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ECESS--AN IBM-704 PROGRAM COMPUTING TRANSPORT EQUATION COEFFICIENTS FOR A MONATOMIC GAS MODERATOR IN THE THERMAL ENERGY REGION

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W. W. Clendenin
G. R. Culpepper

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Abstract

The ECESS code calculates transport equation coefficients for the thermal energy monatomic gas model of a physical moderator. The parameters of the model are the ratio (M/m) of atomic mass to neutron mass, and the temperature t'. Coefficients for these parameters are obtained through the P_3 approximation. In addition the code calculates infinite medium spectra of the scalar flux. The scalar flux and neutron current spectra in large geometry may also be obtained, and based on these, constants for a one group treatment of thermal neutrons are computed.

ECESS--An IBM-704 CODE COMPUTING TRANSPORT EQUATION COEFFICIENTS FOR A MONATOMIC GAS MODERATOR IN THE THERMAL ENERGY REGION

W. W. Clendenin and G. R. Culpepper

I. FORMULAS FOR THE COEFFICIENTS

The ECESS code obtains transport equation coefficients through the P_3 approximation for the monatomic gas model of a physical moderator in the thermal energy region. A description of the physical background of the model is given in WAPD-T-1109. The present report will be restricted to the computational aspects of the code.

The transport equation for neutrons in a monatomic gas medium may be expressed in the form

$$\vec{\nabla} \cdot \vec{\Omega}\, v\, F(\vec{r},\vec{\Omega},E) + \mathcal{N} \sigma_S^{eff}\, v\, F(\vec{r},\vec{\Omega},E)$$

$$+ \mathcal{N} \sigma_A^{eff}\, v\, F(\vec{r},\vec{\Omega},E) = S(\vec{r},\vec{\Omega},E)$$

$$+ \mathcal{N} \iiint v'\, \sigma(E' \to E, \theta)\, F(\vec{r},\vec{\Omega}',E')\, dE'\, d\vec{\Omega}' \quad . \qquad (1)$$

Here $F(\vec{r},\vec{\Omega},E)$ is the number density of neutrons in the direction of the unit vector $\underline{\Omega}$ having energy $E = (1/2)\, m\, v^2$, with m the neutron mass. The parameter $\mathcal{N}$ is the number density of atoms of mass M.

The effective cross sections are

$$\sigma_S^{eff} = v^{-1} \iint v_{rel}\, \sigma_S(v_{rel})\, p(U, \Psi)\, dU\, d\Psi \quad , \tag{2}$$

$$\sigma_A^{eff} = v^{-1} \iint v_{rel}\, \sigma_A(v_{rel})\, p(U, \Psi)\, dU\, d\Psi \quad , \tag{3}$$

in which v_{rel} is the relative velocity of a neutron moving with velocity $\vec{\Omega}\, v$ and an atom moving with speed U at an angle Ψ with $\vec{\Omega}$. The function $p(U, \Psi)$ is the probability

$$p(U, \Psi) = 2\pi^{-1/2}\, \beta^3 \left[U^2 \exp(-\beta^2 U^2) \right] \sin \Psi \quad , \tag{4}$$

with $\beta^2 = M/2kT$, that the atom have this velocity. The cross section $\sigma(E' \rightarrow E, \theta)$ is

$$\sigma(E' \rightarrow E, \theta) = (v')^{-1} \iint v'_{rel}\, \sigma_S(v'_{rel})\, q(E', E, \theta, U, \Psi) \cdot p(U, \Psi)\, dU\, d\Psi \quad . \tag{5}$$

In this equation Ψ is to be measured relative to $\vec{\Omega}'$; the differential cross section $\sigma_S(v'_{rel})\, q(E', E, \theta, U, \Psi)$ is the cross section for scattering through an angle θ with energy change from E' to E.

For scattering and absorption cross sections of arbitrary analytic form it would be necessary to evaluate (2) and (3) numerically. For a monatomic gas having constant $\sigma_S(v_{rel}) = \sigma_S$ and $\sigma_A(v_{rel}) = \sigma'/v_{rel}$ the effective total cross sections are

$$\sigma_S^{eff} = \sigma_S \left[\left\{ 1 + (2\beta^2 v^2)^{-1} \right\} \text{Erf } (\beta v) + (\pi^{1/2} \beta v)^{-1} \exp (-\beta^2 v^2) \right] , \quad (6)$$

$$\sigma_A^{eff} = \sigma'/v \quad . \quad (7)$$

Eq. (6) is obtained by a straightforward evaluation; Eq. (7) follows from the fact that $p(U, \Psi)$ is normalized.

In solving the transport equation, it is usually convenient to expand the cross section $\sigma(E' \rightarrow E, \theta)$ in a series of Legendre polynomials.

$$\sigma(E' \rightarrow E, \theta) = (4\pi)^{-1} \sum_{\ell} (2\ell + 1) \ \sigma_{\ell}(E' \rightarrow E) \ P_{\ell}(\cos \theta) . \quad (8)$$

The evaluation of the coefficients $\sigma_{\ell}(E' \rightarrow E)$ is discussed in WAPD-T-1109. These may be expressed in terms of the quantities z and z' where

$$z^2 = E/kT \ , \ z'^2 = E'/kT \quad . \quad (9)$$

It is convenient to define the parameters

$$y_1 = (1/2)\ (M/m)^{1/2}\ \left[(1 - m/M)\ z' + (1 + m/M)\ z\right] ,$$

$$y_2 = (1/2)\ (M/m)^{1/2}\ \left[(1 - m/M)\ z' - (1 + m/M)\ z\right] ,$$

$$y_3 = (1/2)\ (M/m)^{1/2}\ \left[(1 + m/M)\ z' - (1 - m/M)\ z\right] ,$$

$$y_4 = (1/2)\ (M/m)^{1/2}\ \left[(1 + m/M)\ z' + (1 - m/M)\ z\right] . \qquad (10)$$

For $E \leq E'$, the cross sections σ_0 through σ_3 are:

$$\sigma_0(E' \rightarrow E) = (1/8)\ (M/m)\ (1 + m/M)^2\ (\sigma_S/E')\ \Big[\ \mathrm{Erf}\ (y_1)$$

$$- \mathrm{Erf}(y_2) + \exp\ (z'^2 - z^2)\ \Big\langle \mathrm{Erf}(y_3) - \mathrm{Erf}(y_4) \Big\rangle \Big] ; \qquad (11)$$

$$\sigma_1(E' \rightarrow E) = (1/8)\ (M/m)^2\ (1 + m/M)^2\ (\sigma_S/E') \Big[\ c_1 \Big\{ \mathrm{Erf}(y_1)$$

$$- \mathrm{Erf}(y_2) \Big\} + 2\pi^{-1/2}\ c_2 \Big\{ y_1 \exp\ (-y_1^2) - y_2 \exp\ (-y_2^2) \Big\}$$

$$+ \exp\ (z'^2 - z^2)\ \Big\langle d_1\ \Big\{ \mathrm{Erf}\ (y_3) - \mathrm{Erf}\ (y_4) \Big\}$$

$$+ 2\pi^{-1/2}\ d_2 \Big\{ y_3 \exp\ (-y_3^2) - y_4 \exp\ (-y_4^2) \Big\} \Big\rangle \Big] , \qquad (12)$$

where

$$c_1 = -\ (1/2)\ (1 - m/M)\ (z'/z) + (1/2)\ (1 + m/M)\ (z/z') - 1/zz' ,$$

$$c_2 = d_2 = 1/zz' ,$$

$$d_1 = (1/2)\ (1 + m/M)\ (z'/z) - (1/2)\ (1 - m/M)\ (z/z') - 1/zz' ; \qquad (13)$$

$$\sigma_2(E' \rightarrow E) = (1/8)\ (M/m)^3\ (1 + m/M)^2\ (\sigma_S/E') \Big[e_1 \Big\{ \mathrm{Erf}(y_1)$$

$$- \mathrm{Erf}(y_2) \Big\} + 2\pi^{-1/2} e_2 \Big\{ y_1 \exp(-y_1^2) - y_2 \exp(-y_2^2) \Big\}$$

$$+ 2\pi^{-1/2} e_3 \Big\{ y_1^3 \exp(-y_1^2) - y_2^3 \exp(-y_2^2) \Big\}$$

$$+ \exp(z'^2 - z^2) \Big\langle f_1 \Big\{ \mathrm{Erf}(y_3) - \mathrm{Erf}(y_4) \Big\}$$

$$+ 2\pi^{-1/2} f_2 \Big\{ y_3 \exp(-y_3^2) - y_4 \exp(-y_4^2) \Big\}$$

$$+ 2\pi^{-1/2} f_3 \Big\{ y_3^3 \exp(-y_3^2) - y_4^3 \exp(-y_4^2) \Big\} \Big\rangle \Big] \quad , \qquad (14)$$

where

$$e_1 = (3/8)\ (1 + 2m/M + m^2/M^2)\ (z^2/z'^2) + m^2/4M^2 - 3/4$$

$$+ (3/8)\ (1 - 2m/M + m^2/M^2)\ (z'^2/z^2)$$

$$- (1/z^2 z'^2) \Big\{ (9/4 + 3m/2M)\ z^2$$

$$- (9/4 - 3m/2M)\ z'^2 - 9/2 \Big\} \quad ,$$

$$e_2 = (1/z^2 z'^2) \Big\{ (9/4 + 3m/2M)\ z^2 - (9/4 - 3m/2M)\ z'^2 - 9/2 \Big\} \quad ,$$

$$e_3 = - 3/z^2 z'^2 \quad , \qquad (15)$$

$$f_1 = (3/8)\ (1 - 2m/M + m^2/M^2)\ (z^2/z'^2) + m^2/4M^2 - 3/4$$

$$+ (3/8)\ (1 + 2m/M + m^2/M^2)\ (z'^2/z^2)$$

$$+ (1/z^2 z'^2)\ \Big\{ - (9/4 - 3m/2M)\ z^2$$

$$+ (9/4 + 3m/2M)\ z'^2 - 9/2 \Big\} \quad ;$$

$$f_2 = (1/z^2 z'^2)\ \Big\{ - (9/4 - 3m/2M)\ z^2$$

$$+ (9/4 + 3m/2M)\ z'^2 - 9/2 \Big\} \quad ,$$

$$f_3 = - 3/z^2 z'^2 \quad ;$$

$$\sigma_3(E' \to E) = (1/8)\ (M/m)^4\ (1 + m/M)^2\ (\sigma_S/E')\ \Big[g_1 \Big\{ \mathrm{Erf}\ y_1$$

$$- \mathrm{Erf}\ y_2 \Big\} + 2\pi^{-1/2}\ g_2\ \Big\{ y_1 \exp(-y_1^2) - y_2 \exp(-y_2^2) \Big\}$$

$$+ 2\pi^{-1/2}\ g_3\ \Big\{ y_1^3 \exp(-y_1^2) - y_2^3 \exp(-y_2^2) \Big\}$$

$$+ 2\pi^{-1/2}\ g_4\ \Big\{ y_1^5 \exp(-y_1^2) - y_2^5 \exp(-y_2^2) \Big\}$$

$$+ \exp(z'^2 - z^2)\ \Big\langle h_1 \Big\{ \mathrm{Erf}(y_3) - \mathrm{Erf}(y_4) \Big\}$$

$$+ 2\pi^{-1/2}\ h_2\ \Big\{ y_3 \exp(-y_3^2) - y_4 \exp(-y_4^2) \Big\}$$

$$+ 2\pi^{-1/2}\ h_3\ \Big\{ y_3^3 \exp(-y_3^2) - y_4^3 \exp(-y_4^2) \Big\}$$

$$+ 2\pi^{-1/2}\ h_4\ \Big\{ y_3^5 \exp(-y_3^2) - y_4^5 \exp(-y_4^2) \Big\} \Big\rangle \Big] \quad , \tag{16}$$

where

$$g_1 = (5/16)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ z^3/z'^3$$

$$+ (3/16)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ z/z'$$

$$+ (3/16)(5 - 5m/M - m^2/M^2 + m^3/M^3)\ z'/z$$

$$+ (5/16)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ z'^3/z^3$$

$$+ (1/z^3z'^3)\ \Big\{ - (15/8)\ (2 - 3m/M + m^2/M^2)\ z'^4$$

$$+ (3/4)\ (10 - 3m^2/M^2)\ z^2z'^2 - (15/8)\ (2 + 3m/M + m^2/M^2)\ z^4$$

$$+ (75/4 + 45m/4M)\ z^2 - (75/4 - 45m/4M)\ z'^2$$

$$- 75/2 \Big\} \quad ,$$

$$g_2 = (1/z^3z'^3)\ \Big\{ (15/8)\ (2 - 3m/M + m^2/M^2)\ z'^4$$

$$- (3/4)\ (10 - 3m^2/M^2)\ z^2z'^2 + (15/8)\ (2 + 3m/M + m^2/M^2)\ z^4$$

$$+ (75/4 - 45m/4M)\ z'^2 - (75/4 + 45m/4M)\ z^2 + 75/2 \Big\} \quad ,$$

$$g_3 = (1/z^3z'^3)\ \Big\{ (25/2 - 15m/2M)\ z'^2 + (-25/2 - 15m/2M)\ z^2$$

$$+ 25 \Big\} \quad ,$$

$$g_4 = 10/z^3z'^3 \quad , \qquad (17)$$

$$h_1 = (5/16)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (3/16)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (3/16)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/16)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3)$$

$$+ (1/z^3 z'^3)\ \Big\{ - (15/8)\ (2 + 3m/M + m^2/M^2)\ z'^4$$

$$+ (3/4)\ (10 - 3m^2/M^2)\ z^2 z'^2 - (15/8)\ (2 - 3m/M + m^2/M^2)\ z^4$$

$$+ (75/4 + 45m/4M)\ z'^2 - (75/4 - 45m/4M)\ z^2 - 75/2 \Big\} ,$$

$$h_2 = (1/z^3 z'^3)\ \Big\{ (15/8)\ (2 + 3m/M + m^2/M^2)\ z'^4$$

$$- (3/4)\ (10 - 3m^2/M^2)\ z^2 z'^2 + (15/8)\ (2 - 3m/M + m^2/M^2)\ z^4$$

$$- (75/4 + 45m/4M)\ z'^2 + (75/4 - 45m/4M)\ z^2 + 75/2 \Big\} ,$$

$$h_3 = (1/z^3 z'^3)\ \Big\{ (-25/2 - 15m/2M)\ z'^2$$

$$+ (25/2 - 15m/2M)\ z^2 + 25 \Big\} ,$$

$$h_4 = 10/z^3 z'^3 .$$

The cross sections for $E \geq E'$ may be expressed by similar formulas. However, since each of the cross sections σ_ℓ obeys the detailed balance condition, these cross sections are most easily obtained from those for $E \leq E'$ by making use of this condition. Thus

$$z_1^2 \exp(-z_1^2)\, \sigma_\ell(E_1 \to E_2) = z_2^2 \exp(-z_2^2)\, \sigma_\ell(E_2 \to E_1) \quad , \tag{18}$$

whatever the magnitude relation between E_1 and E_2.

Each of the formulas (11), (12), (14), (16) for $\sigma_\ell(E' \to E)$ is made up of four terms, each one of which involves only one of the y_k, $k = 1 \ldots 4$. The forms for these terms given in (11), (12), (14) and (16) are suitable for computation only for $1 \leq y_k \leq 3$. For values of y_k outside this range, the large cancellation of terms belonging to a given y_k prevents accurate computation with the formulas in this form. For $y_k \leq 1.1$ and $k = 1$ or 2 the terms in y_k inside the square brackets of (12) are replaced by the series

$$\begin{aligned}
\pm\, 2\pi^{-1/2} \Big\{ & c_1 y_k - (c_1/3 + c_2)\, y_k^3 + (c_1/10 + c_2/2)\, y_k^5 \\
& - (c_1/42 + c_2/6)\, y_k^7 + (c_1/216 + c_2/24)\, y_k^9 \\
& - (c_1/1{,}320 + c_2/120)\, y_k^{11} + (c_1/9{,}360 + c_2/720)\, y_k^{13} \\
& - (c_1/75{,}600 + c_2/5{,}040)\, y_k^{15} + (c_1/685{,}440 + c_2/40{,}320)\, y_k^{17} \\
& - (c_1/6{,}894{,}720 + c_2/362{,}880)\, y_k^{19} \\
& + (c_1/76{,}204{,}800 + c_2/3{,}628{,}800)\, y_k^{21} \\
& - (c_1/91{,}808{,}640 \times 10 + c_2/39{,}916{,}800)\, y_k^{23} \\
& + (c_1/11{,}975{,}040 \times 10^3 + c_2/47{,}900{,}160 \times 10)\, y_k^{25}
\end{aligned}$$

$$- (c_1/16,812,956 \times 10^4 + c_2/62,270,208 \times 10^2)\; y_k^{27}$$

$$+ (c_1/25,281,704 \times 10^5 + c_2/87,178,291 \times 10^3)\; y_k^{29} \Big\} , \qquad (19)$$

where the upper sign is used for y_1 and the lower sign for y_2. The parameter C_1 is

$$C_1 = (1/2) \left[(1 + m/M)\,(z/z') - (1 - m/M)\,(z'/z) \right] . \qquad (20)$$

For y_3 and y_4 a series of the same form as (19) is used but with the factor ± 1 replaced by $\pm \exp\,(z'^2 - z^2)$, the parameter c_1 by d_1, and the parameter C_1 by D_1, where

$$D_1 = (1/2) \left[(1 + m/M)\,(z'/z) - (1 - m/M)\,(z/z') \right] . \qquad (21)$$

The upper sign is to be used for y_3 and the lower sign for y_4.

The terms in y_k in the square brackets of (14) are replaced for $y_k \leq 1.1$ and for $k = 1$ or 2 by the series

$$\pm\, 2\pi^{-1/2} \Big\{ E_1 y_k - E_2 y_k^3 + (3E_2/5 - E_1/10 - 2e_3/5)\; y_k^5$$

$$- (3E_2/14 - E_1/21 - 2e_3/7)\; y_k^7$$

$$+ (e_1/216 + e_2/24 - e_3/6)\; y_k^9$$

$$- (e_1/1,320 + e_2/120 - e_3/24)\; y_k^{11}$$

$$+ (e_1/9,360 + e_2/720 - e_3/120)\; y_k^{13}$$

$$\mp (e_1/75{,}600 + e_2/5{,}040 - e_3/720)\, y_k^{15}$$

$$+ (e_1/685{,}440 + e_2/40{,}320 - e_3/5{,}040)\, y_k^{17}$$

$$\mp (e_1/6{,}894{,}720 + e_2/362{,}880 - e_3/40{,}320)\, y_k^{19}$$

$$+ (e_1/76{,}204{,}800 + e_2/3{,}628{,}800 - e_3/362{,}880)\, y_k^{21}$$

$$\mp (e_1/91{,}808{,}640 \times 10 + e_2/39{,}916{,}800 - e_3/3{,}628{,}800)\, y_k^{23}$$

$$+ (e_1/11{,}975{,}040 \times 10^3 + e_2/47{,}900{,}160 \times 10 - e_3/39{,}916{,}800)\, y_k^{25}$$

$$\mp (e_1/16{,}812{,}956 \times 10^4 + e_2/62{,}270{,}208 \times 10^2 - e_3/47{,}900{,}160 \times 10)\, y_k^{27}$$

$$+ (e_1/25{,}281{,}704 \times 10^5 + e_2/87{,}178{,}291 \times 10^3 - e_3/62{,}270{,}208 \times 10^2)\, y_k^{29} \Big\} , \qquad (22)$$

where the upper sign is used for y_1 and the lower sign for y_2. The parameters E_1 and E_2 are

$$E_1 = (3/8)\ (1 + 2m/M + m^2/M^2)\ (z^2/z'^2) + m^2/4M^2$$
$$- 3/4 + (3/8)\ (1 - 2m/M + m^2/M^2)\ (z'^2/z^2) ,$$

$$E_2 = (1/8)\ (1 + 2m/M + m^2/M^2)\ (z^2/z'^2) + m^2/12M^2$$
$$- 1/4 + (1/8)\ (1 - 2m/M + m^2/M^2)\ (z'^2/z^2)$$
$$+ (2/3\ z^2 z'^2)\ \Big\{ (9/4 + 3m/2M)\, z^2$$
$$- (9/4 - 3m/2M)\, z'^2 \Big\} . \qquad (23)$$

In the case of y_3 and y_4 the terms in the square brackets of (14) are replaced by a series of the same form as (22) but with the factor ± 1 replaced by $\pm \exp(z'^2 - z^2)$, the parameter e_1 by f_1, the parameter e_2 by f_2, and the quantities E_1 and E_2 respectively by F_1 and F_2 where

$$F_1 = (3/8)\ (1 - 2m/M + m^2/M^2)\ (z^2/z'^2) + m^2/4M^2 - 3/4$$
$$+ (3/8)\ (1 + 2m/M + m^2/M^2)\ (z'^2/z^2)\ ,$$

$$F_2 = (1/8)\ (1 - 2m/M + m^2/M^2)\ (z^2/z'^2) + m^2/12M^2 - 1/4$$
$$+ (1/8)\ (1 + 2m/M + m^2/M^2)\ (z'^2/z^2)$$
$$+ (2/3\ z^2 z'^2) \Big\{ - (9/4 - 3m/2M)\ z^2$$
$$+ (9/4 + 3m/2M)\ z'^2 \Big\}\ . \qquad (23')$$

The upper sign is to be used for y_3 and the lower sign for y_4.

For the cross section of (16), the terms in y_k with k = 1 or 2 in the square brackets are replaced for $y_k \leq 1.1$ by

$$\pm 2\pi^{-1/2} \Big\{ G_1 y_k - G_2 y_k^3 + G_3 y_k^5$$
$$- (G_1/42 - 3G_2/14 + 5G_3/7 + 2g_4/7)\ y_k^7$$
$$+ (G_1/72 - G_2/9 + 5\ G_3/18 + 2g_4/9)\ y_k^9$$
$$- (g_1/1{,}320 + g_2/120 - g_3/24 + g_4/6)\ y_k^{11}$$
$$+ (g_1/9{,}360 + g_2/720 - g_3/120 + g_4/24)\ y_k^{13}$$

$$- (g_1/75,600 + g_2/5,040 - g_3/720 + g_4/120)\ y_k^{15}$$

$$+ (g_1/685,440 + g_2/40,320 - g_3/5,040 + g_4/720)\ y_k^{17}$$

$$- (g_1/6,894,720 + g_2/362,880 - g_3/40,320 + g_4/5,040)\ y_k^{19}$$

$$+ (g_1/76,204,800 + g_2/3,628,800 - g_3/362,880 + g_4/40,320)\ y_k^{21}$$

$$- (g_1/91,808,640 \times 10 + g_2/39,916,800 - g_3/3,628,800 + g_4/362,880)\ y_k^{23}$$

$$+ (g_1/11,975,040 \times 10^3 + g_2/47,900,160 \times 10 - g_3/39,916,800 + g_4/3,628,800)\ y_k^{25}$$

$$- (g_1/16,812,956 \times 10^4 + g_2/62,270,208 \times 10^2 - g_3/47,900,160 \times 10 + g_4/39,916,800)\ y_k^{27}$$

$$+ (g_1/25,281,704 \times 10^5 + g_2/87,178,291 \times 10^3 - g_3/62,270,208 \times 10^2 + g_4/47,900,160 \times 10)\ y_k^{29} \Big\} \quad , \qquad (24)$$

where the upper sign is used for y_1 and the lower sign for y_2. The parameters G_1, G_2, G_3 are

$$G_1 = (5/16)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (3/16)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (3/16)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/16)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3) \quad ,$$

$$G_2 = (5/48)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (1/16)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (1/16)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/48)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3)$$

$$+ (2/3\ z^3 z'^3)\ \Big\{ (15/8)\ (2 - 3m/M + m^2/M^2)\ z'^4$$

$$- (3/4)\ (10 - 3m^2/M^2)\ z^2 z'^2$$

$$+ (15/8)\ (2 + 3m/M + m^2/M^2)\ z^4 \Big\} \quad , \tag{25}$$

$$G_3 = (5/160)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (3/160)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (3/160)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/160)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3)$$

$$+ (2/5\ z^3 z'^3)\ \Big\{ (15/8)\ (2 - 3m/M + m^2/M^2)\ z'^4$$

$$- (3/4)\ (10 - 3m^2/M^2)\ z^2 z'^2$$

$$+ (15/8)\ (2 + 3m/M + m^2/M^2)\ z^4 \Big\}$$

$$+ (1/z^3 z'^3)\ \Big\{ (5 + 3m/M)\ z^2 - (5 - 3m/M)\ z'^2 \Big\} \quad .$$

For y_3 and y_4, a series of the same form as (24) replaces the terms in y_k in the square brackets of (16) for $y_k \leq 1.1$, with the factor ± 1 replaced by

$\pm \exp(z'^2 - z^2)$, the parameters g_1, g_2, g_3, g_4 replaced by h_1, h_2, h_3, h_4 respectively, and the parameters G_1, G_2, G_3 by H_1, H_2, H_3 respectively. These quantities are

$$H_1 = (5/16)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (3/16)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (3/16)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/16)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3) \quad ,$$

$$H_2 = (5/48)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (1/16)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (1/16)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/48)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3)$$

$$+ (2/3\ z^3 z'^3)\ \Big\{ (15/8)\ (2 + 3m/M + m^2/M^2)\ z'^4$$

$$- (3/4)\ (10 - 3m^2/M^2)\ z^2 z'^2 + (15/8)\ (2 - 3m/M + m^2/M^2)\ z^4 \Big\} \quad ,$$

$$H_3 = (5/160)\ (-1 + 3m/M - 3m^2/M^2 + m^3/M^3)\ (z^3/z'^3)$$

$$+ (3/160)\ (5 - 5m/M - m^2/M^2 + m^3/M^3)\ (z/z')$$

$$+ (3/160)\ (-5 - 5m/M + m^2/M^2 + m^3/M^3)\ (z'/z)$$

$$+ (5/160)\ (1 + 3m/M + 3m^2/M^2 + m^3/M^3)\ (z'^3/z^3)$$

$$+ (2/5\, z^3 z'^3) \left\{ (15/8)\ (2 + 3m/M + m^2/M^2)\ z'^4 \right.$$

$$- (3/4)\ (10 - 3m^2/M^2)\ z^2 z'^2$$

$$\left. + (15/8)\ (2 - 3m/M + m^2/M^2)\ z^4 \right\}$$

$$+ (1/z^3 z'^3) \left\{ (5 + 3m/M)\ z'^2 - (5 - 3m/M)\ z^2 \right\} . \qquad (26)$$

The upper sign is used for y_3 and the lower sign for y_4.

For $y_k \geq 3$, the error function which appears in the formulas must be replaced by its asymptotic expansion. Since the first term in this expansion is independent of y_k, accuracy may be increased by treating the terms in y_1 and y_2 together, and the terms in y_3 and y_4 together. For $y_2 \geq 3$, the error functions in y_1 and y_2 are each replaced by

$$\mathrm{Erf}\ (y_k) \rightarrow -\pi^{-1/2}\ y_k^{-1}\ \exp\ (-y_k^2)\ S(y_k) \quad , \qquad (27)$$

where

$$S(y_k) = 1 - 1/2y_k^2 + 3/(2y_k^2)^2 - 15/(2y_k^2)^3$$

$$+ 105/(2y_k^2)^4 - 945/(2y_k^2)^5 + 10{,}395/(2y_k^2)^6$$

$$- 135{,}135/(2y_k^2)^7 + 2{,}027{,}025/(2y_k^2)^8$$

$$- 34{,}459{,}425/(2y_k^2)^9 \quad . \qquad (28)$$

For $y_3 \geq 3$, the error functions in y_3 and y_4 are replaced by

$$\exp\ (z'^2 - z^2) \left\{ \mathrm{Erf}\ (y_3) \right\} \rightarrow -\pi^{-1/2}\ y_3^{-1}\ \exp\ (-y_2^2)\ S(y_3) \quad ,$$

$$\exp\ (z'^2 - z^2) \left\{ \mathrm{Erf}\ (y_4) \right\} \rightarrow -\pi^{-1/2}\ y_4^{-1}\ \exp\ (-y_1^2)\ S(y_4) \quad . \qquad (29)$$

Since the error functions in y_1 and y_2 always occur with opposite signs, as is also true of the error functions in y_3 and y_4, the first term in each of the asymptotic series of (27) and (29) has been omitted.

The directional flux of Eq. (1) may be expanded in a series of Legendre polynomials of the angles with a polar axis. For slab geometry this has the form

$$v\ F(\vec{r},\vec{\Omega},E) = (4\pi)^{-1} \sum_{\ell} (2\ell + 1)\ \varphi_{\ell}(x,E)\ P_{\ell}(\mu) \quad ,$$

$$v'F(\vec{r},\vec{\Omega}',E') = (4\pi)^{-1} \sum_{\ell} (2\ell + 1)\ \varphi_{\ell}(x,E')\ P_{\ell}(\mu') \quad , \tag{30}$$

where μ and μ' are direction cosines with the polar axis, and x is the position coordinate along the axis. The cross section of (8) may be expressed in terms of μ, μ' and the corresponding azimuths χ and χ' by means of the addition theorem for Legendre polynomials

$$P_{\ell}(\cos\theta) = P_{\ell}(\mu)\ P_{\ell}(\mu') + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!}\ P_{\ell}^{m}(\mu)\ P_{\ell}^{m}(\mu')$$

$$\cdot \cos m\,(\chi - \chi') \quad . \tag{31}$$

With the use of (30) and (31), the integration over $\vec{\Omega}'$ in Eq. (1) may be carried out. The usual resolution of the transport equation through expansion of the flux in Legendre polynomials reduces it to the set of equations,

$$\frac{\ell+1}{2\ell+1}\frac{\partial\varphi_{\ell+1}(x,E)}{\partial x}+\frac{\ell}{2\ell+1}\frac{\partial\varphi_{\ell-1}(x,E)}{\partial x}$$

$$+\mathcal{N}\left[\sigma_S^{eff}+\sigma_A^{eff}\right]\varphi_\ell(x,E)=S_\ell(x,E)$$

$$+\mathcal{N}\int_0^\infty \sigma_\ell(E'\rightarrow E)\,\varphi_\ell(x,E')\,dE' \quad . \tag{32}$$

Here the direct source term $S(\bar{r},\bar{\Omega},E)$ has been expanded as

$$S(\vec{r},\vec{\Omega},E)=(4\pi)^{-1}\sum_\ell (2\ell+1)\,S_\ell(x,E)\,P_\ell(\mu) \quad . \tag{33}$$

In order to solve the equations (32) it is necessary to evaluate the scattering-in integral on the right side of each equation. For application to the thermal energy range, this range may be specified by an upper energy limit E_0. For energies above E_0, the flux component $\varphi_\ell(x,E)$ is assumed to have an asymptotic form which specifies this part of the scattering-in integral. The thermal energy range $0 \leq E \leq E_0$ is divided by means of the N values E_n ($E_{n+1} < E_n$) into N + 1 energy intervals. In each interval the integrand of (32) is taken to vary linearly with energy, corresponding to a trapezoid rule integration. The integral corresponding to $E = E_n$ is then replaced by the sum

$$\sum_{j=1}^{N} c_\ell^{j\rightarrow n}\,\varphi_\ell^j(x) \tag{34}$$

in which

$$\varphi_\ell^j(x)=\varphi_\ell(x,E_j) \quad ,$$

$$c_\ell^{1\rightarrow n}=(1/2)\left\{E_0-E_2+(E_0-E_1)\,(E_1/E_0)^2\right\}\sigma_\ell(E_1\rightarrow E_n) \quad ,$$

$$c_\ell^{j\rightarrow n}=(1/2)\,(E_{j-1}-E_{j+1})\,\sigma_\ell(E_j\rightarrow E_n),\; j=2\,\ldots\,N \quad . \tag{35}$$

Eqs. (32) for $E = E_n$ with the integral evaluated by (34) are a set of ℓN equations in the variables $\varphi_\ell^n(x)$ which may be solved by iterative methods.

It is also necessary to compute σ_S^{eff} of Eq. (6). Since the essential characteristic of the cross section is the fact that it obeys the detailed balance condition, it is useful to retain this property in the form of the equations used for numerical solution. The parameter σ_S^{eff} for a particular energy E_n and temperature is replaced by

$$p_0(z_n) = \left[z_n^2 \exp(-z_n^2) \right]^{-1} \sum_{j=1}^{N} C_0^{j \to n} z_j^2 \exp(-z_j^2) \quad . \tag{36}$$

The similar sums p_ℓ in which $C_0^{j \to n}$ is replaced by $C_\ell^{j \to n}$ are also computed. As a check on p_0 the parameter σ_S^{eff} is computed from Eq. (6). This serves primarily to verify that the group structure values E_n are sufficiently closely spaced.

The part

$$\int_{E_0}^{\infty} \sigma_0(E' \to E)\ \varphi_0(x,E')\ dE' \tag{37}$$

of the scattering-in integral is a source term. For the thermal problem this source, which represents the neutrons which have had collisions in the moderator, will in the usual case be the principal one. The direct source $S_0(x,E)$ must be added if it is not negligible. For high energies $\varphi_0(x,E')$ will have the asymptotic form $k(x) \left\{ \lambda/E' \right\}$ where λ is a constant. The energy dependence of the source term is given by the source integral

$$s(z_n) = \int_0^\infty \left\{ \lambda/E' \right\} \sigma_0(E' \rightarrow E_n) \, dE' \quad . \tag{38}$$

This is computed numerically by the code for each value of z_n. Since the normalization of the source is immaterial, the constant λ is chosen so that $s(z_0) = 1$.

The quantities needed for solution of Eq. (32) are recorded on tape as one form of output of the ECESS code (Section V.). These quantities are

$$z_n^2 \exp(-z_n^2) \ , \ n = 1 \ldots N \ ;$$

$$s(z_n) \ , \ n = 0 \ldots N \ ,$$

$$p_0(z_n) \ , \ n = 1 \ldots N \ ;$$

$$C_\ell^{j \rightarrow n} \ , \ n = 1 \ldots N \ , \ j = 1 \ldots N \ , \ \ell = 0 \ldots 3 \quad . \tag{39}$$

II. SPECIAL SOLUTIONS OF THE TRANSPORT EQUATION

A second purpose of the code, in addition to computing the quantities of Eq. (39), is to solve Eqs. (32) for the cases of an infinite medium or a geometry large compared with a mean free path. For an infinite medium, Eqs. (32) reduce to the neutron moderation equations for $\ell = 0$,

$$\left[p_0(z_n) + \sigma_A^{eff}(E_n) \right] \varphi_0^n = s(z_n) + \sum_{j=1}^{N} C_0^{j \rightarrow n} \varphi_0^j \ , \ n = 1 \ldots N \ . \tag{40}$$

These equations are solved for the fluxes φ_0^n with the GDSR subroutine (Ref. 1), an iterative technique. For convenience $\sigma_A^{eff}(E_n)$ is expressed as

$$\sigma_A^{eff}(E_n) = \sigma_0 / \left\{ E_n/.0253 \right\}^{1/2} , \tag{41}$$

where E_n is in electron-volts. The parameter σ_0 used as input is the absorption cross section at 2200 m./s.

In order to accelerate the convergence of the iterative process, both renormalization and extrapolation techniques are used. The starting flux has a Maxwell form,

$$\varphi_0^n = A\, z_n^2 \exp(-z_n^2) , \tag{42}$$

in which the constant A is determined by requiring equality of the number of neutrons absorbed to the number introduced by the source. The value of this constant is

$$A = \left[\left\{ kT/.0253 \right\}^{1/2} \int_0^{z_0} s(z_n)\, z_n dz_n \right] \Big/ \left[\sigma_0 \right.$$

$$\left. \cdot \left\{ (\pi^{1/2}/4)\, \mathrm{Erf}(z_0) - (1/2)\, z_0 \exp(-z_0^2) \right\} \right] , \tag{43}$$

where kT is in electron-volts. This normalization is repeated after each iteration in which the largest fractional change in the flux is greater than a preset parameter δ, usually set at .01. The normalization factor B differs from A of (43) only in that the term in z_0 in the denominator is replaced by

$$\int_0^{z_0} \varphi_0(z_n)\, dz_n \quad .$$

In addition, a trial function is obtained by extrapolation for each iteration from the formula

$$ {}^{i}\varphi_0^n \text{ (trial)} = {}^{i}\varphi_0^n + \theta_1 \left\{ {}^{i}\varphi_0^n - {}^{i-1}\varphi_0^n \right\} \quad . \tag{44}$$

Here θ_1 is a preset parameter, usually .8, the parameters i and i-1 are the indices of the iterations, and the quantities φ_0^n are the normalized fluxes.

Since the error of trapezoid rule integration is inherent in the normalization factor, the normalization process is discontinued when the fractional change in fluxes is less than δ. The extrapolation process is then continued with unnormalized fluxes.

In the case of large geometry, Eqs. (32) are approximated sufficiently accurately with a P_1 approximation in which flux components with $\ell \geq 2$ are neglected. In this case, the flux component $\varphi_\ell(x,E)$ is separable,

$$\varphi_\ell(x,E) = f_\ell(x) \ \psi_\ell(E) \quad . \tag{45}$$

Under these conditions, Eqs. (32) reduce to the two equations

$$\left\{ df_1/dx \right\} \psi_1(E) + \mathcal{N} \left\{ \sigma_S^{eff} + \sigma_A^{eff} \right\} f_0 \psi_0(E)$$

$$= \mathcal{N} f_0 \int_0^\infty \sigma_0(E' \to E) \ \psi_0(E')\, dE' \quad , \tag{46}$$

$$(1/3)\left\{df_0/dx\right\}\psi_0(E) + \mathcal{N}\left\{\sigma_S^{eff} + \sigma_A^{eff}\right\} f_1\psi_1(E)$$

$$= \mathcal{N} f_1 \int_0^\infty \sigma_1(E' \rightarrow E)\psi_1(E')\, dE' \quad , \tag{47}$$

applicable when the direct source terms $S_\ell(x,E)$ are negligible. Eqs. (46) and (47) are solved for the large geometry limit in which the first term in (46) is neglected so that this equation reduces to Eq. (40). Eq. (47) is put into a similar form. Since the normalization of the ψ_1 spectrum is immaterial, it is written as

$$\left[p_0(z_n) + \sigma_A^{eff}(E_n)\right] \psi_1^n = \psi_0^n$$

$$+ \sum_{j=1}^{N} G_1^{j\rightarrow n}\, \psi_1^j \, , \; n = 1 \ldots N \, , \tag{48}$$

in which the integral $\int_{E_0}^\infty \sigma_1(E' \rightarrow E)\ \psi_1(E')\ dE'$ has been neglected. These equations are also solved using the GDSR subroutine, and the extrapolation technique, without normalization, of Eq. (44). After they have been computed both the spectra ψ_o^n and ψ_1^n are renormalized so that

$$\int_0^{E_0} \left\{.0253/E\right\}^{1/2} \psi_\ell(E)\, dE = 1 \, . \tag{49}$$

A one energy group description of thermal neutrons is obtained by integration of Eq. (32) over energies. This equation then takes the form

$$\frac{\ell+1}{2\ell+1}\frac{\partial\Phi_{\ell+1}(x)}{\partial x} + \frac{\ell}{2\ell+1}\frac{\partial\Phi_{\ell-1}(x)}{\partial x}$$

$$+ \mathcal{N}(Q_\ell + R_\ell - P_\ell)\,\Phi_\ell(x) = T_\ell(x) \quad . \tag{50}$$

in which

$$\Phi_\ell(x) = \int_0^{E_0} \varphi_\ell(x,E)\, dE \quad , \tag{51}$$

$$Q_\ell(x) = \int_0^{E_0} \sigma_S^{eff}\, \varphi_\ell(x,E)\, dE/\Phi_\ell(x) \quad , \tag{52}$$

$$R_\ell(x) = \int_0^{E_0} \sigma_A^{eff}\, \varphi_\ell(x,E)\, dE/\Phi_\ell(x) \quad , \tag{53}$$

$$P_\ell(x) = \int_0^{E_0} dE \int_0^{E_0} \sigma_\ell(E' \rightarrow E)\, \varphi_\ell(x,E')\, dE'/\Phi_\ell(x) \quad , \tag{54}$$

$$T_\ell(x) = \int_0^{E_0} S_\ell(x,E)\, dE + \mathcal{N}\int_0^{E_0} dE \int_{E_0}^{\infty} \sigma_\ell(E' \rightarrow E)\, \varphi_\ell(x,E')\, dE' \quad . \tag{55}$$

Using the fluxes $\psi_0(E)$ and $\psi_1(E)$, obtained from Eqs. (40) and (48), the integrals of (51) through (55) are computed. The notation for these integrals is

$$N_\ell = \sum_{n=0}^{N} (z_n - z_{n+1}) \left[z_n\, \psi_\ell^n + z_{n+1}\, \psi_\ell^{n+1} \right]$$

$$= (kT)^{-1} \int_0^{E_0} \psi_\ell(E)\, dE \quad , \tag{56}$$

$$J_\ell = \sum_{n=0}^{N} (z_n - z_{n+1}) \left[z_n p_0(z_n) \ \psi_\ell^n + z_{n+1} p_0(z_{n+1}) \ \psi_\ell^{n+1} \right]$$

$$= (kT)^{-1} \int_0^{E_0} \sigma_S^{eff} \ \psi_\ell(E) \ dE \quad , \tag{57}$$

$$I_\ell = \sum_{n=0}^{N} (z_n - z_{n+1}) \left[z_n \sum_{j=1}^{N} C_\ell^{j \to n} \ \psi_\ell^j + z_{n+1} \sum_{j=1}^{N} C_\ell^{j \to n+1} \ \psi_\ell^j \right]$$

$$= (kT)^{-1} \int_0^{E_0} dE \int_0^{E_0} \sigma_\ell(E' \to E) \ \psi_\ell(E') \ dE' \quad . \tag{58}$$

Here the quantities at E_0 are taken to be

$$\psi_\ell^0 = (E_1/E_0) \ \psi_\ell^1 \quad ,$$

$$p_0(z_0) \ \psi_\ell^0 = (E_1/E_0) \ p_0(z_1) \ \psi_\ell^1 \quad , \tag{59}$$

$$\sum_{j=1}^{N} C_\ell^{j \to 0} \ \psi_\ell^j = (E_1/E_0) \sum_{j=1}^{N'} C_\ell^{j \to 1} \ \psi_\ell^j \quad .$$

The integrals N_0, J_0, I_0, N_1, J_1, I_1 are computed. In addition the integrals I_{20} and I_{30} are obtained from $C_2^{j \to n}$ and $C_3^{j \to n}$, approximating ψ_2 and ψ_3 with ψ_0. The integrals I_{21} and I_{31} are obtained from $C_2^{j \to n}$ and $C_3^{j \to n}$, approximating ψ_2 and ψ_3 with ψ_1. The parameters of Eqs. (52) through (54) are given in terms of the integrals by

$$Q_\ell = J_\ell / N_\ell \quad ,$$

$$R_\ell = \sigma_0 / (kT) N_\ell \quad ,$$

$$P_\ell = I_\ell / N_\ell \quad . \tag{60}$$

Two computational checks on the problem are provided by the relations implied by Eq. (40) and Eq. (48),

$$J_0 = I_0 \;,$$

$$J_1 + \sigma_0/(kT) = I_1 + N_0/P_1 \quad . \tag{61}$$

In this equation P_1 is a normalization constant for $\psi_1(E)$ which is printed out.

The quantity Q_ℓ is an effective scattering cross section for the thermal group, R_ℓ is an effective absorption cross section, and P_ℓ/Q_ℓ is the average Legendre polynomial. All are spectrum-dependent. The diffusion coefficient of the monatomic gas is

$$D = 1/\left\{3\mathcal{N}(Q_1 + R_1 - P_1)\right\} \;, \tag{62}$$

and the diffusion length is

$$L = \left[1/\left\{3\mathcal{N}^2 R_0(Q_1 + R_1 - P_1)\right\}\right]^{1/2} \quad . \tag{63}$$

Since the coefficients $C_2^{j\to n}$ and $C_3^{j\to n}$ are not relevant to the solution of Eq. (40) and Eq. (48), one form of the code omits their calculation. This form has been labeled ECES3. The form which includes calculation of $C_2^{j\to n}$ and $C_3^{j\to n}$ has been labeled ECES2.

III. INPUT

The field format of the input cards for ECESS includes quantities in both fixed point and floating point notation. The quantities in fixed point notation are positive integers listed as such. The quantities in floating point notation are listed in a form containing ten or fewer digits. The first two digits are the sum of a power of ten and the number fifty; the remaining eight or fewer digits make up the number specified with the decimal point understood as preceding the first of the eight digits. The first field on each card is the total number N of groups (fixed point). The remaining fields of the five cards are as follows:

Card, Type 1

Field	Information
2	Centigrade temperature $t > 0$ to nearest degree (fixed point).
3	Total number K of absorption cross sections σ_0 (fixed point).
4	Atomic mass M (floating point).
5	Neutron mass m (floating point).
6	Asymptotic scattering cross section σ_S (floating point).

Cards, Type 2

Field	Information
2-7	Energy levels E_n in ev. (floating point). There will be N+1 numbers in descending order $E_0 \ldots E_N$. A maximum of six values on a card.

If the number K on Card 1 is zero, the rest of the cards after Card 2 are omitted.

Cards, Type 3

Field	Information
2-7	The K values of the absorption cross section σ_0 (floating point), six or fewer to a card.

Card, Type 4

Field	Information
2	Normalization criterion δ (floating point).
3	Extrapolation factor θ_1 (floating point) for equations in ψ_0.

Card, Type 5

Field	Information
2	Extrapolation factor θ_2 (floating point) for equations in ψ_1. A separate card must be used for each value of σ_0. Solution of these equations may be omitted by using a blank card in place of Card 5.

The unused part of each card is filled in with zeroes.

It is possible to run consecutive problems with the same group structure and same temperature but with a different mass ratio, M/m, by using only Cards 1, 3, 4, 5. Decks for consecutive problems are placed directly after one another. For consecutive problems with the same number of groups but different temperatures, Cards 1, 2, 3, 4, 5 must be used. No blank cards are used except at the end or in place of Card 5 as described above. Three blanks are placed at the end of the input deck(s).

A sample input deck is shown below. This is for a 36-group problem at 21°C., with one absorption cross section σ_0. The atomic mass is M = 2.75, the neutron mass is m = 1.00 (only the ratio M/m is significant), and the scattering cross section is 35.75 barns. The energy E_0 = .680 ev. and the energy E_N = .0005 ev. The cross section σ_0 = .33 barns. The parameters involved in acceleration of the iterative process are δ = .01, θ_1 = .8 and θ_2 = .8.

```
+ 36 + 21 + 1 + 51275 + 511 + 523575 +
+ 36 + 5068 + 50648 + 50612 + 50578 + 50544 + 50512 +
+ 36 + 5048 + 5045 + 5042 + 50392 + 50364 + 50338 +
+ 36 + 50312 + 50288 + 50264 + 50242 + 5022 + 502 +
+ 36 + 5018 + 50162 + 50144 + 50128 + 50112 + 4998 +
+ 36 + 4984 + 4972 + 496 + 495 + 494 + 4932 +
+ 36 + 4924 + 4918 + 4913 + 488 + 484 + 482 +
+ 36 + 475 +
+ 36 + 5033 +
+ 36 + 491 + 508 +
+ 36 + 508 +
```

(Three blank cards)

IV. OPERATING INSTRUCTIONS

Place the ECESS program tape on logical tape 1 and blanks on logical tapes 3 and 5.

Place the input deck(s) in card hopper.

Push CLEAR, LØAD TAPE.

End of run programmed stop is <u>10425</u>.

Save tape 5 for printing off-line. Tape is not rewound.

Save tape 3 if indicated by requestor. An EOF is written on tape 3 after all problems have been run and it is rewound.

Error stops

00603	GLØUT2.	Machine error.
00662	GLØUT2.	Machine error.
01435	WHOO1.	Machine error.
01470	WHOO1.	Machine error.
01553	WHOO1.	Input error. Double punch, blank column.
01766	WHOO1.	Input error. Range error. Floating decimal number out-of-range.
03315	GDSR.	Solution to set of equations not converged after 999 iterations. Push start to continue for another 999 iterations. Problem probably no good.
04367	WHOO1 return.	Bad count end-of-file. Machine error.
04737	SORT error return.	Machine error or negative mass specified.
05024	WHOO1 return.	Blank card.
05025	WHOO1 return.	Count end-of-file.
05050	SORT error return.	Machine error or negative energy specified.
05055	EXP error return.	Machine error. Negative arguments only.
05171	EXPC error return.	Machine error since negative arguments only.
05307	EXPC error return.	Argument too large. Machine or specified energy error.

06752	EXPC error return.	Argument too large. Machine or specified energy error.
07426	SQRT error return.	Machine error.
07546	EXP error return.	Same as 5055.
07623	PWT5 error return.	Impossible end-of-file return. Writing tape 3.
07624	PWT5 error return.	Writing tape 3. Machine error.
07651	WH001 return.	Same as 5024.
07652	WH001 return.	Same as 5025.
07667	WH001 return.	Same as 5024.
07670	WH001 return.	Same as 4367.
07705	SQRT error return.	Machine error.
10034	WH001 return.	Same as 4367.
10040	Group number on Card Type 5 is incorrect.	
10447	AC overflow.	While initializing matrix and vector for GDSR to solve set of equations.
10450	MQ overflow.	Same as 10447.
10451	AC overflow.	While solving second set of equations.
10452	MQ overflow.	Same as 10451.
10453	AC overflow.	While solving first set of equations.
10454	MQ overflow.	Same as 10453.
10455	AC overflow.	While computing C_ℓ matrices.
10456	MQ overflow.	Same as 10455.
10457	AC overflow.	While computing p_ℓ and p_0 (analytic).
10460	MQ overflow.	Same as 10457.

10461	AC overflow.	While computing the source term, $s(z_n)$.
10462	MQ overflow.	Same as 10461.
10637	Group number on Card Type 1 doesn't agree with preceding problem(s).	
10640	Group number on Card Type 2 is incorrect.	
10641	Temperature number is less than that of preceding problem.	
10642	Energy levels not in proper sequence. One energy is not less than the preceding one.	
10653	Group number on Card Type 3.	
10754	EXPC error return. Argument too large.	
10775	CL INT3 error return. Minus AC indicates underflow or overflow. Plus AC indicates n = 0 or 1: Machine error.	
11013	EXPC error return. Argument too large.	
11020	Group number on Card Type 4 is incorrect.	

V. OUTPUT

The BCD output is on logical tape 5 and the binary output on logical tape 3.

Tape 5 is printed off-line. After printing out the information on Card 1 as an identification, the sums $p_\ell(z_n)$ for each group are printed out. The analytic check of Eq. (6) for σ_S^{eff} is also printed together with the difference between this and p_0. The spectra $\psi_0(E_n)$ and $\psi_1(E_n)$ are printed for values of E_n in the order $E_1 \ldots E_N$. Finally the sums N_0, J_0, I_0, N_1, J_1, I_1, I_{20}, I_{21}, I_{30}, I_{31} are printed out, and in addition the normalization factor P_1 of Eq. (61).

If K = 0 on Card 1, no spectra are computed and only the values of p_ℓ and σ_S^{eff} are printed out. If Card 5 is blank, the spectrum $\psi_1(E_n)$ and the sums are omitted. The printout of the spectra and sums is repeated for each value of σ_0 specified.

Tape 3 contains the matrices and auxiliary terms to be used for space and energy dependent problems. After these have been computed corresponding to a given Card 1, a record is written on Tape 3 with the temperature t used as the record number. Each record consists of four blocks of information:

1. $z_n^2 \exp(-z_n^2)$, $n = 1 \ldots N$.
2. $s(z_n)$, $n = 0 \ldots N$.
3. $p_0(z_n)$, $n = 1 \ldots N$.
4. $C_\ell^{j \to n}$, $\ell = 0 \ldots 3$, $j = 1 \ldots N$, $n = 1 \ldots N$.

This record is used by LTP 7 as input data for the library-program tape of the SLOP-1 code (Ref. 2), and may be similarly used for other codes.

REFERENCES

1. L. Hageman, Letter WAPD BS-62, January 20, 1958.
2. H. Bohl et al, "A Thermal Multigroup P-1 Code for the IBM-704," WAPD-TM-188, to be issued.