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RICM 2

A Codo for Solving the Slowing Downs of Neutrons over Many Resonance Levels in Two-Region Lattices

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日本原子力研究所

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正　誤　表

頁,	行	誤	正
表	紙	A Codo for.....	A Code for.....
偶数頁,	ハシラ	RICM2-A : Code for.....	RICM2 : A Code for.....
6,	9 ↓	$E>E_2(E_n=\cdots$	$E\geq E_2(E_n=\cdots\cdots$
10,	4 ↓	IEGID	IEGID$\begin{pmatrix}\mathrm{A}\\ \mathrm{D}\\ \mathrm{P}\end{pmatrix}$
〃	〃	.....E. R.	.....E. R. to be added, deleted or printed out.
10,	10 ↓	ISID	ISID$\begin{pmatrix}\mathrm{A}\\ \mathrm{D}\\ \mathrm{P}\end{pmatrix}$
〃	〃	.....isotope.	.....isotope to be added, deleted or printed out.
11,	8 ↓	$=1:\sigma_S$	$=1:\sigma_T$
11,	9 ↓	$=2:\sigma_T$	$=2:\sigma_S$
11,	13 ↓	$=1:\sigma_f$	$=1:\sigma_c$
11,	14 ↓	$=2:\sigma_c$	$=2:\sigma_f$

RICM2 : A Code for Solving the Slowing Downs of Neutrons over Many Resonance Levels in Two-Region Lattices

Summary

A new code RICM2 is programed which solves the neutron slowing downs continuously over a wide energy range covering many resonances of no more than two kinds of nuclides in a two-region lattice.

In this report descriptions are given of the followings : resonance cross sections, collision probabilities in two-region lattices, numerical solution of the slowing down equations and clear-cut definitions of various reaction rates, average cross sections and effective resonance integrals. An interesting parameter which indicates relative distributions of absorptions by two nuclides are also introduced.

A brief description of the programs and directions for their use conclude the report together with sample problems.

July, 1968

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RICM2：２領域格子系における多数レベル連続減速計算コード

要　　旨

２種までの共鳴核種を含む２領域格子系で，多数の共鳴レベルを含む広いエネルギー範囲にわたって，中性子の減速を連続的に解く計算コード RICM２ を作成した．

この報告には，共鳴断面積，２領域での衝突確率，減速方程式の解法と各種反応率，平均断面積，実効共鳴積分等の明確な定義が記され，２核種による吸収の相対的分布を示す興味深いパラメータも導入されている．最後にプログラムの簡単な内容および使用法が例題と共に記されている．

この計算コードは日本原子力研究所の原子力コード委員会において開発された．

１９６８年７月

日本原子力研究所原子力コード委員会

非均質炉解析コード開発小委員会

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1. Introduction

A series of efforts made for the calculation of the resonance absorption in heterogeneous systems seems to have come to an end when appearances were made of such computer codes as ZUT[1] and RICM[2], which solve numerically the integral transport equations formulated by use of collision probabilities.

These programs, however, were meant mainly for the calculation of the ^{238}U resonance absorption which is an important quantity for slightly enriched uranium thermal reactors. Only one kind of resonant nuclide is allowed in a lattice and resonances are treated level by level separately. In order to estimate the resonance overlapping effect of such combinations of two kinds of nuclides as, ^{235}U-^{238}U in highly enriched uranium fuels, or ^{239}Pu-^{238}U and ^{239}Pu-^{240}Pu in irradiated or PuO_2-UO_2 fuels, the above restrictions had to be removed. Another problem of solving the neutron slowing down equations over a wide range of energies containing many resonance levels, also interested us in connection with the calculation of the ^{235}U or ^{239}Pu resonance absorptions.

A new code RICM2 was programed so that it can handle the slowing down of neutrons over a wide energy range in a two-region lattice consisting of a fuel and a moderator region. The number of regions is limited to two, compared with five in the RICM, because of the consideration on computer memories. Not more than two resonant nuclides are permitted in the fuel region by the same reason and only one of them can be fissionable.

In the following chapters 2, 3 and 4, expressions for various cross sections, a solution of resonance neutron flux in the lattice, and definitions of reaction rates, effective cross sections and resonance integrals are presented in the above order.

The descriptions, and manuals for use, of the two programs RICM2-MAIN and RICM2-LTE are given in the last two chapters 6 and 5, the latter preparing the cross section library for the former's use.

2. Cross sections

Various models have been proposed to reproduce the resonance cross sections obtained experimentally by use of level parameters. They originate from the multilevel-multichannel formula based on the theory of nuclear physics. But it is desirable to assign parameters to each level separately to calculate the Doppler-broadened cross sections analytically to some extent. Along this line, there is well known Breit-Wigner's single level formula, and resonance parameters for its use are compiled in BNL-325 2nd ed. suppl. No. 2. The level parameters evaluated and compiled by SCHMIDT *et al.*[3] are also trusted. Independent of the above approach, ADLER-ADLER[4,5] have made successful efforts to obtain single-level type resonance parameters for each level by trial and error starting from the Wigner-Eisenbud formalism.

In section 2.1, two calculation methods of the resonance cross sections adopted in the RICM2 are presented;

(a) Superpositions of interfering Breit-Wigner type line shapes.

(b) Multilevel method introduced by ADLER-ADLER.

In section 2.2, the approximate calculation methods of Doppler functions $\psi(\xi, x)$ and $\chi(\xi, x)$ will be discussed.

2.1 Various reaction cross sections

(a) Superpositions of interfering Breit-Wigner type line shapes

With the assumption that the cross sections at energy E are made up of the superpositions of single-level line shapes, each reaction cross section is expressed as follows, notations here being the same as those generally used.

$$\sigma_c(E) = \mathop{\mathrm{Sum}}_{i=1}^{NLVL} \sqrt{\frac{E_{ri}}{E}} \sigma_0^i \frac{\Gamma_{ri}}{\Gamma_i} \psi(\xi_i, x_i)$$

$$\sigma_f(E) = \mathop{\mathrm{Sum}}_{i=1}^{NLVL} \sqrt{\frac{E_{ri}}{E}} \sigma_0^i \frac{\Gamma_{fi}}{\Gamma_i} \psi(\xi_i, x_i)$$

$$\sigma_s(E) = \mathop{\mathrm{Sum}}_{i=1}^{NLVL} \sigma_0^i \left\{ \frac{\Gamma_{ni}}{\Gamma_i} \psi(\xi_i, x_i) + \gamma_i \chi(\xi_i, x_i) \right\} + \sigma_p$$

$$\sigma_T(E) = \sigma_c(E) + \sigma_f(E) + \sigma_s(E)$$

with

$$\sigma_0^i = 2.60 \times 10^6 \cdot g_J \frac{\Gamma_{ni}}{E_{ri} \Gamma_i}$$

$$\gamma_i = \sqrt{g_J \frac{\Gamma_{ni}}{\Gamma_i} \sigma_p / \sigma_0^i}$$

$$\xi_i = \Gamma_i / \Gamma_D^i \quad , \qquad \Gamma_D^i = \sqrt{4\, kT\, E_{ri} / A}$$

$$x_i = 2\,(E - E_{ri}) / \Gamma_i \quad , \qquad g_J = \frac{2J+1}{2\,(2I+1)}$$

Where $\mathop{\mathrm{Sum}}_{i=1}^{NLVL}$ signifies the superposition of resonance level which contribute to the cross section at energy E. The definition and some properties of the Doppler functions ψ and χ are given in section 2.2.

(b) Multilevel method

As discussed in (a) of the same section, the single level Breit-Wigner formula is, strictly speaking, valid only when a nuclide, like ^{238}U, has a small Γ/D ratio. A fissionable nuclide, however, has Γ/D frequently larger than 0.1. So, it arises the necessity of the multilevel-multichannel analysis for the expression of the cross sections for such a nuclide.

Starting from the Wigner-Eisenbud theory, Adler-Adler obtained a cross section shape consisting of the superposition of interfering Breit-Wigner type resonances. The cross section for a reaction (x) is,

$$\sqrt{E}\, \sigma^{(x)}(E) = \frac{C}{\sqrt{E}} 2\,(1 - \cos\omega)$$
$$+ C \cdot \mathop{\mathrm{Sum}}_{i=1}^{NLVL} \frac{\nu_i (G_i^{(x)} \cos\omega + H_i^{(x)} \sin\omega) + (\mu_i - E)(H_i^{(x)} \cos\omega - G_i^{(x)} \sin\omega)}{(\mu_i - E)^2 + \nu_i^2}$$
$$+ C\,(A_1^{(x)} + A_2^{(x)}/E + \cdots\cdots + B_1^{(x)} E + B_2^{(x)} E^2 + \cdots\cdots)$$

where

$$C = 6.52 \times 10^5 \text{ barns} \times \text{eV}$$

Here $\mu_i - i\nu_i$ represents the i-th pole of the collision matrix, so that μ_i represents the resonance energy and ν_i the corresponding half-width of the i-th level. The variable ω represents the phase shift of the hard-sphere potential scattering and is set equal to zero, except for the total cross section.

The above expansion lends itself to a formally equivalent expansion for the Doppler-broadened cross sections. When the third term of the above equation is neglected except the term $CA_1^{(x)}$, Doppler-broadened cross section becomes as follows,

$$\sqrt{E}\cdot\sigma^{(x)}(E)=\mathop{\mathrm{Sum}}_{i=1}^{NLVL}\frac{C}{2\beta_i\sqrt{E}}\left\{G_i^{(x)}[\psi(y_1^i)-\psi(y_2^i)]-H_i^{(x)}[\chi(y_1^i)+\chi(y_2^i)]\right\}+CA_1^{(x)} \qquad (2\cdot 1)$$

$$y_1^i=(\sqrt{E}-\alpha_i)/\beta_i \quad , \quad y_2^i=(\sqrt{E}+\alpha_i)/\beta_i$$

where quantities α_i and β_i satisfy $\mu_i-i\nu_i=(\alpha_i-i\beta_i)^2$. ψ and χ are the Doppler functions and χ is defined as a half of the one generally used, but the variable $\xi_i(=2\beta_i\sqrt{A/kT})$ is suppressed in the expressions of the ψ and χ. The values of G^T, H^T, G^F, H^F and background term $A_1^{(x)}$ are evaluated and compiled by Adler-Adler for the energy range 1.8 eV to 37.0 eV.

2.2 Doppler functions $\psi(\xi, x)$ and $\chi(\xi, x)$

The probability for a neutron to be captured by a target nucleus depends on the relative velocity between the neutron and the target nucleus. Therefore, the effective cross sections are obtained by taking the average of the cross section over the velocity distribution of the target nucleus.

In calculating the function ψ and χ, rational approximations are provided in the RICM2 in addition to the "Gelbard method" used in the RICM. As the Gelbard method[6] was described in detail in reference 2), we will give only a brief explanation of the rational approximations.

$$\psi(\xi, x)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{dy}{1+y^2}e^{-\frac{\xi^2}{4}(x-y)^2}$$

$$\chi(\xi, x)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{ydy}{1+y^2}e^{-\frac{\xi^2}{4}(x-y)^2}$$

(χ here is also a half of the one generally used.)
These ψ and χ have the following properties;

$$\int_{-\infty}^{\infty}\psi\, dx=\pi \quad , \quad \int_{-\infty}^{\infty}\psi^2\, dx=\frac{\pi}{2}M(\theta)$$

$$\int_{-\infty}^{\infty}\frac{\chi}{x}dx=\pi a(\theta) \quad , \quad \int_{-\infty}^{\infty}\left(\frac{\chi}{x}\right)^2dx=\frac{\pi}{2}N(\theta)$$

$$\psi(\xi, 0)=a(\theta) \quad , \quad \lim_{x\to 0}\frac{\chi(\xi, x)}{x}=\gamma(\theta)$$

where

$$a(\theta)=\psi(\xi, 0)=\frac{\sqrt{\pi}\xi}{2}\exp\left(\frac{\xi^2}{4}\right)\left\{1-\mathrm{erf}\left(\frac{\xi}{2}\right)\right\}=\xi e^{\xi^2/4}\cdot\mathrm{Erfc}(\xi/2)$$

$$M(\theta)=a(\theta/2) \quad , \quad \gamma(\theta)=\{1-a(\theta)\}/2\theta$$

$$N(\theta)=\{2a(\theta)-M(\theta)-(a(\theta))^2\}/\theta$$

with $\theta=\xi^{-2}$ and

$$\mathrm{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}du\equiv 1-\frac{2}{\sqrt{\pi}}\mathrm{Erfc}(x)$$

We consider the followihg approximate formula for ψ and χ/x, and will determine constants a, b, c and d so as to conserve the above properties.[7]

$$\psi(\xi, x)=\frac{x^2+aa^2b^2}{(x^2+a^2)(x^2+b^2)} \quad , \quad \frac{\chi(\xi, x)}{x}=\frac{x^2+\gamma c^2d^2}{(x^2+c^2)(x^2+d^2)}$$

As shown in Appendix 1, we finally obtain the following solutions,

$$a+b=\frac{1-a}{M-a} \quad , \quad a\,b=\frac{1-M}{a(M-a)}$$

$$c+d=\frac{a^2-\gamma}{N-a\gamma} \quad , \quad c\,d=\frac{a^3-N}{\gamma(N-a\gamma)}$$

Errors introduced into J-function by using the approximate ψ function thus obtained are tabulated in Appendix 2.

As ψ and χ are calculated towards the both tails from the resonance center with a constant step Δx in the Gelbard method, the energy mesh point E_i and the energy E_n corresponding the mesh point x_n for the calculation of ψ would generally not agree. Therefore, the values of ψ and χ by the Gelbard method at any energy mesh point E_i are obtained by interpolation, whereas those by the rational approximation are calculated directly at the point with less computing time.

3. Resonance neutron flux

When both the collision probabilities as functions of the cross section in the fuel region and the microscopic cross sections of the resonant nuclides as functions of the energy are given, we can obtain the neutron spectrum by solving slowing down equations as was done in the RICM. As the collision probabilities in two-region lattices are fairly easily calculated, that part of the calculation is done in the main program.

In the next chapter 3.1, a brief account on the two-region collision probabilities is given. The microscopic cross sections described in the previous chapter being prepared by the separate program RICM2-LTE, they are used as given quantities in the following. In chapter 3.2, the method of solving the slowing down equations in two-region system is described. This part, however, is essentially the same as the RICM.

3.1 Collision probability

A great number of papers has been published concerning the escape probability $P_0(E)$ from a fuel rod into a moderator region in a two-region system. The escape probabilities $P_0(E)$ from an isolated infinite slab and cylinder are expressed analytically, and the tables of them are prepared by CASE *et al.*[8] These escape probabilities for the isolated systems are extended to those for the corresponding lattices using the approximation formula $P_0^L(E)$ proposed by Nordheim;

$$P_0^L(E)=\frac{P_0G_\infty}{1-(1-G_0)(1-G_\infty)} \quad , \qquad G_0=\Sigma l\cdot P_0 \tag{3-1}$$

This approximation, which makes use of the Dancoff coefficient G_∞, is known to give a considerably good accuracy. Where Σ and l are respectively the total macroscopic cross section in the fuel region and the mean chord length of the fuel, $l=4V_1/S$, V_1 and S representing the volume and the surface area of it.

Next, we will touch on the Dancoff coefficient G_∞. When we define the total macroscopic cross section Σ_2 and the mean chord length $l_2(=4V_2/S)$ of the moderator, the G_∞ of a slab lattice is given rigorously by use of the exponential integral function $E_3(x)$ as follows,

$$G_\infty^{slab}=1-2E_3(\Sigma_2 l_2/2) \tag{3-2}$$

The G_∞ of a cylindrical lattice depends on $\Sigma_2 l_2$, V_2/V_1 and lattice arrangement — hexagonal or square — and a numerical calculation is necessary for obtainning the exact value. In this program, the following approximate formula by SAUER[9] is used,

$$G_\infty^{cyl}=1-\exp(-\tau\Sigma_2 l_2)/\{1+(1-\tau)\Sigma_2 l_2\} \tag{3-3}$$

$$\tau=\begin{cases}(\sqrt{\pi/4}\cdot\sqrt{1+V_2/V_1}-1)/(V_2/V_1)-0.08 & \text{(Sq.)}\\ (\sqrt{\pi/2\sqrt{3}}\cdot\sqrt{1+V_2/V_1}-1)/(V_2/V_1)-0.12 & \text{(Hex.)}\end{cases}$$

if the same quantity is not fed by input. The following formula known as the Bell approximation is also provided.

$$G_\infty = \Sigma_2 l_2 / (1 + \Sigma_2 l_2) \tag{3-4}$$

As the tables of the escape probabilities P_0 for an isolated slab and a cylindrical lattices are stored in this program, the P_0^L for the lattice are obtained by formula (3-1) with (3-2) through (3-4). A provision is also made for G_∞ and P_0 to be read in from input cards in case one wants more accurate values or the same quantities for geometry other than the slab or the cylinder.

The values of G_∞^{slab}, P_c^{slab} and P_c^{cyl} $(P_c = 1 - P_0)$ stored in the program are listed in the following table against a variable z or x.

$$z = \begin{cases} \Sigma_1 l_1/2 & \text{for } P_c \\ \Sigma_2 l_2 & \text{for } G_\infty \end{cases} \tag{3-5}$$

$$x = \begin{cases} z & (z \leqq 1) \\ 2 - z^{-1} & (z > 1) \end{cases} \tag{3-5'}$$

n	z	x	G_∞^{slab}	P_c^{slab}	P_c^{cyl}
1	0.0	0.0	0.00000	0.0000	0.00000
2	0.2	0.2	0.16742	0.2597	0.20697
3	0.4	0.4	0.29611	0.3932	0.34838
4	0.6	0.6	0.39992	0.4859	0.45225
5	0.8	0.8	0.48543	0.5554	0.53126
6	1.0	1.0	0.55679	0.6097	0.59285
7	1.25	1.2	0.63042	0.6629	0.65249
8	$1.\dot{6}$	1.4	0.72440	0.7275	0.72342
9	2.5	1.6	0.84286	0.8065	0.80677
10	$3.\dot{3}$	1.7	0.90832	0.8518	0.85273
11	5	1.8	0.96741	0.9002	0.90077
12	10	1.9	0.98824	0.9500	0.95009
13	50	1.98	1.00000	0.9900	0.99000

A value for an arbitrary x is obtained by three-point interpolation as is done in the RICM.

Now, we use suffixes i and j to indicate regions, 1 and 2 corresponding to the fuel and moderator regions respectively. P_{ij} is the probability that a neutron born uniformly and isotopically in region i makes its first collision in region j. Utilizing the reciprocity relation and the conservation law, $P_{ij}(i, j = 1, 2)$ are obtained as follows.

$$P_{12} = P_0^L \quad , \quad P_{11} = 1 - P_{12}$$

$$P_{21} = \frac{V_1 \Sigma_1}{V_2 \Sigma_2} P_{12} \quad , \quad P_{22} = 1 - P_{21}$$

These P_{ij} are used in the slowing down calculation in the next section.

3.2 Slowing down calculation

This part is similar to that in the RICM in the following points: The equation solved is the Chernick's equation, and the slowing down source integral is evaluated by applying the modified and extended Simpson's quadrature rule. Only the outline of the calculation, therefore, is given here.

Using the same notations as those in reference 2), our starting equation is

$$V_i \Sigma_i(E) \phi_i(E) = \underset{j=1,2}{\text{Sum}} P_{ji}(E) V_j S_j(E) \qquad (i = 1, 2) \tag{3-6}$$

where

$$S_j(E)=\mathop{\mathrm{Sum}}_{k=1}^{k_j} S_{jk}(E) \tag{3-7}$$

$$S_{jk}(E)=\int_E^{E/\alpha_{jk}} \Sigma_{sjk}(E')\phi_j(E')\frac{dE'}{(1-\alpha_{jk})E'} \tag{3-8}$$

k_j being the number of isotopes in region j.

With the help of the reciprocity relation

$$V_i\Sigma_i(E)P_{ij}(E)=V_j\Sigma_j(E)P_{ji}(E) \tag{3-9}$$

We can rewrite Eq. (3-6) into

$$\phi_i(E)=\mathop{\mathrm{Sum}}_{j=1,2} P_{ij}(E)S_j(E)/\Sigma_j(E) \tag{3-10}$$

We solved this equation starting from a given energy E_1 towards the lower energy E_n (n=2, ……, N) with the assumption that $\phi_j(E)=1/E$ at energies $E>E_2$ ($E_n=E_1-(n-1)\cdot\Delta E$).

When we calculate the neutron flux $\phi_j(E_n)$ ($n\geqq 3$), $\phi_j(E_m)$ ($m\leqq n-1$), are known quantities. And making use of the modified and extended Simpson's quadrature rule, the slowing down integral (3-8) is approximately given by

$$S_{jk}(E_n)=A_{jk}\phi_j(E_n)+B_{jk} \tag{3-11}$$

where A_{jk} and B_{jk} are composed of known quantities. With the introduction of the following notations

$$A_j=\mathop{\mathrm{Sum}}_{k=1}^{k_j} A_{jk} \quad , \quad B_j=\mathop{\mathrm{Sum}}_{k=1}^{k_j} B_{jk}$$

Eq. (3-10) can be rearranged into the following coupled equation for $\phi_j(E_n)$ at energy E_n;

$$\mathop{\mathrm{Sum}}_{j=1,2} a_{ij}\phi_j(E_n)=b_i \qquad (i=1,\ 2) \tag{3-12}$$

where

$$a_{ij}=\delta_{ij}-P_{ij}(E_n)\cdot A_j/\Sigma_j(E_n) \tag{3-13}$$

$$b_i=\mathop{\mathrm{Sum}}_{j=1,2} P_{ij}(E_n)\cdot B_j/\Sigma_j(E_n)$$

The solutions of the Eq. (3-12) are well known.

$$\phi_1(E_n)=(b_1\cdot a_{22}-b_2\cdot a_{12})/\Delta \tag{3-14}$$

$$\phi_2(E_n)=(b_2\cdot a_{11}-b_1\cdot a_{21})/\Delta$$

$$\Delta=a_{11}\cdot a_{22}-a_{12}\cdot a_{21}$$

Although the above discussion is limitted to two-region cases, the same procedure can be also applied for one-region (homogeneous) cases, the solution of Eq. (3-12) being given by $\phi_1(E_n)=b_1/a_{11}$.

4. Reaction rates

When neutron spectrum $\phi_1(E)$ in the fuel region is obtained, various reaction rates, average cross sections and effective resonance integrals can be calculated with the use of microscopic cross sections.

We must pay attention to the fact that the effects of one isotope on the other in the presence of two kinds of absorbers give rise not only to the local depression of neutron flux due to the presence of the resonances of the other but also to the decrease of neutron flux level at lower energies due to the absorption by the same. When we define the resonance integral using the reaction rates, a special attention are paid to the above point. It is also taken into consideration that the relation between the effective resonance integral and the resonance escape probability be simple and consistent.

4.1 Average cross sections

Considering the reactions only in the fuel region, we will use the following simplified notations,

$$\phi_n=\phi_1(E_n) \qquad (n=1,\ \cdots\cdots,\ N)$$

The suffix $i(i=1,\ 2)$ is used to distinguish two kinds of resonance absorbers as is shown in the examples like $\sigma_{an}^i\ (=\sigma_a^i(E_n))$, N_i and $Q_i\equiv\overline{N_i}/\overline{\xi\Sigma_s}$. Notations N, $\xi\Sigma_s$ etc. are those commonly used. The definition of average cross section $\bar{\sigma}$ at energies $E_{l+1}\leqq E\leqq E_m$ is defined by

$$\bar{\sigma}_a^i=\sum_{n=m}^{l} A_n^i/(Q_i\cdot\sum_{n=m}^{l}\Phi_n) \tag{4-1}$$

$$A_n^i=Q_i\cdot\sigma_{an}^i\phi_n\cdot\Delta E \tag{4-2}$$

$$\Phi_n=\phi_n\cdot\Delta E$$

Although the quantities σ_{an}^i and ϕ_n are the values at $E=E_n$, they are regarded as the average value at energies $E_{n+1}\leqq E\leqq E_n$ by reason of smallness of energy mesh ΔE. When one of the nuclides is fissionable, the fission and capture cross sections are, respectively,

$$\bar{\sigma}_f^1=\sum_{n=m}^{l}\frac{A_n^1}{1+\alpha_n}\Big/(Q_1\cdot\sum_{n=m}^{l}\Phi_n) \tag{4-3}$$

$$\bar{\sigma}_c^1=\bar{\sigma}_a^1-\bar{\sigma}_f^1 \tag{4-4}$$

$$(\bar{\sigma}_c^2=\bar{\sigma}_a^2,\ \ \bar{\sigma}_f^2=0)$$

These definitions can be quite easily accepted.

4.2 Effective resonance integrals

By use of the definition A_n^i, the slowing down density P_n at energy E_n and the resonance escape probability $\tilde{P}_n$ in the energy interval $E_{n+1}\leqq E\leqq E_n$ are obtained as follows.

$$P_1=1,\qquad P_{n+1}=P_n-A_n \qquad (A_n=A_n^1+A_n^2) \tag{4-5}$$

$$\tilde{P}_n=P_{n+1}/P_n=1-A_n/P_n\equiv 1-\bar{A}_n \qquad (\bar{A}_n^i=A_n^i/P_n) \tag{4-6}$$

Now that the resonance escape probability is expressed by the product of $\tilde{P}_n$, it is desirable to define the following new quantity ${}^0A_n^i$ so that the effective resonance integral RI^i for each nuclide may be obtained by summing up the corresponding RI_n^i over n.

$$\tilde{P}_n=1-\tilde{A}_n=1-\tilde{A}_n^1-\tilde{A}_n^2\equiv(1-{}^0A_n^1)(1-{}^0A_n^2) \tag{4-7}$$

$$1-{}^0A_n^i\equiv\exp(-Q_i\cdot RI_n^i)\qquad,\qquad RI_n^i=-\ln(1-{}^0A_n^i)/Q_i \tag{4-8}$$

A little more detailed investigation leads to

$$1-\tilde{A}_n^1-\tilde{A}_n^2=1-{}^0A_n^1(1-{}^0A_n^2\alpha)-{}^0A_n^2(1-{}^0A_n^1\beta) \tag{4-9}$$

$$\alpha+\beta=1$$

When the absorption by nuclide 1 occurs above in energy than that by nuclide 2, $\alpha=0$ and $\beta=1$ will result, and in the reverse situation, $\alpha=1$ and $\beta=0$. Within a narrow energy mesh ΔE considered here, $\alpha=\beta=1/2$ would be appropriate.

$$\tilde{A}_n^1={}^0A_n^1(1-{}^0A_n^2/2) \tag{4-10}$$

$$\tilde{A}_n^2={}^0A_n^2(1-{}^0A_n^1/2)$$

${}^0A_n^1$ and ${}^0A_n^2$ are solved in Eq. (4-10), and RI_n^i is calculated by Eq. (4-8).

Now, let's make sure of the relations between the P, A and RI defined above at energies $E_{l+1}\leqq E\leqq E_m$;

$$P=P_{l+1}/P_m=\prod_{n=m}^{l}\tilde{P}_n$$

$$=\prod_{n=m}^{l}(1-\tilde{A}_n)=\prod_{n=m}^{l}(1-\tilde{A}_n^1-\tilde{A}_n^2)$$

$$=\prod_{n=m}^{l}(1-{}^0A_n^1)\cdot\prod_{n=m}^{l}(1-{}^0A_n^2)$$

$$=\exp(-Q_1\cdot\mathop{\mathrm{Sum}}_{n=m}^{l}RI_n^1)\cdot\exp(-Q_2\cdot\mathop{\mathrm{Sum}}_{n=m}^{l}RI_n^2)$$

Finally, we show the formula for the parameters α and β, an extension of the same quantities in Eq. (4-9) over a wider energy interval, which indicate the relative position of the absorptions in the energy interval $E_{l+1}\leqq E\leqq E_m$.

$$A^i\equiv\mathop{\mathrm{Sum}}_{n=m}^{l}A_n^i/P_m$$

$$RI^i\equiv\mathop{\mathrm{Sum}}_{n=m}^{l}RI_n^i$$

$${}^0A^i\equiv 1-\exp(-Q_i\cdot RI^i)$$

$$1-A^1-A^2=(1-{}^0A^1)(1-{}^0A^2)$$

$$=1-{}^0A^1(1-{}^0A^2\cdot\alpha)-{}^0A^2(1-{}^0A^1\cdot\beta)$$

$$A^1={}^0A^1(1-{}^0A^2\cdot\alpha)$$

$$\alpha=({}^0A^1-A^1)/({}^0A^1\cdot{}^0A^2)$$

in the same way, or from $\beta=1-\alpha$,

$$\beta=({}^0A^2-A^2)/({}^0A^1\cdot{}^0A^2)$$

are derived.

5. RICM2-LTE

5.1 Structure of the program

The block diagram of the RICM2-LTE program is shown in Fig. 1 and the function of each subprogram is given below.

1. MAIN : Reads in control instructions and calls each subroutine according to these instructions.
2. DELET : Delets disused isotopes from the old tape.
3. TAPREA : Rewrites the contents of one tape onto another.
4. CROSS : Calls subroutines RATION and GELBAR which prepare cross sections, respectively, by rational approximation to the Doppler functions and by the Gelbard method.
5. ADLER : Computes the Adler type cross sections by use of the level parameters prepared by Adler.
6. GELBAR : Computes the cross sections using the Doppler functions ψ and χ obtained by the Gelbard method.
7. DFUNC : Prepares the the tables of the ψ and χ by use of the Gelbard method.
8. RATION : Computes the cross sections using the ψ and χ obtaind by rational approximation.
9. PSI : Computes the ψ and χ by use of rational approximation.
10. PSI0 : Gives the value of $\psi(\xi,\ 0)$.

11. NOMALI : Makes such nomalizations as described at the section of input specification.
12. ADDIT :
13. ADI2 : } Adds new isotopes onto the library tape.
14. PRINT :
15. PRINT2 : } Prints out the cross sections stored on the tape.
16. ERROR2 : Prints out error messages and stops the execution, when a certain input error is encountered.

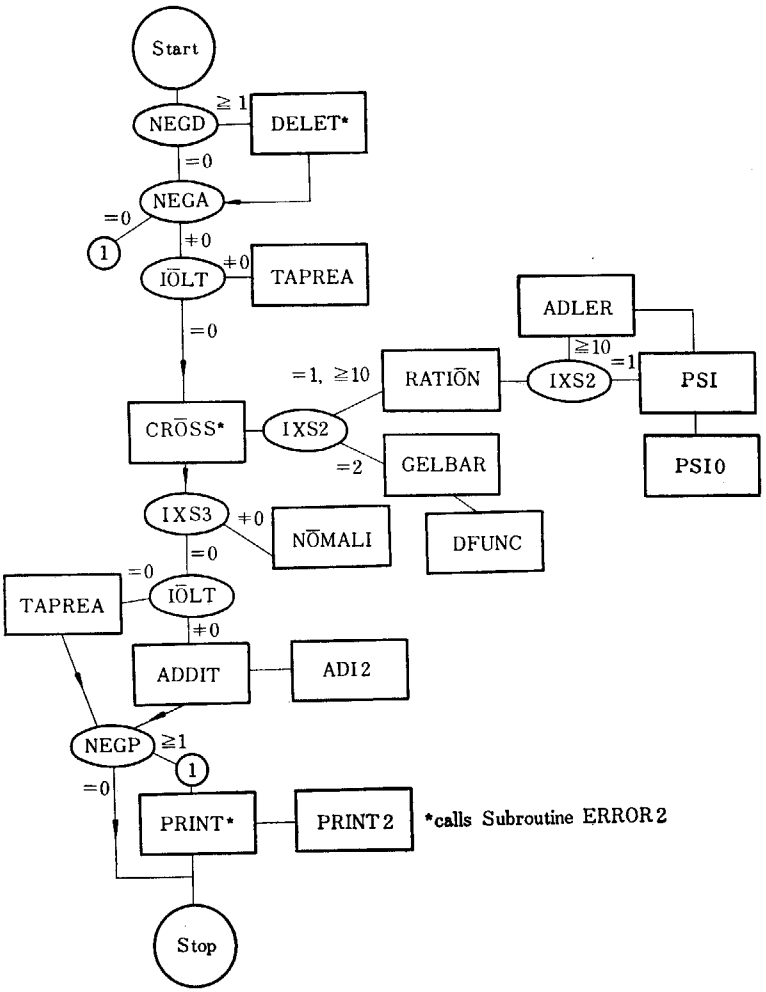

Fig. 1 Block diagram of the RICM2-LTE

5.2 Input specification

The input information necessary for the operation of the program will be written on the data sheets at the end of this report.

The notations used are as follows.

Variables	Description
TID	Tape identification. (I. D.)
IOLT	= 0 : Old library tape is not necessary. ≥ 1 : Old library tape is necessary.
NEGA	No. of energy ranges (E. R.) containing isotopes to be newly added. ≦20
NEGD	No. of E. R. containing isotopes to be deleted. ≦20
NEGP	No. of E. R. containing isotopes to be printed out. ≦20

Variables	Description
NA	$=0$: New TID is used. $\geqq 1$: Old TID is used.
IEGID	I.D. of the E.R.
NIS $\begin{pmatrix} A \\ D \\ P \end{pmatrix}$	No. of isotopes to be added, deleted or printed out. $\leqq 30$
NTA	No. of energy meshes of the E.R. $\leqq 2001$
EAA	E_a, lower limit of the E.R.
EBA	E_b, upper limit of the E.R.
DEA	ΔE, energy-mesh interval.
ISID	I.D. of the isotope.
ISCMT	Comments on the isotope.
ISCF	$=1$: Fertile. $=2$: Fissile.
NLVL	Total no. of input levels.
TEMP	T(°K), temperature.
AMAS	A, atomic mass.
SP	$\sigma_p(b)$, potential scattering cross section.
SPIN	I, nuclear spin.
IXS1	Comments on the source of the level parameters. $=1$: BNL 325 (2nd ed. suppl. no. 2) $=2$: Schmidt. $=3$: Adler. $\geqq 4$: Blank at present.
IXS2	Choice of calculation method for the ψ and χ. $=1$: Rational approximation. $=2$: Gelbard method. $=11$: Rational approximation coupled with Adler type cross sections.
IXS3	Choice of meteod for normalization of the cross sections. $=0$: No normalization. $=1$: $1/v$ type σ is added in the entire E.R. so as to normalize the calculated $\sigma_a(E)$ ($\sigma_f(E)$) to given values at $E=E_{th}=0.0253$ eV. $=2$: $1/v$ type σ is added in the entire E.R. so that the calculated RI_c*(RI_f*) over the energies E_c to E_d may coincide with the given one. *) $RI_c(RI_f)$ is the resonance integral at infinite dilution over the specified energy interval. $=3$: After the normalization of IXS3=1, $1/v$ type σ is added between energies E_v and E_d so that $RI_c(RI_f)$ over the energies E_c to E_d may coincide with the given one.
EC	E_c, cut off energy for the use of normalization of σ.(see IXS3)
EV	E_v, intermediate energie for the use of the normalization of σ.(see IXS3)
XSCO	$\sigma_c(E_{th})$
RICO	$RI_c(E_c \sim E_d)$
XSFO	$\sigma_f(E_{th})$
RIFO	$RI_f(E_c \sim E_d)$
ERA, GNA, GGA, GFA, GJA	E_r, Γ_n, Γ_γ, Γ_f and g_J respectively. If g_J is not fed by the input, $g_J=1$ ($I=0$) or $g_J=1/2$($I\geq 1/2$).
IXS	IXS2 for this particular level. $=0$: No change in IXS2. >0 : IXS supersedes IXS2 for this level.

Variables	Description
ANU, GT, HT, GFM, HF	Adler-Adler type level parameters : μ, G^T, H^T, G^F and H^F, respectively.
C, AT, AF	Coefficient C in Eq.(2-1) (usually 6.52×10^5), total- and fission-background cross sections, respectively.
ITS	Control for print out(σ_S and σ_T). = 0 : none. = 1 : σ_S = 2 : σ_T = 3 : σ_S and σ_T
ICF	Control for print out(σ_f and σ_c). = 0 : none. = 1 : σ_f = 2 : σ_c = 3 : σ_f and σ_c
IP1(N), IP2(N), IP3(N)	Specification of the mesh points to be printed out. Prints out the cross sections from IP1(N) to IP2(N) in every IP3(N) mesh points.

5.3 Contents of the library tape

Quantities arranged together compose one record on the tape.

1. NEG, (TID(K), K=1, 10)
2. (IEGID(N), EAA(N), EBA(N), DEA(N), NISA(N), N=1, NEG)
3. NEG times of 3.1 and 3.2
   - 3.1 EA, EB, DE, NT, NIS
     (ISIDA(N), ISCFA(N), (ISCMT(N, K), K=1, 10), N=1, NIS)
   - 3.2 NIS times of 3.2.1 and 3.2.2
     - 3.2.1 ISID, ISCF, IXS1, IXS2, IXS3, NLVL, TEMP, AMAS, XI, SP, (ST(N), SS(N), N=1, NT)
     - 3.2.2 (SC(N), N=1, NT) ····· (ISCF=1)
       (SC(N), SF(N), N=1, NT) ····· (ISCF=2)

As the most of the notations here have already appeared in Section 5.2, descriptions are given only for the new variables.

Variables	Description
EA, EB, DE, NT, NIS	Correspond to EAA, EBA, DEA, NTA and NISA, respectively.
ISIDA	Corresponds to ISID.
ISCFA	Corresponds to ISCF.
ST, SS, SC, SF	σ_T, σ_s, σ_c and σ_f, respectively.
XI	Average increase in lethargy per elastic collision. $\xi = 1 + \frac{\alpha}{1-\alpha}\ln\alpha$, $\alpha = \left(\frac{A-1}{A+1}\right)^2$

5.4 Output print

(a) Output on the way of calculation.
The input quantities are mostly printed out.

(b) Outputs of the quantities on the library tape.
The values of the cross sections specified by ITS and ICF are printed out.

Cross sections are tabulated towards low energies in a row begining from the energy given in the first column.

6. RICM2-MAIN

6.1 Structure of the program

```
        ┌── INP*
        ├── IRG*
        ├── PCC*
        ├── LIB*
MAIN────┼── OP1**
        ├── FLX─AIJ─AEX
        ├── OP2**
        ├── EDT
        └── OP3**
```

* calls Subroutine IMIS
** calls Subroutine PGCG

RICM2-MAIN consists of a main program and thirteen subroutines.
The main function of each subroutine is given below.

- MAIN : Calls each subroutine.
- INP : Reads in input information.
- IRG : Assigns isotopes to each region.
- PCC : Computes the escape probabilities.
- LIB : Reads in the microscopic cross sections from the library tape.
- OP1 : Prints out the input information, contents of the library tape and the escape probabilities.
- FLX : Computes the flux $\phi_1(E)$ and $\phi_2(E)$.
- AIJ : Computes the coefficient a_{ij} and b_i of the coupled equation (3-12).
- AEX : Computes the constants A_{jk} and B_{jk} of the slowing down integral (3-11).
- OP2 : Prints out the following quantities E, $E\phi_1$, $E\phi_2$, $E\Sigma_T\phi_1$, $\sigma_{S1}\phi_1$, $\sigma_{S2}\phi_1$, $\sigma_{c1}\phi_1$, $\sigma_{f1}\phi_1$ and $\sigma_{c2}\phi_1$.
- EDT : Computes the following quantities : $\int\sigma_c\phi_1\,dE$, $\int\sigma_f\phi_1\,dE$, RI_c and RI_f.
- OP3 : Prints out the quantities calculated in the EDT.
- IMIS : Stops the calculation when an input miss was encountered.
- PGCG : Changes the page and prints out the I. D. of the problem at the head.

6.2 Input specification

The input information necessary for the operation of the program will be written on the data sheet at the end of this report.
The notations used are as follows.

Variables	Description
1 CSID(12)	Case identification. (I. D.)
2-1 IGM	Geometry. $\leqq 0$: Homo, 1 : Slab, 2 : Cylinder, $\geqq 3$: Others.
Not necessary if IGM=0. IDC	Dancoff coefficient. $\leqq 1$: Bell, 2 : Sauer(Sq.), 3 : Sauer(Hex.), $\geqq 4$: (INPUT).
Not necessary if IGM=0. IE1, IE2	$=0$: (ϕ)-region; The flux of this region, ϕ_j, is calculated with a slowing down approximation specified by ISSD. $=1$: $(1/E)$-region; $\phi_j=1/E$ in this region.

Variation	Description
Not necessary if IGM=0.	
IPD	$\geqq 1$: Prints the table of the collision probabilities.
PD	Dancoff coefficient. It is computed in this program if PD$\leqq 0$ and IGM=1, 2(IDC$\leqq 3$). PD is set to 1 if PD>1.
R1	>0 : Distance from the center to the outer boundary of the region 1, or half mean chord length l' (only for IGM$\geqq 3$). <0 : R1$=-\lvert$R1$\rvert$ (If R1<0, the later input data than 2-2 are not necessary. And the data of the previous case are used.)
R2	>0 : Distance from the center to the outer boundary of the region 2. <0 : $-$(lattice pitch). (not necessary for IGM$\geqq 3$).
V1, V2	Volume of the region 1 and 2, respectively. (necessary only for IGM$\geqq 3$).
NXR	No. of X_n for which the values of P_c are read in.
Necessary only if IGM$\geqq 3$	
2-2 GMCT (6)	Comments on geometry.
DCCT (6)	Comments on Dancoff coefficient.
2-3 XR(21)	X_n, $(=Z_n \cdots\cdots (Z_n \leqq 1)$ or $= 2-Z_n^{-1} \cdots\cdots (Z_n > 1)$; $Z_n = \Sigma_1 \cdot l')$
2-4 PC(21)	$P_c(X_n)$ $(=1-P_0(X_n))$, Self collision probability.
3 IEGID	I.D. (Identification) of the energy range.
LM	>0 : Total no. of isotopes.($\lvert$LM$\rvert \leqq 10$) This corresponds to the no. of the cards for input 4. <0 : Change the data of the first $\lvert$LM$\rvert$ isotopes.
NOP2	>0 : no. of the input cards for input 5. (NOP2$\leqq 9$) <0 : Input 5 is not necessary. Use the data for the previous problem.
NBK	>0 : No. of energy groups for edit (NBK$\leqq 21$). <0 : Input 6 is not necessary. Use the data for the previous problem.
4 ISID(L)	I.D. of the isotope.
ISCF(L)	$\leqq 0$: No resonance, σ_s=const., $\sigma_a=0$. 1 : Fertile. (cross sections are fed from the library tape) 2 : Fissile. (〃)
ISSD(L)	Option for slowing down treatment. 0 : Exact, 1 : NR approx., 2 : WR approx.
AM(L), SP(L)	A(mass number) and σ_D, respectively.
ON1(L), ON2(L)	Number density N_i in region 1 and 2, respectively (10^{24}/cm^3).
5 ··· not necessary if NOP2$\leqq 0$	
IFXS(L)	Control of outputs. 1 : E, 2 : $E\phi_1$, 3 : $E\phi_2$, 4 : $\Sigma_T E\phi_1$, 5 : $\sigma_{s1}\phi_1$, 6 : $\sigma_{s2}\phi_1$, 7 : $\sigma_{c1}\phi_1$, 8 : $\sigma_{f1}\phi_1$, 9 : $\sigma_{c2}\phi_1$
ISET(L)	No. of sets of (IP1, IP2, IP3). (1$\leqq$ISET(L)$\leqq 4$)
IP1(L,K), IP2(L,K), IP3(L,K) (K=1, ISET)	Specifications of the mesh points to be printed out. Print out the cross sections from IP1(N) to IP2(N) in every IP3(N) mesh point(s).
6 ··· not necessary if NBK$\leqq 0$ (if NBK$=0$, the total energy interval is divided into approximately equal five groups. (NBK$=5$))	
EBK(21)	The lower limit (eV) of each energy group used in the EDT.

6.3 Output print

Only a brief account is necessary for the quantities printed out because the outputs accompany almost self-evident symbols with them.

* Dancoff coefficient
  PD; G_∞, Dancoff coefficient.
  XP2; Σ_2, Macroscopic cross section of the region 2.
  CL2; l_2, Mean chord length of the region 2.
* OP2 control
  10(5)150; Corresponds to IP1(IP3) IP2 in input 5.
* Collision probability
  XR; x.....Eq.(3-5)
  P1, P2, P3; The coefficients which are necessary for the interpolation of $P_0(x)$.
* OP2
  E; Energy at each mesh point(eV).
  E * F1; $E\phi_1(E)$
  E * F2; $E\phi_2(E)$
  XT * E * F1; $\Sigma_T \cdot E\phi_1$
  SS1 * F1; $\sigma_{s1}\phi_1$
  SS2 * F1; $\sigma_{s2}\phi_1$
  SC1 * F1; $\sigma_{c1}\phi_1$
  SF1 * F1; $\sigma_{f1}\phi_1$
  SC2 * F1; $\sigma_{c2}\phi_1$
  The quantities are tabulated towards low energies in a row begining from the energy given in the first column.
* OP3
  EBK(NP); Energy at the breaking point.
  P, A(12), A(1A), A(2C), A(1C), A(1F); P, A^1+A^2, A^1, A^2, A^1_{cap} and A^1_{fiss}, respectively.
  PHI, S(1A), S(2C), S(1C), S(1F); Φ, $\bar{\sigma}^1_a$, $\bar{\sigma}^2_c$, $\bar{\sigma}^1_c$ and $\bar{\sigma}^1_f$, respectively.
  U, RI(1A), RI(2C), RI(1C), RI(1F); U, RI^1_a, RI^2_c, RI^1_c and RI^1_f ($U=\int\frac{dE}{E}$), respectively.
  PO, AO(1A), AO(2C), ALPHA, BETA; $\tilde{P}$, ${}^0A^1$, ${}^0A^2$, α and β, respectively.
  The values written below the dotted line correspond to the values for all the energy ranges lying above the line.

The program also prints out "stop numbers" and some quantities (either integers (INT) or floatings (FLO)) connected with them if certain input errors are encountered, the stop numbers corresponding to the following input errors.

STOP NO.	Input errors	Quantities
1	NXR is less than 5 or greater than 21.	NXR
2	Either V1 or V2 is negative.	V1*V2
3	|LM| is greater than 10.	LM
4	NOP2 is greater than 6.	NOP2
6	NBK is greater than 21.	NBK
9	ISCF(L) is negative or greater than 2.	L

10	No resonant isotopes in region 1.	K1R
11	More than 1 fissionable isotopes.	K1F
12	More than 2 resonance isotopes.	K1R
13	More than 5 isotopes in region 1.	K1
15	Resonant isotopes in region 2.	L
16	More than 5 isotopes in region 2.	K2
18	V1 is zero or negative.	V1
19	V2 is zero or negative.	V2
20	CL is zero or negative.	CL
23	PD is zero or negative.	PD
26	Specified energy range not in the library.	NEG
27	The first isotope not in the library.	N1
28	The second isotope not in the library.	N2
29	The second isotope is fissionable.	ISCF (2)

7. Sample calculations

The effects of overlapping on the resonance integrals of the 21.84 eV and 23.48 eV resonances of ^{232}Th for an oxide rod in a water moderated cell are picked up in these sample calculations. The problem is divided into three cases.

(1) Both resonances are present.

(2) Only the 23.48 eV resonance is present.

(3) Only the 21.84 eV resonance is present.

The difference between the sum of the resonance integrals in the problem (2) and (3) and that in the problem (1) is accounted as a self overlapping effect between the two resonances.

In the first, the code RICM2-LTE is run to prepare the library tape containing the above three microscopic cross sections. In the next, the RICM2-MAIN is run to calculate resonance integrals etc. by use of the library tape. In the data sheets at the end of this report, the inputs for the LTE and the MAIN for the above three problems are given. Those pages of the outputs from the MAIN where resonance integrals are printed out are shown together with the output from the LTE of the microscopic cross sections for the problem (1). About 12 sec. of execution time including the loading time is required for the preparation of the library tape by the LTE on the computor GE-635. As for the calculations in the MAIN, the total execution time is about 20 sec. inclusive of the loading time. The LTE and the MAIN require approximately 26K and 32K memory spaces, respectively.

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Appendix 1 Rational approximations of the ψ and χ

The Doppler functions $\psi(\xi,\ x)$ and $\chi(\xi,\ x)$ are defined by

$$\psi(\xi,\ x)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{dy}{1+y^2}e^{-\frac{\xi^2}{4}(x-y)^2}$$

$$\chi(\xi,\ x)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{y\ dy}{1+y^2}e^{-\frac{\xi^2}{4}(x-y)^2}$$

where χ is a half of the one commonly used. For the integration of expressions including the ψ and χ over x, the following definitions are convenient,

$$\psi(\xi,\ x)=\int_0^{\infty}e^{-y-\theta y^2}\cdot\cos xy\ dy$$

$$\chi(\xi,\ x)=\int_0^{\infty}e^{-y-\theta y^2}\cdot\sin xy\ dy$$

where $\theta=\xi^{-2}$,

To obtain the above equalities, the following Gaussian summation is conveniently used.

$$\frac{1}{\pi}\int_0^{\infty}e^{-y^2/\lambda^2}\left[\int_{-\infty}^{\infty}f(t)\ \cos y(x-t)\ dt\right]dy=\frac{\lambda}{2\sqrt{\pi}}\int_{-\infty}^{\infty}f(t)\ e^{-\frac{\lambda^2}{4}(x-t)^2}dt$$

If we set $\lambda=\xi$ and $f(t)=1/(1+t^2)$,

$$\psi(\xi,\ x)=\frac{1}{\pi}\int_0^{\infty}e^{-y^2/\xi^2}\left[\int_{-\infty}^{\infty}\frac{\cos yx\cdot\cos yt}{1+t^2}dt\right]dy$$

$$=\frac{1}{\pi}\int_0^{\infty}e^{-y^2/\xi^2}\cos yx\cdot\pi e^{-y}dy=\int_0^{\infty}e^{-y-\theta y^2}\cos xy\ dy$$

Similarly, if we sets $\lambda=\xi,\ f(t)=t/(1+t^2)$,

$$\chi(\xi,\ x)=\frac{1}{\pi}\int_0^{\infty}e^{-y^2/\xi^2}\left[\int_{-\infty}^{\infty}\frac{t\sin yx\cdot\sin yt}{1+t^2}\ dt\right]dy$$

$$=\frac{1}{\pi}\int_0^{\infty}e^{-y^2/\xi^2}\cdot\sin yx\cdot\pi e^{-y}dy=\int_0^{\infty}e^{-y-\theta y^2}\cdot\sin xy\ dy$$

Integrations of some expressions including the ψ and χ.

(i) $$\int_{-\infty}^{\infty}\psi(\xi,\ x)\ dx=\lim_{a\to 0}2\int_0^{\infty}e^{-ax}\left[\int_0^{\infty}e^{-y-\theta y^2}\cdot\cos xy\ dy\right]dx \qquad (a>0)$$

$$=\lim_{a\to 0}2\int_0^{\infty}e^{-y-\theta y^2}\frac{a}{a^2+y^2}\ dy$$

$$=\lim_{a\to 0}2\int_0^{\infty}e^{-at-\theta(at)^2}\frac{dt}{1+t^2}=\pi$$

(ii) $$\int_{-\infty}^{\infty}\{\psi(\xi,\ x)\}^2dx=\lim_{a\to 0}2\int_0^{\infty}e^{-ax}\left[\int_0^{\infty}e^{-y-\theta y^2}\cdot\cos xy\ dy\right]\left[\int_0^{\infty}e^{-t-\theta t^2}\cdot\cos xt\ dt\right]dx$$

$$=2\int_0^{\infty}e^{-y-\theta y^2}dy\int_0^{\infty}e^{-t-\theta t^2}dt\left[\lim_{a\to 0}\int_0^{\infty}e^{-ax}\cos xy\cdot\cos xt\ dx\right]$$

The integration of the term in the [ ] is

$$\int_0^\infty e^{-ax}\cos xy\cdot\cos xt\,dx=\frac{1}{2}\left[\frac{a}{a^2+(y+t)^2}+\frac{a}{a^2+(y-t)^2}\right]$$

Utilizing the following relation

$$\lim_{a\to 0}\int_0^\infty f(t)\frac{a}{a^2+(t\pm y)^2}\,dt=\lim_{a\to 0}\int_{\pm y/a}^\infty f(a\omega\mp y)\frac{d\omega}{1+\omega^2}$$

$$\text{L. H. S.}=\begin{cases}0 & \frac{\pi}{2}f(0) \quad (+)\\ \pi f(y) & \frac{\pi}{2}f(0) \quad (-)\end{cases}$$

$$(y>0)\quad (y=0)$$

we finary obtain

$$\int_{-\infty}^\infty \psi^2\,dx=\pi\int_0^\infty e^{-y-\theta y^2}\cdot e^{-y-\theta y^2}\,dy=\frac{\pi}{2}\int_0^\infty e^{-u-\frac{\theta}{2}u^2}\cdot du$$

$$=\frac{\pi}{2}\psi(\sqrt{2}\xi,\ 0)=\frac{\pi}{2}a\left(\frac{\theta}{2}\right)\equiv\frac{\pi}{2}M(\theta)$$

$$(a(\theta)=\psi(\xi,\ 0)=\xi e^{\xi^2/4}\cdot\mathrm{Erfc}(\xi/2)\ ;\quad cf.\ 2.2)$$

(iii) $$\int_{-\infty}^\infty\frac{\chi(\xi,\ x)}{x}\,dx=2\int_0^\infty e^{-y-\theta y^2}\left[\int_0^\infty\frac{\sin xy}{x}\,dx\right]dy=\pi\int_0^\infty e^{-y-\theta y^2}\,dy$$

$$=\pi\psi(\xi,\ 0)\equiv\pi a(\theta)$$

(iv) $$\int_{-\infty}^\infty\left[\frac{\chi(\xi,\ x)}{x}\right]^2dx=2\int_0^\infty e^{-y-\theta y^2}\,dy\int_0^\infty e^{-t-\theta t^2}\,dt\left[\int_{-\infty}^\infty\frac{\sin xy\cdot\sin xt}{x^2}\,dx\right]$$

Now that the integral in the [ ] is $\pi\cdot\min(y,\ t)$,

$$\text{L. H. S.}=2\pi\int_0^\infty y\cdot e^{-y-\theta y^2}\,dy\int_y^\infty e^{-t-\theta t^2}\,dt$$

Introducing new variables $u=\sqrt{\theta}\left(y+\frac{1}{2\theta}\right)$ and $v=\sqrt{\theta}\left(t+\frac{1}{2\theta}\right)$

$$\text{L. H. S.}=\frac{2\pi\cdot e^{\frac{1}{2\theta}}}{\theta}\cdot\int_{\frac{1}{2\sqrt{\theta}}}^\infty\frac{1}{\sqrt{\theta}}\left(u-\frac{1}{2\sqrt{\theta}}\right)e^{-u^2}\,du\int_u^\infty e^{-v^2}\,dv$$

$$=2\pi\xi^3\cdot e^{\xi^2/2}\left[\int_{\xi/2}^\infty u\cdot e^{-u^2}\,\mathrm{Erfc}(u)\,du-\frac{\xi}{2}\int_{\xi/2}^\infty e^{-u^2}\,\mathrm{Erfc}(u)\,du\right]$$

where $\mathrm{Erfc}(u)=\int_u^\infty e^{-u^2}\,du$ is the error function.

Utilizing the following relations

$$\int_x^\infty u\cdot e^{-u^2}\,\mathrm{Erfc}(u)\,du=\frac{1}{2}\left[e^{-x^2}\,\mathrm{Erfc}(x)-\frac{1}{\sqrt{2}}\,\mathrm{Erfc}(\sqrt{2}x)\right]$$

$$\int_x^\infty e^{-u^2}\,\mathrm{Erfc}(u)\,du=\frac{1}{2}\left[\mathrm{Erfc}(x)\right]^2$$

we finally obtain

$$\int_{-\infty}^{\infty}\left[\frac{\chi}{x}\right]^2 dx=\pi\xi^3 e^{\xi^2/2}\left[e^{-\xi^2/4}\,\mathrm{Erfc}(\xi/2)-\frac{1}{\sqrt{2}}\mathrm{Erfc}\left(\frac{\xi}{\sqrt{2}}\right)-\frac{\xi}{2}\left\{\mathrm{Erfc}\left(\frac{\xi}{2}\right)\right\}^2\right]$$

$$\equiv\frac{\pi}{2}N(\theta)$$

Summing up, the Doppler functions ψ and χ have the following properties.

$$\int_{-\infty}^{\infty}\psi\,dx=\pi \quad , \quad \int_{-\infty}^{\infty}\psi^2\,dx=\frac{\pi}{2}M(\theta) \quad , \quad \psi(\xi,\ 0)\sim a(\theta) \quad , \quad \psi(\xi,\ \infty)\sim\frac{1}{x^2}$$

$$\int_{-\infty}^{\infty}\frac{\chi}{x}dx=\pi a(\theta) \quad , \quad \int_{-\infty}^{\infty}\left(\frac{\chi}{x}\right)^2 dx=\frac{\pi}{2}N(\theta) \quad , \quad \chi(\xi,\ 0)\sim x\cdot\gamma(\theta) \quad , \quad \chi(\xi,\ \infty)\sim\frac{x}{x^2}$$

We determine constants a, b, c and d of the following approximate formulae so as to conserve the above properties.

$$\psi(\xi,\ x)=\frac{x^2+aa^2b^2}{(x^2+a^2)(x^2+b^2)} \quad , \quad \frac{\chi(\xi,\ x)}{x}=\frac{x^2+\gamma c^2d^2}{(x^2+c^2)(x^2+d^2)}$$

After some tedious calculations, we have

$$a+b=(1-a)/(M-a) \quad , \quad ab=(1-M/a(M-a)$$

$$c+d=(a^2-\gamma)/(N-a\gamma) \quad , \quad cd=(a^3-N)/\gamma(N-a\gamma)$$

a and b (c and d) being complex conjugate each other.

Appendix 2 Errors in J function due to the use of the rational approximation of the ψ function

Here we study the accuracy of $J(\xi,\ \beta)=\int_0^{\infty}\frac{\psi(\xi,\ x)}{\psi(\xi,\ x)+\beta}dx$ over the range of $\beta=(1\sim2^{20})\times10^{-5}$ and $\xi=0.01\sim1.00$ instead of the direct examination for the ψ mentioned in section 2.2. Now that the ψ in rational approximation is given by

$$\psi=\frac{x^2+aa^2b^2}{(x^2+a^2)(x^2+b^2)}$$

we have

$$J_{\mathrm{rat}}=\frac{1}{2}\int_{-\infty}^{\infty}\frac{x^2+aa^2b^2}{\beta(x^2+a^2)(x^2+b^2)+x^2+aa^2b^2}dx\equiv\frac{1}{2}\int_{-\infty}^{\infty}I(x)\,dx \tag{2-1}$$

If we rewrite $I(x)$ to the following expression

$$I(x)=\frac{x^2+A}{\beta\{x^2-(B+Ci)\}\{x^2-(B-Ci)\}}$$

we see that $I(x)$ has the following four poles.

$$x_{1,2}^2=\sqrt{B^2+C^2}\cdot e^{i\theta}\equiv D\cdot e^{i\theta}$$

$$x_{3,4}^2=\sqrt{B^2+C^2}\cdot e^{-i\theta}\equiv D\cdot e^{-i\theta}$$

$$x_1=\sqrt{D}\cdot e^{i\theta/2} \quad , \quad x_2=-\sqrt{D}\cdot e^{i\theta/2}$$

$$x_3=\sqrt{D}\cdot e^{-i\theta/2} \quad , \quad x_4=-\sqrt{D}\cdot e^{-i\theta/2}$$

where

$$A=\alpha a^2b^2 \quad , \quad B^2+C^2=(\alpha+\beta)\,a^2b^2/\beta$$

$$B=-\frac{1}{2\beta}\{\beta(a^2+b^2)+1\} \quad , \quad \tan\theta=C/B$$

Two of the four poles lie above the x-axis on the complex plane and the residue theorem gives

$$J_{\mathrm{rat}}=\frac{\pi}{4}\,\frac{A+D}{\beta D^{3/2}}\cdot\sqrt{\frac{2D}{D-B}}=\frac{\pi}{2\beta}\,\frac{1+\alpha ab/\sqrt{(\alpha+\beta)/\beta}}{\sqrt{(a^2+b^2+\beta^{-1})+2ab\sqrt{(\alpha+\beta)/\beta}}} \tag{2-2}$$

Comparison of J_{rat} thus obtained with J_{ex} which are obtained by numerical integration of the definition equation utilizing the exact ψ by Gelbard method, is made in **Tables A2-1** and **2**.

TABLE A2-1 The function $J(\xi,\ \beta)$ for $\xi=(0.01,\ 1.00)$ and $\beta=2^i\times10^{-5}$

i	$J\ (\xi,\ \beta)$						
	$\xi=0.010$	0.020	0.050	0.100	0.200	0.500	1.000
0	6.9359 E 02	5.4786 E 02	5.0364 E 02	4.9829 E 02	4.9709 E 02	4.9678 E 02	4.9674 E 02
1	5.8634 E 02	4.2086 E 02	3.6131 E 02	3.5349 E 02	3.5176 E 02	3.5132 E 02	3.5125 E 02
2	5.1160 E 02	3.3715 E 02	2.6281 E 02	2.5161 E 02	2.4912 E 02	2.4847 E 02	2.4839 E 02
3	4.5428 E 02	2.8116 E 02	1.9564 E 02	1.8027 E 02	1.7669 E 02	1.7578 E 02	1.7565 E 02
4	4.0495 E 02	2.4153 E 02	1.5048 E 02	1.3072 E 02	1.2570 E 02	1.2440 E 02	1.2423 E 02
5	3.5783 E 02	2.1060 E 02	1.2011 E 02	9.6709 E 01	8.9935 E 01	8.8120 E 01	8.7875 E 01
6	3.0934 E 02	1.8350 E 02	9.9000 E 01	7.3572 E 01	6.5012 E 01	6.2521 E 01	6.2182 E 01
7	2.5760 E 02	1.5726 E 02	8.3158 E 01	5.7741 E 01	4.7773 E 01	4.4495 E 01	4.4029 E 01
8	2.0269 E 02	1.3023 E 02	6.9926 E 01	4.6484 E 01	3.5890 E 01	3.1834 E 01	3.1212 E 01
9	1.4760 E 02	1.0211 E 02	5.7673 E 01	3.7829 E 01	2.7590 E 01	2.2967 E 01	2.2169 E 01
10	9.8018 E 01	7.4168 E 01	4.5603 E 01	3.0471 E 01	2.1530 E 01	1.6753 E 01	1.5792 E 01
11	5.9390 E 01	4.9163 E 01	3.3751 E 01	2.3693 E 01	1.6756 E 01	1.2347 E 01	1.1286 E 01
12	3.3391 E 01	2.9750 E 01	2.2926 E 01	1.7322 E 01	1.2683 E 01	9.1188 E 00	8.0762 E 00
13	1.7836 E 01	1.6713 E 01	1.4210 E 01	1.1660 E 01	9.0808 E 00	6.6286 E 00	5.7436 E 00
14	9.2388 E 00	8.9231 E 00	8.1329 E 00	7.1790 E 00	6.0137 E 00	4.6241 E 00	3.9970 E 00
15	4.7047 E 00	4.6207 E 00	4.3953 E 00	4.0905 E 00	3.6582 E 00	3.0216 E 00	2.6629 E 00
16	2.3743 E 00	2.3527 E 00	2.2922 E 00	2.2047 E 00	2.0675 E 00	1.8288 E 00	1.6656 E 00
17	1.1928 E 00	1.1872 E 00	1.1716 E 00	1.1480 E 00	1.1088 E 00	1.0325 E 00	9.7216 E -01
18	5.9779 E -01	5.9640 E -01	5.9240 E -01	5.8628 E -01	5.7575 E -01	5.5385 E -01	5.3482 E -01
19	2.9925 E -01	2.9890 E -01	2.9789 E -01	2.9633 E -01	2.9360 E -01	2.8770 E -01	2.8229 E -01
20	1.4971 E -01	1.4962 E -01	1.4937 E -01	1.4898 E -01	1.4828 E -01	1.4675 E -01	1.4530 E -01

TABLE A2-2 Relative error in J_{rat}, $(J_{\mathrm{rat}}-J_{\mathrm{ex}})/J_{\mathrm{ex}}$ $(J(\xi,\ \beta),\ \beta=2^i\times10^{-5})$

i \ ξ	0.01	0.02	0.05	0.1	0.2	0.5	1.0
0	65.06%	40.50%	10.62%	2.41%	0.41%	0.03%	0.00%
1	60.33	45.89	15.40	4.01	0.74	0.06	0.01
2	51.55	46.94	20.73	6.34	1.30	0.11	0.01
3	41.02	43.37	25.49	9.41	2.21	0.20	0.03
4	30.56	36.51	28.17	12.89	3.56	0.37	0.05
5	21.25	28.24	27.72	16.02	5.36	0.64	0.09
6	13.64	20.11	24.29	17.73	7.40	1.08	0.17
7	7.92	13.10	19.04	17.25	9.20	1.70	0.29
8	4.07	7.67	13.37	14.71	10.06	2.46	0.48
9	1.80	3.96	8.36	10.97	9.52	3.20	0.72
10	0.68	1.76	4.58	7.13	7.73	3.64	1.00
11	0.22	0.67	2.15	4.00	5.33	3.53	1.21
12	0.07	0.22	0.86	1.90	3.10	2.84	1.25
13	0.02	0.07	0.30	0.77	1.50	1.88	1.06
14	0.01	0.01	0.09	0.26	0.61	1.00	0.72
15	0.00	0.00	0.03	0.08	0.21	0.43	0.39
16	0.00	0.00	0.01	0.02	0.07	0.16	0.17
17	0.00	0.00	0.00	0.01	0.02	0.05	0.06
18	0.00	0.00	0.00	0.00	0.01	0.02	0.02
19	0.00	0.00	0.00	0.00	0.00	0.01	0.01
20	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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INPUT DATA (1–80); COMMENT (73–80)

1	1	2	3	4	5	(TID(K), K = 1, 10)															
	(5I2, 10A6)					1...IOLT,		2...NEGD, 3...NEGA, 4...NEGP, 5...NA													
2-1	IEGIDD					NISD															NEGD times
	(A6, 4X, I5)																				
2-2	ISIDD(M)																(M = 1, NISD)				
	(A6)																				
3-1	IEGIDA(N)					NISA(N)		EAA(N)		EBA(N)		DEA(N)					(N = 1, NEGA)				
	(A6, 4X, I5, 5X, 3E10.3)																				
3-2	ISIDA(M)					(ISCMT(M, K), K = 1, 10)											(M = 1, NISA(N))				NEGA times
	(A6, 4X, 10A6)																				
3-3	ISID		ISCF		NLVL		IXS1	IXS2		IXS3	TEMP		AMAS		SP		SPIN				
	(A6, I4, 4I5, 4E10.3)																				
3-4	EC				ED			EV			XSCO		RICO		XSFO		RIFO				NISA times
	(7E10.3)																				
3-5	ER				GM			GG			GF		GJ				IXS	(L=1, NLVL)			
	(5E10.3, 10X, I5)																				
3-5'	ER				AND			GF			HT		GFM		HF			(L=1, NLVL)			
	(6E10.3)																				
3-6	C				AT			AF													
	(3E10.3)																				

PROBLEM RICM2-LTE INPUT FORMAT WRITTEN BY DATE PAGE 2 OF 2

INPUT DATA (1–80); COMMENT (73–80)

4-1	IEGIDP					NISP															NEGP times
	(A6, 4X, I5)																				
4-2	ISIDP(M)	ITS	IDF			(IP1(K), IP2(K), IP3(K), K = 1, 4)											(M=1, NISP)				
	(A6, 2I2, 12I5)																				

(Note) If NEGD = 0, no input 2-x.
If NEGA = 0, no input 3-x.
If NEGA > 0, input 3-4 is always necessary.
If IXS2 ≤ 10, no input 3-5' and 3-6'.
If IXS2 > 10 no input 3-5.

If NEGP = 0, no input 4-x.
EAA in input 3-1 should be in ascending order.
(The same order should apply for EBA if EAA's are same and for NTA if both EAA's and EBA's are same.)

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INPUT DATA (1–80); COMMENT (73–80)

1	(CSID(K), K=1, 12)																				
	(12A6)																				
2-1	IGM		IDC		IE1	IE2	IPD		PD		R1		R2		V1		V2		NXR		
	(4I5, I2, F8.6, 4E10.5, I2)																				
2-2	(GMCT(K), K=1, 6)												(DCCT(K), K=1, 6)								
	(12A6)																				
2-3	(XR(N), N=1, NXR)																				
	(7E10.5)																				
2-4	(PC(N), N=1, NXR)																				
	(7E10.5)																				
3	IEGID				LM		NOP2	NBK													
	(A6, 4X, 3I5)																				
4	ISID(L)	1	2		AM(L)	SP(L)		OM1(L)			OM2(L)		1...ISCF(L)		2...ISSD(L)						(L=1, LM)
	(A6, 2I2, 2F5.2, 2E10.5)																				
5	IFXS(N)	ISET(N)				(IP1(N,K), IP2(N,K), IP3(N,K), K=1, 4)															(N=1, NOP2)
	(14I5)																				
6	(EBK(N), N=1, NBK)																				
	(7E10.5)																				

PROBLEM RICM2-LTE Sample Problem WRITTEN BY DATE PAGE 1 OF 2

INPUT DATA — COMMENT

1 5	10	15	20	25	30	35	40	45	50	55	60	65	70	73 75	80
0 0 1 1															
ENER 1		3		15.0		30.0		0.025							
TH232A		TWO LEVELS		ER=23.48 AND ER=21.84											
TH232B		ONE LEVEL		ER=23.48											
TH232C		ONE LEVEL		ER=21.84											
TH232A 1		2	4	2		300.		232.		10.5					
(BLANK CARD)															
23.48		.004		.03											
21.84		.0024		.03											
TH232B 1		1	4	2		300.		232.		10.5					
(BLANK CARD)															
23.48		.004		.03											
TH232C 1		1	4	2		300.		232.		10.5					
(BLANK CARD)															
21.84		.0024		.03											
ENER 1		3													
TH232A 3 1		1	601	4	260	360	1								
TH232B 3 1		1	601	4	310	360	1								
TH232C 3 1		1	601	4	260	290	1								

PROBLEM RICM2-MAIN Sample Problem WRITTEN BY DATE PAGE 2 OF 2

INPUT DATA — COMMENT

1 5	10	15	20	25	30	35	40	45	50	55	60	65	70	73 75	80
EFFECT OF OVERLAP ON RI OF TWO TH232 RES. H2O-OXIDE CELL BOTH RES.															
2	2	0	0	1		0.5		1.							
ENER 1		3	5	2											
TH232A 1		232.	10.5	0.0137											
0.16		16.	3.8	0.0274		0.0334									
H 1		1.	20.0			0.0668									
2	1	1	601	2											
3	1	1	601	2											
4	1	1	601	2											
5	1	1	601	2											
7	1	1	601	2											
22.5		15.0													
EFFECT OF OVERLAP ON RI OF TH232 RES. H2O-OXIDE CELL 23.48EV RES.															
2	2	0	0	1		0.5		1.							
ENER 1		-1	-5	-2											
TH232B 1		232.	10.5	0.0137											
EFFECT OF OVERLAP ON RI OF TH232 RES. H2O-OXIDE CELL 21.84EV RES.															
2	2	0	0	1		0.5		1.							
ENER 1		-1	-5	-2											
TH232C 1		232.	10.5	0.0137											

OUT PUT OF RICM2-LTE

SELECTED ENERGY GROUP ****ENER 1**** (EA= 1.5000E 01 EB= 3.0000E 01 DE= 2.5000E-02 NMPT= 601)

SELECTED ISOTOPE ***TH232A***

ISID	ISCF	IXS1	IXS2	IXS3	NLVL	TEMP	AMAS	XI	SP
TH232A	1	4	2	0	2	300.00	232.00	0.01	10.50

*** ST *** 1(4) 601

E(EV)	1	2	3	4	5	6	7	8	9	10
30.00 I	1.1600E 01	1.1618E 01	1.1636E 01	1.1655E 01	1.1675E 01	1.1695E 01	1.1716E 01	1.1738E 01	1.1761E 01	1.1784E 01
29.00 I	1.1809E 01	1.1834E 01	1.1860E 01	1.1888E 01	1.1916E 01	1.1946E 01	1.1977E 01	1.2009E 01	1.2043E 01	1.2078E 01
28.00 I	1.2115E 01	1.2154E 01	1.2195E 01	1.2238E 01	1.2283E 01	1.2330E 01	1.2380E 01	1.2433E 01	1.2489E 01	1.2548E 01
27.00 I	1.2611E 01	1.2678E 01	1.2749E 01	1.2825E 01	1.2907E 01	1.2995E 01	1.3 89E 01	1.3190E 01	1.3300E 01	1.3420E 01
26.00 I	1.3550E 01	1.3692E 01	1.3848E 01	1.4021E 01	1.4212E 01	1.4425E 01	1.4665E 01	1.4935E 01	1.5243E 01	1.5597E 01
25.00 I	1.6007E 01	1.6489E 01	1.7062E 01	1.7753E 01	1.8604E 01	1.9675E 01	2.1 57E 01	2.2902E 01	2.5474E 01	2.9273E 01
24.00 I	3.5341E 01	4.6297E 01	7.1266E 01	1.8895E 02	1.1211E 03	3.1312E 03	1.9294E 03	3.2254E 02	6.2906E 01	3.2060E 01
23.00 I	2.3067E 01	1.9412E 01	1.7936E 01	1.7646E 01	1.8218E 01	1.9668E 01	2.2351E 01	2.7269E 01	3.7455E 01	6.9090E 01
22.00 I	3.2665E 02	1.6080E 03	1.8673E 03	4.4130E 02	6.1559E 01	2.4550E 01	1.6178E 01	1.2759E 01	1.1066E 01	1.0139E 01
21.00 I	9.5988E 00	9.2719E 00	9.0708E 00	8.9475E 00	8.8740E 00	8.8332E 00	8.8144E 00	8.8106E 00	8.8170E 00	8.8306E 00
20.00 I	8.8491E 00	8.8709E 00	8.8949E 00	8.9203E 00	8.9466E 00	8.9733E 00	9.0000E 00	9.0267E 00	9.0531E 00	9.0790E 00
19.00 I	9.1045E 00	9.1295E 00	9.1538E 00	9.1776E 00	9.2007E 00	9.2233E 00	9.2452E 00	9.2665E 00	9.2872E 00	9.3073E 00
18.00 I	9.3268E 00	9.3458E 00	9.3643E 00	9.3822E 00	9.3996E 00	9.4166E 00	9.4330E 00	9.4490E 00	9.4646E 00	9.4797E 00
17.00 I	9.4944E 00	9.5088E 00	9.5227E 00	9.5363E 00	9.5495E 00	9.5624E 00	9.5750E 00	9.5872E 00	9.5991E 00	9.6108E 00
16.00 I	9.6221E 00	9.6332E 00	9.6440E 00	9.6546E 00	9.6649E 00	9.6749E 00	9.6848E 00	9.6944E 00	9.7038E 00	9.7129E 00
15.00 I	9.7219E 00									

*** SS *** 1(4) 601

E(EV)	1	2	3	4	5	6	7	8	9	10
30.00	1.1503E 01	1.1518E 01	1.1533E 01	1.1549E 01	1.1565E 01	1.1582E 01	1.1599E 01	1.1617E 01	1.1635E 01	1.1654E 01
29.00	1.1674E 01	1.1695E 01	1.1716E 01	1.1738E 01	1.1760E 01	1.1784E 01	1.1808E 01	1.1834E 01	1.1860E 01	1.1888E 01
28.00	1.1916E 01	1.1946E 01	1.1978E 01	1.2010E 01	1.2044E 01	1.2080E 01	1.2118E 01	1.2157E 01	1.2199E 01	1.2242E 01
27.00	1.2288E 01	1.2337E 01	1.2388E 01	1.2442E 01	1.2500E 01	1.2561E 01	1.2627E 01	1.2697E 01	1.2771E 01	1.2852E 01
26.00	1.2938E 01	1.3031E 01	1.3132E 01	1.3242E 01	1.3362E 01	1.3493E 01	1.3638E 01	1.3798E 01	1.3976E 01	1.4177E 01
25.00	1.4403E 01	1.4662E 01	1.4960E 01	1.5308E 01	1.5719E 01	1.6215E 01	1.6824E 01	1.7594E 01	1.8599E 01	1.9974E 01
24.00	2.1978E 01	2.5203E 01	3.1446E 01	5.2481E 01	1.7487E 02	3.9000E 02	2.0609E 02	2.4006E 01	3.6286E 00	4.4337E 00
23.00	5.8257E 00	7.0277E 00	8.0770E 00	9.0479E 00	1.0014E 01	1.1062E 01	1.2313E 01	1.3996E 01	1.6655E 01	2.2444E 01
22.00	4.9420E 01	1.4530E 02	1.3150E 02	2.0121E 01	7.1149E-01	1.9033E 00	3.2324E 00	4.1809E 00	4.8846E 00	5.4289E 00
21.00	5.8641E 00	6.2213E 00	6.5208E 00	6.7762E 00	6.9971E 00	7.1904E 00	7.3614E 00	7.5138E 00	7.6508E 00	7.7746E 00
20.00	7.8873E 00	7.9902E 00	8.0848E 00	8.1720E 00	8.2527E 00	8.3277E 00	8.3975E 00	8.4627E 00	8.5238E 00	8.5811E 00
19.00	8.6350E 00	8.6859E 00	8.7339E 00	8.7793E 00	8.8224E 00	8.8633E 00	8.9021E 00	8.9391E 00	8.9744E 00	9.0081E 00
18.00	9.0402E 00	9.0710E 00	9.1004E 00	9.1286E 00	9.1557E 00	9.1817E 00	9.2067E 00	9.2308E 00	9.2539E 00	9.2762E 00
17.00	9.2977E 00	9.3184E 00	9.3384E 00	9.3578E 00	9.3765E 00	9.3946E 00	9.4120E 00	9.4290E 00	9.4454E 00	9.4613E 00
16.00	9.4767E 00	9.4917E 00	9.5063E 00	9.5204E 00	9.5341E 00	9.5474E 00	9.5604E 00	9.5730E 00	9.5853E 00	9.5972E 00
15.00	9.6088E 00									

*** SC *** 1(4) 601

E(EV)	1	2	3	4	5	6	7	8	9	10
30.00	9.6624E-02	9.9648E-02	1.0281E-01	1.0613E-01	1.0960E-01	1.1324E-01	1.1707E-01	1.2109E-01	1.2531E-01	1.2975E-01
29.00	1.3443E-01	1.3937E-01	1.4457E-01	1.5007E-01	1.5588E-01	1.6203E-01	1.6854E-01	1.7546E-01	1.8279E-01	1.9060E-01
28.00	1.9890E-01	2.0776E-01	2.1722E-01	2.2733E-01	2.3815E-01	2.4976E-01	2.6224E-01	2.7567E-01	2.9015E-01	3.0581E-01
27.00	3.2276E-01	3.4115E-01	3.6117E-01	3.8300E-01	4.0688E-01	4.3308E-01	4.6190E-01	4.9371E-01	5.2895E-01	5.6814E-01
26.00	6.1191E-01	6.6109E-01	7.1632E-01	7.7901E-01	8.5045E-01	9.3239E-01	1.0270E 00	1.1372E 00	1.2665E 00	1.4199E 00
25.00	1.6037E 00	1.8269E 00	2.1017E 00	2.4458E 00	2.8853E 00	3.4598E 00	4.2324E 00	5.3084E 00	6.8754E 00	9.2989E 00
24.00	1.3363E 01	2.1094E 01	3.9820E 01	1.3647E 02	9.4623E 02	2.7412E 03	1.7233E 03	2.9854E 02	5.9277E 01	2.7626E 01
23.00	1.7241E 01	1.2384E 01	9.8589E 00	8.5985E 00	8.2036E 00	8.6066E 00	1.0038E 01	1.3270E 01	2.0800E 01	4.6646E 01
22.00	2.7723E 02	1.4627E 03	1.7358E 03	4.2118E 02	6.0847E 01	2.2646E 01	1.2945E 01	8.5778E 00	6.1812E 00	4.7103E 00
21.00	3.7347E 00	3.0506E 00	2.5501E 00	2.1714E 00	1.8769E 00	1.6428E 00	1.4530E 00	1.2968E 00	1.1663E 00	1.0560E 00
20.00	9.6182E-01	8.8965E-01	8.1009E-01	7.4832E-01	6.9388E-01	6.4560E-01	6.0256E-01	5.6401E-01	5.2930E-01	4.9794E-01
19.00	4.6949E-01	4.4359E-01	4.1993E-01	3.9825E-01	3.7833E-01	3.5998E-01	3.4303E-01	3.2734E-01	3.1278E-01	2.9924E-01
18.00	2.8664E-01	2.7487E-01	2.6387E-01	2.5357E-01	2.4391E-01	2.3484E-01	2.2630E-01	2.1827E-01	2.1068E-01	2.0352E-01
17.00	1.9676E-01	1.9035E-01	1.8428E-01	1.7852E-01	1.7306E-01	1.6786E-01	1.6292E-01	1.5822E-01	1.5374E-01	1.4946E-01
16.00	1.4538E-01	1.4149E-01	1.3776E-01	1.3420E-01	1.3079E-01	1.2753E-01	1.2440E-01	1.2139E-01	1.1851E-01	1.1575E-01
15.00	1.1309E-01									

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EFFECT OF OVERLAP ON RI OF TH232 RES. H2O-OXIDE CELL 21.84EV RES. PAGE 12

)TOPE 1 ... TH232C

A...ABSORPTION, C...CAPTURE, F...FISSION, ONR1= 0.13700E-01 ONR2= 0. XIXP= 0.40663E 01
P=1-A=EXP(-Q*RI) Q=ONR/XIXP Q1= 0.33691E-02 Q2= 0.

N	NP	EBK(NP)	P	A(12)	A(1A)	A(2C)	A(1C)	A(1F)
1	301	2.25000E 01	9.99600E-01	3.99040E-04	3.99040E-04	0.	3.99040E-04	0.
2	601	1.50000E 01	9.92331E-01	7.26731E-03	7.26731E-03	0.	7.26731E-03	0.
			---	---	---	---	---	---
			9.92331E-01	7.66635E-03	7.66635E-03	0.	7.66635E-03	0.

N	NP	EBK(NP)		PHI	S(1A)	S(2C)	S(1C)	S(1F)
1	301	2.25000E 01	0.	2.86113E-01	4.13964E-01		4.13964E-01	0.
2	601	1.50000E 01	0.	3.75899E-01	5.73833E 00	0. 0.	5.73833E 00	0.
			---	---	---	---	---	---
			0.	6.62012E-01	3.43721E 00	0.	3.43721E 00	0.

N	NP	EBK(NR)		U	RI(1A)	RI(2C)	RI(1C)	RI(1F)
1	301	2.25000E 01	0.	2.87682E-01	1.18464E-01	0.	1.18464E-01	0.
2	601	1.50000E 01	0.	4.05465E-01	2.16578E 00	0.	2.16578E 00	0.
			---	---	---	---	---	---
			0.	6.93147E-01	2.28424E 00	0.	2.28424E 00	0.

N	NP	EBK(NP)	P0		A0(1A)	A0(2C)	ALPHA	BETA
1	301	2.25000E 01	9.99600E-01	0.	3.99042E-04	0.	0.	0.
2	601	1.50000E 01	9.92729E-01	0.	7.27021E-03	0.	0.	0.
			---	---	---	---	---	---
			9.92331E-01	0.	7.66635E-03	0.	0.	0.

EFFECT OF OVERLAP ON RI OF TWO TH232 RES. H2O-OXIDE CELL BOTH RES. PAGE 12

)TOPE 1 ... TH232A

A...ABSORPTION, C...CAPTURE, F...FISSION, ONR1= 0.13700E- 1 ONR2= 0. XIXP= 0.40663E 01
P=1-A=EXP(-Q*RI) Q=ONR/XIXP Q1= 0.33691E- 2 Q2= 0.

N	NP	EBK(NP)	P	A(12)	A(1A)	A(2C)	A(1C)	A(1F)
1	301	2.25000E 01	9.91674E-01	8.32444E-03	8.32444E-03	0.	8.32444E-03	0.
2	601	1.50000E 01	9.84236E-01	7.43771E-03	7.43771E-03	0.	7.43771E-03	0.
			---	---	---	---	---	---
			9.84236E-01	1.57622E-02	1.57622E-02	0.	1.57622E-02	0.

N	NP	EBK(NP)		PHI	S(1A)	S(2C)	S(1C)	S(1F)
1	301	2.25000E 01	0.	2.58849E-01	9.54537E 00		9.54537E 00	0.
2	601	1.50000E 01	0.	3.69822E-01	5.96940E 00	0. 0.	5.96940E 00	0.
			---	---	---	---	---	---
			0.	6.28670E-01	7.44177E 00	0.	7.44177E 00	0.

N	NP	EBK(NP)		U	RI(1A)	RI(2C)	RI(1C)	RI(1F)
1	301	2.25000E 01	0.	2.87682E-01	2.48115E 00	0.	2.48115E 00	0.
2	601	1.50000E 01	0.	4.05465E-01	2.23454E 00	0.	2.23454E 00	0.
			---	---	---	---	---	---
			0.	6.93147E-01	4.71569E 00	0.	4.71569E 00	0.

N	NP	EBK(NP)	P0		A0(1A)	A0(2C)	ALPHA	BETA
1	301	2.25000E 01	9.91674E-01	0.	8.32445E-03	0.	0.	0.
2	601	1.50000E 01	9.92499E-01	0.	7.50015E-03	0.	0.	0.
			---	---	---	---	---	---
			9.84236E-01	0.	1.57622E-02	0.	0.	0.

ISOTOPE 1 ... TH232B

A...ABSORPTION, C...CAPTURE, F...FISSION, ONR1= 0.13700E- 1 ONR2= 0. XIXP= 0.40663E 01
P=1-A=EXP(-Q*RI) Q=ONR/XIXP Q1= 0.33691E- 2 Q2= 0.

N	NP	EBK(NP)	P	A(12)	A(1A)	A(2C)	A(1C)	A(1F)
1	301	2.25000E 01	9.91965E-01	8.03437E-03	8.03437E-03	0.	8.03437E-03	0.
2	601	1.50000E 01	9.91458E-01	5.05210E-04	5.05210E-04	0.	5.05210E-04	0.
			9.91458E-01	8.53958E-03	8.53958E-03	0.	8.53958E-03	0.

N	NP	EBK(NP)		PHI	S(1A)	S(2C)	S(1C)	S(1F)
1	301	2.25000E 01	0.	2.60015E-01	9.17142E 00	0.	9.17142E 00	0.
2	601	1.50000E 01	0.	3.97888E-01	3.76872E-01	0.	3.76872E-01	0.
			0.	6.57904E-01	3.85263E 00	0.	3.85263E 00	0.

N	NP	EBK(NP)		U	RI(1A)	RI(2C)	RI(1C)	RI(1F)
1	301	2.25000E 01	0.	2.87682E-01	2.39434E 00	0.	2.39434E 00	0.
2	601	1.50000E 01	0.	4.05465E-01	1.51206E-01	0.	1.51206E-01	0.
			0.	6.93147E-01	2.54555E 00	0.	2.54555E 00	0.

N	NP	EBK(NP)	P0		A0(1A)	A0(2C)	ALPHA	BETA
1	301	2.25000E 01	9.91965E-01	0.	8.03438E-03	0.	0.	0.
2	601	1.50000E 01	9.99490E-01	0.	5.09304E-04	0.	0.	0.
			9.91458E-01	0.	8.53959E-03	0.	0.	0.