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PEACO-II: A CODE FOR CALCULATION OF EFFECTIVE CROSS SECTIONS IN HETEROGENEOUS SYSTEMS

January 1974

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JAERI-M 5527

PEACO-II : A Code for Calculation of Effective Cross Sections in Heterogeneous Systems

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(Received December 26, 1973)

The methods used in the PEACO-II code to solve the integral transport equations in heterogeneous systems are summarized; the systems consist of an infinite number of cells with slab, cylindrical, square or hexagonal geometry. The RABBLE Method is used to calculate the neutron slowing-down source, and the heterogeneity is treated by the first-flight collision probability method. For calculation of the collision probability, an interpolation method is introduced.

PEACO-II is a revised version of the PEACO code, and it is coded in FORTRAN-IV of the FACOM-230/60 machine. A core memory of 100 K bytes will be required for a problem having 30 regions in the cell, 10 materials including 3 resonance-absorbing materials, and 10 compositions.

JAERI－M 5527

PEACO－Ⅱ：非均質系における実効共鳴断面積計算コード

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石黒幸雄

（1973年12月26日受理）

平板，円筒，六方および正方格子非均質系で，衝突確率を用いて中性子減速方程式を解くPEACO－Ⅱコードに用いられている方法が要約される。衝突確率の計算に対して，精度・計算時間が共に優れた新しい内ソウ法が開発される。いわゆるRABBLE法が中性子の減速源を計算するのに用いられる。

PEACO－ⅡコードはFACOM－230／60計算機用FORTRAN－Ⅳで書かれており，次の問題を行うには100Kバイトのコアー・メモリーを必要とする。

30領域，10核種，3共鳴核種，10組成。

TABLE OF CONTENTS

LIST OF FIGURE

LIST OF TABLES

I. INTRODUCTION

Several computer codes have been developed for the purpose of directly and accurately evaluating resonance absorption, average neutron fluxes, and group cross sections in heterogeneous systems[1) - 7)]. However some codes, prepared for the computers with smaller core memories, need complicated preparation of input data and usage of some codes is restricted to special geometry. Other codes for general purpose require a considerable amount of computer time and would be too expensive to be used for practical problems.

Anyhow, Kier developed an excellent calculation-method of slowing-down source, the RABBLE Method, which saves largely running time and core memory of computer.[4), 5), 6)] In this method, the "fine-group" scattering rate is approximated by the "intermediate-group" scattering rate divided by the number of the fine group. It was shown by using the PEACO code that this approximation was very accurate when an adequate group structure was used for representing the fine and intermediate groups.[7)] It was also shown that the effect of the "self-scatter" neglected in the RABBLE code was quite insignificant.

The original PEACO code adopted the RABBLE Method but the usage of this code was rather complex. The neutron balance between different regions in a lattice cell was treated by a collision-probability method, and an interpolation method was used for calculating the collision probability. Since the most computer time is generally spent on the calculation of the regional neutron balance, an interpolation scheme is extremely useful for the calculation of the collision probability, in particular when the variety of the compositions with heavy resonance absorbers is few. In the revised code, PEACO-II, a new interpolation method is introduced for calculating the collision probability of two fuel-composition problem. The interpolation method introduced is

quite time-saving and accurate, and is extremely useful when the moderator cross sections are constant over the energy range under study. The microscopic scattering cross sections of sodium and iron below 25 KeV are self-contained in the Block Data form.

II. NUMERICAL METHOD OF CALCULATING NEUTRON FLUX DISTRIBUTION

We assume that heterogeneous systems are built up of an infinite number of "unit cells" and the neutron balance in a heterogeneous system can be described by using the first-flight collision probabilities. To reduce the numerical errors caused by the flat-flux assumption, each region of the system may be divided into subregions as many as necessary or possible. Then, assuming the isotropic elastic scattering, the neutron balance in a cell may be written by the neutron slowing down equation

$$V_i \Sigma_i(u) \psi_i(u) = \sum_{j=1}^{J} P_{ji}(u)\, V_j \sum_{k=1}^{K} S_{jk}(u) \tag{1}$$

$$S_{jk}(u) = \frac{1}{1-\alpha_k} \int_{u-\varepsilon_k}^{u} \exp\{-(u-u')\} \Sigma_{sjk}(u') \psi_j(u')\, du' \tag{2}$$

with

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 \quad \text{and} \quad \varepsilon = -\ln\alpha . \tag{3}$$

Here, the subscript i or j stands for the subregion number and the k corresponds to the nuclear species. P_{ji} is the effective probability in a unit cell that a neutron scattered isotropically in region j, into lethargy u, will have its first collision in region i, and other notation has the customary meanings.

By letting $V_i \psi_i(u) \exp(u) = \phi_i(u)$, we have

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By letting $V_i \psi_i(u) \exp(u) = \phi_i(u)$, we have

$$\Sigma_i(u)\phi_i(u) = \sum_{j,k} P_{ij}(u)\, S^o_{jk}(u) \tag{4}$$

with

$$S^o_{jk}(u) = \frac{1}{1-\alpha_k}\int_{u-\varepsilon_k}^{u} F_{jk}(u')\,du' \tag{5}$$

$$F_{jk}(u) = \Sigma_{sjk}(u)\phi_j(u)\ . \tag{6}$$

Here, note that the equations (4) and (5) for $\phi(u)$ is more simple than Eqs. (1) and (2). The factor exp(u) multiplied to $\psi_i(u)$ may serve to reduce round errors appeared in the recurrence formula introduced later for the numerical calculation of slowing-down source, since the energetic depletion of $\phi_i(u)$ due to resonance absorption is more slow than that of $\psi_i(u)$.

For the computation of the neutron spectra $\phi_i(u)$ on discretes lethargy meshes, we use the RABBLE Method developed by Kier [4), 5)]. Hence, the lethargy meshes used are assumed to be extremely narrow compared to the maximum lethargy gain per collision with the heaviest nuclei in the system under consideration. Furthermore, we assume that the resonance cross sections are given at the mid point of this fine group and the collision probabilities $P_{ij}(u)$ is constant over a fine group. Now define

$$\phi^m_i = \int_{u_o}^{u_+} \phi_i(u)\,du \tag{7}$$

$$F^m_{jk} = \int_{u_o}^{u_+} F_{jk}(u)\,du = \Sigma^m_{sjk}\phi^m_i \tag{3}$$

where u_+ and u_o are upper and lower lethargy bounds, respectively, corresponding to

the fine group m. Then, the integration of Eq. (4) over the lethargy range from u_o to u_+ gives

$$\Sigma_i^m \phi_i^m = \sum_{j,k} P_{ji}^m Q_{jk}^m \tag{9}$$

where

$$Q_{jk}^m = \frac{1}{1-\alpha_k} \int_{u_o}^{u_+} du \int_{u-\xi_k}^{u} F_{jk}(u')\, du' \tag{10}$$

$$\cong \frac{\Delta u_m}{1-\alpha_k} \int_{u_o-\xi_k}^{u_o} F_{jk}(u)\, du$$

$$= Q_{jk}^{m-1} + \frac{\Delta u_m}{1-\alpha_k} \left\{ F_{jk}^m - (F_{jk})_{m-L_k^m}^m \right\} \tag{11}$$

with

$$(F_{jk})_{m-L_k^m}^m = \int_{u_- -\xi_k}^{u_o-\xi_k} F_{jk}(u)\, du. \tag{12}$$

Here, u_- is the lower bound of the $(m-1)$th fine group and L_k^m is an integral number of groups which corresponds to the maximum lethargy gain by elastic collision. Note that the self-scatter was neglected in deriving the above equations because the effect of the self-scatter was shown to be quite insignificant[7]. It is assumed that the scattering rate given by Eq. (12) can be approximated by using the intermediate-group scattering rate[4]. The accuracy of this approximation was also investigated and shown to be quite satisfactory when an adequate group structure is adopted for representing the fine and intermediate groups[7]. Assuming the asympotic flux distribution below the lethargy range under consideration, the neutron flux distribution can recussively be calculated, until the entire energy range of interest is covered.

III. INTERPOLATION METHOD FOR COLLISION-PROBABILITY CALCULATION

We consider a heterogeneous system built up of an infinite number of lattice cells. This cell may consist of several compositions and each number referring to the compositions corresponds generally to few different region-numbers. The resonance-absorbing isotopes are contained in some compositions (fuel-compositions) and other compositions are assumed to have constant cross sections. Now, for such a system we select a resonance absorber, say ^{238}U, and define the microscopic resonance cross per the absorber under consideration in the fuel compositions by

$$\overline{\sigma}_l(E) = \frac{1}{N_l} \sum_k N_{lk} \sigma_k(E) \qquad (N_l \neq 0) \tag{13}$$

where l corresponds to the fuel composition, the summation on k is extended over all the resonance absorbers, $\sigma_k(E)$ is the microscopic total cross section of the k'th absorber, and N_l and N_{lk} are the atomic number densities of the absorber under consideration and of the k'th resonance absorber in the l'th composition, respectively.

Some fuel compositions may have the same relative densities N_{lk}/N_l, hence the same value for $\overline{\sigma}_l(E)$. In such compositions, the value of $\overline{\sigma}_l(E)$ can be considered as a common variable to express the macroscopic total cross sections. There may be another possibility to find such an independent variable in other fuel compositions. In the present treatment, it is assumed that the macroscopic total cross sections can be expressed or be approximated by using at most two such independent variables.

Now, let us denote by Σ_{oJ} the smallest macroscopic total cross section made by the nonresonance isotopes in the fuel compositions belonging to the independent variable $\overline{\sigma}_J(E)$. Let us introduce new variables defined by

$$X_J = (N_J \overline{\sigma}_J + \Sigma_{oJ}) \bar{\ell}_J \qquad J = 1, \ IMAX, \tag{14}$$

where IMAX is the number of the independent variables (IMAX $\leqq$ 2) and $\bar{\ell}_J$ is the averaged value of double widthes of the regions which belong to the variable $\overline{\sigma_J}(E)$. Then, the collision probability, P_{ji} (u), in Eq. (1) or (5) can be considered to be a function of X_J (J=1, IMAX).

In the PEACO-II, two kinds of computational methods are adopted for the calculation of the collision probability, P_{ji} (X_1, X_2): The first method is based on the interpolation of P_{ji} (X_1, X_2), which is used for X_1, $X_2 \leqq 9$. The calculation of the values of P_{ji} (X_1, X_2) needed for the interpolation is made by using the codes PATH-S and PATH-C, developed by Tsuchihashi, for slab and cylindrical geometries, respectively [8]. The second one uses the asymptotic expansion of P_{ji} (X_1, X_2) when X_1 or $X_2 \gtrsim 9$.

III-1 ONE RESONANCE-ABSORBING COMPOSITION PROBLEM (IMAX = 1)

It is easy to show [9, 10]

$$P_{ij}(X) \cong \eta_{ij} + \gamma_{ij} / X \qquad \text{for } X \Rightarrow \infty, \tag{15}$$

with

$$\eta_{ij} \equiv P_{ij} \ (X = \infty) \tag{16}$$

and

$$\gamma_{ij} \equiv \begin{cases} \left[P_{ij}(X) - \eta_{ij} \right] X & X \Rightarrow \infty \quad \text{if } i \in \text{RAC} \\ 0 & \text{otherwise,} \end{cases} \tag{17}$$

where RAC stands for the resonance-absorbing composition.

The above equation (15) is used for $X > 9$ and the generalized Dancoff factor γ_{ij}, given by Eq. (17), is calculated at $X = 9$, while η_{ij} is obtained as the value of $P_{ij}(X)$ at $X = 10^4$.

On the other hand, for the range of $X < 9$ we introduce a new variable

$$Z \equiv \frac{X}{X+1} \quad \text{or} \quad X = \frac{Z}{1-Z} . \tag{18}$$

The interpolation of the collision probability is made by using the values of $P_{ij}(X)$ calculated on ten points of the variable Z with $\Delta Z = 0.1$ and the Lagrangian three points interpolation formula [11]

$$f(Z_o + \delta Z) = \frac{1}{2} u (u-1) f_{-1} + (1-u^2) f_o + \frac{1}{2} u (u+1) f_1 \tag{19}$$

where

$$u = \frac{\delta Z}{\Delta Z} \quad \text{and} \quad |u| \leqq 1 . \tag{20}$$

The values of Z and X used for the interpolation are shown in TABLE 1.

III-2 TWO RESONANCE-ABSORBING COMPOSITION PROBLEM (IMAX=2)

We can prove also for the two resonance-absorbing composition problem

$$P_{ij}(X_1, X_2) \cong \begin{cases} P_{ij}(\infty, X_2) - \gamma^1_{ij}(X_2)/X_1 & X_1 > 9 , \ X_2 \leqq 9 \quad (21) \\ (\gamma^1_{ij}(X_2) \equiv 0 \quad \text{if } i \notin X_1) & \\ P_{ij}(X_1, \infty) - \gamma^2_{ij}(X_1)/X_2 & X_1 \leqq 9 , \ X_2 > 9 \quad (22) \\ (\gamma^2_{ij}(X_1) \equiv 0 \quad \text{if } i \notin X_2) & \end{cases}$$

$$P_{ij}(X_1, X_2) \begin{cases} P_{ij}(\infty,\infty) - \gamma_{ij}^{\infty}/X_1 & (i \in X_1) \\ P_{ij}(\infty,\infty) - \gamma_{ij}^{\infty}/X_2 & (i \in X_2) \\ P_{ij}(\infty,\infty) & (\text{otherwise}) \end{cases} \qquad X_1, X_2 > 9 \tag{23}$$

Here, P_{ij} and γ_{ij} in Eqs. (21) and (22) are calculated by the exact same way as the case of the interpolation of $P_{ij}(X)$ for $X \leq 9$ in the one resonance-absorbing composition problem.

For the range of X_1, $X_2 \leqq 9$, we again introduce two variables

$$Z_I = \frac{X_I}{1 + X_I} \quad \text{or} \quad X_I = \frac{Z_I}{1 - Z_I} \qquad (I = 1, 2) \tag{24}$$

and $P_{ij}(X_1, X_2)$ is interpolated on these variables by using one of the following formulae[11]

ⓒ
$$f(Z_{10} + \delta Z_1, Z_{20} + \delta Z_2) = \left\{ 1 - \frac{1}{2}(3 - u - v)(u+v) \right\} f_{oo} + (2 - u - v)(uf_{10} + vf_{01}) + uvf_{11} + \frac{1}{2}u(u-1)f_{20} + \frac{1}{2}v(v-1)f_{02}, \tag{25}$$

with $$u = \frac{\delta Z_1}{\Delta Z}, \quad v = \frac{\delta Z_2}{\Delta Z}, \quad |u|, |v| \leqq 1, \tag{26}$$

ⓒ
$$f(Z_{10} + \delta Z_1, Z_{20} + \delta Z_2) = \frac{1}{2}u(u-1)f_{-10} + \frac{1}{2}v(v-1)f_{0-1} + (1 - uv - u^2 - v^2)f_{oo} + \frac{1}{2}u(u - 2v - 1)f_{10} + \frac{1}{2}v(v - 2u + 1)f_{01} + uvf_{11}, \tag{27}$$

ⓒ
$$f(Z_{10} + \delta Z_1, Z_{20} + \delta Z_2) = (1-u)(1-v)f_{oo} + u(1-v)f_{10} + v(1-u)f_{01} + uvf_{11}. \tag{28}$$

The choice of Eq. (25), (27) or (28) depends on the values of Z_1, Z_2 on which the P_{ij} (X_1, X_2) is to be interpolated.

III-3 CONSERVATION AND RECIPROCITY OF COLLISION PROBABILITY

The first-flight collision probability must satisfy two important relations, that is, the conservation law

$$\sum_i P_{ij} = 1 \qquad \text{for all } i \tag{29}$$

and the reciprocity relation [9, 10]

$$V_i \Sigma_i P_{ij} = V_j \Sigma_j P_{ji} \quad \text{for all } i, j . \tag{30}$$

In the PEACO-II, at first, the values of P_{ij} are calculated only for $j \leqq i$ by Eqs. from (15) to (28). Then, the collision probabilities satisfying Eqs. (29) and (30) are successively obtained by the following equations starting from i=1.

$$P_{ij}^* = \frac{1-\beta_1}{\beta_0} P_{ij} \quad , \quad P_{ji}^* = \frac{1-\beta_1}{\beta_0} P_{ji} \quad (j=i, J) \tag{31}$$

where

$$\beta_0 = \sum_{j=i}^{J} P_{ij} \quad \text{and} \quad \beta_1 = \sum_{i=1}^{j-1} P_{ij}^* \tag{32}$$

with

$$P_{ij} = V_j \Sigma_j P_{ji} / (V_i \Sigma_i) \qquad \text{for } j > i . \tag{33}$$

The collision probabilities P_{ij}^* given by Eq. (31) will readily be known to satisfy Eqs. (29) and (30).

Using the interpolation and the asymptotic expansion, combined with the method mentioned above, we can guarantee the accuracy of 0.1% for the calculation of the collision probability, including the one resonance-absorbing composition problem.

III-4 CONSIDERATION OF RESONANCE SCATTERING BY LIGHT AND INTERMEDIATE WEIGHT NUCLEI

In a fast reactor, the Doppler coefficient of reactivity comes from rather higher energies, where all the cross sections are in general considered to vary with energy. Especially an accurate Doppler coefficient can not be estimated without taking account of the resonance scattering by light or intermediate weight nuclei, such as sodium and iron. Hence, for an accurate estimation of the effective cross sections in resonance energy, the variation with energy should be considered for all the cross sections in the system under consideration.

The variation of the cross sections of these nuclei is usually quite slow, compared to those of heavy resonance-absorbers. This slow variation will bring also a slowly energetic variation in the collision probability P_{ij}. We assume that this slow variation of the collision probability can be considered by representing the resonance-scattering cross sections by step function of energy. New calculation is performed for $P_{ij}(Z_{1\ell}, Z_{2m})$ (ℓ, m=1, 10) on the each intermediate group where the resonance-scattering cross sections change by step. This is what is done in the PEACO-II code for the treatment of the resonance scattering cross section. Figure 1 shows the resonance-scattering cross sections, represented by step function, which were taken from the ENBF/B version III and is stored as a Block Date in the code.

IV. RESONANCE CROSS SECTIONS AND GROUP STRUCTURE

Considerable amount of computing time is usually spent on the calculation of resonance cross sections in a spectrum calculation code. Moreover, the cross sections for a fixed energy range and temperature have to be repeatedly calculated if both the calculating parts of the cross sections and of the flux are included in one code. Hence, in order to eliminate the wastefulness the PEACO-II code reads the resonance cross sections from the library tapes prepared beforehand. We can use the code, MCROSS-2, developed by Takano [12] for the preparation of the library tapes. This code adopts a modified Vogt's expression for the resonance cross section representation. For unresolved resonance region, the resonance parameters needed for calculating the resonance cross sections can be generated by a ramdom sampling technique [13]. For this purpose, we can use a code, BABEL [14], which generates sequences of the resonance parameters over the energy range of interest and writes them in a library tape for later use to the MCROSS-2 code.

From the experience gained by the use of the PEACOand PEACO-II codes, we recommend a group structure for the fine and intermediate groups, which is shown in TABLE II.

V. INPUT AND OUTPUT DESCRIPTION

The PEACO-II code is written by FACOM-230/60 FORTRAN which is a standard FORTRAN commonly used. The following general restrictions must be noted for the use of a computer with core memories less than 128 K bytes.

Parameter	Range
Regions	$1 \leqq KREG \leqq 30$
Materials	$1 \leqq KMAT \leqq 10$
Resonant materials	$1 \leqq KRES \leqq 3$
Compositions	$1 \leqq KCOMP \leqq 10$
Resonance-absorbing compositions	$1 \leqq KCOMPF \leqq 2$
Geometries	homogeneous, plan, cylindrical, square, hexagonal

Card	FORMAT	Variables	Description
1	18A4	TIL (I)	Problem identification
2	1216	KREG	No. of regions ($\leqq 30$)
		KMAT	No. of materials ($\leqq 10$)
		KRES	No. of resonance-absorbing nuclides ($\leqq 3$)
		KCOMP	No. of compositions ($\leqq 10$)
		KCOMPF	No. of fuel compositions ($\leqq 2$)
		KTEMP	No. of temperatures ($\leqq 3$)
		KBG	No. of broad groups ($\leqq 40$)
3	1216	ISH	-2 : Homogeneous
			-1 : Plane
			0 : Cylindrical
			1 : Square

Card	FORMAT	Variables	Description
			2 : Hexagonal
		NSYM	0 : Nonsymmetrical geometry
			1 : Symmetrical plane geometry
		NCELL	No. of unit cells which is considered in the calculation of P_{ij}.
		LIMIT	Maximum path length in unit of integral number of cm beyond which the neutron path is neglected.
		IBOUND	0 : Isotropic boundary condition at the outer boundary of the cell.
			1 : Perfect reflection boundary condition.
			2 : Fixed reflection boundary condition.
4	1216	NPLOT	$\neq 0$: Intermediate group flux is plotted by the CALCOMP graph plotter.
		LISTR	$\neq 0$: Intermediate group flux in each region is printed.
		LISTS	$\neq 0$: Intermediate group flux in each sub-region is printed.
		MORE	$= 0$: For the last problem, otherwise MORE $\neq 0$

For the case of ISH = -2, the following cards of No. 5~7 are not necessary.

5	1216	(MAIN (I), I=1, KCOMPF)	No. of the main resonance material in the I'th fuel composition.
6	1216	(NCORS (I), I=1, KCOMP)	$= 0$: Nonresonant composition (moderator composition)
			$\leqq 2$: The I'th composition corresponds to the NCORS (I)'th resonance-absorbing composition.

Card	FORMAT	Variables	Description
7	216, E12.5	(NCOMP (I),	Composition number of the I'th region.
		NSUBR (I),	Subregion number of the outer boundary of the I'th region.
		RMAX (I), I=1, KREG)	Distance from center to the outer boundary of the I'th region.
8	1216	(NTEMP (I), I=1, KCOMP)	Assignation of temperature number to each composition.
9	6E12.5	(TEMP (I), N=1, KTEMP)	Temperature (°K)
10	6E12.5	(EN (I), I=1, KBG+1)	Energy boundaries of coarse groups.
11	A4, 8X, 5E12.5, I6	(NUCLID (I),	Nuclide identification
		AMU (I),	Atomic mass (AMU)
		SIGA (I),	Capture,
		SIGF (I),	Fission,
		SIGS (I),	Scattering cross sections for E ≥ starting energy
		VCAP (I),	2200-m/sec value of I/V absorption cross section
		MAOPT (I),	=1 corresponds to natural iron, =2 to sodium
12	6E12.5	(DEN (I, J), J=1, KCOMP), I=1, KMAT)	Atomic number density (atoms/(barns-cm)) of the J'th composition.

The following card is not needed for NPLOT=0.

13	1216	(NREGP (I), I=1, KREG)	≠0 : The neutron flux is plotted.

Each output quantity has its own self-evident description and their notation will be

seen in Ref. (7). We can plot the results for the intermediate group fluxes and the plotting is made using a subroutine GPLOT 1 [15].

ACKNOWLEDGMENT

The author wishes to thank Messrs. H. Takano and A. Hasegawa for their valuable suggestions on the coding. Thanks are also due to Dr. S. Katsuragi for his kind advice in English translation.

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ACKNOWLEDGMENT

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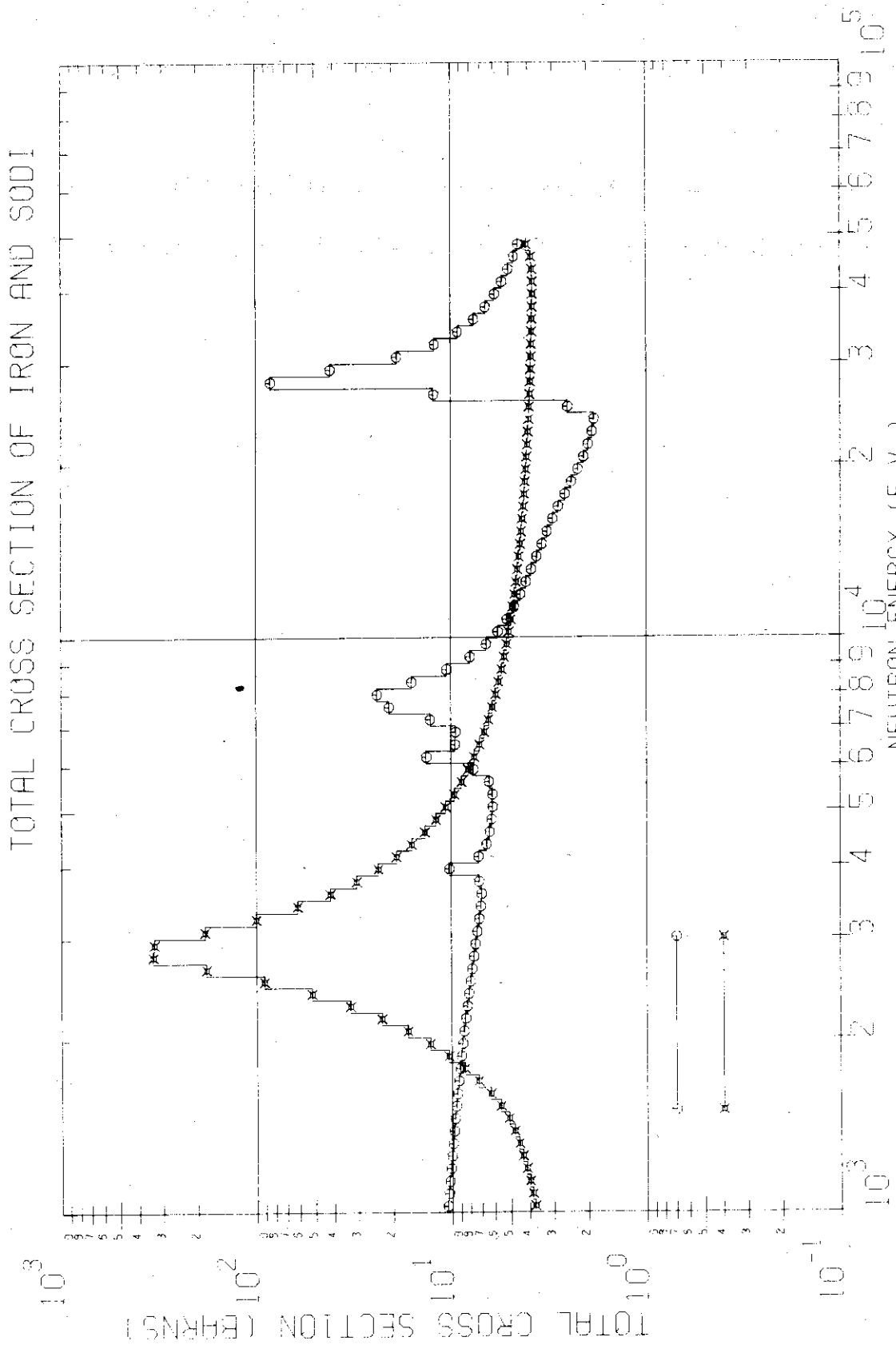

FIG. Total Cross Sections of Natural Iron and Sodium, taken from ENDF/B-II

TABLE I The values of Z and X used for the interpolation of collision probability

No.	Z	X
1	0	0
2	0.1	0.111111
3	0.2	0.25
4	0.3	0.428571
5	0.4	0.666667
6	0.5	1.
7	0.6	1.5
8	0.7	2.333333
9	0.8	4.
10	0.9	9.
11	0.9999	10^4

TABLE II A recommended structure of intermediate and fine groups for the use of the PEACO-II code

Upper energy (eV)	Lower energy (eV)	Lethargy [a]	No. of intermediate groups	No. of fine groups [b]	Mesh width of intermediate groups	Mesh width of fine groups
23250	4650	1.1513	2303	10	0.0005	0.00005
4650	465	2.3026	2303	10	0.001	0.0001
465	46.5	"	767	10	0.003	0.0003
46.5	4.65	"	460	5	0.005	0.001
4.65	0.465	"	230	2	0.01	0.005

a) These lethargy widths except for the first group are selected to not exceed the maximum lethargy gain per collision with deuteron.

b) This shows the number of fine groups in an intermediate one.