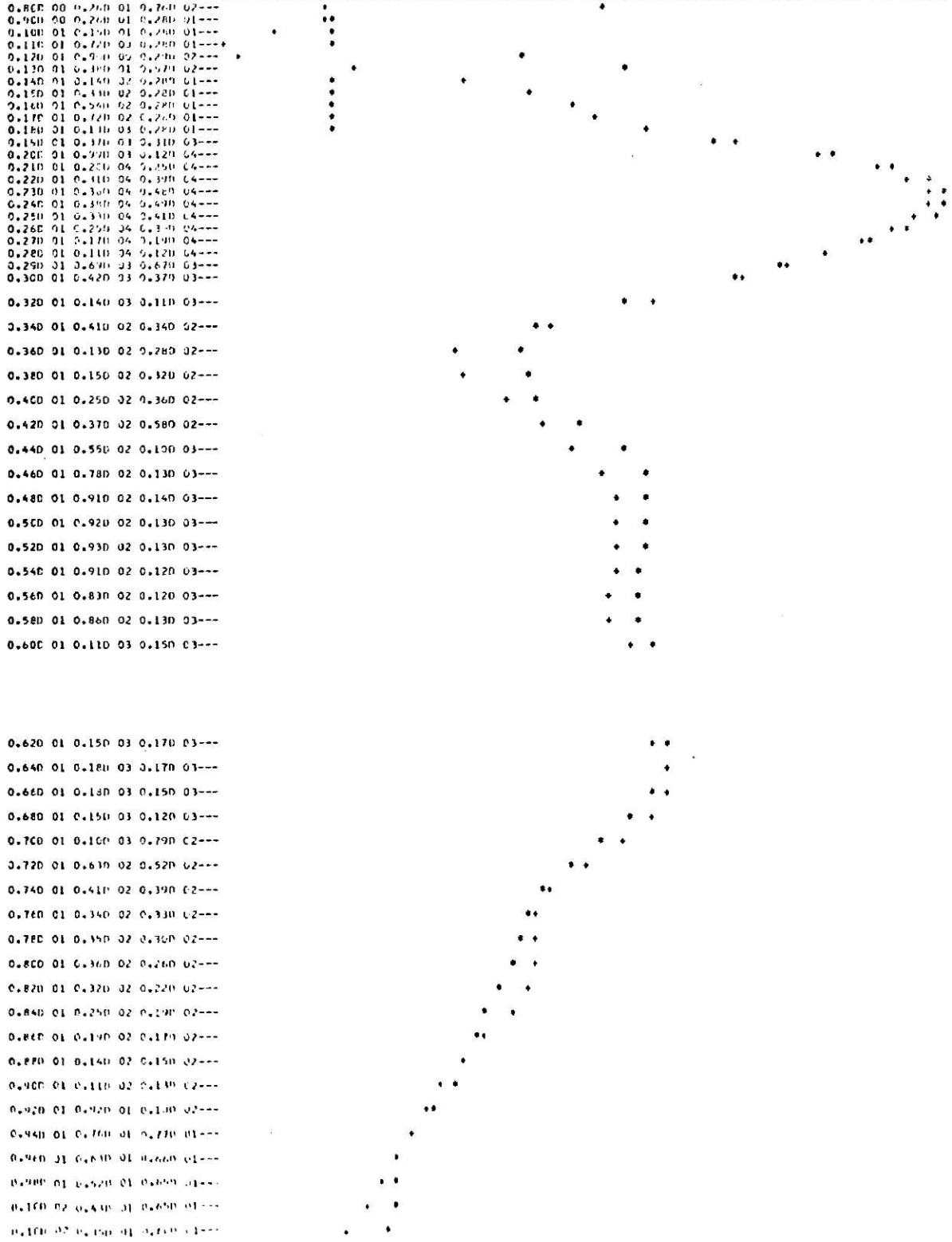
THE CALCULATED, SMOOTHED TRANSMITTED SPECTRA IS:

ENERGY	FLUX TRANSMITTED
0.8	0.259010 01
0.9	0.256180 01
1.0	0.145410 01
1.1	0.716730 00
1.2	0.900500 00
1.3	0.377750 01
1.4	0.139190 02
1.5	0.330040 02
1.6	0.542280 02
1.7	0.723830 02
1.8	0.132630 03
1.9	0.370940 03
2.0	0.993240 03
2.1	0.212110 04
2.2	0.311190 04
2.3	0.378750 04
2.4	0.377720 04
2.5	0.326080 04
2.6	0.249120 04
2.7	0.172700 04
2.8	0.112020 04
2.9	0.693750 03
3.0	0.417690 03
3.2	0.141500 03
3.4	0.435110 02
3.6	0.133300 02
3.8	0.147600 02
4.0	0.251670 02
4.2	0.368990 02
4.4	0.546380 02
4.6	0.779380 02
4.8	0.910850 02
5.0	0.918580 02
5.2	0.933080 02
5.4	0.911210 02
5.6	0.825820 02
5.8	0.861460 02
6.0	0.111530 03
6.2	0.149610 03
6.4	0.178340 03
6.6	0.177990 03
6.8	0.146750 03
7.0	0.102270 03
7.2	0.633860 02
7.4	0.407120 02
7.6	0.337650 02
7.8	0.349330 02
8.0	0.355560 02
8.2	0.318580 02
8.4	0.253850 02
8.6	0.190870 02
8.8	0.144280 02
9.0	0.113170 02
9.2	0.919160 01
9.4	0.758840 01
9.6	0.626570 01
9.8	0.517800 01

PLOT OF LOG(FLUX) VS ENERGY

ENERGY CAL. FLUX EXP. FLUX * = CALCULATED + = EXPERIMENTAL

THE SCALE OF THIS GRAPH IS 1 LEVISTOR = 1.0000E-00 UNITS



0.800 00 0.260 01 0.260 02---
0.900 00 0.260 01 0.280 01---
0.100 01 0.150 01 0.260 01---
0.110 01 0.720 00 0.280 01---
0.120 01 0.900 00 0.280 02---
0.130 01 0.300 01 0.970 02---
0.140 01 0.140 02 0.280 01---
0.150 01 0.430 02 0.280 01---
0.160 01 0.560 02 0.280 01---
0.170 01 0.720 02 0.260 01---
0.180 01 0.110 03 0.280 01---
0.190 01 0.370 01 0.310 03---
0.200 01 0.990 03 0.120 04---
0.210 01 0.250 04 0.850 04---
0.220 01 0.410 04 0.390 04---
0.230 01 0.360 04 0.460 04---
0.240 01 0.390 04 0.690 04---
0.250 01 0.330 04 0.410 04---
0.260 01 0.250 04 0.330 04---
0.270 01 0.170 04 0.190 04---
0.280 01 0.110 04 0.120 04---
0.290 01 0.690 03 0.670 03---
0.300 01 0.420 03 0.370 03---
0.320 01 0.140 03 0.110 03---
0.340 01 0.410 02 0.340 02---
0.360 01 0.130 02 0.280 02---
0.380 01 0.150 02 0.320 02---
0.400 01 0.250 02 0.360 02---
0.420 01 0.370 02 0.580 02---
0.440 01 0.550 02 0.100 03---
0.460 01 0.780 02 0.130 03---
0.480 01 0.910 02 0.140 03---
0.500 01 0.920 02 0.130 03---
0.520 01 0.930 02 0.130 03---
0.540 01 0.910 02 0.120 03---
0.560 01 0.830 02 0.120 03---
0.580 01 0.860 02 0.130 03---
0.600 01 0.110 03 0.150 03---
0.620 01 0.150 03 0.170 03---
0.640 01 0.180 03 0.170 03---
0.660 01 0.180 03 0.150 03---
0.680 01 0.150 03 0.120 03---
0.700 01 0.100 03 0.790 02---
0.720 01 0.630 02 0.520 02---
0.740 01 0.410 02 0.390 02---
0.760 01 0.340 02 0.330 02---
0.780 01 0.350 02 0.360 02---
0.800 01 0.360 02 0.260 02---
0.820 01 0.320 02 0.220 02---
0.840 01 0.250 02 0.190 02---
0.860 01 0.190 02 0.170 02---
0.880 01 0.140 02 0.150 02---
0.900 01 0.110 02 0.130 02---
0.920 01 0.920 01 0.130 02---
0.940 01 0.760 01 0.770 01---
0.960 01 0.630 01 0.660 01---
0.980 01 0.520 01 0.650 01---
0.100 02 0.430 01 0.650 01---
0.102 02 0.350 01 0.630 01---

NE213RES

This program determines the resolution of the NE-213 detection system from the measured and unfolded responses to the monoenergetic neutrons. The code is based upon the expressions derived in Appendix B for gaussian resolution fitting using weighted least squares. Input to the program includes the upper and lower bounds of each point in the unfolded spectrum over which the gaussian is to be fit. Output includes the FWHM and the standard deviation on this value along with the comparison between the actual data and the calculated data based on the gaussian fit. The matrix inversion required in the calculation is done by the subroutine MATINV.

INPUT

Card	Format	
1	I10	1) NDS = Number of data sets to be analyzed
2	F10.0,I10	1) ENEUT = Nominal energy of the monoenergetic neutrons
		2) NDP = Number of data points in this set to be fit to the gaussian
3 (Deck)	8F10.0	1) EN(I) = Energies in the unfolded spectrum (MeV) ⋮
4 (Deck)	8F10.0	1) PLO(I) = Lower bound of each point in the unfolded spectrum ⋮
5 (Deck)	8F10.0	1) PUP(I) = Upper bound of each point in the unfolded spectrum ⋮

NE213RES Listing

```
FORTRAN IV G LEVEL  18                  MAIN                DATE = 71159          22/12/23

            C**** THIS PROGRAM DETERMINES THE RESOLUTION OF A DETECTION SYSTEM FROM
            C**** THE MEASURED AND UNFOLDED RESPONSES TO THE MONOENERGETIC NEUTRONS
 0C01               IMPLICIT REAL*8 (A-H,O-Z)
 0C02               DOUBLE PRECISION DLOG,DEXP
 0C03               DIMENSION Y(25),EN(25),A(3,3),B(3),VAR(25),PLO(25),PUP(25)
                   1,NDUM(3,1)
 0C04              1 FORMAT(8F10.0)
 0005              2 FORMAT(I10)
 0C06              3 FORMAT(F10.0,I10)
 0C07              4 FORMAT(/4X,27HEXPERIMENTAL NEUTRON ENERGY,5X,F5.2,2X,3HMEV)
 0C08              5 FORMAT(/4X,17HUNFOLDED ENERGIES)
 0C09              6 FORMAT(1X,12F10.1)
 0C10              7 FORMAT(5X,17HUNFOLDED SPECTRUM)
 0C11              8 FORMAT(5X,9HVARIANCES)
 0C12              9 FORMAT(/4X,12HPEAK ENERGY=,F5.2,1X,3HMEV,3X,4H+OR-,F5.2,4H MEV)
 0C13             10 FORMAT(/4X,8HPEAK HT=,F10.0,3X,4H+OR-,F10.0)
 0C14             11 FORMAT(/,4X,20HFULL WIDTH HALF MAX=,F6.3,4H MEV,3X,4H+OR-,F6.3,
                   14H MEV/)
 0C15            556 FORMAT(1HO,20HNORMALIZED PEAK HT.=,D15.6,1X,11HN/CM-CM-SEC)
 0C16            557 FORMAT(1HO,3HRO=,D15.6,1X,7HMEV-MEV)
            C**** NDS IS THE NUMBER OF DATA SETS TO BE ANALYZED
 0C17               READ(1,2)NDS
 0018               DO 100 K=1,NDS
            C
            C**** ENEUT IS THE NOMINAL ENERGY OF THE MONOENERGETIC NEUTRONS
            C*** NDP IS THE NUMBER OF DATA POINTS IN THIS SET
            C
 0019               READ(1,3)ENEUT,NDP
 0C20               DO 20 II=1,NDP,8
 0C21            20 READ(1,1)(EN(II-1+I),I=1,8)
            C
            C**** EN(I) ARE THE ENERGIES IN MEV IN THE UNFOLDED SPECTRUM
            C
 0C22               DO 21 II=1,NDP,8
 0023            21 READ(1,1)(PLO(II-1+I),I=1,8)
 0C24               DO 22 II=1,NDP,8
 0C25            22 READ(1,1)(PUP(II-1+I),I=1,8)
 0026               DO 321 I=1,NDP
 0027               PLO(I)=PLO(I)*10000.
 0028           321 PUP(I)=PUP(I)*10000.
            C
            C**** PLO AND PUP ARE THE LOWER AND UPPER BOUNDS OF EACH POINT ON THE
            C     UNFOLDED SPECTRUM
            C
 0029               DO 200 I=1,NDP
 0030               Y(I)=(PLO(I)+PUP(I))/2.
 0C31           200 VAR(I)=((PUP(I)-PLO(I))/2.)**2
 0C32               DO101 I=1,3
 0033               B(I)=0.
 0C34               DO 101 J=1,3
 0C35           101 A(I,J)=0.
 0036               DO 102 I=1,NDP
 0C37               RATIO=Y(I)*Y(I)/VAR(I)
 0C38               A(1,3)=A(1,3)+RATIO
 0039               A(2,3)=A(2,3)+RATIO*EN(I)
 0040               A(2,2)=A(2,2)+RATIO*EN(I)*EN(I)
 0C41               A(2,1)=A(2,1)+RATIO*(EN(I)**3)
 0C42               A(1,1)=A(1,1)+RATIO*(EN(I)**4)
```

```
FORTRAN IV G LEVEL  18                  MAIN                    DATE = 71109          22/12/23

0043                  B(1) = B(1)+RATIO*DLOG(Y(I))*EN(I)*EN(I)
0044                  B(2) = B(2)+RATIO*DLOG(Y(I))*EN(I)
0045              102 B(3) = B(3)+RATIO*DLOG(Y(I))
0046                  A(3,2)=A(2,3)
0047                  A(3,1)=A(2,2)
0048                  A(1,3)=A(2,2)
0049                  A(1,2)=A(2,1)
0050                  DO 176 I=1,3
0051              176 BDUM(I,1)=B(I)
0052                  N1 = 1
0053                  N3 = 3
0054                  CALL MATINV(A,N3,BDUM,N1,DETERM,N3)
0055                  DO 177 I=1,3
0056              177 B(I)=BDUM(I,1)
0057                  BO=-1./B(1)
0058                  EO=BO*B(2)/2.
0059                  YO = DEXP(B(3)+EO*EO/BO)
0060                  DUM = DLOG(.2001)
0061                  FWHM = 2.*(BO*DUM)**.5
0062                  VARBO=A(1,1)/(B(1)*B(1))
0063                  SDVBO = VARBO**.5
0064                  VAREO=(B(2)*B(2)*VARBO+BO*BO*A(2,2))/4.
0065                  SDVEO = VAREO**.5
0066                  VARYO=YO*YO*(A(3,3)+4.*EO*EO*VAREO/(BO*BO)+(VARBO*(EO**4))/
                     1(BO**4))
0067                  SDVYO = VARYO**.5
0068                  VARFW=VARBO*DUM/BO
0069                  SDVFW = VARFW**.5
0070                  PI=3.1415927
0071                  YNORM = 1./(BO*PI)**.5
0072                  WRITE(3,4)ENEUT
0073                  WRITE(3,5)
0074                  WRITE(3,6)(EN(I),I=1,NDP)
0075                  WRITE(3,7)
0076                  WRITE(3,6)(Y(I),I=1,NDP)
0077                  WRITE(3,8)
0078                  WRITE(3,6)(VAR(I),I=1,NDP)
0079                  WRITE(3,9)EO,SDVEO
0080                  WRITE(3,10)YO,SDVYO
0081                  WRITE(3,556)YNORM
0082                  WRITE(3,557)BO
0083              100 WRITE(3,11)FWHM,SDVFW
0084                  STOP
0085                  END
```

```
FORTRAN IV G LEVEL  18                  MATINV              DATE = 71109          22/12/23

0001                  SUBROUTINE MATINV (A,N,B,M,DETERM,NMAX)
                C
                C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
                C        A  INPUT-COEFFICIENT MATRIX
                C           RETURN-INVERSE MATRIX
                C        N  NUMBER OF EQUATIONS
                C        B  INPUT-RIGHT HAND SIDE VECTOR(S)
                C           RETURN-SOLUTION VECTOR(S)
                C        M  NUMBER OF RIGHT HAND SIDE VECTOR(S)
                C        DETERM  RETURN-DETERMINATE OF A
                C        NMAX  MAXIMUM NUMBER OF EQUATIONS AS DIMENSIONED IN MAIN PROGRAM
                C
                C**** REMOVE NEXT STATEMENT IN SINGLE PRECISION VERSION
0002                  IMPLICIT REAL*8 (A-H,O-Z)
0003                  REAL*4 PIVOT
0004                  DOUBLE PRECISION DABS
0005                  DIMENSION A(NMAX,NMAX),B(NMAX,1)
0006                  COMMON /F402/ PIVOT(100), INDEX(100)
                C
                C     INITIALIZE DETERMINANT AND PIVOT ELEMENT ARRAY
                C
0007                  DETERM=1.0
0008                  DO 20 I=1,N
0009                  PIVOT(I)=0.0
0010               20 CONTINUE
                C
                C     PERFORM SUCCESSIVE PIVOT OPERATIONS (GRAND LOOP)
                C
0011                  DO 550 I=1,N
                C
                C     SEARCH FOR PIVOT ELEMENT AND EXTEND DETERMINANT PARTIAL PRODUCT
                C
0012                  AMAX=0.0
0013                  DO 105 J=1,N
0014                  IF (PIVOT(J).NE.0.0) GO TO 105
0015                  DO 100 K=1,N
0016                  IF (PIVOT(K).NE.0.0) GO TO 100
0017                  TEMP=DABS(A(J,K))
0018                  IF (TEMP.LT.AMAX) GO TO 100
0019                  IROW=J
0020                  ICOLUM=K
0021                  AMAX=TEMP
0022               100 CONTINUE
0023               105 CONTINUE
0024                  INDEX(I)=4096*IROW+ICOLUM
0025                  J=IROW
0026                  AMAX=A(J,ICOLUM)
0027                  DETERM=AMAX*DETERM
                C
                C     RETURN IF MATRIX IS SINGULAR (ZERO PIVOT) AFTER COLUMN INTERCHANGE
                C
0028                  IF (DETERM.EQ.0.0) GO TO 600
                C
0029                  PIVOT(ICOLUM)=AMAX
                C
                C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
                C
0030                  IF (IROW.EQ.ICOLUM) GO TO 260
```

```
FORTRAN IV G LEVEL  18                  MATINV              DATE = 71109          22/12/23

0031                  DETERM=-DETERM
0032                  DO 200 K=1,N
0033                  SWAP=A(J,K)
0034                  A(J,K)=A(ICOLUM,K)
0035                  A(ICOLUM,K)=SWAP
0036            200 CONTINUE
0037                  IF (M.LE.0) GO TO 260
0038                  DO 250 K=1,M
0039                  SWAP=B(J,K)
0040                  B(J,K)=B(ICOLUM,K)
0041                  B(ICOLUM,K)=SWAP
0042            250 CONTINUE
                C
                C     DIVIDE PIVOT ROW BY PIVOT ELEMENT
                C
0043            260 K=ICOLUM
0044                  A(ICOLUM,K)=1.0
0045                  DO 350 K=1,N
0046                  A(ICOLUM,K)=A(ICOLUM,K)/AMAX
0047            350 CONTINUE
0048                  IF (M.LE.0) GO TO 380
0049                  DO 370 K=1,M
0050                  B(ICOLUM,K)=B(ICOLUM,K)/AMAX
0051            370 CONTINUE
                C
                C     REDUCE NON-PIVOT ROWS
                C
0052            380 DO 550 J=1,N
0053                  IF (J.EQ.ICOLUM) GO TO 550
0054                  T=A( J,ICOLUM)
0055                  A( J,ICOLUM)=0.0
0056                  DO 450 K=1,N
0057                  A( J,K)=A( J,K)-A(ICOLLM,K)*T
0058            450 CONTINUE
0059                  IF (M.LE.0) GO TO 550
0060                  DO 500 K=1,M
0061                  B( J,K)=B( J,K)-B(ICOLLM,K)*T
0062            500 CONTINUE
0063            550 CONTINUE
                C
                C     INTERCHANGE COLUMNS AFTER ALL PIVOT OPERATIONS HAVE BEEN PERFORMED
                C
0064            600 DO 710 I=1,N
0065                  II=N+1-I
0066                  K=INDEX(II)/4096
0067                  ICOLUM=INDEX(II)-4096*K
0068                  IF (K.EQ.ICOLUM) GO TO 710
0069                  DO 705 J=1,N
0070                  SWAP=A(J,K)
0071                  A(J,K)=A(J,ICOLUM)
0072                  A(J,ICOLUM)=SWAP
0073            705 CONTINUE
0074            710 CONTINUE
                C
0075                  RETURN
0076                  END
```

Sample Input Data - NE213RES

```
 1
.90      0
 0.7    0.8      0.9      1.0      1.1      1.2      1.3      1.4
1.5
016    8915    13464    10949     5530     2057      578      134
 22
208    6290    13743    11191     5682     2096      607      140
 35
```

POLYFIT

This program fits a given resolution function to a polynomial of degree m by a weighted least squares procedure. The program was written to perform the calculations derived in Appendix B on polynomial fitting. Input to the program includes the upper and lower bounds on the resolution data to be fitted. Output includes the variance of the mth order polynomial fit, the coefficients of the fit, and a comparison between the input values and the values calculated by the polynomial. Again, the matrix inversion required by the calculation is done by the subroutine MATINV.

INPUT

Card	Format		
1	I3	1) N	= number of data points to be fit
2 (Deck)	3F10.4	1) E(I)	= Energy of the ith data point (MeV)
		2) SPCT(I)	= The FWHM at energy i (MeV)
		3) SDEV(I)	= The standard deviation of the FWHM at energy i
3	I10	1) NA	= Number of fits to be attempted
4	I10	1) M	= Order of the approximation for the first fit
5	I10	1) M	= Order of the approximation for the second fit
.	.	.	
.	.	.	
.	.	.	
.	.	1) M	= Order of the approximation for the NA fit

POLYFIT Listing

```
FORTRAN IV G LEVEL  18                  MAIN                DATE = 71109          22/07/41

            C**** THIS PROGRAM FITS A GIVEN RESOLUTION FUNCTION TO A POLYNOMIAL OF
            C**** DEGREE M BY A WEIGHTED LEAST SQUARES PROCEDURE.
 0001               IMPLICIT REAL*8 (A-H,O-Z)
 0002               DIMENSION E(100),PLO(100),PUP(100),SPCT(100),VAR(100),SDEV(100),
                   1CSPCT(100),A(15,15),B(15,1),C(15),SDEVC(15)
 0003                1 FORMAT(I5)
 0004                2 FORMAT(I3)
 0005                3 FORMAT (3F10.4)
 0006                4 FORMAT(72HORDER OF APPROXIMATION TOO LARGE FOR THE NUMBER OF DATA
                    1POINTS AVAILABLE)
 0007                5 FORMAT(6X,23HORDER OF APPROXIMATION=,I3)
 0008                6 FORMAT(11X,6HENERGY,6X,14HINPUT FWHM     ,4X,7HSTD DEV,6X,
                    114HCALC. FWHM     /)
 0009                7 FORMAT(6X,4D17.6)
 0010                8 FORMAT(//6X,28HRESULTS OF LEAST SQUARES FIT//)
 0011                9 FORMAT(6X,11HCOEFFICIENT,15X,5HVALUE,9X,7HSTD DEV/)
 0012               10 FORMAT(11X,1HC,I2,12X,2D17.9//)
 0013               14 FORMAT(//6X,20HVARIANCE OF THE FIT=,D15.6//)
 0014               15 FORMAT(4F10.4)
                    C
                    C**** N=NUMBER OF DATA POINTS
                    C**** NA=NUMBER OF APPROXIMATIONS USED
                    C**** M=ORDER OF APPROXIMATION
                    C**** PLO,PUP=LOWER AND UPPER BOUNDS OF THE SPECTRUM
                    C**** E=ENERGY
                    C
 0015                    READ 2,N
 0016                    DO 100 I=1,N
 0017                    READ 3,E(I),SPCT(I),SDEV(I)
 0018                100 VAR(I)=(SDEV(I))**2.
 0019                    READ 1,NA
 0020                    DO 101 K=1,NA
 0021                    READ 1,M
 0022                    IF(N.LT.(M+1))GO TO 102
 0023                    M1=M+1
 0024                    DO 103 I=1,M1
 0025                    B(I,1)=0.
 0026                    DO 103 J=1,M1
 0027                103 A(I,J)=0.
 0028                    DO 104 J=1,M1
 0029                    I=1
 0030                    NP=I-1+J-1
 0031                    DO 104 L=1,N
 0032                104 A(I,J)=A(I,J)+(E(L)**NP)/VAR(L)
 0033                    DO 105 I=2,M1
 0034                    J=M+1
 0035                    NP=I-1+J-1
 0036                    DO 105 L=1,N
 0037                105 A(I,J)=A(I,J)+(E(L)**NP)/VAR(L)
 0038                    DO 106 I=1,M1
 0039                    DO 106 L=1,N
 0040                106 B(I,1)=B(I,1)+SPCT(L)*((E(L))**(I-1))/VAR(L)
 0041                    DO 107 I=2,M1
 0042                    DO107 J=2,M1
 0043                107 A(I,J-1)=A(I-1,J)
 0044                    CALL MATINV(A,M1  ,B,1,DETERM,15)
 0045                    DO 108 I=1,M1
 0046                    C(I)=B(I,1)
```

```
FORTRAN IV G LEVEL  18                  MAIN                    DATE = 71109          22/07/41

0047          108 SDEVC(I)=DSQRT(A(I,I))
0048              DO 109 J=1,N
0049          109 CSPCT(J)=0.
0050              DO 110 J=1,N
0051              DO 110 I=1,M1
0052          110 CSPCT(J)=CSPCT(J)+C(I)*(E(J)**(I-1))
0053              DEV=0.
0054              DO 111 I=1,N
0055          111 DEV=DEV+((CSPCT(I)-SPCT(I))**2)/(DFLOAT(N-M-1))
0056              PRINT 5,M
0057              PRINT 8
0058              PRINT 9
0059              DO 113 I=1,M1
0060          113 PRINT 10,I,C(I),SDEVC(I)
0061              PRINT 6
0062              DO 112 I=1,N
0063          112 PRINT 7,E(I),SPCT(I),SDEV(I),CSPCT(I)
0064              PRINT 14,DEV
0065              GO TO 101
0066          102 PRINT 4
0067          101 CONTINUE
0068              STOP
0069              END
```

```
FORTRAN IV G LEVEL  18                  MATINV              DATE = 71109          22/07/41

0001                  SUBROUTINE MATINV (A,N,B,M,DETERM,NMAX)
                C
                C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
                C        A  INPUT-COEFFICIENT MATRIX
                C           RETURN-INVERSE MATRIX
                C        N  NUMBER OF EQUATIONS
                C        B  INPUT-RIGHT HAND SIDE VECTOR(S)
                C           RETURN-SOLUTION VECTOR(S)
                C        M  NUMBER OF RIGHT HAND SIDE VECTOR(S)
                C        DETERM  RETURN-DETERMINATE OF A
                C        NMAX  MAXIMUM NUMBER OF EQUATIONS AS DIMENSIONED IN MAIN PROGRAM
                C
                C**** REMOVE NEXT STATEMENT IN SINGLE PRECISION VERSION
0002                  IMPLICIT REAL*8 (A-H,O-Z)
0003                  REAL*4 PIVOT
0004                  DIMENSION A(NMAX,NMAX),B(NMAX,1)
0005                  COMMON /F402/ PIVOT(100), INDEX(100)
                C
                C     INITIALIZE DETERMINANT AND PIVOT ELEMENT ARRAY
                C
0006                  DETERM=1.0
0007                  DO 20 I=1,N
0008                  PIVOT(I)=0.0
0009               20 CONTINUE
                C
                C     PERFORM SUCCESSIVE PIVOT OPERATIONS (GRAND LOOP)
                C
0010                  DO 550 I=1,N
                C
                C     SEARCH FOR PIVOT ELEMENT AND EXTEND DETERMINANT PARTIAL PRODUCT
                C
0011                  AMAX=0.0
0012                  DO 105 J=1,N
0013                  IF (PIVOT(J).NE.0.0) GO TO 105
0014                  DO 100 K=1,N
0015                  IF (PIVOT(K).NE.0.0) GO TO 100
0016                  TEMP=DABS(A(J,K))
0017                  IF (TEMP.LT.AMAX) GO TO 100
0018                  IROW=J
0019                  ICOLUM=K
0020                  AMAX=TEMP
0021               100 CONTINUE
0022               105 CONTINUE
0023                  INDEX(I)=4096*IROW+ICOLUM
0024                  J=IROW
0025                  AMAX=A(J,ICOLUM)
0026                  DETERM=AMAX*DETERM
                C
                C     RETURN IF MATRIX IS SINGULAR (ZERO PIVOT) AFTER COLUMN INTERCHANGE
                C
0027                  IF (DETERM.EQ.0.0) GO TO 560
                C
0028                  PIVOT(ICOLUM)=AMAX
                C
                C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
                C
0029                  IF (IROW.EQ.ICOLUM) GO TO 260
0030                  DETERM=-DETERM
```

```
FORTRAN IV G LEVEL  18                  MATINV              DATE = 71109          22/07/41

0031                  DO 200 K=1,N
0032                  SWAP=A(J,K)
0033                  A(J,K)=A(ICOLUM,K)
0034                  A(ICOLUM,K)=SWAP
0035              200 CONTINUE
0036                  IF (M.LE.0) GO TO 260
0037                  DO 250 K=1,M
0038                  SWAP=B(J,K)
0039                  B(J,K)=B(ICOLUM,K)
0040                  B(ICOLUM,K)=SWAP
0041              250 CONTINUE
                  C
                  C     DIVIDE PIVOT ROW BY PIVOT ELEMENT
                  C
0042              260 K=ICOLUM
0043                  A(ICOLUM,K)=1.0
0044                  DO 350 K=1,N
0045                  A(ICOLUM,K)=A(ICOLUM,K)/AMAX
0046              350 CONTINUE
0047                  IF (M.LE.0) GO TO 380
0048                  DO 370 K=1,M
0049                  B(ICOLUM,K)=B(ICOLUM,K)/AMAX
0050              370 CONTINUE
                  C
                  C     REDUCE NON-PIVOT ROWS
                  C
0051              380 DO 550 J=1,N
0052                  IF (J.EQ.ICOLUM) GO TO 550
0053                  T=A( J,ICOLUM)
0054                  A( J,ICOLUM)=0.0
0055                  DO 450 K=1,N
0056                  A( J,K)=A( J,K)-A(ICOLUM,K)*T
0057              450 CONTINUE
0058                  IF (M.LE.0) GO TO 550
0059                  DO 500 K=1,M
0060                  B( J,K)=B( J,K)-B(ICOLUM,K)*T
0061              500 CONTINUE
0062              550 CONTINUE
                  C
                  C     INTERCHANGE COLUMNS AFTER ALL PIVOT OPERATIONS HAVE BEEN PERFORMED
                  C
0063              600 DO 710 I=1,N
0064                  I1=N+1-I
0065                  K=INDEX(I1)/4096
0066                  ICOLUM=INDEX(I1)-4096*K
0067                  IF (K.EQ.ICOLUM) GO TO 710
0068                  DO 705 J=1,N
0069                  SWAP=A(J,K)
0070                  A(J,K)=A(J,ICOLUM)
0071                  A(J,ICOLUM)=SWAP
0072              705 CONTINUE
0073              710 CONTINUE
                  C
0074                  RETURN
0075                  END
```

Sample Input Data - POLYFIT

```
21
     1.0       0.463        .025
     1.3       0.437        .019
     1.5       0.529        .013
     1.6       0.480        .022
     1.7       0.487        .023
     1.8       0.541        .018
     2.0       0.527        .022
     2.1       0.577        .015
     2.4       0.560        .017
     2.7       0.521        .029
     3.0       0.673        .009
     3.3       0.622        .021
     3.6       0.648        .009
     3.9       0.678        .010
     4.2       1.010        .014
     4.6       0.896        .010
     4.9       0.886        .007
     6.0       1.110        .014
     7.0       1.329        .006
     8.0       1.316        .008
     9.0       1.000        .009
       5
       6
       7
       8
       9
      10
```

APPENDIX B

DERIVATIONS

TRANSMITTED FLUX INTEGRAL

GAUSSIAN RESOLUTION FITTING

POLYNOMIAL FITTING

APPENDIX B

DERIVATIONS

TRANSMITTED FLUX INTEGRAL

$$\phi_{trans}(E) = \int_0^\infty \phi_I(E')e^{-\Sigma(E')t}\, R(E,E')\, dE' \tag{1}$$

$$\text{where } R(E,E') = y_o(E)\, \exp\left[\frac{-(E' - E)^2}{b_o(E)}\right] \tag{2}$$

$$\therefore \phi_{trans}(E) = \int_0^\infty \phi_I(E')\, \exp(-\Sigma(E')t)\, y_o(E)\, \exp\left[\frac{(E' - E)^2}{b_o(E)}\right] dE' \tag{3}$$

Assume $\text{Log}[\phi_I(E')]$ is linear between discrete energy points; between E_i and E_{i+1}:

$$\phi_I(E') = \phi_I^i + \exp\left[\left(\frac{\ln\phi_I^{i+1} - \ln\phi_I^i}{E_{i+1} - E_i}\right)(E' - E_i)\right]$$

where ϕ_I^i = incident flux at E_i

$$\text{now let } P_i = \left(\frac{\ln\phi_I^{i+1} - \ln\phi_I^i}{E_{i+1} - E_i}\right)$$

$$\therefore \phi_I(E') = \phi_I^i + \exp[(P_i)(E' - E_i)]$$

$$= \phi_I^i + \exp(P_iE')\, \exp(-P_iE_i) \tag{4}$$

Assume $\Sigma(E')$ is linear between discrete energy points; between E_i and E_{i+1}:

$$\Sigma(E')t = \Sigma_i\, t + \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i}\right)(E' - E_i)t$$

where Σ_i = cross-section at E_i

$$\text{now let } X_i = \left(\frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i}\right)t$$

$$\text{and } S_i = \Sigma_i t$$

$$\therefore \Sigma(E')t = S_i - X_i(E' - E_i)$$

$$\therefore \exp[-\Sigma(E')t] = \exp(-S_i + X_iE_i)\exp(-X_iE') \tag{5}$$

$$\text{Also, } \exp\left[\frac{-(E' - E)^2}{b_o}\right] = \exp\left[-\frac{E^2}{b_o}\right]\exp\left[-\frac{E'^2}{b_o} + \frac{2E'E}{b_o}\right] \tag{6}$$

$$y_o = \frac{1}{\sqrt{b_o\pi}} = \text{normalization factor for gaussian} \tag{7}$$

Now, if there exists a ϕ_I^i and Σ_i for each E_i, the integral of equation (3) can be integrated piecewise:

$$\phi_{trans}(E) = \int_0^{E_1}[\ ]\,dE' + \int_{E_1}^{E_2}[\ ]\,dE' + \ldots + \int_{E_i}^{E_{i+1}}[\ ]\,dE'$$

$$+\ldots+\int_{E_n}^{\infty}[\ ]\,dE' \tag{8}$$

$$\text{or } \phi_{trans}(E) = \sum_{i=0}^{\infty}\int_{E_i}^{E_{i+1}}[\ ]\,dE' \tag{9}$$

$$\text{where } [\ ] = \phi_I(E')\exp[-\Sigma(E')t]\,y_o(E)\exp\left[-\frac{(E' - E)^2}{b_o(E)}\right] \tag{10}$$

Now, substituting equation (4), (5), (6), and (7) into (10), each term of equation (9) will be:

$$\int_{E_i}^{E_{i+1}}\{\phi_I^i + \exp(P_iE')\exp(-P_iE_i)\}\{\exp(-S_i + X_iE_i)\exp(-X_iE')\}\left\{\frac{1}{b_o\pi}\right\}$$

$$\left\{\exp\left(-\frac{E^2}{b_o}\right)\exp\left(-\frac{E'^2}{b_o} + \frac{2E'E}{b_o}\right)\right\}dE'$$

$$= \frac{1}{\sqrt{b_o\pi}}\exp\left(-S_i + X_iE_i - \frac{E^2}{b_o}\right)\int_{E_i}^{E_{i+1}}\{\phi_I^i + \exp(P_iE')\exp(-P_iE_i)\}$$

$$\left\{\exp\left(-\frac{E'^2}{b_o} + \frac{2E'E}{b_o} - X_iE'\right)\right\}dE' \tag{11}$$

$$\text{let } C_i = \frac{1}{\sqrt{b_o \pi}} \exp(-S_i + X_i E_i - \frac{E^2}{b_o}) \tag{12}$$

$$= C_i \phi_I^i \int_{E_i}^{E_{i+1}} \exp(-\frac{E'^2}{b_o} + \frac{2E'E}{b_o} - X_i E')\, dE'$$

$$+ C_i \exp(-P_i E_i) \int_{E_i}^{E_{i+1}} \exp(-\frac{E'^2}{b_o} + \frac{2EE'}{b_o} - X_i E' + P_i E')\, dE' \tag{13}$$

These two integrals are of the form:

$$\int_{x_1}^{x_2} e^{-(ax^2 + 2bx + c)}\, dx = \frac{1}{\sqrt{a}} (\frac{b^2 - ac}{a}) \int_{y_1}^{y_2} e^{-y^2}\, dy \tag{14}$$

$$\text{where } y = \sqrt{a}(x + \frac{b}{a})$$

$$\text{Note } \int_{y_1}^{y_2} e^{-y^2}\, dy = \frac{\sqrt{\pi}}{2} [\text{erf}(y_2) - \text{erf}(y_1)]$$

For first integral $a = \frac{1}{b_o}$, $b = \left(\frac{X_i}{2} - \frac{E}{b_o}\right)$, $c = 0$, $y_i = \frac{1}{\sqrt{b_o}}\left(E_i - E + \frac{X_1 b_o}{2}\right)$

Now, substituting these constants into (14), and combining (13) and (14)

$$\therefore \text{ first integral} = \frac{\phi_I^i}{2} \exp\left(\frac{X_i^2 b_o}{4} + X_i(E_i - E) - S_i\right)[\text{erf}(y_{i+1}) - \text{erf}(y_i)] \tag{15}$$

For second integral

$$a = \frac{1}{b_o} \text{ , } b = \frac{X_i}{2} - \frac{E}{b_o} - \frac{P_i}{2} \text{ , } c=0, \; z_i = \frac{1}{\sqrt{b_o}}\left(E_i - E + \frac{X_i b_o}{2} - \frac{P_i b_o}{2}\right)$$

Substituting these constants into (14) and combining (13) and (14)

second integral =

$$\frac{1}{2} \exp\left(\frac{X_i^2}{4} b_o + X_i(E_i - E) + P_i(E - E_i) - \frac{X_i P_i b_o}{2} - \frac{P_i^2}{4} b_o - S_i\right)$$

Adding (15) and (16), equation (11) is now equal to:

$$\left[\frac{1}{2}\exp\left(\frac{X_i^2}{4}b_o + X_i(E_i - E) - S_i\right)\right]\left[\phi_I^i(\mathrm{erf}(y_{i+1}) - \mathrm{erf}(y_i))\right.$$

$$\left. + \exp\left[P_i(E - E_i) - \frac{X_i P_i b_o}{2} - \frac{P_i^2}{4}b_o\right](\mathrm{erf}(Z_{i+1}) - \mathrm{erf}(Z_i))\right] \qquad (17)$$

$$\therefore \phi_{trans}(E) =$$

$$\sum_{i=1}^{\infty}\left\{\left[\frac{1}{2}\exp\left(\frac{X_i^2}{4}b_o + X_i(E_i - E) - S_i\right)\right]\left[\phi_I^i(\mathrm{erf}(y_{i+1}) - \mathrm{erf}(y_i))\right.\right.$$

$$\left.\left. + \exp\left(P_i(E - E_i) - \frac{X_i P_i b_o}{2} - \frac{P_i^2}{4}b_o\right)(\mathrm{erf}(Z_{i+1}) - \mathrm{erf}(Z_i))\right]\right\} \qquad (18)$$

where ϕ_I^i = incident flux at E_i

Σ_i = cross-section at E_i

$S_i = \Sigma_i t$

$X_i = (\Sigma_{i+1} - \Sigma_i)/(E_{i+1} - E_i)$

$P_i = (\ln\phi_I^{i+1} - \ln\phi_I^i)/(E_{i+1} - E_i)$

$y_i = \frac{1}{\sqrt{b_o}}(E_i - E + \frac{X_i b_o}{2})$

$Z_i = \frac{1}{\sqrt{b_o}}(E_i - E + \frac{X_i b_o}{2} - \frac{P_i b_o}{2})$

b_o = function of the resolution = $\frac{(FWHM)^2}{4 \cdot \ln 2}$

GAUSSIAN RESOLUTION FITTING

Using Weighted Least Squares

Gaussian:

$$y_i = y_o \, e^{\frac{-(x_i - x_o)^2}{b_o}} \tag{1}$$

Definition: FWHM

$$\tfrac{1}{2} y_o = y_o \exp\left[\frac{-(x - x_o)}{b_o}\right]^2$$

$$\ln y_o = \ln 2 = \ln y_o - \frac{(x - x_o)^2}{b_o}$$

$$\ln 2 = \frac{(x - x_o)^2}{b_o}$$

$$(x - x_o)^2 = b_o \cdot \ln 2$$

$$x - x_o = (b_o \ln 2)^{\frac{1}{2}}$$

Now,
$$FWHM = 2(x - x_o) = 2(b_o \ln 2)^{\frac{1}{2}} \tag{2}$$

also,
$$b_o = \frac{(FWHM)^2}{4 \ln 2} \tag{3}$$

Determine y_o so total area under Gaussian is equal to 1

$$1 = \int_0^\infty y_o \exp\left[\frac{-(x_i - x_o)^2}{b_o}\right] dx_i \simeq y_o \int_{-\infty}^{\infty} \exp\left[\frac{-(x_i - x_o)^2}{b_o}\right] dx_i \tag{4}$$

since the gaussian curves are on the positive real axis, and at some distance from the origin.

$$\text{Let } z = x_i - x_o \,, \; dx_i = dz$$

$$\therefore \simeq y_o \int_{-\infty}^{\infty} e^{-z^2/b_o} \, dz = y_o \left\{2 \int_0^\infty e^{-z^2/b_o} \, dz\right\} \tag{5}$$

$$\int_0^\infty e^{-z^2/b_o}\,dz = \sqrt{b_o}\int_0^\infty e^{-z^2}\,dz = \sqrt{b_o}\;\frac{\pi}{2}\,[\mathrm{erf}(z)]_0^\infty$$

$$\therefore \int_0^\infty e^{-z^2/b_o}\,dz = \frac{\sqrt{b_o\pi}}{2}\,(1-0) = \frac{\sqrt{b_o\pi}}{2} \tag{6}$$

$$\therefore 1 \simeq 2y_o\,\frac{\sqrt{b_o\pi}}{2}$$

or
$$y_o = \frac{1}{\sqrt{b_o\pi}} \quad \text{Normalized} \tag{7}$$

Using Weighted Least Squares

Taking the ln( ) of equation 1.

$$\ln y_i = \ln y_o - \frac{(x_i - x_o)^2}{b_o} \tag{8}$$

let $z_i = \ln y_i$

$$\therefore \sigma_{z_i}^2 = \left(\frac{\delta_{z_i}}{\delta_{y_i}}\right)^2 \sigma_{y_i}^2 = \left(\frac{1}{y_i}\right)^2 \sigma_{y_i}^2 = \frac{\delta_{y_i}^2}{y_i^2}$$

Thus, weight the function z_i by $\frac{1}{\sigma_{z_i}^2} = \frac{y_i^2}{\sigma_{y_i}^2}$

$$\therefore W = \begin{pmatrix} \frac{y_1^2}{\sigma_{y_1}^2} & 0 & 0 & \cdot \\ 0 & \frac{y_2^2}{\sigma_{y_2}^2} & \cdot & \cdot \\ 0 & 0 & \cdot & \frac{y_n^2}{\sigma_{y_n}^2} \end{pmatrix} \tag{9}$$

Now, using equation 8

$$\ln y_i = \ln y_o - \frac{x_i^2}{b_o} + \frac{2x_i x_o}{b_o} - \frac{x_o^2}{b_o} \tag{10}$$

Let
$$\ln y_o - \frac{x_o^2}{b_o} = S_3 \tag{11}$$

$$\frac{2X_o}{b_o} = S_2 \tag{12}$$

$$-\frac{1}{b_o} = S_1 \tag{13}$$

Thus

$$\begin{pmatrix} X_1^2 & X_1 \cdot 1 \\ X_2^2 & X_2 \cdot 1 \\ \vdots & \vdots \\ X_n^2 & X_n \cdot 1 \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \\ \\ S_3 \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix} \tag{14}$$

This is of the form: $A \cdot X = B$

For least square solution: $A^T A \cdot X = A^T B$

Now, applying weighting function:

$$W A^T A \cdot X = W A^T B \tag{15}$$

Since W is a diagonal matrix, equation 15 can be written as:

$$A^T W A X = A^T W B$$

or
$$X = (A^T W A)^{-1} A^T W B \tag{16}$$

Defining the term of equation 16:

$$A^T = \begin{pmatrix} x_1^2 & x_2^2 \ldots x_n^2 \\ x_1 & x_2 \ldots x_n \\ 1 & 1 \ldots 1 \end{pmatrix}$$

$$W\,A = \begin{pmatrix} \frac{x_1^2 y_1^2}{\sigma_{y_1}^2} & \frac{x_1 y_1^2}{\sigma_{y_1}^2} & \frac{y_1^2}{\sigma_{y_1}^2} \\ \frac{x_2^2 y_2^2}{\sigma_{y_2}^2} & \frac{x_2 y_2^2}{\sigma_{y_2}^2} & \frac{y_2^2}{\sigma_{y_2}^2} \\ \vdots & \vdots & \vdots \\ \frac{x_n^2 y_n^2}{\sigma_{y_n}^2} & \frac{x_n y_n^2}{\sigma_{y_2}^2} & \frac{y_1^2}{\sigma_{y_n}^2} \end{pmatrix}$$

$$A^T\,W\,A = \begin{pmatrix} \sum_{i=1}^{n} \frac{x_i^4 y_i^2}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i^3 y_i^2}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma_{y_i}^2} \\ \sum_{i=1}^{n} \frac{x_i^3 y_i^2}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma_{y_i}^2} \\ \sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{y_i^2}{\sigma_{y_i}^2} \end{pmatrix}$$

$$W\,B = \begin{Bmatrix} \frac{y_1^2}{\sigma_{y_1}^2} z_1 \\ \frac{y_2^2}{\sigma_{y_2}^2} z_2 \\ \vdots \\ \frac{y_n^2}{\sigma_{y_n}^2} z_n \end{Bmatrix} \qquad A^T\,W\,B = \begin{Bmatrix} \sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma_{y_i}^2} z_1 \\ \sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma_{y_i}^2} z_i \\ \sum_{i=1}^{n} \frac{y_i}{\sigma_{y_i}^2} z_i \end{Bmatrix}$$

Substituting these quantities into equation 16, get solution of the form:

$$X = \begin{Bmatrix} S_1 \\ S_2 \\ S_3 \end{Bmatrix}$$

where S_1, S_2 and S_3 are given by equations 11, 12, and 13.

Also

$$\sigma_{S_1}^2 = (A^T W A)^{-1}_{11}$$

$$\sigma_{S_2}^2 = (A^T W A)^{-1}_{22}$$

$$\sigma_{S_3}^2 = (A^T W A)^{-1}_{33}$$

Therefore:

$$b_o = -\frac{1}{S_1}$$

$$\text{and } \sigma_{b_o}^2 = \left(\frac{\partial b_o}{\partial S_1}\right)^2 \sigma_{S_1}^2 = \frac{1}{S_1^2}\sigma_{S_1}^2$$

$$x_o = \frac{b_o S_2}{2}$$

$$\text{and } \sigma_{x_o}^2 = \left(\frac{\partial x_o}{\partial b_o}\right)^2 \sigma_{b_o}^2 + \left(\frac{\partial x_o}{\partial S_2}\right)^2 \sigma_{S_2}^2 = \frac{S_2^2}{4}\sigma_{b_o}^2 + \frac{b_o^2}{4}\sigma_{S_2}^2$$

$$\ln y_o = S_3 + \frac{x_o^2}{b_o}$$

$$\sigma_{y_o}^2 = \left(\frac{\partial y_o}{\partial S_3}\right)^2 \sigma_{S_3}^2 + \left(\frac{\partial y_o}{\partial X_o}\right)^2 \sigma_{X_o}^2 + \left(\frac{\partial y_o}{\partial b_o}\right)^2 \sigma_{b_o}^2$$

$$= \left(e^{S_3 + \frac{x_o^2}{b_o}}\right)^2 \sigma_{S_3}^2 + \left(\frac{2X_o}{b_o} e^{S_3 + \frac{x_o^2}{b_o}}\right)^2 \sigma_{x_o}^2 + \left(-\frac{x_o^2}{b_o} e^{S_3 + \frac{x_o^2}{b_o}}\right)^2 \sigma_{b_o}^2$$

Note, expoentials may get large, causing overflows on the computer

Therefore, let $z = \ln y_o = S_3 + \frac{x_o^2}{b_o}$

$$\sigma_3^2 = \left(\frac{1}{y_o}\right) \sigma_{y_o}^2 = \left(\frac{\partial 3}{\partial S_3}\right) \sigma_{S_3}^2 + \left(\frac{\partial 3}{\partial x_o}\right)^2 \sigma_{x_o}^2 + \left(\frac{\partial 3}{\partial b_o}\right)^2 \sigma_{b_o}^2$$

$$= \sigma_{S_3}^2 + \left(\frac{2x_o}{b_o}\right)^2 \sigma_{x_o}^2 + \left(-\frac{x_o^2}{b_o}\right)^2 \sigma_{b_o}^2$$

$$\therefore \sigma_{y_o}^2 = y_o^2\left(\sigma_{S_3}^2 + \frac{4x_o^2}{b_o^2} \sigma_{x_o}^2 + \frac{x_o^4}{b^4} \sigma_{b_o}^2\right)$$

POLYNOMIAL FITTING

Using Weighted Least Squares

The method used for this problem is the same as that used for the gaussian fitting problem. In this case, data is fit to a polynomial of degrees m:

$$y_i = a_o + a_1 x_i + a_2 x_i^2 + a_3 x_i^3 + \ldots a_m x_i^m \qquad (1)$$

For this function, the weighting function W is the variance of y_i, that is:

$$W = \begin{pmatrix} \frac{1}{\sigma_{y_1}^2} & \cdot & \cdot & 0 \\ & \frac{1}{\sigma_{y_2}^2} & & \cdot \\ 0 & & \cdot & \frac{1}{\sigma_{y_n}^2} \end{pmatrix} \qquad (2)$$

Rewriting equation 1:

$$\begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^m \\ 1 & x_2 & x_2^2 & \cdots & x_2^m \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & x_n & x_n^2 & \cdots & x_n^m \end{pmatrix} \begin{Bmatrix} a_o \\ a_1 \\ a_2 \\ \\ a_m \end{Bmatrix} = \begin{Bmatrix} y_i \\ y_2 \\ y_3 \\ \\ y_n \end{Bmatrix} \qquad (3)$$

This is of the form $A \cdot X = B$

If $n > m$, which is normally the case, the set of equations in equation 3 is over determined, and the least squares solution is:

$$A^T A\, X = A^T B$$

Now, applying the weighting function W and rearranging as before:

$$X = (A^T W A)^{-1}\, A^T W B \qquad (4)$$

This is the same equation as used in the gaussian fitting problem, where A and B are defined by equation 3, and

$$A^T = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ x_1^2 & x_2^2 & \cdots & x_n^2 \\ \cdot & \cdot & \cdots & \cdot \\ x_1^m & x_2^m & \cdots & x_n^m \end{pmatrix}$$

$$WA = \begin{pmatrix} \frac{1}{\sigma_{y_1}^2} & \frac{x_1}{\sigma_{y_1}^2} & \cdots & \frac{x_1^m}{\sigma_{y_1}^2} \\ \frac{1}{\sigma_{y_2}^2} & \frac{x_2}{\sigma_{y_2}^2} & \cdots & \frac{x_2^m}{\sigma_{y_2}^2} \\ \cdot & \cdot & \cdots & \cdot \\ \frac{1}{\sigma_{y_n}^2} & \frac{x_n}{\sigma_{y_n}^2} & \cdots & \frac{x_n^m}{\sigma_{y_n}^2} \end{pmatrix}$$

$$A^TWA = \begin{pmatrix} \sum_{i=1}^{n} \frac{1}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i}{\sigma_{y_i}^2} & \cdots & \sum_{i=1}^{n} \frac{x_i^m}{\sigma_{y_i}^2} \\ \sum_{i=1}^{n} \frac{x_i}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i^2}{\sigma_{y_i}^2} & \cdots & \sum_{i=1}^{n} \frac{x_i^{m+1}}{\sigma_{y_i}^2} \\ \cdot & \cdot & \cdots & \cdot \\ \sum_{i=1}^{n} \frac{x_i^m}{\sigma_{y_i}^2} & \sum_{i=1}^{n} \frac{x_i^{m+1}}{\sigma_{y_i}^2} & \cdots & \sum_{i=1}^{n} \frac{x_i^{m+m}}{\sigma_{y_i}^2} \end{pmatrix}$$

$$WB = \begin{pmatrix} \frac{y_1}{\sigma_{y_1}^2} \\ \frac{y_2}{\sigma_{y_2}^2} \\ \vdots \\ \frac{y_n}{\sigma_{y_n}^2} \end{pmatrix} \qquad A^T WB = \begin{pmatrix} \sum_{i=1}^{n} \frac{y_i}{\sigma_{y_i}^2} \\ \sum_{i=1}^{n} \frac{x_i y_i}{\sigma_{y_i}^2} \\ \vdots \\ \sum_{i=1}^{n} \frac{x_i^m y_i}{\sigma_{y_i}^2} \end{pmatrix}$$

Substituting these quantities into equation (4), the solution is of the term

$$X = \begin{pmatrix} a_o \\ a_1 \\ a_2 \\ \vdots \\ a_m \end{pmatrix}$$

where the a_i's are the coefficients of the polynomial of degree m.

APPENDIX C

SAMPLE CONTAINERS

OXYGEN SAMPLE CONTAINER DESIGN

LIQUID SODIUM SAMPLE CONTAINER DESIGN

APPENDIX C

SAMPLE CONTAINERS

OXYGEN SAMPLE CONTAINER DESIGN

A rectangular tank was the sample (liquid oxygen) vessel and had an inner box of 2" x 2" x 36", an outer box of 4" x 4" x 40", and the void in between was filled with Vermiculite insulating material. A double walled cylinder (1 1/2" I.D., 3 1/2" O.D., 8" high) acted as a vent at the top of the oxygen reservoir. The inner pipe extended 12" beyond the double walled cylinder for venting purposes. The entire insulating chamber was sealed to prevent exposure to the liquid oxygen.

Due to the flammable and sometimes explosive nature of materials in the presence of high concentrations of oxygen, several precautions were necessary. The sample tank was cleaned several times both inside and out during construction with trichlorethylene to remove any contamination, especially oil, and was checked using a black light. The insulating material, Vermiculite, is known for its inert properties, but a further check was made to determine if oxygen is absorbed to a great extent by the material. The Vermiculite was also "outgassed" at 600°F for several hours to remove contaminates. All equipment was grounded so that static electricity would not cause a spark. The venting tube on top of the sample tank had a "goose-neck" shape to prevent foreign material from falling into the oxygen reservoir. The venting tube was large enough to reduce the number of fillings necessary during an experiment. Evaporation of O_2 was estimated to be ≈500 liters/hr of gas (≈6 liters/hr liquid) which was dispersed into the volume of the reactor bay. This created a rise of .005%/hour in oxygen concentration in the bay. Total increase in oxygen concentration during a single experiment was less than .01% since the initial filling of the sample

was carried out outside the reactor bay; thus, the large evolution of gaseous oxygen associated with "cooling down" of the sample tank took place out of doors.

As a final precaution, before any large volumes of oxygen were introduced into the bay, a small sample ($\simeq$.5 liter) of liquid oxygen in an aluminum dewar was placed in the neutron beam from the reactor to insure that no unforeseen reactions would take place.

LIQUID SODIUM SAMPLE CONTAINER DESIGN

Due to the high chemical reactivity of sodium, especially with water, several precautions were taken to insure that the sodium was kept under an inert atmosphere. To achieve this, a double walled stainless steel container of 1/16" stock was used. The inner container, 2" x 2" x 36" long, held the sodium and was heated with resistance heating wire. A funnel shaped reservoir provided an expansion chamber for the sodium as it was heated. The outer container was 4" x 6" x 40", with the void between the inner and outer chamber being filled with Vermiculite for insulation to a depth of 4". The top two inches of the void were filled with an inert gas (nitrogen) which was constantly passed over the sodium, and maintained at a pressure of approximately 2 psi gage. Directly over the sodium expansion chamber, the outer chamber had a removable section so that calcium carbonate could be added in case of fire at the sodium interface. Exposure of the sodium to the neutron beam resulted in a radiation hazard with the formation of ≈15 millicuries of Na^{24}, which resulted in a dose rate of ≈15 mr/hr. at 1 foot. Therefore, the sample had to be stored in a dry, shielded area until the Na^{24} decayed.

THE EVALUATION OF MINIMA IN TOTAL NEUTRON CROSS-SECTION BY TRANSMISSION OF FISSION SPECTRA THROUGH THICK SAMPLES

by

WILLIAM HOWARD MILLER

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Department of Nuclear Engineering

KANSAS STATE UNVIVERSITY
Manhattan, Kansas

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ABSTRACT

An evaluation of minima in total neutron cross-sections was performed for several materials by comparing an experimentally measured transmitted spectrum with the corresponding calculated result. Published cross-section data were evaluated for iron, lead, liquid oxygen, and solid and liquid sodium. Since thick samples (three or more mean free paths thick) were used, the analysis was very sensitive to minima in the cross-section.

The incident neutron spectrum was obtained from the Triga Mark II reactor and was detected using an NE-213 liquid scintillator spectrometer system. Computer codes were used to unfold the raw data and to calculate the transmitted spectrum (which was a function of published cross-section data, the measured incident flux on the sample and the resolution of the detector). The results of this study demonstrate the usefulness of this technique in evaluating total neutron cross-section.

Several experimental geometry conditions were used in this work to obtain valid results and to study the effects of forward scattering and multiple scattering in the thick samples. The results showed that there is a question as to the accuracy of published angular cross-section data near the zero scattering angle.