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August, 1973

日本原子力研究所
Japan Atomic Energy Research Institute

編集兼発行　日 本 原 子 力 研 究 所

印　　刷　日立高速印刷株式会社

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Cross Section Data and Specifications of AGLI/0 for Fast Reactor Analysis (Adjusted Group Library by Integral data)

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Received November 28, 1972

Abstract

In order to satisfy the accuracy required in the recent analysis of integral data within a reasonable computer time, the cross section library AGLI which mediates between the usual concept of group constants and nuclear data such as ENDF/B is produced.

Two major features are imposed upon the AGLI-library, one is that can be used as input to the spectrum generating code without any time-consuming procedures and the other is that should be convenient form to adjust the cross section by utilizing various integral data measured in critical assemblies.

In the library, the total, fission and absorption cross sections are given by 1950-energy groups equi-lethargy width with the so-called histogram representation of self-shielding correction factor; and the inelastic scattering cross sections are given by level-wise with the same energy group structure as in the other cross sections. The number of neutron per fission and the Legendre coefficient of angular distribution of scattering are expanded by the Chebychev polynomials with respect to the lethargy; and these expansion coefficients are stored on the file.

The nuclides provided so far are U-235, U-238, Pu-239, Pu-240, Pu-241, Fe, Cr, Ni, Na, Al, O, C, Mn, Mo, Pb, Cu, B-10, B-11 and H.

The AGLI/0-th version has been produced and used together with the computer code system DOYC for the analysis of various integral data, and has been connected with the on-line adjusting system ARCADIA. As the results the AGLI-library is shown to satisfactorily fulfil the requirement mentioned above.

This report belongs among serial reports which describe the DOYC computer software system developed for analyses relative to the fast reactor physics.

高速炉系解析用核断面積データーライブラリ：AGLI/0

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黒井　英雄　・　東稔　達三

1972年11月28日受理

要　　旨

現在要求されている積分測定値の解析精度を妥当な計算時間内で求めるため，いわゆる群定数と呼ばれているデーターと核データーの中間的な核断面積データーAGLIライブラリが作成された。AGLIに課せられた主な特徴は，スペクトル解析コードに複雑な処理を行なわずに直接入力可能なこと及び積分測定値による修正が簡単に行なわれる事等である。この為全断面積，核分裂及び吸収断面積は等レサジ間隔の1950群構造を持ち，自己遮蔽因子はヒストグラム表示によって表わされている。非弾性散乱は各レベルごとに上記群数で与えられている。核分裂当りの中性子数及び散乱の異方性は，レサジに関しチェビシェフ展開されその係数がデーターとして与えられている。本AGLIは計算コードシステムDOYC及びオンライン修正システムARCADIAと結合され，解析修正が行なわれ上記要求を充分満たすものであることが示され，今後の利用が期待できる。本報告書は高速炉の炉物理解析の為に開発された計算コード及びデータシステムDOYCに関する報告書の一部である。

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1. Introduction

Nuclear cross section data for fast reactor analysis which have been used in JAERI, are in principle, classified into two types, one consists of the so-called group cross section set (1),(2) in which effective cross sections in 18~35 energy groups weighted by an appropriate neutron spectrum are given together with their self-shielding factors. The other type consists of point-wise or parametric expression of microscopic cross sections such as given in ENDF/B (3) or the UK-nuclear data (4) file.

The former type is convenient for a survey of reactor physics parameters, but neither sufficient for precise analysis of experimental results obtained in critical experiments nor for obtaining accurate information of reactor design parameters, especially for a fine neutron spectrum, fine structure of power distribution, heterogeneity effects and reactivity perturbation mainly due to light elements.

For a fine analysis, calculations have been carried out using point-wise data on ENDF/B or the UK-nuclear data file, but these are too time-consuming for ordinary purposes. Considering the present trend in reactor physics, analysis of large amount of integral data is required with high accuracy to squeeze any useful systematic information on cross sections from those data obtained by integral experiments.

As a consequence, development of an appropriate cross section library together with a computer code system used for analysis of integral data with sufficient accuracy and reasonable computer time is intensively desired. To fulfil these requirements, the fine-group cross section library AGLI/0 has been developed for the purpose of providing cross section input data of Modular Coding System DOYC (5) which was provided for fine analysis of integral data.

This report describes the philosophy, data format and procedures how to use the data on the AGLI/0 file.

2. Description of Cross Section Data on AGLI/0

For an accurate analysis of integral data, the most essential are to generate accurate neutron spectra. Precise analysis must be made on heterogeneity effect and competition between slowing down due to resonance scatterers and absorption due to heavy nuclides.

The treatment based on the integral transport theory in an ultra-fine group structure (about 10^5 energy groups) is considered as the most accurate method, but is not practical for routine analysis of integral data. The histogram representation in the resonance energy region used in the AGLI-library make it possible to reduce the number of energy group (about 2000 energy groups) extensively without loss of accuracy of analysis.

The AGLI-library is designed to be a convenient form for data adjustment by a cathode ray tube and light-pen system or card input. The library is also designed to be used as cross section input to various computer codes for fast reactor analysis without any time-consuming procedures.

2.1 Outline of AGLI/0

The cross section library AGLI is similar to FGL-Library[6], which has been developed in UK, but unfortunately detailed knowledge can not easily be obtained from any published documents. The library of AGLI developed here has been constructed conveniently for adjusting the cross sections on the library by using various integral data. The nuclear cross sections used for providing AGLI/0 have been selected to be as same as possible those in JAERI-Fast set[2], preserving a consistency among our analysis of integral data.

The library consists of two files in which one contains 1950-group constants of total, absorption and fission cross sections with their self-shielding factors; and the other file contains data of inelastic scattering, the number of neutrons per fission, fission neutron spectrum, and angular distribution of scattered neutrons.

These two files have been produced by various codes using data given in ENDF/B, UK-data and CONCOCT-1[7]. Those nuclear data used for each nuclide are listed in Table 1. Since the library is destined to be adjusted by integral data soon to produce AGLI/1, no special efforts have been made for evaluating these nuclear data other than the efforts already done in JAERI-Fast set.

The energy range covered by the library depends on the group lethargy

Table 1 Nuclear data used in AGLI/0

U-235	JAERI-1195, JAERI-1199
U-238	JAERI-1195, JAERI-1199
U-239	JAERI-1195, JAERI-1199
U-240	JAERI-1195, JAERI-1199
Pu-241	UKNDL(1967)
Fe	UKNDL(1967)
Cr	UKNDL(1967)
Ni	UKNDL(1967)
Mn	ENDF/B Version 2
Mo	ENDF/B Version 1
Pb	UKNDL(1970)
Cu	ENDF/B Version 2
Al	UKNDL(1967)
Na	JAERI-1195
O	UKNDL(1967)
C	UKNDL(1967)
H	UKNDL(1967)
B-10	UKNDL(1967)
B-11	UKNDL(1967)

width used, and in AGLI/0, the highest energy was fixed at 10.5 MeV and 1950 energy groups with 0.0085 lethargy width were used. Elements which have been stored on the data file so far, are ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, Fe, Cr, Ni, Mn, Mo, Pb, Cu, Al, Na, O, C, H, ^{10}B and ^{11}B. Three different data of the first file are provided at three temperatures of 300, 900 and 2100°K.

2.2 Description of data on File A

The fine group cross sections of the total, absorption and fission are given on File A, and those self-shielding factors are also given on File A. The data stored on the file are obtained as follows.

(a) Group number

The negative flag is assigned on a group number when the energy group envisaged is so narrow that the effect of self-shielding correction is less than 0.5% for practical cases. In this case, the self-shielding correction factors to be described in (c) are not given.

(b) Fine group cross section

The fine group cross sections of the total $\bar{\sigma}_t$, absorption $\bar{\sigma}_a$ and fission $\bar{\sigma}_f$ obtained by the following integration are given on File A

$$\bar{\sigma}_i = \frac{1}{U_l - U_u} \int_{U_u}^{U_l} \sigma_i (U) \, dU \tag{1}$$

where i : i-th type of reaction

U_l : lethargy at lower boundary of the energy group

U_u : lethargy at upper boundary of the energy group.

(c) Self-shielding factor

A histogram representation of a resonance structure proposed in the reference[8] is applied to give self-shielding factors within an energy group. In the reference, J.L. Rowlands and J.D. Macdougall recommended to vary the number of histogram points depending on the different groups and elements. However, the physical significance of the histogram representation more than two points is not clear so that the two point histogram was used for all energy groups and all elements in the AGLI library.

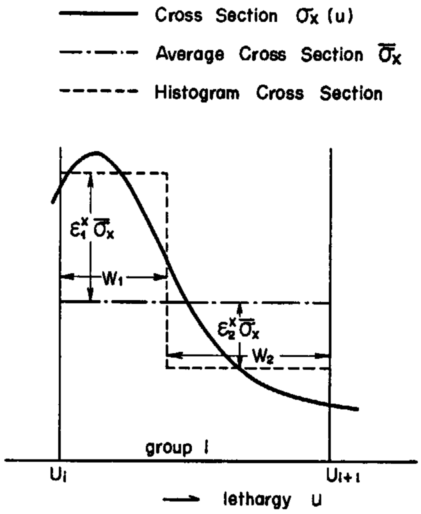

Fig. 1 Histogram Representation of Cross Section $\sigma_x(u)$

A model of the two point histogram is shown in Fig. 1, and the self-shielded effective cross section $\tilde{\sigma}_x$ is expressed using this model as follows;

$$\tilde{\sigma}_x = \frac{\bar{\sigma}_x \left[\dfrac{W_1}{\sigma_0 + \bar{\sigma}_t (1+\varepsilon_1^t)} + \dfrac{W_2}{\sigma_0 + \bar{\sigma}_t (1+\varepsilon_2^t)} + \dfrac{W_1 \ \varepsilon_1^x}{\sigma_0 + \bar{\sigma}_t (1+\varepsilon_1^t)} + \dfrac{W_2 \ \varepsilon_2^x}{\sigma_0 + \bar{\sigma}_t (1+\varepsilon_2^t)} \right]}{\dfrac{W_1}{\sigma_0 + \bar{\sigma}_t (1+\varepsilon_1^t)} + \dfrac{W_2}{\sigma_0 + \bar{\sigma}_t (1+\varepsilon_2^t)}} \tag{2}$$

where σ_0 is the same quantity defined in the ABBN set[1].

Thus the self-shielding factor f^x is given by

$$f^x = \frac{\tilde{\sigma}_x}{\bar{\sigma}_x} = 1 + \frac{\dfrac{\bar{\sigma}_t W_2 \varepsilon_2^x(\varepsilon_1^t - \varepsilon_2^t)}{\sigma_0 + \bar{\sigma}_t(1+\varepsilon_2^t)}}{1 + \dfrac{\bar{\sigma}_t W_2(\varepsilon_1^t - \varepsilon_2^t)}{\sigma_0 + \bar{\sigma}_t(1+\varepsilon_2^t)}} \tag{3}$$

Considering physical significance of the histogram representation of cross section, the following conditions must be satisfied,

$$\begin{aligned} W_1 + W_2 &= 1 \\ \varepsilon_1^x W_1 + \varepsilon_2^x W_2 &= 0 \end{aligned} \tag{4}$$

When the total, absorption and fission cross sections are considered, the number of unknown parameters is 8 and the number of equations given by Eq. (4) is 4. Therefore, four additional equations can be used to obtain unknown parameters of W's and ε's. In the AGLI library, the fission and total cross sections are fitted to those exact values at one value of σ_0 in Eq. (3) and the absorption cross section is fitted to exact ones at two values of σ_0. The value of σ_0 used for fitting the total and fission cross sections is 20 barns and; 20 and 300 barns for absorption. In AGLI/0, W_1, ε_1^t, ε_2^t, ε_2^f and ε_2^a are stored on File A, if the group number given in (a) is possitive.

2.3 Description of data on File B

File B contains data for inelastic scattering, angular distribution of scattered neutron, the number of neutrons per fission and fission neutron spectrum. All smooth quantities with respect to the incident neutron lethargy are expanded using Chebyshev polynomials up to 12 terms and the expansion coefficients are stored on File B.

(a) Angular distribution of elastic scattering cross section

The angular distribution of elastic scattering are represented by Legendre polynomials $P_\ell(\mu)$ as fcllows,

$$\frac{d\sigma_s(\Omega,\mu)}{d\Omega} = \frac{\sigma_s(u)}{2\pi}\sum_{\ell=0}^{L}\frac{2\ell+1}{2} f_\ell(u) P_\ell(\mu) \tag{5}$$

where μ : cosine of scattering angle in either the laboratory or the center of mass system

u : lethargy of incident neutron in the laboratory system

$\sigma_s(u)$: elastic scattering cross section at u

$f_\ell(u)$: the ℓ-th coefficient of Legendre polynomials

The coefficients both in the center of mass system $f_\ell^C(u)$ and in the laboratory system $f_\ell^L(u)$ are expanded using Chebyshev polynomials in the lethargy range from UA to UB as follows,

$$f_\ell^C(u) = \sum_{j=0}^{11} A_{\ell j}^C u^j$$
$$f_\ell^L(u) = \sum_{j=0}^{11} A_{\ell j}^L u^j \tag{6}$$

The values of $f_\ell^C(u)$ and $f_\ell^L(u)$ out-side the lethargy range UA~UB are assumed to be constant and these constant values are also stored on File B. The maximum number of expansion terms in Eq. (5) is seven in the AGLI library and the constant values which are used out-side the lethargy range UA~UB are usually set equal zero except the 0-th and 1st terms of the Legendre expansion in the laboratory system.

(b) The number of neutrons per fission

The average number of neutrons emitted per fission $\nu(u)$ is expanded using Chebyshev polynominals in the lethargy interval between UA and UB as follows;

$$\nu(u) = \sum_{j=0}^{11} A_j u^j \tag{7}$$

In the outside from the lethargy range between UA and UB, a constant value ν_c is used for $\nu(u)$. The error caused by using this expansion of $\nu(u)$ has been examined to be less than ±0.2%. The expansion coefficient A_j, lethargy interval UB and UA; and the constant value ν_c are stored on File B.

(c) Fission neutron spectrum

The simple Maxwellian distribution is assumed and the nuclear temperature is given on the File B as a function of the average number of neutrons per fission;

$$n(E) = C\sqrt{E}\,\exp(-E/\theta(\tilde{\nu})) \tag{8}$$

where $n(E)$: fission neutron spectrum

C : normalization constant

$\theta(\tilde{\nu})$: nuclear temperature given in Mev.

The linear extrapolation or interpolation is recommended to obtain θ at arbitrary values of $\tilde{\nu}$ from the data given on the File B.

(d) Inelastic scattering cross section

Since the source calculations of inelastically scattered neutrons due to discrete levels or the continuum (continuum region of levels) are performed individually in DOYC as explained later, inelastic scattering cross sections are stored on File B individually for discrete levels and the continuum. The fine group cross sections were obtained by interpolation of nuclear data given at arbitrary energy points. There are no limitations on the number of discrete levels of each element.

Data of the excitation energy ω_n of the n-th level and the nuclear temperature T_c in the evaporation model are stored on File B, which are used for obtaining the inelastic scattering matrices in fine group representation. To reduce computing time for calculating the source due to excitation of the continuum, the fraction scattered into the self-group, which is necessary in the recurrence equation (46), is stored on File B.

The numerical procedures for calculating the source due to inelastic scattering will be described in the section 4.3 .

3. Organization of Data Files

Two data files, A and B, have been provided in binary mode. The organization of these binary data disks (or tapes) is described in this section.

3.1 Organization of File A

In the first physical record on File A, the title of the data disk used, two values of σ_0 used for the histogram representation, the upper energy of the first group, the fine group lethargy width, the number of fine groups and the code number of each element on the file are stored. In the second record, the group cross sections and self-shielding factors are given by blocking 50 energy groups into one record. The code number of each element on the file and the nuclear data used are given in Table 2.

(a) 1st physical record

TITLE(15), SO, S1, EM, DELU, MAXG, LCODE(20)

Table 2 Code number of each nuclide

U-235	935
U-238	928
Pu-239	939
Pu-240	940
Pu-241	941
Fe	26
Cr	24
Ni	28
Mn	25
Mo	42
Pb	82
Cu	29
Al	13
Na	11
O	8
C	6
H	1
B-10	105
B-11	115

TITLE : Title of the file

SO, S1 : Values of σ_0 used for histogram representation

EM : The upper energy of the 1st group

DELU : Group width in lethargy

MAXG : The number of energy groups

LCODE : Code numbers of elements, for which data are stored on the data file

(b) 2nd physical record

In the second physical record, the group cross sections of the first 50 energy groups of the first element are given as follows.

IGI : Group number; if flagged negative, no self-shielding corrections are given.

FX(K, 1) : $\bar{\sigma}_t$

FX(K, 2) : $\bar{\sigma}_f$

FX(K, 3) : $\bar{\sigma}_{ab}$

FX(K, 4) : $\bar{\sigma}_e$ (not given in AGLI/O)
FX(K, 5) : W_2
FX(K, 6) : ε_1^t
FX(K, 7) : ε_2^t
FX(K, 8) : ε_2^a
FX(K, 9) : ε_2^f
FX(K,10) : not used

where K indicates the energy group number.

(c) 3rd physical record

IGI and FX of the first 50 energy groups of the second element are given in the third record.

The similar records for all elements are repeated, then the data of the second 50 groups are stored in the same manner until the lowest energy group is reached as schematically shown in Fig. 2.

3.2 Organization of File B

The first physical record on File B contains the data of the angular distribution of elastic scattering which are expanded up to twelve terms by Chebychev's polynomials. In the second record, data of the number of neutrons emitted per fission are contained, which are also expanded up to twelve terms by the Chebyshev polynomials and the nuclear temperatures used for fission

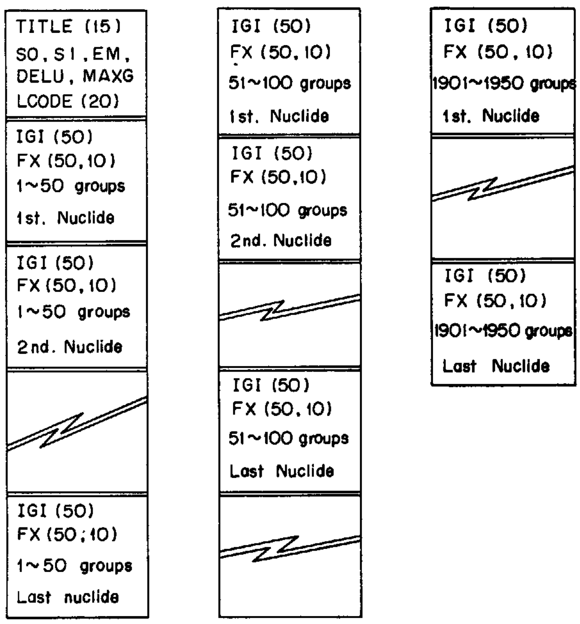

Fig. 2 Arrangement of File A in AGLI/O

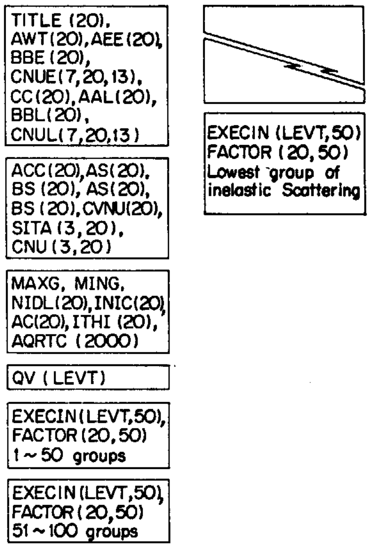

Fig. 3 Arrangement of File B in AGLI/0

neutron spectrum are given with corresponding values of ν (the average number of neutrons per fission). In the third, fourth and fifth records, the data of inelastic scattering cross sections are stored.

(a) 1st physical record

TITLE(20), AWT(20), AEE(20), BBE(20), CNUE(7,20,13), CC(20), ALL(20), BBL(20), CNUL(7,20,13)

TITLE	:	Title of the file.
AWT	:	Atomic weight.
AAE	:	The lowest lethargy at which the Chebychev's expansion is applied for calculating μ_c of the elastic scattering in the center of mass system, usually 0.0
BBE	:	The highest lethargy of the interval where the above expansion is applied.
CNUE	:	Expansion coefficients of μ_c .
CC	:	Constant value of μ_ℓ in the laboratory system.
AAL	:	The lowest lethargy at which the Chebysheve expansion is applied for μ_ℓ of the elastic scattering in the laboratory system, usually 0.0.
BBL	:	The highest lethargy of the interval where the above expansion is applied.
CNUL	:	Expansion coefficients of μ_ℓ .

where the number of dimensions given in the bracket means; 20= the maximum number of nuclides, 13= the maximum number of terms in the Chebyshev expansion, 7= the maximum number of terms in the Legendre expansion.

(b) 2nd physical record

ACC(20), AS(20), BS(20), CVNU(20,13), SITA(3,20), CNU(3,20)

ACC : Constant value of ν (the number of neutrons per fission).

AS : The lowest lethargy of the interval where the Chebyshev expansion is applied for ν, usually 0.0.

BS : The highest lethargy of the interval where the above expansion is applied.

CVNU : Expansion coefficients of ν.

SITA : Nuclear temperature used for fission neutron spectrum in Mev at the corresponding value of ν given by CNU.

CNU : Value of ν at which the nuclear temperature is given.

where the number of dimensions given in the bracket means; 20= the maximum number of nuclides stored on the file, 10= the maximum number of fissile nuclides stored on the file, 3= the maximum number of different values of ν at which the value of nuclear temperature is given.

(c) 3rd physical record

MAXG, MING, NIDL(20), INIC(20), AC(20), ITHI(20), AQRTC(2000)

MAXG : The highest energy group above which the inelastic scattering does not occur; usually 1.

MING : The lowest energy group below which the inelastic scattering does not occur.

NIDL : Indication representing the presence of discrete levels

INIC : Indication representing the presence of the continuum

AC : The value of a in Eq. (42).

ITHI : The lowest energy group below which the transfer cross section due to the continuum is ignored.

AQRTC : The value of $\sqrt{E}$ (E: upper energy of each fine groups in Mev).

(d) 4th physical record

QV(LEVT)

QV : Level energy (positive value).

LEVT : Aggregate number of discrete levels and the continuum for all elements in AGLI/O.

(e) 5th physical record

EXECIN(LEVT, 50), FACTOR(20, 50)

EXECIN : Fine group cross sections of discrete levels and the continuum.

FACTOR : The source due to the continuum into the self-group.

The fifth record is repeated for every fifty energy groups until the inelastic scattering cross section in the lowest group is stored. The organization of these data is schematically shown in Fig. 3.

4. Procedures to Use the Data on AGLI/0

Since many of necessary procedures how to use data on the library are self-explanatory in the previous sections of 2.2 and 2.3, brief descriptions of the procedure to obtain effective cross section in homogeneous and heterogeneous media, and to obtain inelastically scattered neutron sources are given in this section.

4.1 Effective group constants in homogeneous media

The group lethargy width of 0.0085 used in the library is not so narrow that effects of self-shielding must be corrected to obtain the effective group constants in some energy groups. The correction is not necessary in the energy groups where the all nuclides in a medium are flagged negative on their group numbers.

The correction is applied for total, absorption and fission cross sections and not for inelastic scattering. The effective elastic scattering cross section is obtained by subtracting all effective cross sections, except elastic one, from the effective total cross section.

Using the value of $\sigma_{o,i}$ defined in the ABBN set[1], the effective group cross section $\tilde{\sigma}_{x,i}$ of the reaction type x of the i-th element is obtained by

$$\tilde{\sigma}_{x,i} = \bar{\sigma}_{x,i}\left[1 + \frac{\dfrac{\bar{\sigma}_{t,i} W_{2,i}\, \varepsilon^{x}_{2,i}(\varepsilon^{t}_{1,i} - \varepsilon^{t}_{2,i})}{\sigma_{o,i} + \bar{\sigma}_{t,i}(1 + \varepsilon_{2,i})}}{1 + \dfrac{\sigma_{o,i} W_{2,i}(\varepsilon^{t}_{1,i} - \varepsilon^{t}_{2,i})}{\sigma_{o,i} + \bar{\sigma}_{t,i}(1 + \varepsilon^{t}_{2,i})}} \right] \tag{9}$$

and

$$\sigma_{o,i}=\frac{1}{N_i}\sum_{j\neq i}N_j\,\tilde{\sigma}_{t,j} \tag{10}$$

where N_i is the atom density of the i-th element. In the first approximation, $\sigma_{o,i}$ in the above equation is obtained by replacing $\tilde{\sigma}_{t,j}$ with $\bar{\sigma}_{t,j}$, then $\tilde{\sigma}_{t,j}$ can be obtained by Eq. (9) and $\sigma_{o,i}$ may be recalculated by using $\tilde{\sigma}_{t,j}$ newly obtained. It is possible to repeat this iterative procedure, if necessary.

4.2 Effective group constants in heterogeneous media

Usually, the heterogeneity correction is carried out by means of the collision probability method. Therefore it is worthwhile to know physical interpretation of collision probability using the histogram representation.

Now consider the collision probability $P_{k\to\ell}$ where neutrons given in the region k suffer their first collision in region ℓ. Let this $P_{k\to\ell}$ be the collision probability calculated using the cross section of $\sum_n N_{i,n}\,\bar{\sigma}_{t,n}$ in the region i, and $P_{k\to\ell}$ (j, m) be the collision probability calculated using the cross section $\sum_{n\neq m} N_{i,n}\,\bar{\sigma}_{t,n}+N_{i,m}(1+\varepsilon^{i}_{j,m})\,\bar{\sigma}_{t,m}$ for the j-th histogram point in region i, where $N_{i,n}$ is the atom density of the n-th element in region i.

It is of course possible to calculate the collision probability $P_{k\to\ell}$(j, m) by using the cross section defined above, but the histogram representation becomes to be insignificant if the $P_{k\to\ell}$(j, m) should be collision probability $P_{k\to\ell}$ (j, m) can be approximately evaluated in connection with $P_{k\to\ell}$, assuming that the mean free path of neutrons is longer as compared with the length of unit cell used for calculation.

The collision probability $P_{k\to\ell}$ is considered to be the product of $\Phi_{k\to\ell}$ and R_ℓ

$$P_{k\to\ell}=\Phi_{k\to\ell}\,R_\ell \tag{11}$$

where $\Phi_{k\to\ell}$ is the volume integrated neutron flux in region ℓ induced from a neutron generated in region k without any collisions; and R_ℓ is the total cross section in region ℓ. Then the change of $P_{k\to\ell}$ due to a cross section variation in each region is expressed by

$$P_{k\to\ell}+\delta P_{k\to\ell}=P_{k\to\ell}\left[1+\frac{\delta\Phi_{k\to\ell}}{\Phi_{k\to\ell}}+\frac{\delta R_\ell}{R_\ell}\right] \tag{12}$$

Now consider the j-th histogram point of nuclide m, then

$$\frac{\delta R_\ell}{R_\ell} \doteqdot \frac{\varepsilon_{j,m}\,\bar{\sigma}_{t,m}}{\sigma^\ell_{o,m} + \bar{\sigma}_{t,m}} \tag{13}$$

Assuming that the mean free path of neutrons is much longer than the length of a unit cell, $\delta\Phi_{k\to\ell}/\Phi_{k\to\ell}$ due to a cross section variation given by histogram representation is approximately evaluated as follows;

$$\frac{\delta\Phi_{k\to\ell}}{\Phi_{k\to\ell}} = \frac{-\sum_k \dfrac{P_{k\to\ell}}{N_{\ell,m}(\sigma^\ell_{o,m}+\bar{\sigma}_{t,m})} V_k N_{k,m}\,\varepsilon^t_{j,m}\,\bar{\sigma}_{t,m}\,\phi_k}{V_\ell\,\phi_\ell} \tag{14}$$

Using the assumption mentioned above, neutron flux ϕ_ℓ in region ℓ does not strongly depend on the region where the neutron is generated. Therefore,

$$\frac{\delta\Phi_{k\to\ell}}{\Phi_{k\to\ell}} = -\sum_k \frac{P_{k\to\ell}}{(\sigma^\ell_{o,m}+\bar{\sigma}_{t,m})N_{\ell,m}}\,\frac{V_k}{V_\ell} N_{k,m}\,\varepsilon^t_{j,m}\,\bar{\sigma}_{t,m} \tag{15}$$

Using the reciprocity relation of collision probability

$$V_k N_{k,m}(\sigma^k_{o,m}+\bar{\sigma}_{t,m})P_{k\to\ell} = V_\ell N_{\ell,m}(\sigma^\ell_{o,m}+\bar{\sigma}_{t,m})P_{\ell\to k} \tag{16}$$

then Eq. (15) is rewritten as follows,

$$\frac{\delta\Phi_{k\to\ell}}{\Phi_{k\to\ell}} = -\sum_k \frac{\varepsilon^t_{j,m}\,\bar{\sigma}_{t,m}}{(\sigma^k_{o,m}+\tilde{\sigma}_{t,m})} P_{\ell\to k} \tag{17}$$

As the consequence, the purturbed collision probability $P_{k\to\ell}(j, m)$ due to the j-th histogram of the m-th element is simply obtained in connection with $P_{k\to\ell}$ as follows;

$$P_{k\to\ell}(j,m) = P_{k\to\ell} + \delta P_{k\to\ell} = P_{k\to\ell}\left[1 + \frac{\varepsilon^t_{j,m}\,\bar{\sigma}_{t,m}}{\sigma^\ell_{o,m}\,\bar{\sigma}_{t,m}} - \sum_k \frac{\varepsilon^t_{j,m}\,\bar{\sigma}_{t,m}}{(\sigma^k_{o,m}+\bar{\sigma}_{t,m})} P_{\ell\to k}\right] \tag{18}$$

Using the above relation between $P_{k\to\ell}(j, m)$ and $P_{k\to\ell}$, the computing time necessary for the calculation of the collision probability $P_{k\to\ell}(j, m)$ is reduced sharply as compared with a direct calculation of $P_{k\to\ell}(j, m)$.

4.3 Slowing down due to inelastic scattering

The fine group inelastic scattering matrices are not provided for File B, because the number of their elements is very vast, more than a few millions for all elements stored on AGLI/0. The recurrence relation given below is recommended to calculate neutron sources due to inelastic scattering.

(a) Inelastic transfer matrices due to discrete level.

Relations among the incident neutron energy E_i, the final neutron energy E_f, the excitation energy ω_n of the n-th level, the cosine of scattering angle in the center of mass system μ_c and that in the laboratory system μ_0 are given as follows[(9)~(11)]

$$\frac{E_f}{E_i}=\frac{\left(\sqrt{A^2-1+\mu_0^2-A(A+1)\omega_n/E_i}+\mu_0\right)^2}{(A+1)^2} \tag{19}$$

$$=\frac{2}{(A+1)^2}\frac{\mu_c}{W}+\frac{1}{(A+1)^2}\left(1+\frac{1}{W^2}\right) \tag{20}$$

$$\mu_0=\frac{1}{2}(A+1)\sqrt{\frac{E_f}{E_i}}-\frac{1}{2}(A-1)\sqrt{\frac{E_i}{E_f}}+\frac{A\,\omega_n}{2\,E_i}\sqrt{\frac{E_i}{E_f}} \tag{21}$$

$$=\frac{W+\mu_c}{\sqrt{W^2+2W\mu_c+1}} \tag{22}$$

where A is the mass number of the target nucleus and

$$W^2=\frac{1}{A^2-A(A+1)\omega_n/E_i} \tag{23}$$

The maximum and minimum energies of a scattered neutron are given by

$$E_{max}=\frac{A^2+1}{(A+1)^2}E_i-\frac{A\omega_n}{A+1}+\frac{2E_i}{(A+1)^2}\sqrt{A^2-A(A+1)\omega_n/E_i} \tag{24}$$

$$E_{min}=\frac{A^2+1}{(A+1)^2}E_i-\frac{A\omega_n}{A+1}-\frac{2E_i}{(A+1)^2}\sqrt{A^2-A(A+1)\omega_n/E_i} \tag{25}$$

Thus the energy interval into which a neutron is scattered is given by

$$E_{max} - E_{min} = \frac{4E_i}{(A+1)^2}\sqrt{A^2 - A(A+1)\omega_n/E_i} = \frac{4E_i}{(A+1)^2}\frac{1}{W} \tag{26}$$

Using a series of Legendre functions $P_\ell(\mu_0)$, the angular and energy dependence of the scattering cross section can be represented as[12]

$$\sigma(E_i \to E_f, \Omega_i \to \Omega_f) = \sum_\ell S_\ell(E_i \to E_f) P_\ell(\mu_0) \tag{27}$$

where Ω_i and Ω_f are the initial and the final neutron directions and

$\mu_0 = \Omega_i \cdot \Omega_f$.

Angular distribution of the scattered neutron in the center of mass system is proportional to

$$1 + \sum_{\ell \geq 1} \frac{\sigma_\ell}{\sigma_0} P_\ell(\mu_c) \tag{28}$$

where the σ_ℓ are the Legendre expansion coefficients. Then the expansion coefficient $S_\ell(E_i \to E_f)$ in Eq. (27) is obtained, as follows;

$$\begin{aligned} S_\ell(E_i \to E_f) &= \frac{2\ell+1}{4\pi}\int d\Omega\sigma(E_i \to E_f, \Omega_i \to \Omega_f) \\ &= \frac{2\ell+1}{4\pi}\int d\Omega\sigma(E_i)\frac{1+\sum_{\ell'} P_{\ell'}(\mu_c)\sigma_{\ell'}/\sigma_0}{4\pi}\frac{d\mu_c}{d\mu_0}P_\ell(\mu_0) \\ &\quad \times \delta\left(E_f - \frac{E_i}{(A+1)^2}\left\{\frac{2}{W}\mu_c + 1 + \frac{1}{W^2}\right\}\right) \\ &= \frac{2\ell+1}{8\pi}\sigma(E_i)\left\{1 + \sum_{\ell'}\frac{\sigma_{\ell'}}{\sigma_0}P_{\ell'}(\mu_c(E_i, E_f)\right\}P_\ell(\mu_0(E_i \cdot E_f)) \\ &\quad \times \frac{(A+1)^2 W}{2E_i}, \end{aligned} \tag{29}$$

where

$$\sigma(E_i) = \int d\Omega dE_f\ \sigma(E_i \rightarrow E_f, \Omega_i \rightarrow \Omega_f). \tag{30}$$

The cross section for scattering into unit energy interval at E_f is

$$\sigma(E_i \rightarrow E_f) = \int d\Omega \sigma(E_i \rightarrow E_f, \Omega_i \rightarrow \Omega_f) = 4\pi S_0(E_i \rightarrow E_f) \tag{31}$$

$$= \sigma(E_i)\{1 + \sum_\ell \frac{\sigma_\ell}{\sigma_0} P_\ell(\mu_c(E_i, E_f))\} \frac{(A+1)^2 W}{2E_i}, \tag{32}$$

and using Eq. (26)

$$= \sigma(E_i)\{1 + \sum_\ell \frac{\sigma_\ell}{\sigma_0} P_\ell(\mu_c(E_i, E_f))\} \frac{1}{E_{max} - E_{min}}. \tag{33}$$

If the scattering is spherically symmetric in the center of mass system,

$$\sigma(E_i \rightarrow E_f) = \sigma(E_i) \frac{1}{E_{max} - E_{min}}. \tag{34}$$

It is noted that in case of $\omega_n = 0$ all the equations derived above are reduced to the equations for energy transfer due to elastic scattering.

From Eq. (34), the transfer cross section from the initial energy to the j-th fine group is given by

$$\sigma(E_i \rightarrow E_j) = \int_{E_{j\ell}}^{E_{ju}} \sigma(E_i \rightarrow E_f) dE_f = \sigma(E_i) \frac{1 - e^{-\Delta u}}{1 - e^{-(m_i - k_i)\Delta u}} \frac{E_{ju}}{E_{max}}$$

$$= \sigma(E_i) \frac{1 - e^{-\Delta u}}{1 - e^{-(m_i - k_i)\Delta u}} e^{-(j_i - k_i)\Delta u}, \tag{35}$$

where E_{ju} and $E_{jl}(=E_{ju}e^{-\Delta u})$ are the upper and lower energies of the j-th group, Δu is the lethargy width of fine groups and,

$$k_i = \frac{\ln(E_i/E_{max})}{\Delta u}, \tag{36}$$

$$m_i = \frac{\ln(E_i/E_{min})}{\Delta u}, \tag{37}$$

$$j_i = \frac{\ln(E_i/E_{ju})}{\Delta u}. \tag{38}$$

The transfer cross section to the energy group including the highest energy of scattered neutrons, E_{max} , is

$$\sigma(E_i)\cdot\frac{1-e^{-\Delta u}}{1-e^{-(m_i-k_i)\Delta u}} \tag{39}$$

The transfer cross sections to the lower group can be easily obtained by multiplying Eq. (39) by a factor $R=e^{-\Delta u}$ successively.

Since the angular distributions of discrete level cross sections used in AGLI/0 are spherically symmetric in the center of mass system, the transfer cross sections are exactly calculated by the above recurrence relation. This relation was initially applied for calculating source below 2 Mev in the code ESELEM-2[13] which calculates the fundamental mode fine spectrum in homogeneous media.

(b) Transfer cross section due to the continuum region.

The neutron slowing down by the continuum inelastic scattering is calculated by means of the evaporation model. In this model, the energy distribution of inelastically scattered neutrons is given by

$$N(E_f)=b(E_i)\,E_f\,e^{-E_f/T_{c,i}} \tag{40}$$

where $N(E_f)$ is the probability that the energy of the scattered neutron will be in a unit interval at E_f , $T_{c,i}$ is the temperature of the residual nucleus, and $b(E_i)$ is a normalization factor. The nuclear temperature used in AGLI/0 is[14]

$$T_{c,i}=a\sqrt{E_i} \tag{41}$$

where

$$a=2/B \tag{42}$$

and B is given by using the mass number as

$$B\doteqdot 0.62\sqrt{A} \tag{43}$$

The source of neutrons scattered by the continuum from group i to group j + 1 is represented by means of the reccurrence relation as follows[13];

$$q^i_{j+1}=b_i\,E_{j+1}\,e^{-E_{j+1}/T_{ci}}\,\Delta E_{j+1}\,\phi_i\,\sigma_i\,\Delta E_i \tag{44}$$

$$= q_j^i e^{\Delta E_j/T_{ci}} \frac{E_{j+1}}{E_j} \cdot \frac{\Delta E_{j+1}}{\Delta E_j} = q_j^i e^{\Delta E_j/T_{ci}} R^2 \tag{45}$$

$$\doteqdot q_j^i \cdot f_c^{ij} \tag{46}$$

where ΔE_i and ΔE_i are the energy intervals of the groups i and j, ϕ_i is the neutron flux of the group i, and

$$f_c^{ij} = \frac{1 + \dfrac{\Delta E_j}{2T_{ci}}}{1 - \dfrac{\Delta E_j}{2T_{ci}}} R^2 \tag{47}$$

The error induced by the expansion of the exponential term in Eq. (45) is small as the order of $(\Delta E_i/2T_{cj})^3/12$, where $\Delta E_j/2T_{cj}$ is about 0.07 for heavy elements at 10.5 Mev. Therefore this reccurrence relation can be applied to whole energy region with satisfactory accuracy.

The source q_j^i is obtained by multiplying the initial source q_i^i by f_c^{ij} successively. To reduce the computing time of q_i^i in DOYC the values of q_i^i without ϕ_i in Eq. (45) are stored on File B.

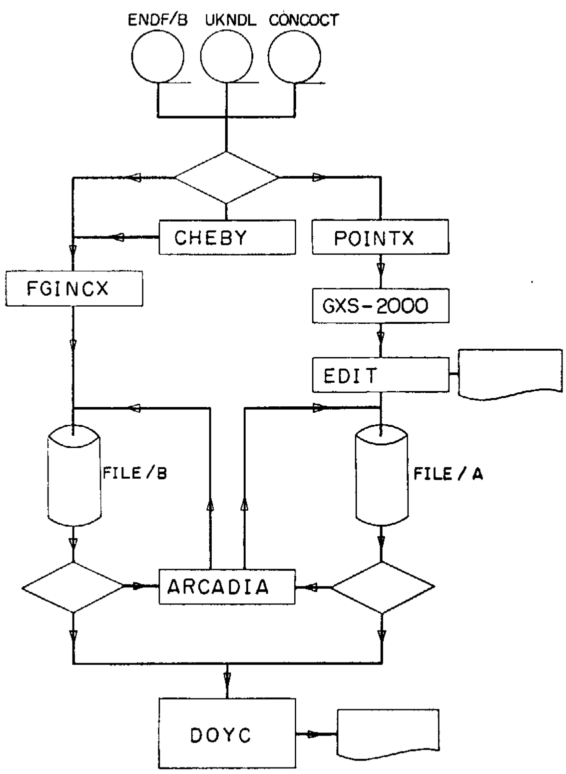

Fig. 4 Flow to Compile AGLI

5. Processing Codes for AGLI-library

Since the cross section library AGLI has been provided to be convenient form for adjusting the cross section by integral data and also to be convenient form as input to a spectrum generating code, the data form stored in the AGLI is quite different from that of the usual nuclear data in ENDF/B or UKNDF. Therefore, a series of processing codes has been developed which read ENDF/B, UKNDF or other source data of cross sections as input and generate the AGLI cross section library.

These processing codes are summarized as follows;

POINTXS

The code POINTXS is a modified version of SIGPLOT suitable for our purposes. The code prepares temperature dependent energy-point-wise cross section of total, fission, capture and elastic scattering cross sections in the whole energy region of interest (covering from 15 Mev to 1 ev). This code has been made which read ENDF/B library as input and generates output results which, in turn, are read as input to the code GXS2000.

CHEBY

The code CHEBY calculates the coefficients of the Chebyshev expansion of f(u), with respect to lethargy, where f is the Legendre expansion coefficients of angular distribution of elastically scattered neutrons at incident lethary u in the center of mass system or in the laboratory system. The ENDF/B library can be used as input to the code. This code is also used to expand $\nu(u)$ with respect to u where ν is the average number of neutrons produced per fission.

GXS2000

The code GXS2000 calculates infinitely dilute fine-group (equi-lethargy width of 0.0085) cross sections and their self-shielding correction factors by means of the so-called "Histogram Representation". The input data to the code are energy-point-wise cross sections of total, fission, capture and elastic scattering which are generated by POINTXS. Any type of point-wise data of cross sections with respect to energy can easily be read in GXS2000.

FGINCX

The code FGINCX calculates infinitely dilute fine-group (equi-lethargy width of 0.0085) inelastic scattering cross sections for discretes and the continuum using energy-point-wise nuclear cross section data according to ENDF/B or /A format or an arbitrary format as input; and the code generates the File B of AGLI cross section library in connection with the output results from CHEBY which provides the information of angular distribution of elastically scattered neutrons and the average number of neutrons per fission. The code is designed to facilitate the addition of new elements to the File B and retrieval of old data on the File B.

EDIT

The code EDIT generates the File A of AGLI cross section library using the output results obtained by GXS2000 as input to the EDIT. This code is also used to retrieve, list and plot the data stored on the File A.

ARCADIA

The code ARCADIA is used to adjust the data on the File A using the on-line graphic display and light pen system.

The most distinctive feature of the code ARCADIA is found in the procedure to adjust cross section data on the AGLI library utilizing information obtained by the so-called LSQ method.[15]

Since this information is given as a ratio of coarse group cross sections (10~15 energy groups) before and after the adjustment, certain human intervention might be necessary to adjust the 1950 energy group cross section data in the AGLI library using such information. This human intervention is achieved by a conversation between man and machine using graphic display and light-pen pointing. Since detailed descriptions of the code are given in the references (16) (17), only brief descriptions which have direct concern with the adjustment by the LSQ method are given below.

Let $\tilde{\sigma}(u)$ and $\sigma(u)$ be the cross section at lethargy u after and before the adjustment respectively, and $\tilde{\sigma}_i$ be the adjusted coarse group cross section by the LSQ method, and σ_i be the unadjusted coarse group cross section. In the code the adjusted cross section $\tilde{\sigma}(u)$ is obtained by

$$\tilde{\sigma}(u) = \sigma(u) \times [\, Au^2 + Bu + C \,] \tag{48}$$

In Eq. (48), the constants A, B and C are fixed within each coarse group i and these are obtained to satisfy the following relations;

$$Au_i^2 + Bu_i + C = \frac{1}{2}\left(\frac{\tilde{\sigma}_i}{\sigma_i} + \frac{\tilde{\sigma}_{i-1}}{\sigma_{i-1}}\right) \tag{49}$$

$$Au_{i+1}^2 + Bu_{i+1} + C = \frac{1}{2}\left(\frac{\tilde{\sigma}_i}{\sigma_i} + \frac{\tilde{\sigma}_{i+1}}{\sigma_{i+1}}\right) \tag{50}$$

$$\int_{u_i}^{u_{i+1}} \sigma(u)\left(Au^2 + Bu + C\right) du = \tilde{\sigma}_i\,(u_{i+1} - u_i) \tag{51}$$

where u_i is the lower lethargy of the coarse group i.

All of necessary information for carring out the adjustment by Eq. (48) are supplied using the light-pen, key board or card reader; and the adjustment is carried out coarse group-wise.

The adjusted and unadjusted cross section data, $\tilde{\sigma}(u)$ and $\sigma(u)$, are displayed on the cathode ray tube simultaneously in order to check the adequacy of the adjustment carried out. An example of the CRT display is shown in Fig. 6.

Figure 4 shows an example of the flow to compile the AGLI cross section library.

6. Example of Neutronic Calculation Using AGLI/0

The AGLI/0 is a sort of the so-called secondary library which is not a direct collection of the results of differential measurements of cross sections, but is reduced to certain effective values and is rearranged conveniently as input to a spectrum calculation code.

The main purpose of AGLI cross section library is to supply neutron cross section data to the neutron spectrum calculation code SP2000 incorporated in the Modular Codeing System DOYC. A typical result of neutron spectrum calculated by using AGLI/0 in connection with DOYC is given in Fig. 5.

The result given in Fig. 5 is a neutron spectrum in FCA V-2 core where 10 different nuclides are contained. The computer CPU time necessary to obtaine the result was about 5 minutes on FACOM 230/60.

The AGLI/0 has also been used for evaluating a heterogeneity effect on criticality due to a plate cell structure in FCA V-1 core, by solving the 1950 energy group collision probability which can be calculated in DOYC.

Typical computer CPU time was about 25 minutes for solving the problem including 10 nuclides in 11 space regions on the same computer.

The neutron spectrum calculated by SP2000 is used as a weighting spectrum for collapsing 1950 energy group cross section of AGLI/0 into 50-100 energy group cross sections which are used for one dimensional criticality calculation.

After this one dimensional calculation, rather conventional method for space dependent group collapsing into fewer energy groups for two or three dimensional analysis is carried out.

The heterogeneity effect on criticality was analysed by the above procedure and the calculated result was 0.35% $\Delta k/k$ coresponding experimental value = 0.37.

From these test calculations, AGLI/0 in connection with DOYC system is considered to be able to solve various problems in reactor physics within a satisfied accuracy and reasonable computer CPU time.

For better understanding of the library and for future use of AGLI/0 to be adjusted, cross section data of infinitely dilute cross sections of fission and absorption stored on the File A and inelastic scattering cross sections stored on the File B are graphically given as the appendix.

Acknowlegements

The authors are grateful for the advice and encouragement from Dr. J. Hirota and wish to thank Dr. S. Katsuragi for various comments on cross section data.

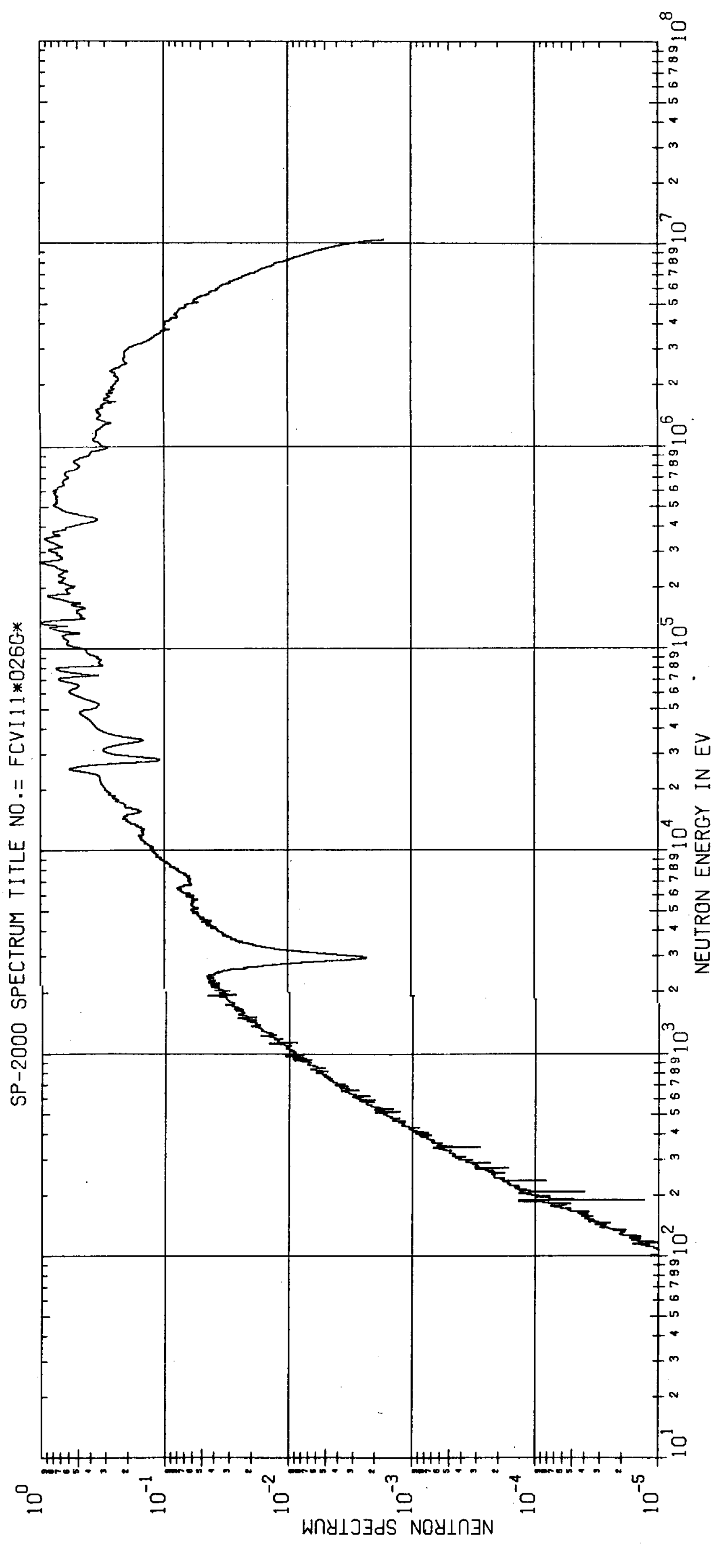

Fig. 5 Typical example of calculated neutron spectrum.

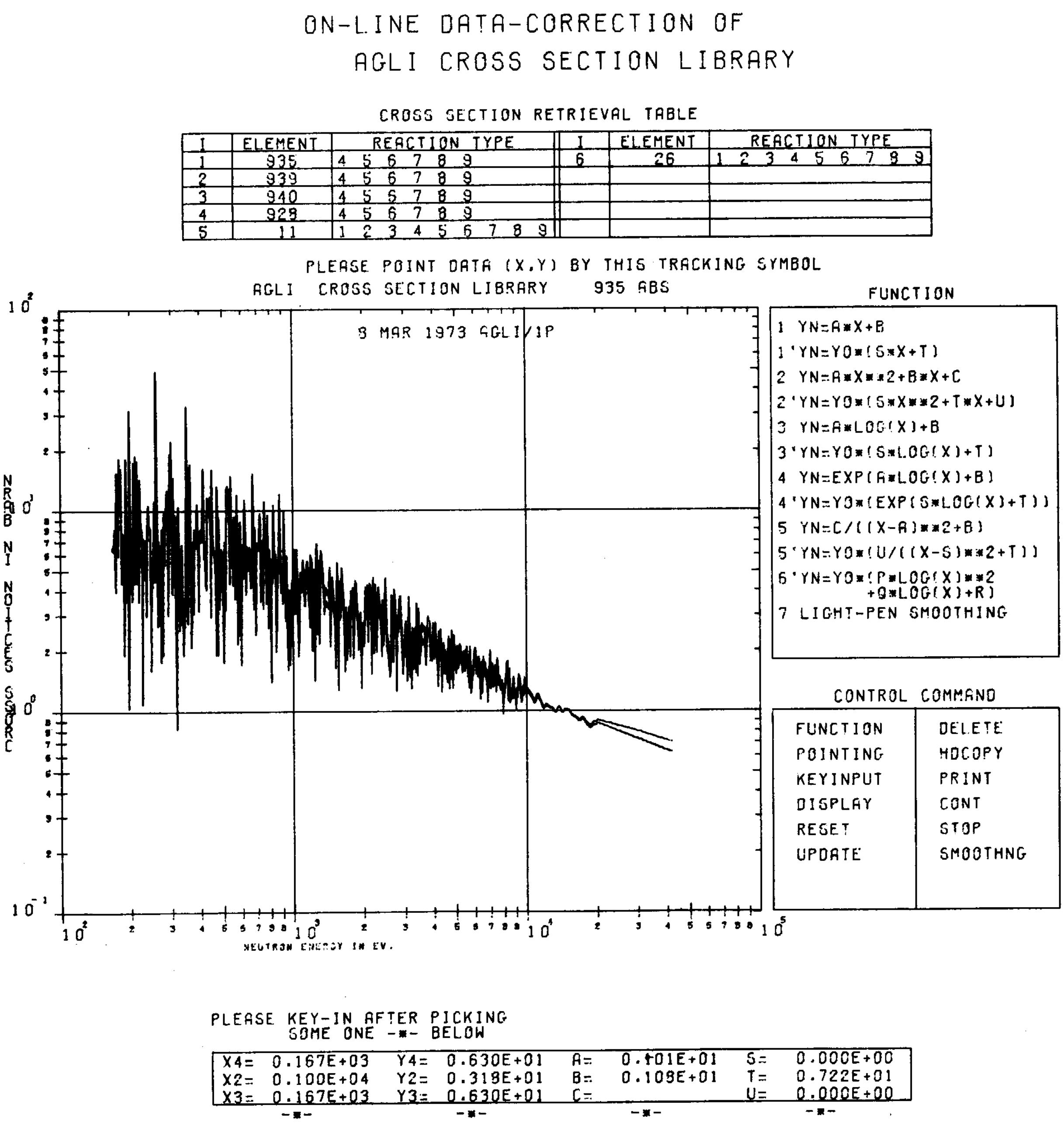

Fig. 6 Cross section display on CRT

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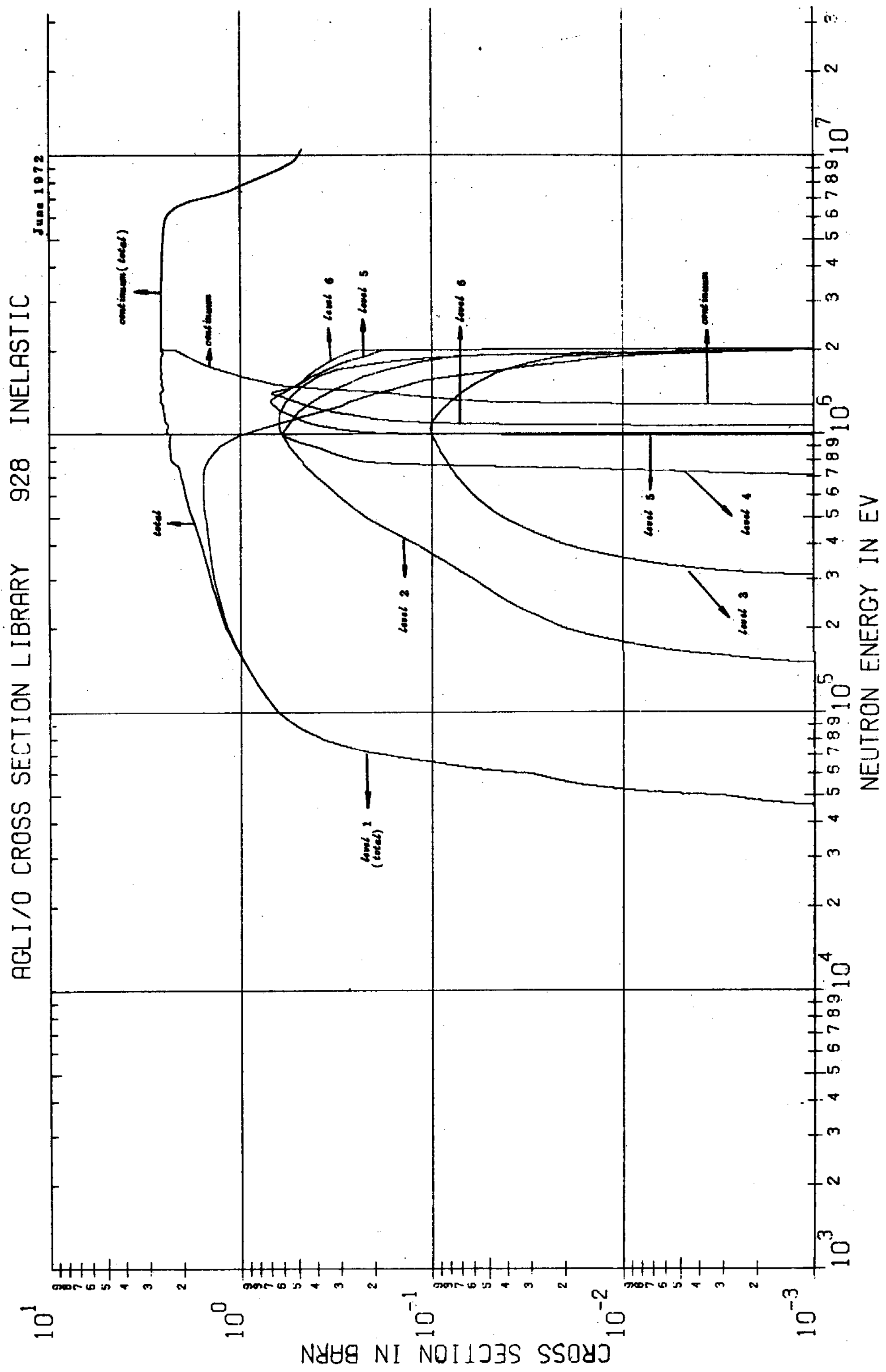
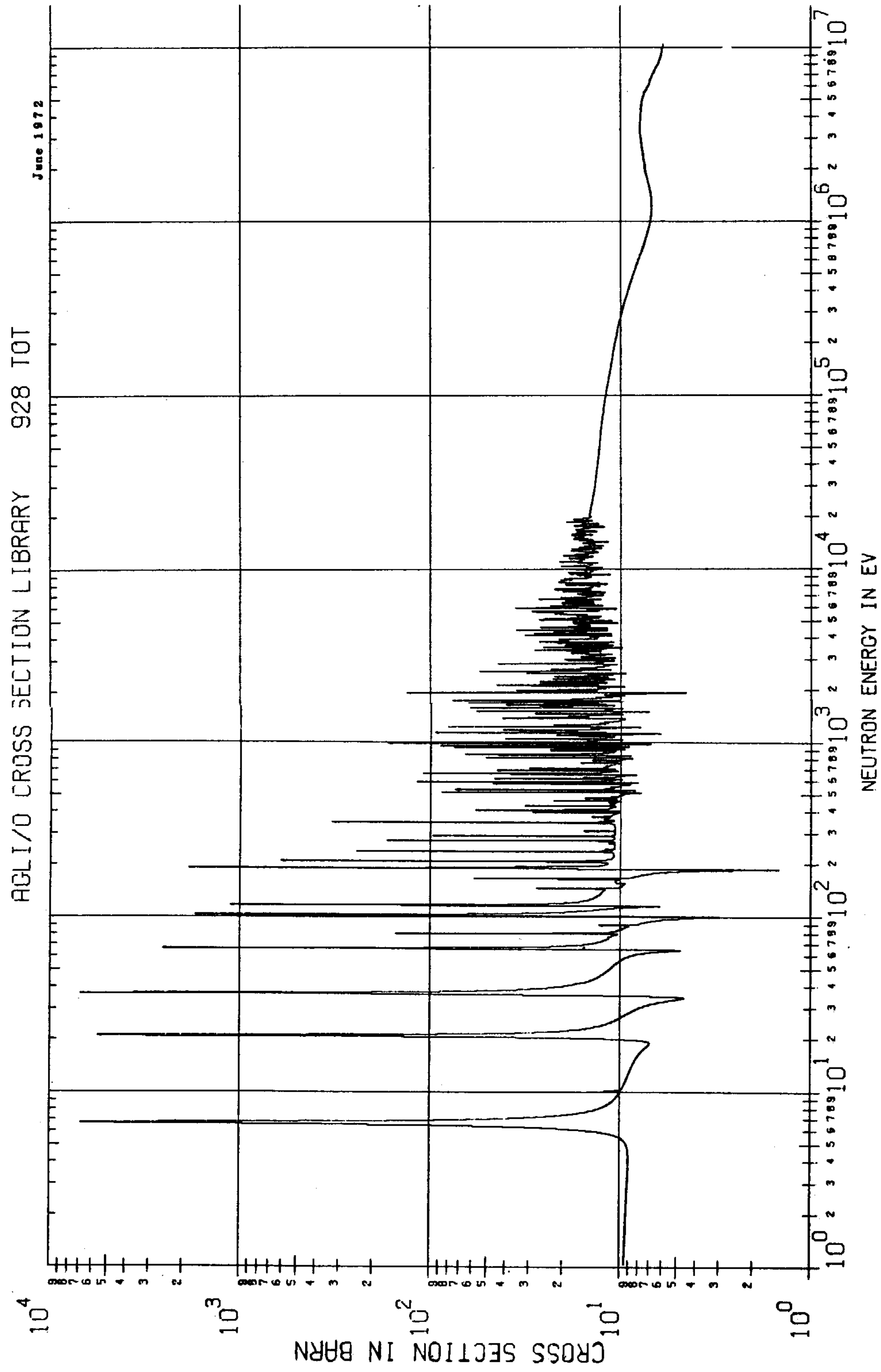
Appendix

Cross Section Data of U-238 and Pu-239 in AGLI/O Library

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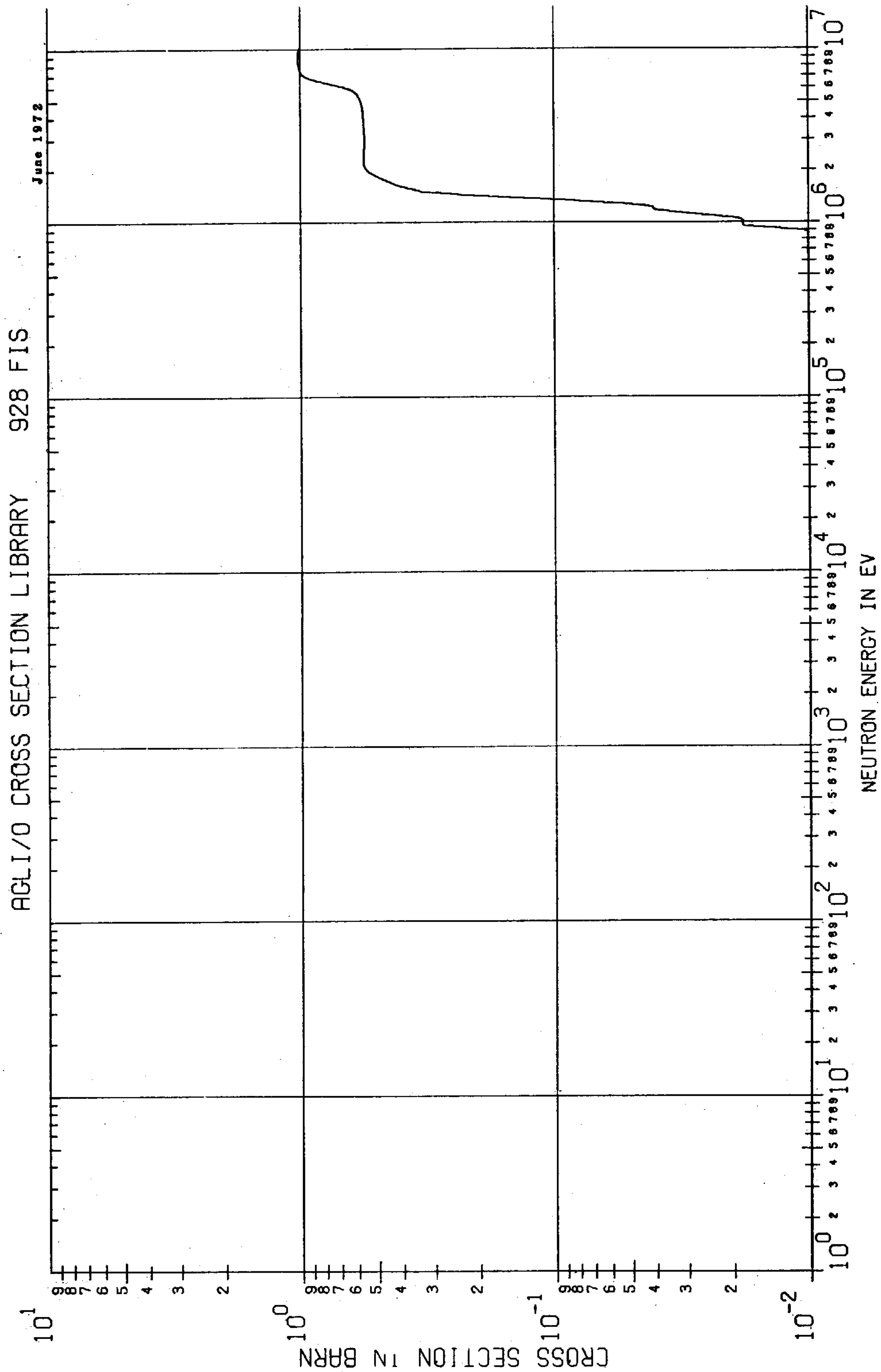
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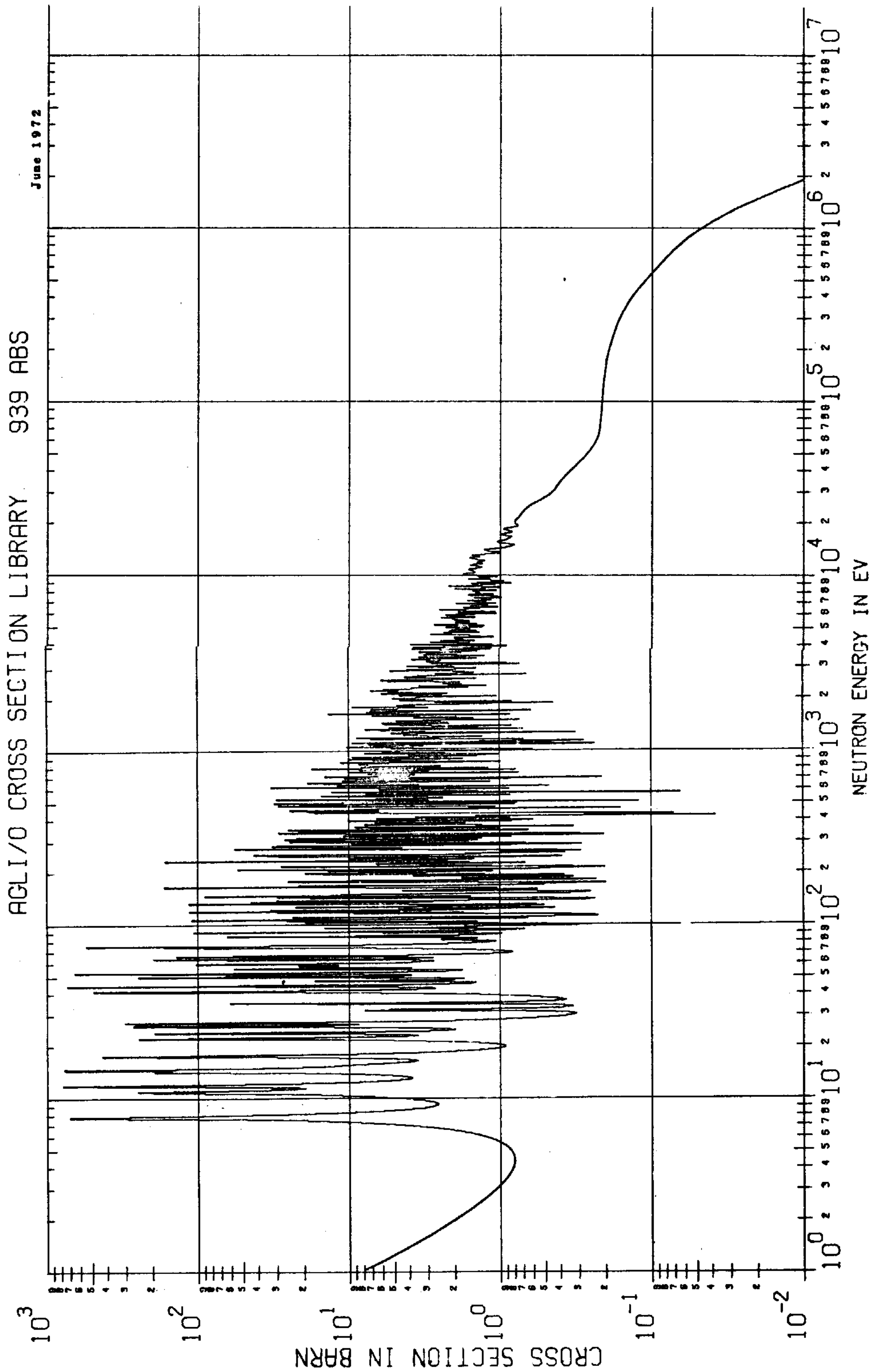
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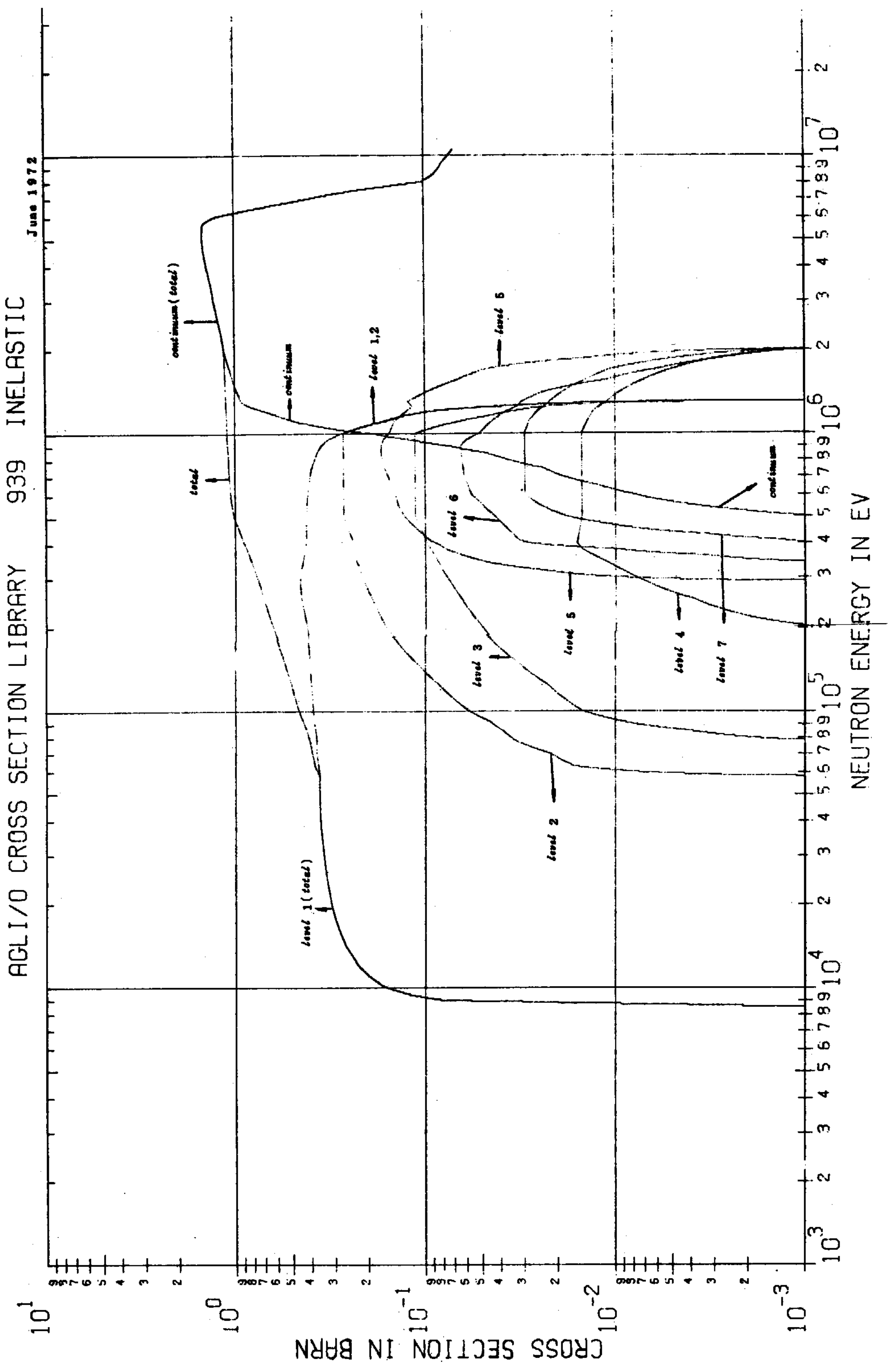
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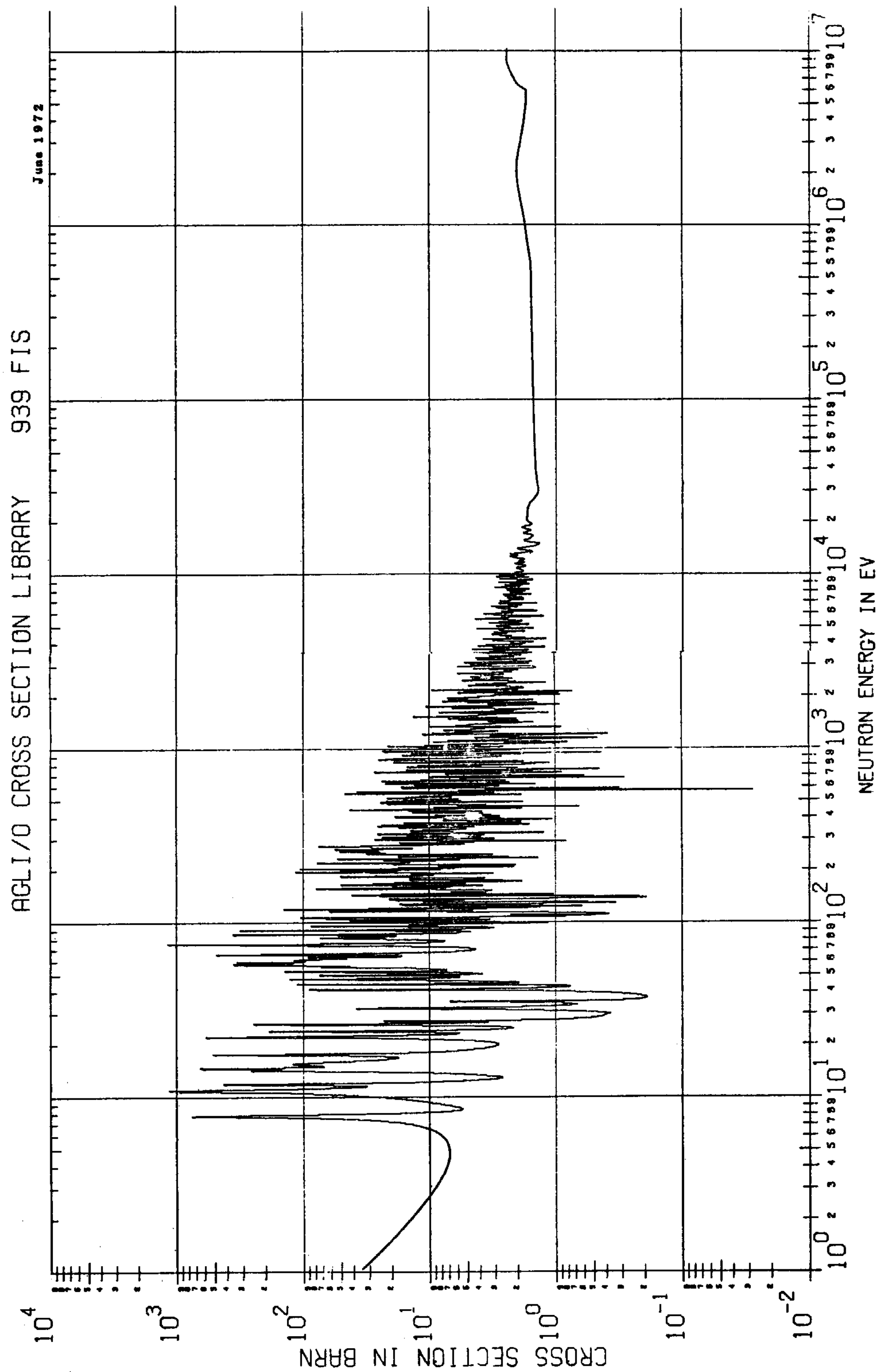
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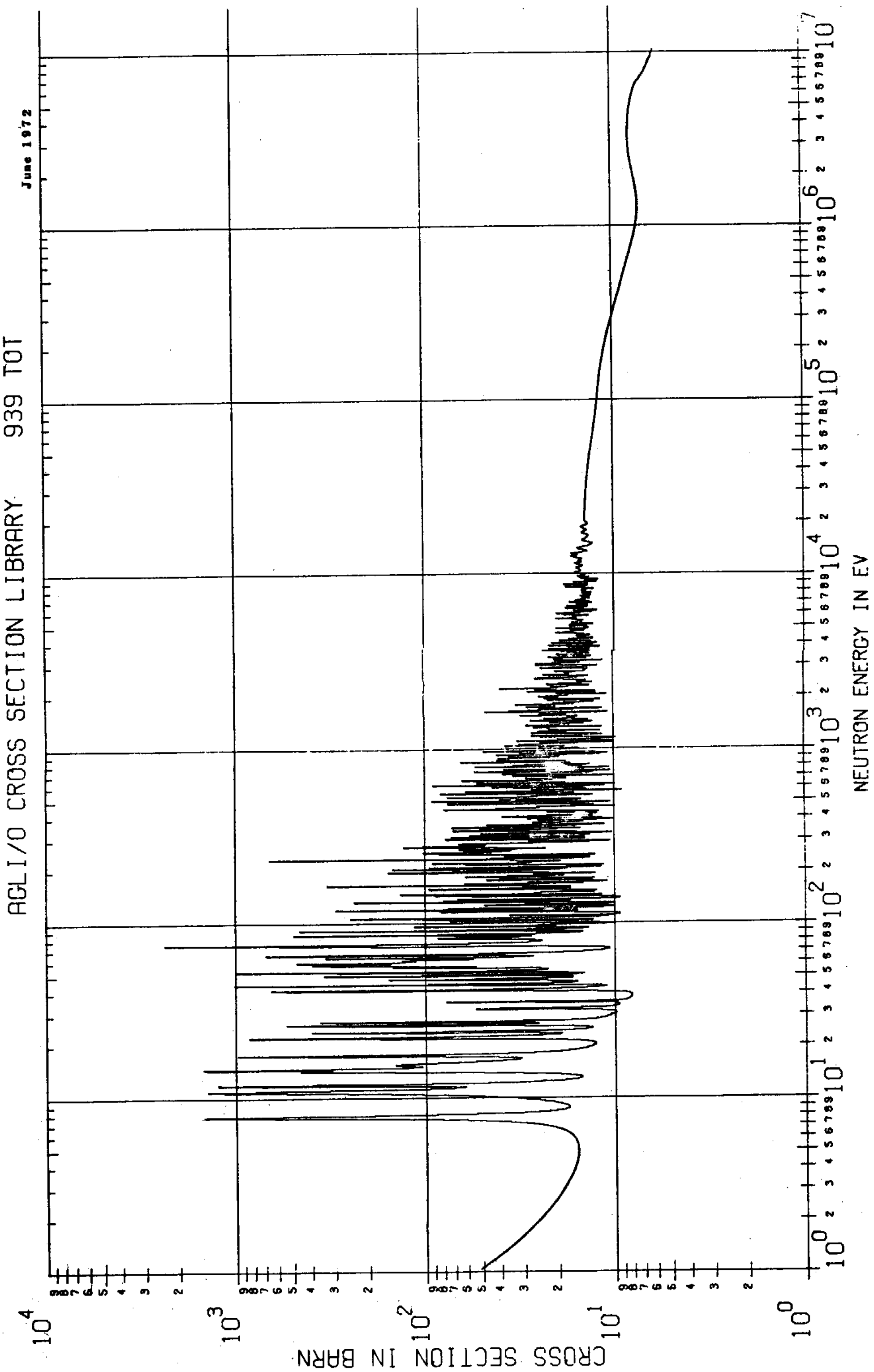
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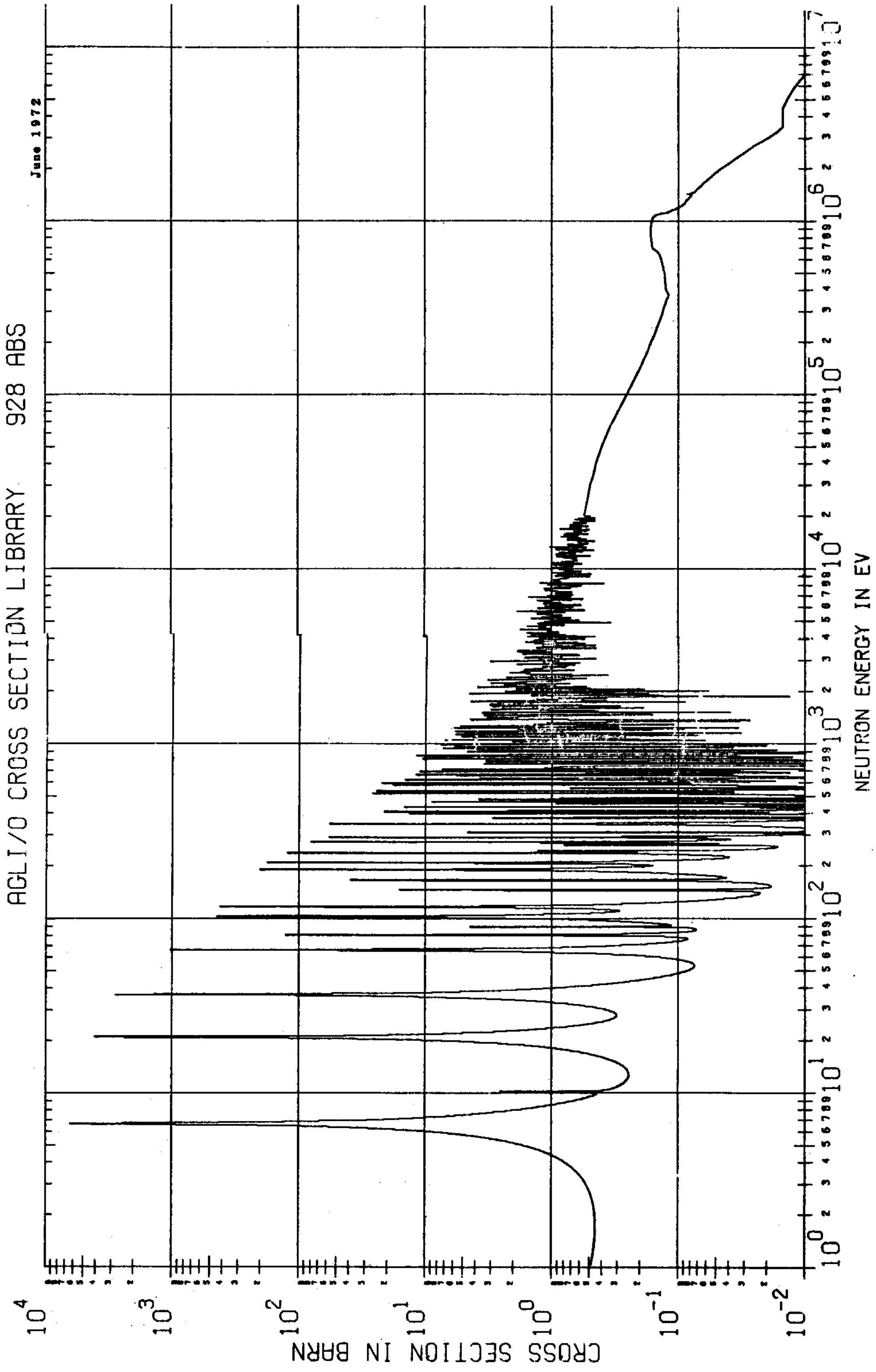
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