

FOREWORD

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The FANTASIA II code was developed and programmed by H. Steinberg. The development of TRIPROD II was carried out by J. Heitner under the supervision of R. Aronson.

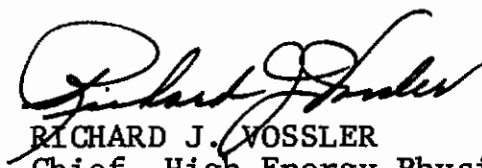
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ABSTRACT

Two codes have been developed for the IBM 7090. FANTASIA II computes neutron transmission through laminated slab shields and slowing down density within the shields by Monte Carlo methods. TRIPROD II is a slowing down code suitable for shielding problems. These codes are based on FANTASIA and TRIPROD, shielding codes for the 1103A Univac. Throughout the text the "II" is omitted in reference to FANTASIA II and TRIPROD II. Operating instructions are included.

This report has been reviewed and is approved.



RICHARD J. VOSSLER
Chief, High Energy Physics Branch
Materials Physics Division
AF Materials Laboratory

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I. INTRODUCTION

This report describes FANTASIA, a slab Monte Carlo program for neutrons, and TRIPROD, a multigroup diffusion program. FANTASIA computes neutron transmission, as well as the slowing down densities due to hydrogen and non-hydrogen scattering at some cutoff energy, usually 300 kev. These programs, originally coded for the 1103A-Univac,^[1] have been recoded for the IBM-7090. FANTASIA is now a production code; TRIPROD is not. The codes were designed to be used together, though they can be used separately. There is a link between them which converts the slowing down densities computed by FANTASIA into input for TRIPROD.

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II. FANTASIA

A. General Description

FANTASIA is a Monte Carlo code designed to calculate neutron shielding data for a multislabs plane shield. The code may be used alone or in conjunction with TRIPROD, which calculates, starting with FANTASIA results, further shielding data.

FANTASIA is divided into two logically distinct sections for operating purposes; these sections are called FANTASIA-CROSS-SECTION (FCS) and FANTASIA-PROPER (FP).

The function of FCS is to take cross-section data in standard form* and modify it to make the data usage in FP as simple as possible. The communication between the two codes is by means of a cross-section tape prepared by FCS.

FP carries out all the Monte Carlo calculations and, if called for, produces a tape containing the slowing down data to be used by TRIPROD, which then computes a thermal flux distribution.

B. FANTASIA-CROSS-SECTION

1. Standard Cross-Sections

FANTASIA-CROSS-SECTION (FCS) has been set up to run with FANTASIA-PROPER (FP) to prepare cross-section data and related information for FP. The output of FCS is a binary tape, which is read by FP. The first logical record on the tape consists of the energy argument table, hydrogen cross-sections, flux

* The form used is that given in a series of reports prepared by the United Nuclear Corporation. See, for example, Reference [2].

to dose conversions, the energy divisions for the Gamma ray production and some miscellaneous parameters. Each additional logical record contains all the data for a given element. These data consist of the total cross-section, the elastic scattering cross-section, the non-elastic neutron-producing cross-section σ_I , given by

$$\sigma_I = \sigma_{n'} + 2 \sigma_{2n} + \nu \sigma_f ,$$

where $\sigma_{n'}$ is the inelastic, σ_{2n} the (n,2n) reaction, and σ_f the fission cross-section, and ν is the (energy dependent) number of neutrons per fission, differential information for elastic scattering angle and inelastic scattering energy, slowing down cross-sections, and gamma production cross-sections, as well as various miscellaneous related data. Since raw cross-sections in the form taken do not directly contain much of this data, these must be calculated. The following is a tabulation of the basic input and the processing in FCS:

- a. Total and elastic (integral) cross-sections:
No processing (except conversion from barn atom^{-1} to $\text{cm}^2 \text{ gm}^{-1}$).
- b. Non-elastic processes: σ_I calculated.
- c. Elastic differential cross-sections: Legendre coefficients converted to coefficients of the polynomial expansion in Δ_c , the cosine of the center of mass scattering angle, normalized to make average = σ_n , the elastic scattering cross-section.

d. Inelastic differential: For continuum levels, use cumulative distributions. Height of curve at energy E' is replaced by $\int_0^{E'}$, with $\int_0^{E_{HI}}$ normalized to 1, where E_{HI} is the highest possible energy of the outgoing neutron. For discrete levels, $\sigma_{Q_i}(E)$, the cross-section for excitation of the target nucleus to energy Q_i by a neutron of energy E , is replaced by (where N is the number of levels)

$$\frac{\sum_{j=1}^i \sigma_{Q_j}(E)}{\sum_{j=1}^N \sigma_{Q_j}(E)}$$

In case fission is possible, the Watt fission spectrum is added to the inelastic differential data. It is assumed that for fissionable elements there are no discrete levels for inelastic scattering.

e. Slowing down cross-section: Calculated from elastic, inelastic, and fission cross-sections (see following section).

f. Gamma ray production: The continuous part is converted to integrals over given energy ranges. Discrete gamma rays are converted to energy deposited within given range.

2. Slowing Down Cross-Sections

The cross-section for slowing down past the FANTASIA cutoff energy E_L is computed as the sum of three terms, due respectively to elastic scattering, inelastic scattering, and fission.

a. Elastic

Calculate $\Delta_{c,M}$, the cosine of the minimum scattering angle for which the energy of the neutron after scattering is below the cutoff energy E_L , where A is the atomic weight of the target divided by the atomic weight of a neutron and E is the incoming neutron energy

$$\Delta_{c,M} = \frac{(A+1)^2 (E_L/E) - (A^2+1)}{2A}$$

If $\Delta_{c,M} > -1$, the contribution $\sigma_{s,n}(E)$ to slowing down is

$$\sigma_{s,n}(E) = \int_{-1}^{\Delta_{c,M}} \sigma_n(E, \Delta_c) d\Delta_c$$

Otherwise $\sigma_{s,n}(E) = 0$. $\sigma_n(E, \Delta_c)$ is the differential elastic scattering cross-section for incident neutron energy E and center of mass scattering cosine Δ_c .

b. Inelastic

Let $\sigma_{s,n'}(E)$ be the contribution to slowing down by a neutron at energy E from an inelastic collision.

1) Continuum distribution

$$\sigma_{s,n'}(E) = \int_0^{E_L} \sigma_{n'}(E, E') dE'$$

where $\sigma_{n'}(E, E')$ is the differential cross-section of a neutron at energy E , non-elastically scattered and producing a neutron of energy E' .

2) Discrete Level

For each level where the excitation energy $Q_i > E$, $\Delta_{c,M}$ is calculated

$$\Delta_{c,M} = \frac{(A+1)^2 (E_L/E) - (\bar{A}^2 + 1)}{2\bar{A}}$$

where $\bar{A} = A \sqrt{\frac{E - Q_i}{E}}$

If $\Delta_{c,M} > -1$

$$\lambda = \min(\Delta_{c,M}, 1)$$

$$\sigma_{s,n'}(E, Q_i) = \frac{(\lambda + 1)}{2} \sigma_{Q_i}(E)$$

Otherwise $\sigma_{s,n'}(E, Q_i) = 0$

Finally $\sigma_{s,n'}(E) = \sum_i \sigma_{s,n'}(E, Q_i)$

c. Fission

The contribution $\sigma_{s,f}(E)$ is given by

$$\sigma_{s,f}(E) = \nu(E) \sigma_f(E) \int_0^{E_L} f(E') dE'$$

where $f(E')$ is the normalized fission spectrum

$$\text{(i.e. } \int_0^{\infty} f(E') dE' = 1).$$

C. FANTASIA-PROPER

1. General

FANTASIA is designed to calculate fast neutron shielding data for multilayer plane slab shields by Monte Carlo. The output is logically broken down into two categories, transmitted and internal. The transmitted results consist of fast neutron current, flux, and dose. The internal results consist of neutron slowing down densities and inelastic scattering gamma ray production.

The code is able to treat either delta function or distributed sources in position, direction, and energy, (see Section 3).

The shield is made up of infinite plane slabs. Internal results are calculated for each slab only, so that to obtain data internal to a given physical slab it is necessary to divide into several logical slabs, each with the same composition. Throughout this report all references to slabs will be to logical slabs.

Incorporated into the code is a multibase feature which allows the calculation of data simultaneously for several different shields, where the thickness of each (logical) slab in each case is prescribed separately.

2. Output Description

a) Transmitted

The current and flux are calculated in spectral (histogram) form as functions of the energy of the emitted neutrons in dimensions of neutrons $\text{cm}^{-2} \text{sec}^{-1}$ for a source strength of one neutron $\text{cm}^{-2} \text{sec}^{-1}$. Total dose is calculated as millirad hour^{-1} for the same source strength.

b) Internal

The slowing down output is divided into hydrogen and non-hydrogen slowing down. Slowing down density for each category is obtained at a given spatial point (double-valued at region changes) as neutrons $\text{cm}^{-3} \text{sec}^{-1}$ and integrated over each region as neutrons $\text{cm}^{-2} \text{sec}^{-1}$. The gamma-ray production (from inelastic scattering) is obtained in integrated energy spectral form, i.e., as $\text{Mev-cm}^{-2} \text{sec}^{-1}$ within each given energy range.

3. Problem Specification

a) Source

The source is considered to be of the form $f_E(E) f_\delta(\delta) f_x(x)$, where any of the functions may be delta functions. The energy source $f_E(E)$ may alternatively be considered to form a fission spectrum.

If none of the above apply, then the source function is specified by giving an argument list and a corresponding function list for the variable. For all three variables, the

function is then assumed to be zero outside the argument range. For initial energy and direction, the function is assumed to be linear between each pair of prescribed points. For initial position, the function is assumed to be exponential between each pair of points.

b) Shield

A shield for FANTASIA consists of a set of infinite plane slabs of finite width. The composition of each slab is arbitrary, within the limitation of available cross-sections. Any element may be used at any density.

The multicas e feature (see Section 10), as used in FANTASIA, permits the specification of a set of problems by varying the thickness of each slab.

4. Analytical Foundations

Let A be any desired quantity to be calculated (e.g., flux, dose, slowing down density, etc.). A can be represented by

$$A = \sum_{n=0}^{\infty} A_n$$

where A_n is the contribution to A due to neutrons undergoing exactly n collisions. Let $P_n(x, \delta, E)$ be the probability density function that a neutron after exactly n collisions will be at position x , with direction cosine δ , and energy E . Then

$$A_n = \int \int \int P_n(x, \delta, E) Q_A(x, \delta, E) dx d\delta dE$$

where $Q_A(x, \delta, E)$ gives the contribution to A for a neutron at x, δ, E and undergoing no further collision. Further

$$P_{n+1}(x', \delta', E') = \int \int \int P_n(x, \delta, E) p(x, \delta, E; x', \delta', E') dx d\delta dE$$

where p is the probability density that a neutron starting at x, δ, E will undergo a collision leading to x', δ', E' with no collision in between. In this description P_0 is the source distribution. p and the Q 's are given as follows:

$$p = e^{-\frac{D(x, x', E)}{|\delta|}} \Sigma(x', E, E', \delta, \delta')$$

A	Q_A
Current	$Q_C = \psi_{(0,1)}(\delta) G_n$
Flux	$Q_F = \frac{Q_C}{\delta}$
Dose	$Q_D = f(E) Q_F$

For the i^{th} slab:

Hydrogen slowing down, left boundary	$S_H(i) F_L(i)$
right boundary	$S_H(i) F_R(i)$
interior	$S_H(i) F_I(i)$
Non-hydrogen slowing down, left boundary	$S_N(i) F_L(i)$
right boundary	$S_N(i) F_R(i)$
interior	$S_N(i) F_I(i)$

Gamma ray production, k^{th} energy interval, slab interior $S_G(i, k) F_I(i)$

Where $\Sigma(x', E, E', \delta, \delta')$ = the cross-section at x' for scattering from E, δ to E', δ' .

For $\delta > 0$: $F_L(i) = \psi_{(0, T_{i-1})}(x) \cdot \frac{G_{i-1}}{\delta}$

$$F_R(i) = \psi_{(0, T_i)}(x) \cdot \frac{G_i}{\delta}$$

For $\delta < 0$:
$$F_L(i) = \psi(T_{i-1}, \infty)(x) \cdot \frac{G_{i-1}}{|\delta|}$$

$$F_R(i) = \psi(T_i, \infty)(x) \cdot \frac{G_i}{|\delta|}$$

For all δ :
$$F_I(i) = \frac{\delta}{\Sigma_i} \left(F_L(i) + \frac{\psi(T_{i-1}, T_i)(x)}{\delta} - F_R(i) \right)$$

Where
$$G_i = e^{-\frac{D(x, T_i, E)}{|\delta|}}$$

and $D(x, y, E)$ = Component of mean free path distance between x and y normal to slab faces.

n = Total number of slabs.

T_i = Distance from origin to i^{th} shield division.
($T_0 = 0$, T_n = shield thickness).

$S_H(i)$ = Hydrogen slowing down cross-section of the i^{th} slab.

$S_N(i)$ = Non-hydrogen slowing down cross-section of the i^{th} slab.

$S_G(i, k)$ = Gamma ray production cross-section of the i^{th} slab for the k^{th} gamma ray energy interval.

$\psi(a, b)(u)$ = Characteristic function of the interval (a, b) , i.e.

$\psi = 1$ for u inside the interval,

$\psi = 0$ otherwise.

5. Statistical Estimation

Statistical estimation is used to obtain all output data. For the external data a special first scattering is made at each collision (see Section 6), and the contribution C to neutron current (with no further collision) is calculated from:

$$C = W e^{-D/\delta}$$

The contributions F to flux and R to dose are obtained by:

$$F = C/\delta$$

$$R = r(E)F$$

where D = number of mean free paths to edge of shield along the normal

W = present neutron weight (after estimate collision)

δ = direction cosine

$r(E)$ = flux to dose conversion factor (a function only of the neutron energy E).

The internal data estimates are made after each true scattering (see Section 6). This is done by first calculating the uncollided flux F_i at the i^{th} slab boundary and the uncollided integral flux I_i in the i^{th} slab by

$$F_i = \frac{W}{|\delta|} e^{-\frac{t_i}{|\delta|}}$$

$$I_i = \frac{\delta}{\Sigma_i} (F_{i-1} - F_i)$$

for each i along the extended uncollided neutron path, where
 Σ_i = the linear total cross-section of the i^{th} slab

t_i = the number of mean free paths, along a normal projection of the neutron path, to the i^{th} slab boundary. The boundaries are indexed so that the far boundary (from the origin) has the same value as the slab index.

In case the neutron is in the i^{th} slab, I_i is given by:

$$I_i = \frac{\delta}{\Sigma_i} \left(\frac{W}{\delta} - F_i \right) \quad , \quad \text{if } \delta > 0$$

$$I_i = \frac{\delta}{\Sigma_i} \left(F_{i-1} - \frac{W}{\delta} \right) \quad , \quad \text{if } \delta < 0$$

The contributions to slowing down by hydrogen are obtained by:

$$H_{L,i} = S_{H,i} F_{i-1}$$

$$H_{R,i} = S_{H,i} F_i$$

$$H_{I,i} = S_{H,i} I_i$$

where $H_{L,i}$, $H_{R,i}$, and $H_{I,i}$ are the contributions to slowing down by hydrogen at the left end, right end, and interior of the i^{th} slab with:

$$S_{H,i} = \Sigma_{H,i} \frac{E_{L/E}}$$

where $\Sigma_{H,i}$ is the linear hydrogen cross-section of the i^{th} slab and E_L is the low energy cutoff. The contributions to slowing down by non-hydrogen and gamma ray production are obtained by:

$$N_{L,i} = S_{N,i} F_{i-1}$$

$$N_{R,i} = S_{N,i} F_i$$

$$N_{I,i} = S_{N,i} I_i$$

$$G_{i,k} = S_{G,i,k} I_i$$

where $N_{L,i}$, $N_{R,i}$, and $N_{I,i}$ are the left, right, and interior contributions to slowing down by non-hydrogen elements for the i^{th} slab and $G_{i,k}$ is the contribution to gamma ray production in the k^{th} energy interval and the i^{th} slab. The conversion factors $S_{N,i}$, $S_{G,i,k}$ are tabulated function of neutron energy (see cross-section description).

6. Scattering Procedure

At each collision, two scatterings are computed. The first is carried out for the purposes of estimating transmission (current, flux, and dose), while the second is used to obtain slowing down density and gamma production estimates and to continue the history.

The first scattering is carried out in the following sequence:

1a. Choose δ' the cosine of the angle with the shield normal. The new direction must be in the forward hemisphere.

1b. Choose ϕ the azimuthal scattering angle.

1c. Calculate Δ the cosine of the angle of scatter.

$$\Delta = \delta\delta' + \sqrt{(1-\delta^2)(1-\delta'^2)} \cos \phi$$

where δ is the previous cosine with the normal.

1d. Choose between hydrogen and other elements.

In this selection, if the cosine of the scattering angle is negative or if small enough to make the neutron energy $E' (= \Delta^2 E$, where E is the energy before collision) after hydrogen scattering to be below the cutoff, hydrogen scattering is forbidden (assuming hydrogen present in this slab).

At this point, if hydrogen had been chosen the process is complete, since E' had already been computed. However, if hydrogen is not chosen, we proceed as follows:

1e. Choose the target element.

1f. Choose between elastic and inelastic scattering. If the scattering is elastic, we calculate Δ_c the cosine of the center of mass scattering angle and E' the resultant energy of the neutron.

$$\Delta_c = (\Delta^2 - 1 + \Delta \sqrt{A^2 + \Delta^2 - 1})/A$$

$$E' = E(A^2 + 2A\Delta_c + 1)/(A + 1)^2$$

where A is the atomic weight of the target nucleus divided by the neutron weight.

If the scattering is inelastic, either E^* the adjusted emitted neutron energy (in the center of mass) or Q^* the adjusted energy level of the target is obtained by a random selection procedure, depending on whether the incident energy is in the discrete or continuum range. The adjustment factor is $(A+1)/A$, so that $E^* + Q^* = E$. \bar{A} is then calculated

$$\bar{A} = A \sqrt{E^*/E}$$

The mechanics branches at this point, depending on whether or not \bar{A} is greater than one. If greater, E' , the emitted laboratory neutron energy, is calculated using Δ_c the cosine of the center of scattering angle.

$$\Delta_c = (\Delta^2 - 1 + \Delta \sqrt{\bar{A}^2 + \Delta^2 - 1})/\bar{A}$$

$$E' = E(\bar{A}^2 + 2 \bar{A} \Delta_c + 1)/(A + 1)^2$$

However if \bar{A} is less than or equal to one, the center of mass scattering angle (which determines the energy and weight) is a two-valued function of the laboratory scattering angle.

$$\Delta_c = (\Delta^2 - 1 \pm \Delta \sqrt{\bar{A}^2 + \Delta^2 - 1})/\bar{A}$$

Furthermore, certain laboratory scattering angles are impossible, i.e. $\Delta < \sqrt{1 - \bar{A}^2}$. Therefore, to complete the collision, a choice

of the two values (if possible) must be made, Δ_c is computed from the above formula where the sign had been chosen at random. E' is then computed from the resultant Δ_c . In case $\Delta < \sqrt{1 - \bar{A}^2}$, E' is made ≈ 0 .

For the second scattering the order of events is as follows:

2a. Choose between hydrogen and other elements. If not hydrogen, steps 1a, 1b, 1c, 1e, and 1f are carried out in order as for the first scattering (except that in 1a, the cosine chosen is for the full sphere).

If hydrogen is chosen, the process continues with:

2b. Choose Δ the cosine of the laboratory scattering angle, restricted to a range determined by the low energy cutoff of the problem, i.e.

$$\sqrt{\frac{E_L}{E}} \leq \Delta \leq 1$$

2c. Choose \emptyset the azimuthal angle.

2d. Calculate E' the energy and δ' the cosine of the angle with the normal.

$$E' = \Delta^2 E$$

$$\delta' = \Delta\delta + \sqrt{(1-\Delta^2)(1-\delta^2)} \cos \emptyset$$

Because of the large overlap of the two procedures, particularly for non-hydrogen scattering, the code contains only one subroutine to carry out the two scatterings (using an indicator to distinguish), with separate sampling formulas for each case.

7. Non-Elastic Neutron Producing Reactions

The reactions considered here are inelastic scattering, (n,2n) reaction, and fission. These reactions are handled by use of a function $\sigma(E,E')$ of the incoming reaction energy E and the outgoing reaction energy E' , where

$$\sigma(E,E') = \sigma_{n'}(E,E') + 2\sigma_{n,2n}(E,E') + \nu(E)\sigma_f(E)f(E')$$

$\sigma_{n'}(E,E')$, $\sigma_{n,2n}(E,E')$ are the differential inelastic and (n,2n) cross-sections respectively, $f(E')$ the fission spectrum normalized to unity, $\nu(E)$ the number of neutrons per fission, and $\sigma_f(E)$ the fission cross-section.

This implies that after a non-elastic reaction, there are on the average λ neutrons produced for each neutron undergoing such a reaction, where $\lambda = (\sigma_{n'} + 2\sigma_{2n} + \nu \sigma_f) / (\sigma_{n'} + \sigma_{2n} + \sigma_f)$. In FANTASIA, this process is handled in effect by multiplying the neutron weight by λ , having chosen the outgoing energy E' from the distribution given by $\sigma(E,E')$.

8. History Termination

In normal operation histories are terminated by either Russian Roulette or low energy. Russian Roulette is used with a survival probability of 1/10 and is called for when the contribution to current from the next collision is estimated to be less than 0.01 times that of the maximum from the history. If (possibly due to underflow) the neutron weight is zero, the history is killed outright. The low energy cutoff for FANTASIA

is 300 kev. In order to increase the amount of information obtained in each history, hydrogen scattering is set up to forbid degradation below the cutoff, sharply limiting the number of occurrences of degradation during operation of the code.

In addition there is the possibility of certain circumstances leading to anomalous results, due to digital imprecision. To avoid destroying useful data, such histories are terminated immediately.

The number of histories terminated by each of the three possibilities (Russian Roulette, low energy, error) are included in the output data (see Section 12-c).

9. Importance Sampling

Importance sampling is carried out in two logically different operations, random variable selection and random decision making. Since the theory and application of importance sampling has been described extensively, we will only present the actual procedure used.

For all random variable selections, a truncated exponential distribution based on a parameter B, depending on the state of the neutron, is used to calculate a normalized random variable u. The corresponding physical variable is obtained from u by a linear transformation. If λ is a physical variable with λ_L , λ_H the minimum and maximum possible values, then u is defined by

$$u = \frac{\lambda - \lambda_L}{\lambda_H - \lambda_L}$$

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In Table I, B , λ_L , and λ_H for each of the physical variables are listed. The choice functions for each of the decisions are presented in Table 2.

TABLE 1
RANDOM VARIABLE PARAMETERS

Physical Variable and Limits	B
Source	
$E_O (E_{MIN}, E_{MAX})$	0
$\delta_O (\delta_{MIN}, \delta_{MAX})$	$.5(\delta_{MAX} - \delta_{MIN})(L + L_H - 1) / (L + 1)$
$x_O (x_{MIN}, x_{MAX})$	0
Collision	
$x (0, D)$	$D_N - D \delta $
For Estimate	
$\delta' (0, 1)$	$\text{MIN}(L+1, \text{MAX}(0, 3(L-.5)))$
$\phi (0, \pi)$	$-(.5 + L_H/L) \sqrt{(1-\delta^2)(1-\delta'^2)}$
For non-hydrogen scattering	
$\delta' (-1, 1)$	$(L + L_H - 1) / (L + 1)$
$\phi (0, \pi)$	$-.5 \sqrt{(1-\delta^2)(1-\delta'^2)}$
For hydrogen scattering	
$\Delta (\sqrt{\frac{E_L}{E}}, 1)$	$2(U-1/U)(1 - \sqrt{E_L/E})^4$ where $U = 1 + (1+\delta)(1.5 + \text{MIN}(9, L_H)) / 3$
$\phi_\Delta (0, \pi)$	$\pi V(L-1) / (L+1)$ where $V = - \sqrt{(1-\delta^2)(1-\Delta^2)} / (\frac{2L}{L+L_H} - \delta\Delta)$ if $\frac{2L}{L+L_H} - \delta\Delta - \sqrt{(1-\delta^2)(1-\Delta^2)} \leq 0$, otherwise $V = - \text{MIN} \left(\frac{\sqrt{(1-\delta^2)(1-\Delta^2)}}{\frac{2L}{L+L_H} - \delta\Delta}, \left(\frac{\sqrt{(1-\delta^2)(1-\Delta^2)}}{\frac{2L}{L+L_H} - \delta\Delta - \sqrt{(1-\delta^2)(1-\Delta^2)}} \right)^{1/2} \right)$

TABLE 2

DECISION FUNCTIONS

<u>Type</u>	<u>At Estimate</u>	<u>At True Collision</u>
P_H	$\Sigma^*/(\Sigma^* + \Sigma_T)$	$\Sigma^*/(\Sigma^* + \Sigma_T)$
	where $\Sigma^* = \text{Max}(0, 4\Delta\Sigma_H(E\Delta^2 - E_L)/(E - E_L))$ where $\Sigma^* = 4\Sigma_H/(4+L)$	
P_E	$\sigma_n/(\sigma_n + \sigma_I)$	$2\sigma_n/(2\sigma_n + \sigma_I)$

Since all random variables and decisions are made using importance sampling it is necessary to adjust the neutron weight. Furthermore the dual scattering procedure makes it necessary to retain the old weight before collision so that the true collision will be properly weighted. When each random variable is chosen, the weight of the neutron is divided by the density function and for the selection, i.e. W' , the new weight is given by:

$$W' = W(e^B - 1)e^{-Bu/B}$$

where W is the old weight. W and W' symbolize previous and present values of the weight. In the above formula and all those below, a W' produced in one formula becomes the W for the next.

In addition the following specific adjustments are made. Let W_0 be the weight before collision. This is calculated, after the collision position is chosen, by (symbols defined at end of section):

$$W_0 = DW/\Sigma_T \mid \delta \mid$$

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At the estimate collision the weight is adjusted in a series of steps.

$$\text{First } W' = W_0/2$$

Second, if the scattering is by hydrogen,

$$W' = 4\Delta \Sigma_H W/P_H$$

In this case no further adjustments are necessary. If the scattering was by a non-hydrogeneous element.

$$W' = W \Sigma_N / \sigma_t (1 - P_H)$$

Then if the scattering (non-hydrogen) was elastic

$$W' = W \sigma_n(\Delta_c) / W$$

If the scattering was inelastic

$$W' = W \sigma_I / (1 - P_E)$$

In the case where $\bar{A} \leq 1$ so that a choice had to be made for a sign in the Δ_c formula, let P_+ be given by:

$$P_+ = .5 + \Delta \sqrt{\bar{A}^2 + \Delta^2 - 1} / (\bar{A}^2 + 2\Delta^2 - 1)$$

Then if a plus sign is chosen:

$$W' = .5W/P_+$$

If a minus sign is chosen

$$W' = .5W/(1 - P_+)$$

Finally, for both elastic and inelastic scattering (where $\bar{A} = A$ for elastic),

$$W' = W(\bar{A}^2 + 2\bar{A} \Delta_c + 1)/\bar{A} \sqrt{\bar{A}^2 + \Delta_c^2 - 1}$$

At the true collision the first step is

$$W' = W_0$$

If the scattering is by hydrogen

$$W' = 2\Delta \Sigma_H (1 - \sqrt{E_L/E}) W/P_H$$

If the scattering is by a non-hydrogenous element, the formulas used for the estimate collision apply. The symbols used herein are defined as follows:

Σ_T = Linear total cross-section, i.e. $[\Sigma_T] = \text{cm}^{-1}$.

Σ_N = Linear non-hydrogen cross-section.

Σ_H = Linear hydrogen cross-section.

σ_t = Macroscopic element total cross-section, i.e.
 $[\sigma_t] = \text{cm}^2/\text{gm}.$

σ_n = Macroscopic elastic cross-section.

$\sigma_n(\Delta_c)$ = Macroscopic elastic differential cross-section,
 normalized to have its average equal σ_n .

σ_I = Macroscopic non-elastic neutron production cross-section (see FCS).

$E_{\text{MIN}}, E_{\text{MAX}}$ = Minimum and maximum values of source energy read in when input distribution is used. If fission

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spectrum, $E_{\text{MIN}} = E_L$ and E_{MAX} given by upper limit of argument for cross-section table.

$\delta_{\text{MIN}}, \delta_{\text{MAX}}$ = Minimum and maximum values of source direction cosine when input distribution is used.

$x_{\text{MIN}}, x_{\text{MAX}}$ = Minimum and maximum values of source position when input distribution is used.

L = Number of mean free paths along normal to outer edge of shield.

L_H = Number of hydrogen mean free paths along normal to outer edge of shield.

D = Number of mean free paths along normal to edge of shield in direction of neutron path.

D_H = Number of hydrogen mean free paths along normal to edge of shield in direction of neutron path.

P_H = Coded probability that hydrogen will be chosen as the target nucleus.

P_E = Coded probability that the scattering will be elastic.

10. Multicase Features

Because of the fundamental role of importance sampling in Monte Carlo codes, where all "natural" properties of matter are treated by weight adjustments, it is possible to carry out calculations for many different shields by using the same tracks, as long as the purely geometric variables (distances and angles) remain unchanged. In addition, with the case of plane slabs, owing to the equivalence of density and thickness changes, only angles must be preserved.

In developing a code to make use of this property, a decision must be made as to how general a multibase procedure to incorporate in the code, weighing the complexity of the code and the added computation time against the value of the added information with the decrease in running time per case.

The complexity in procedure falls into two logical categories, source variations and shield variations. Source variations may be made in angular distribution (for distributed as opposed to monodirectional sources) or in energy. The former was not included since it was felt that distributed angular sources other than isotropic have limited value. Many energy sources might be more useful, but the greater complexity did not appear warranted by this program, since the fission source would be used most of the time.

Shield variations can be made in different degrees of complexity. The simplest is a constant density change for the entire shield (the similarity transform). Somewhat more complex is having each slab in the shield vary in density separately. Even more generality may be obtained by varying the proportions of various elements in each slab or even using different shielding materials (taking into account the special position of hydrogen). In deciding how complex a procedure to use, the principal criterion used was what kinds of problems to which FANTASIA would be applied. On this basis, it was decided that varying the density of each slab would be sufficient for most studies and that further complexity (with increased coding complexity and running time) would not have enough value to be incorporated into the program.

11. Generalized Quota Sampling

Given a sampling scheme in a Monte Carlo calculation, if the standard deviation of a quantity calculated on the basis of one history is σ , then if N independent samples are chosen, the deviation of the quantity would be σ/\sqrt{N} . However if a correlation sampling procedure is used it is possible to obtain a more rapid reduction of the standard deviation of any quantity. The particular correlation scheme described here has the property that for a sample of size N , the standard deviation σ_N of a quantity can be shown^[3] to satisfy

$$\sigma_N < \sqrt{\frac{k}{N^2} + \frac{\sigma^{*2}}{N}},$$

where k is independent of N , and $\sigma^* < \sigma$.

The procedure is a method of independent quota sampling for each variable called generalized quota sampling. For each variable, the unit interval is divided into N equal subintervals, where N is the number of histories per group. When a random number is generated to obtain the desired random variable, it is forced to lie in one of the subintervals not used in a previous history, with the choice among the unused intervals not subject to any biasing, and independent for each variable. This procedure satisfied the requirements of generalized quota sampling described in^[3]. As used in the code, N has a practical limit of 216. If a larger N is prescribed, the generalized quota sampling is carried out on subgroups of histories of size at most 216.

12. Operation

a. General Description

FANTASIA and TRIPROD have been written to be operated under the 7090 FORTRAN Monitor System. To avoid tape setup, all Monitor intermediate tapes were used as program intermediates. If FANTASIA is used alone, no further tapes are required. If TRIPROD is used with FANTASIA logical tape 9 is needed in addition. To operate the code, it is then only necessary to place the decks on the input tape in the following order:

Binary:

- a) FANTASIA links
- b) TRIPROD links (if used)

Data:

- a) all FANTASIA input
- b) all TRIPROD input (if used)

Tapes 1-8 are needed for FANTASIA alone, 1-9 if run together.

The logical tape assignments are:

- 1, system
- 2,3,4,8,9 (if needed), intermediate
- 5, input
- 6, output
- 7, binary card images (in case of
recompiling)

b. Input Data

The input for FANTASIA problem is from standard IBM cards. The format is given below and the quantities described

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subsequently. For a series of problems the input for each is self-contained and may be loaded sequentially.

	<u>QUANTITY</u>	<u>RANGE</u>	<u>FORMAT</u>	<u>NO. COLUMNS</u>
Card 1				
	Problem number and date		A	24
	Comment		A	48
Card 2				
	N_C	(1,8)	I	3
	N_M	(1,7)	I	3
	N_S	(1,30)	I	3
	I_T	--	I	3
	N_H	(1,1000)	I	6
	N_E	≥ 0	I	6
	N_D	≥ 0	I	6
	M_C	≥ 0	I	6
	G_P	$\geq 1.$	F(0)	3
	R_O	--	\emptyset	13
	E_U	--	F(0)	6
	E_Δ	--	F(0)	6
Card 3				
	x_O	(0.,T)	F(2)	9
	N_1	0 or (2,20)	I	3
	δ_O	(-1.,1.)	F(2)	9
	N_2	0 or (2,20)	I	3
	E_O	0 or (.3,14.)	F(2)	9
	N_3	0 or (2,20)	I	3

Card 1 is self explanatory.

Card 2

N_C = Number of cases (described in section 10).

N_M = Number of different physical compositions used to make up the various slabs.

N_S = Number of slabs in shield.

I_T = TRIPROD indicator; if <0 , then TRIPROD is used and this is the last FANTASIA problem; $= 0$, then TRIPROD is not used for this problem; >0 , then TRIPROD is used for this problem, more FANTASIA problems follow. If TRIPROD is used at all, it must be used in the last FANTASIA problem.

N_H = Number of histories per group; set = 1000, if input greater.

N_E = Limit on number of errors; set = 40, if input ≤ 0 ; problem terminates at end of printout if number of errors exceed N_E .

N_D = Number of debugging printouts, i.e. first N_D collisions are traced.

M_C = Maximum number of collisions; problem terminates at end of printout if number of collisions exceed M_C .

G_P = Number of groups between printout; code sets to positive integer.

R_O = Initial random number; codes sets odd.

Distributed source blocks. For each value of k ($k = 1, 2, 3$ in order), the following two sets.

<u>QUANTITY</u>	<u>RANGE</u>	<u>FORMAT</u>	<u>NO. COLUMNS</u>
L_k Cards			
$A_{j,k}$	-	F(2)	9 each
L_k Cards			
$F_{j,k}$	-	F(2)	9 each
Shield geometry block.			
N_S Cards			
T_i	-	F(2)	7
M_i	(1, N_M)	I	5
$r_{i,l}$	-	F(3)	5 each
Composition block.			
1 Card			
N_L	(0, 7)	I	2
ρ_p	-	F(3)	7 each
N_L Cards			
I_q	(1, 5)	I	2
$\omega_{p,q}$	-	F(3)	7 each

DESCRIPTION OF INPUT

Format designations are A for alphanumeric, I for integer, \emptyset for octal and F for floating point, where the number in parenthesis indicates the number of decimal places assumed to the right of the decimal point if no decimal point is inserted.

E_U = Upper energy for flux and current transmission spectra.

E_Δ = Width of energy division for transmission spectra.

Card 3

x_0 = Source position; ignored if $N_1 \neq 0$; T = shield thickness.

N_1 = Number of points for source position distribution; 0 indicates delta function at x_0 .

δ_0 = Cosine of angle with normal of source; ignored if $N_2 \neq 0$.

N_2 = Number of points for source direction cosine distribution; 0 indicates delta function at δ_0 .

E_0 = Source energy; ignored if $N_3 \neq 0$; if $N_3 = 0$, $E_0 = 0$ indicates fission spectrum source distribution.

N_3 = Number of points for source energy distribution; 0 indicates delta function at E_0 or fission spectrum.

Distributed source blocks.

For each k , L_k is given by:

$$L_k = 0, \text{ if } N_k = 0$$

$$L_k = 1 + \left[\frac{N_k - 1}{8} \right], \text{ if } N_k \neq 0$$

where $k = 1, 2, 3$ refer to source position, direction, energy, respectively.

$A_{j,k}$ is the argument table and $F_{j,k}$ the function table, where j ranges from 1 to N_k . The $A_{j,k}$ are in increasing order of

magnitude. Both $A_{j,k}$ and $F_{j,k}$ have at most 8 items per card. All $F_{j,1}$ (source position) are made $\geq 10^{-30}$ since the function is assumed exponential in between. For $K = 2$ or 3 , linear interpolation is used.

Shield Geometry block.

For the i^{th} slab (numbered in order of increasing distance from origin):

T_i = Nominal thickness (cm).

M_i = Number denoting composition of slab; i.e. M_i = mixture number (see below).

$r_{i,\ell}$ = thickness ratio for the ℓ^{th} case where $1 \leq \ell \leq N_C$;

the true thickness for the ℓ^{th} case is then $T_i r_{i,\ell}$; N_C

items on card.

Composition block.

First card

N_L = Number of non-hydrogeneous elements used in problem.

ρ_p = Density (gm-cm^{-3}) of hydrogen in mixture number p , where $1 \leq p \leq N_M$; N_M items on card, with p 's in consecutive order.

Subsequent Cards

For the q^{th} non-hydrogeneous element used (no ordering required, but $I_q < I_{q+1}$ suggested).

I_q = Position on tape of element cross-section table, see section 12-d for element list.

$\omega_{p,q}$ = Density of element in mixture number p ; see comments on ρ_p .

c. Output Format

The following are examples of typical first page, error, and data page printouts. The data are as follows.

First Page:

- (1) Comment from input.
- (2) Number of histories per group.
Initial random number.
- (3) Number of different slab compositions (mixtures).
Number of elements used (hydrogen included even if not used).
- (4) Mixture numbers.
- (5) Element symbol.
Density of element in mixture indicated at head of column.
- (6) Number of slabs.
Number of cases.
- (7) Case numbers.
- (8) Slab number.
Mixture number indicating composition of slab.
Slab thickness for case indicated at head of column.
- (9) Nominal thickness of each slab (see input description).
- (10) Source position (delta function distribution).
- (11) Number of points of source direction distribution.
- (12) Factor used to renormalize function table to make
average value unity.
- (13) Point number.

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- (14) Argument of point.
- (15) Function at point, after normalization.
- (16) Source energy distribution given by fission spectrum, normalized to make average value unity.

Error Printout block.

- (1) Type indicator (at extreme left of line), see note 1.
- (2) Argument for error, see note 1.
 - Present group number.
 - Present history number in group.
 - Present collision number in history.
 - Total number of collisions to present.
 - Value of latest parameter used in random variable routine.
 - Value of latest random variable calculated.
 - Value of latest random number generated.
- (3) Part of weight independent of case, see note 2.
 - Part of weight associated with first case, see note 2.
 - Number of mean free paths from source to present position along path, for first case.
 - Number of mean free paths from present position to edge, along perpendicular, used for statistical estimation, for first case.
 - Number of mean free paths from present position to edge, along perpendicular, used for slowing down estimates, for first case.
 - Factor used for Russian Roulette test.

(4) Slab number of present position.

Nominal distance from origin of present position (cm).

Linear cross-section minus hydrogen cross-section of
slab containing present position.

Present value of cosine of angle with normal.

Value of cosine of angle with normal before present
collision.

Cosine of scattering angle at latest collision.

Cosine of azimuthal angle at latest scattering.

Present value of neutron energy.

Value of neutron energy before present collision.

Output data page.

Data from (1) - (8) is separate for each case.

Remainder applies to all cases.

(1) Case number.

Group of histories.

(2) Upper energy limits for gamma rays produced.

For items (3) - (6) and (9), the data in each row is for a
slab. The order of the rows corresponds to the order of the
slabs from the origin.

(3) Total gamma ray energy produced in each energy
interval (column).

(4) Total gamma ray energy produced.

Slab thickness.

(5) Slowing down density due to hydrogen collisions
at left end point.

Slowing down density due to hydrogen collisions
at right end point.

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Slowing down density due to other element collisions at left end point.

Slowing down density due to other element collisions at right end point.

- (6) Slowing down flux due to hydrogen collisions.

Slowing down flux due to other element collisions.

- (7) Neutron number current transmitted through shield in energy interval.

Neutron number flux transmitted through shield.

Upper limit of energy interval.

- (8) Total current transmitted.

Total flux transmitted.

Total dose transmitted.

The data in (9) and (10) are accumulated for an entire problem.

- (9) Slab number.

Number of collisions.

Number of collisions (not necessarily in particular slab) for which an estimate of gamma ray production and/or slowing down flux was made.

- (10) Number of collisions.

Number of histories terminated by degradation.

Number of histories terminated by Russian Roulette.

Number of histories terminated by Errors.

Latest random number generated.

Note 1. Error Indications

<u>Type Indicator</u>	<u>Argument</u>	<u>Place</u>	<u>Reason</u>
0	-	Slowing down estimate	Called for by input
1	Number of mean free paths past edge of shield	Collision posi- tion calcula- tion	Particle escape
2	Excess of cross- section over total of non- hydrogen	Scattering for estimate	No non-hydrogen elements selectable
3	Excess of cross- section over total of non- hydrogen	Scattering for collision	No non-hydrogen elements selectable
4	Function argu- ment	Exponential subroutine	Exponential argu- ment too large
5	-	Random number subroutine	Random number routine bug

Note 2. The neutron weight, for the first case, is the product of the first two items of (3).

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MAY 29, 1963 TEST 27 FANTASIA PAGE 1
H2O THICK 200 F/G IN. R.N. CC0C00000001
200 FIS./GP. (1)
1 MIXTURES 2 ELEMENTS (2)
DENSITY (GM/CC) OF ELEMENT IN MIXTURE (3)
ELEM. 1 (4)
H 0.112 (5)
Ø 0.688
2 SLABS 1 CASES (6)
SLAB THICKNESS (CM) FOR EACH CASE (7)
SLAB MIX 1 (8)
1 1 10.00
2 1 90.00
UNNORMALIZED THICKNESS FOR EACH SLAB
10.00 90.00 (9)
SOURCE POSITION -0. (10)
2 POINT SOURCE DIRECTION DISTRIBUTION (11)
NORMALIZATION FACTOR = 1.0000 (12)
POINT 1 2 (13)
NORM.COS. 0.0100 1.0000 (14)
HEIGHT 1.00 1.00 (15)
FISSION SOURCE NORMALIZED BY 3.5515 (16)

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FANTASIA PAGE 2

O	CAUSE	GP	FIST	CØL	TØTCØL	RV	PARAMETER	RVAR	RNUM	
-4.7274E 01		1	1	0	0	8.5455E-01		0.930	0.101	(1)
WT	FIXED									(2)
5.7159E 00		1.0000E 00		0.		44.0141	44.0141	1.2100E 00		(3)
SLB	PØSIT	XSEC-H		CØS-N	CØS-NH	CØS-SC	CØS-AZ	ENER	ENER-H	(4)
1	-0.	0.		0.931	0.	0.	0.	0.787	0.	

O	CAUSE	GP	FIST	CØL	TØTCØL	RV	PARAMETER	RVAR	RNUM
-1.3225E 02		1	2	0	1	8.0924E-01		0.259	0.813
WT	FIXED								
5.6645E 00		1.0000E 00		0.		35.2554	35.2554	4.9210E-18	
SLB	PØSIT	XSEC-H		CØS-N	CØS-NH	CØS-SC	CØS-AZ	ENER	ENER-H
1	-0.	0.093		0.267	0.931	0.734	0.830	1.379	0.787

O	CAUSE	GP	FIST	CØL	TØTCØL	RV	PARAMETER	RVAR	RNUM
-1.4685E 01		1	3	0	2	6.6468E-01		0.700	0.373
WT	FIXED								
6.2747E-03		1.0000E 00		0.		10.3205	10.3205	3.9894E-01	
SLB	PØSIT	XSEC-H		CØS-N	CØS-NH	CØS-SC	CØS-AZ	ENER	ENER-H
1	-0.	0.102		0.703	0.267	-0.748	-0.788	10.891	1.379

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FANTASIA PAGE 7

CASE 1

GROUP 5 (1)

GAMMA RAY PRODUCTION SPECTRUM (MEV/CM2)

HIGH E	1.00	2.00	3.00	4.00	(2)
	6.90E-06(5)	3.10E-05(5)	6.10E-05(5)	9.61E-05(6)	(3)
	1.68E-06(7)	7.51E-06(7)	1.47E-05(8)	2.3CE-05(9)	

HIGH E	6.00	14.00
	1.20E-04(6)	5.92E-03(3)
	2.85E-05(9)	1.35E-03(4)

TOTAL GAMMA RAY PRODUCTION SLAB THICKNESS (CM)

6.233E-03(3)	10.00	(4)
1.424E-03(4)	90.00	

SLOWING DOWN DENSITY (N/CM3) AT INTERVAL ENDP0INT

HYDROGEN COLLISION		OTHER COLLISION	
AT LEFT END	AT RIGHT END	AT LEFT END	AT RIGHT END
3.67E-01(21)	3.95E-03(33)	5.55E-03(14)	4.49E-06(20)
3.95E-03(33)	1.89E-08(35)	4.49E-06(20)	5.68E-10(54)

(5)

SLOWING DOWN FLUX (N/CM2) IN INTERVAL

HYDROGEN COLLISION	OTHER COLLISION
3.071E-01(20)	6.504E-03(10)
1.545E-02(30)	1.464E-05(8)

(6)

TRANSMISSION DATA

CURRENT SPECTRUM	FLUX SPECTRUM	ENERGY MAX
2.58E-09(47)	2.84E-09(48)	14.00
1.39E-08(44)	1.55E-08(45)	12.00
1.31E-07(34)	1.45E-07(34)	10.00
7.36E-08(62)	7.88E-08(61)	8.00
3.31E-07(43)	5.15E-07(38)	6.00
2.42E-07(75)	3.03E-07(68)	4.00
8.93E-08(41)	1.28E-07(31)	2.00

(7)

TOTAL	CURRENT
8.828E-07(33)	

FLUX
1.188E-06(36)

D0SE
2.515E-08(37)

(8)

COLLISION DATA

SLAB	COLLISIONS	N0N-H ESTIMATES
1	1601	773
2	2040	931

(9)

COLLISION

TOTAL	LOW ENERGY	HISTORY TERMINATIONS	KILLED	ERROR	LAST	RAND0M NUMBER
3641	32	968	0	0	C76467051401	(10)

13. Cross-Section Tables

The code at present contains (in order) cross-sections for the following elements (in addition to hydrogen, which is treated separately).

1. Oxygen
2. Aluminum
3. Iron
4. Silicon
5. Carbon

The following is a description of the data and format needed for additional elements. An excerpt from a typical table is given where the cards are numbered to correspond to the text.

Element Cross-Section Table Prologue

- (1) 37 data words, each consisting of a decrement part, denoting the lengths of tables 2.-38. described below. The use of the macro QTBL generates 9 items given the first location of each of nine consecutive tables and the location of the next datum after the ninth table.
- (2) 1 word, containing the element symbol (left adjusted). For fissionable elements, an F must be inserted as the third character.

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- (3) 8 words, containing in order the following:
 - a. Atomic weight (floating).
 - b. Continuous to discrete crossover energy, i.e.
 - a. to b. crossover for tables 13.-38.

The remaining items are all FORTRAN integers.

- c. Number of Legendre coefficient tables.
 - d. Number of continuous inelastic arguments.
 - e. Number of discrete inelastic levels.
 - f. Number of continuous gamma production arguments.
 - g. Number of discrete gamma rays produced by arguments above crossover energy.
 - h. Number of discrete gamma rays produced by arguments below crossover energy.
- (4) 10 words, continuous inelastic arguments.
- (5) 7 words, discrete inelastic arguments.
- (6) 16 words, continuous gamma ray production arguments and energies of discrete gamma rays produced for arguments above crossover.
- (7) 11 words, energies of discrete gamma rays produced for arguments below crossover.

In tables (4) - (7), the numbers are in increasing order of magnitude, except that the two parts of (6) each are in order of magnitude and are consecutive. If the number of entries do not fill a table, zeros must be inserted at the end.

The macro QALI may be used for this purpose with an address of the form A+B, where A is the location of the beginning of the table and B is the desired total length.

Element Cross-Section Table Body

1. Total cross-sections.
2. Elastic scattering cross-sections.
3. Inelastic scattering cross-sections.
4. (n,2n) cross-sections.
- 5-12. Coefficients of first eight Legendre polynomials for elastic scattering differential cross-sections.
- 13a. Table of values $\sigma_n(E,E')$ for first value of E' .
- 13b. Table of values of $\sigma_{Q_i}(E)$ for first value of Q_i .
- 14-22. Same as 13 for second through tenth values of E' and/or Q_i , where the arguments for the a. parts are given in item (4) and for the b. parts in item (5) of the prologue.
- 23a. Table of values of $\sigma_\gamma(E,E')$, the continuous gamma production differential cross-section, for first value of E' .
- 23b. Table of values of $\sigma_{\gamma,Q_i}(E)$, the cross-section for production of gamma ray of energy Q_i , for first value of Q_i for low energy part of E argument table.

24-38. Same as 23 for second through sixteenth values of E' and/or Q_i . If any Q_i have a non-zero $\sigma_{\gamma, Q_i}(E)$ at high energy part of E argument table, these are placed after all $\sigma_{\gamma}(E, E')$ have been exhausted and are tabulated in the same manner as the $\sigma_{\gamma}(E, E')$, where the arguments for the a. parts are given in item (6) and for the b. parts in item (7) of the prologue.

The following items are included for fissionable elements only, where $\nu(E)$, the number of neutrons for fission, is assumed to be of the form:

$$\nu(E) = \nu_0 + \nu' E$$

39. Fission cross-sections.

40. ν_0 (one item).

41. ν' (one item).

Table 1 and if present, table 39, are assumed to be full, i.e. equal in length to the argument table. All other tables begin at a point corresponding to the highest entry of the energy argument table. Table 2 ends at the lowest energy for which the value differs from the corresponding value of Table 1. Tables 3.-38. each end at the lowest energy for which its value is not zero. For those tables where there are a. and b. parts (13.-38.) if the b. part is not empty, the a. part must be included (by inserting zeros if necessary) for all energy arguments above the cross-over point.

Finally a table is included, indicating which elements are present and where. A FAP card of the form,

HTR XXEL

where XXEL is the location of the first entry in item 2. (The elastic cross-sections) of the body of the table, must be inserted just before a card,

NNH SYM *-ADA

positioned six locations before the energy argument table in the cross-section data subroutine, MOVDA, source deck.

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	PZE	0,0,ØIN-ØEL	
	QTBL	ØIN,ØNT,ØL1,ØL2,ØL3,ØL4,ØL5,ØL6,ØL7,ØL8	
	QTBL	ØL8,ØI1,ØI2,ØI3,ØI4,ØI5,ØI6,ØI7,ØI8,ØI9	(1)
	QTBL	ØI9,ØIA,ØG1,ØG2,ØG3,ØG4,ØG5,ØG6,ØG7,ØG8	
	QTBL	ØG8,ØG9,ØGA,ØGB,ØGC,ØGD,ØGE,ØGF,ØGG,ØEN	
	BCI	1,Ø	(2)
	DEC	16.,10.,6B17,8B17,2B17,6B17,2B17,2B17	(3)
ØENC	DEC	.5,1.,1.5,2.,3.,4.,6.,8.,0,0	(4)
ØQT	DEC	6.1,7.	(5)
	QALI	ØQT+7	
ØCGA	DEC	1.,2.,3.,4.,5.,6.,6.1,7.	(6)
	QALI	ØCGA+16	
ØDGA	DEC	6.1,7.	(7)
	QALI	ØDGA+11	
ØTØT	DEC	1.58,1.57,1.54,1.5,1.43,1.33	1.
		:	
		:	
		:	
ØG8	DEC	.064,.067,.07,.075,.076,.077,.08	30.
ØG9	SYN	*	
ØGA	SYN	*	
ØGB	SYN	*	
ØGC	SYN	*	
ØGD	SYN	*	
ØGE	SYN	*	
ØGF	SYN	*	
ØGG	SYN	*	
ØEN	SYN	*	38.

III. TRIPROD

A. Difference Equation Formulation

The derivation of the TRIPROD difference equations from the original Boltzmann equation is standard.^[1] The equations apply to slab, cylindrical, and spherical geometries.

The difference equations are

$$-a_{ni}\phi_{n+1,i} + b_{ni}\phi_{n,i} - c_{ni}\phi_{n-1,i} = Q_{ni} \quad (3.1)$$

Here

$\phi_{n,i}$ = average flux per unit lethargy in i^{th} lethargy group at space point (slab and cylinder)
 = radius times average flux per unit lethargy in i^{th} lethargy group at space point n (sphere)

The actual solution of eqs. (3.1) is a recursive one involving two auxiliary quantities Z and W . Thus the equations actually solved by the machine are:

$$\phi_{ni} = W_{ni} + Z_{ni} \phi_{n+1,i} \quad (3.2)$$

with

$$Z_{ni} = \frac{a_{ni}}{b_{ni} - c_{ni} Z_{n-1,i}}, \quad 0 \leq n \leq N \quad (3.3)$$

$$W_{ni} = \frac{c_{ni} W_{n-1,i} + Q_{ni}}{b_{ni} - c_{ni} Z_{n-1,i}}, \quad 0 \leq n \leq N \quad (3.4)$$

$$\phi_{n,i} = h_{ik} \tilde{\phi}_{n,i}^- + f_{ik} \tilde{\phi}_{n,i}^+ \quad (3.5)$$

$$\phi_{n,i-1}^+ = \phi_{n,i}^- \quad (3.6)$$

$$\begin{aligned} Q_{ni} = & \left[\tau_{1n} S_{n,i}^- + \tau_{2n} S_{n,i}^+ \right] + \frac{1-e^{-\Delta u_i}}{u_i} \left[\tau_{1n} \eta(n, u_{i-1}^-) + \tau_{2n} \eta(n, u_{i-1}^+) \right] + \\ & + \frac{\tau_{1n}}{\Delta u_i} \sum_{j=1}^{i-1} g_{n,j \rightarrow i}^{\Delta u_j} \phi_{n,j} + \frac{\tau_{2n}}{\Delta u_i} \sum_{j=1}^{i-1} g_{n,j \rightarrow i}^{\Delta u_j} \phi_{n,j} \\ & + e_{ni} \tilde{\phi}_{n,i}^- \end{aligned} \quad (3.7)$$

$$a_{ni} = \frac{\mu_{2n} K_{i1}^1(n^+)}{\Delta r_n^+} \quad (3.8)$$

$$\begin{aligned} b_{ni} = & \sigma_{1n} c_{ni} + \sigma_{2n} a_{ni} + \tau_{2n} \left[K_{i1}^4(n^+) + K_{i1}^3(n^+) \right] \\ & + \tau_{1n} \left[K_{i1}^4(n^-) + K_{i1}^3(n^-) \right] + \alpha_{i1}(n) \end{aligned} \quad (3.9)$$

$$c_{ni} = \frac{\mu_{1n} K_{i1}^1(n^-)}{\Delta r_n^-} \quad (3.10)$$

$$e_{ni} = \tau_{2n} K_{i2}^3(n^+) + \tau_{1n} K_{i2}^3(n^-) \quad (3.11)$$

$$\eta(n^+, u_i) = e^{-\Delta u_i} \eta(n^+, u_{i-1}) + \Delta u_i K_{i1}^4(n^+) \phi_{ni} \quad (3.12a)$$

$$\eta(n^-, u_i) = e^{-\Delta u_i} \eta(n^-, u_{i-1}) + \Delta u_i K_{i1}^4(n^-) \phi_{ni} \quad (3.12b)$$

$$\mu_{1n} = 1 - \frac{\rho(2-\rho)\Delta r_n^-}{2r_n} \quad (3.13a)$$

$$\mu_{2n} = 1 + \frac{\rho(2-\rho)\Delta r_n^+}{2r_n} \quad (3.13b)$$

$$\tau_{1n} = \frac{\Delta r_n^-}{2} \left[1 - \frac{\rho(4-\rho)\Delta r_n^-}{12r_n} \right] \quad (3.14a)$$

$$\tau_{2n} = \frac{\Delta r_n^+}{2} \left[1 + \frac{\rho(4-\rho)\Delta r_n^+}{12r_n} \right] \quad (3.14b)$$

$$\sigma_{1n} = 1 - \frac{\rho(\rho-1)\Delta r_n^-}{2r_n} \quad (3.15a)$$

$$\sigma_{2n} = 1 + \frac{\rho(\rho-1)\Delta r_n^+}{2r_n} \quad (3.15b)$$

The μ 's, τ 's, and σ 's are geometrical factors, with the value of ρ depending on the geometry.

$\rho = 0$, slab

$= 1$, cylinder

$= 2$, sphere

The K 's are kernel functions, involving the cross-sections which are computed according to either of two options

and are discussed below. The $g_{n,j \rightarrow i}$ are group transfer coefficients for inelastic scattering and are also discussed below.

In the equations, $n^+ = n^-$ except at boundary points, at which the notation indicates that discontinuous quantities are to be evaluated in the region to the left of the boundary (n^-) or in the region to the right (n^+), where n is a boundary point. Also,

$$\Delta r_n^+ = r_{n+1} - r_n \quad (3.16a)$$

$$\Delta r_n^- = r_n - r_{n-1} \quad (3.16b)$$

$$\Delta u_i = u_i - u_{i-1} \quad (3.17)$$

u_i = upper lethargy boundary of i^{th} group

$S_{n,i}$ = average source strength per unit lethargy and volume in i^{th} group at n^{th} space point.

$\alpha_{i1}(n)$ is a parameter related to the boundary conditions and will be discussed later.

Suppose we are given the following:

1. The geometry, by specifying ρ and the boundary points.
2. The mesh structure, by specifying r_n , u_i .
3. The kernels K_{i1}^1 , K_{i1}^3 , K_{i1}^4 , and K_{i2}^3 ; the parameter $\alpha_{i1}(n)$; and the sources $S_{n^+,i}$.
4. The region of interest, say $0 \leq n \leq N$, $1 \leq i \leq I$.
5. The boundary conditions in the form Z_{oi} , W_{oi} , ϕ_{Ni} .

6. The initial conditions $\tilde{\phi}_{n,1}^-$ and $\eta(n^+, u_0)$.

7. f_{ni} and h_{ni} are given.

The eqs. (3.2 - 17) determine the flux for $0 \leq n \leq N$, $1 \leq i \leq I$.

We compute as follows:

1. Δr_n^+ , Δr_n^- , Δu_i for the problem from eqs. (3.16a - 17).
2. μ_{1n} , μ_{2n} , σ_{1n} , σ_{2n} , τ_{1n} , τ_{2n} from eqs. (3.13a - 15b),
for $1 \leq n \leq N-1$.
3. a_{ni} , b_{ni} , c_{ni} , e_{ni} from eqs. (3.8 - 11).
4. For $i = 1$, Q_{ni} from eq. (3.7) for $1 \leq n \leq N-1$.
5. For $i = 1$, Z_{ni} and W_{ni} recursively from eqs. (3.3 - 4),
first for $n = 1$ and then for successively higher n to
 $n = N-1$.
6. For $i = 1$, ϕ_{ni} recursively from eq. (3.2), first for
 $n = N-1$ and then for successively lower n to $n = 0$.
7. For $i = 1$, $\eta(n^+, u_i)$ from eqs. (3.12a,b), $0 \leq n \leq N$.
8. $\tilde{\phi}_{n,i}^+$ from eq. (3.5) and $\tilde{\phi}_{n,i+1}^-$ from eq. (3.6), having
already computed $\tilde{\phi}_{n,i}^-$ and $\bar{\phi}_{n,i}$.
9. Repeat steps 4-8, letting $i+1 \rightarrow i$, until ϕ has been
computed for all groups.

Here

$\tilde{\phi}_{n,i}^-$ = flux per unit lethargy at the point lethargy
value u_{i-1} and the space point n (r_n times the
flux, for a sphere)

$\eta(n, u_i)$ = slowing down density at n and u_i due to scattering by hydrogen (r_n times as much, for a sphere)

$g_{n,j \rightarrow i}$ = macroscopic cross-section at n for inelastic scattering from lethargy group j to group i

f_{ni}, h_{ni} = constants relating the average flux per unit lethargy at space point n in lethargy group i to the flux per unit lethargy at the endpoints of the group.

We will generally choose either $f_{ni} = h_{ni} = \frac{1}{2}$ or

$f_{ni} = 1, h_{ni} = 0.$

B. Cross-Section Averaging and Kernel Computation

There are two different cross-section averaging procedures that will be described here. The definitions of the kernels in terms of cross-sections depends on the procedure used. One wants to enter the computation either at the beginning by giving the microscopic cross-sections or later by giving the group-averaged cross-sections. In either case one has to specify the averaging option and group structure used and in the latter case make sure that the scheme and the group structure are the same in the group-averaged cross-section input as in the body of the problem.

Option I:

For all cross-sections $\Sigma = \Sigma_t, \Sigma_a, \Sigma_{SH}, \Sigma_{tr}$

$$\Sigma^i = \frac{1}{\Delta u_i} \int_{u_{i-1}}^{u_i} \Sigma(u) du \quad (3.18)$$

Σ^{*i} will be defined later.

$$K_{i1}^1 = \frac{1}{3\Sigma_{tr}^i} \quad (3.19)$$

$$K_{i1}^3 = \Sigma_a^i + \Sigma^{*i} + \frac{\xi \Sigma_t^i}{f_i \Delta u_i} + \frac{B^2}{3\Sigma_{tr}^i} \quad (3.20)$$

$$K_{i1}^4 = \frac{1 - e^{-\Delta u_i}}{\Delta u_i} \quad (3.21)$$

$$K_{i2}^3 = \frac{\xi \Sigma_t^{i-1} + \frac{h_i}{f_i} \xi \Sigma_t^i}{\Delta u_i} \quad (3.22)$$

$$\Sigma^{*i} = \frac{1}{\Delta u_i} \int_{u_{i-1}}^{u_i} \Sigma_{in}(u) f(u, u_i) du \quad (3.23)$$

$$g_{h,j \rightarrow i} = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \Sigma_{in}(u) [f(u, u_{i-1}) - f(u, u_i)] du \quad (3.24)$$

Option II:

For all cross-sections $\Sigma = \Sigma_t, \Sigma_a, \Sigma_{SH}, \Sigma_{tr}$

$$\Sigma^i = \frac{\int_{u_{i-1}}^{u_i} \frac{\Sigma(u)}{\xi \Sigma_t(u)} du}{\int_{u_{i-1}}^{u_i} \frac{\Sigma_{in}(u)}{\xi \Sigma_t(u)} du} \quad (3.25)$$

$$\Sigma^{*i} = \frac{\int_{u_{i-1}}^{u_i} \frac{\Sigma_{in}(u)}{\xi \Sigma_t(u)} f(u, u_{i+}) du}{\int_{u_{i-1}}^{u_i} \frac{du}{\xi \Sigma_t(u)}} \quad (3.26)$$

$$g_{k,j \rightarrow i} = \frac{\int_{u_{j-1}}^{u_j} \frac{\Sigma_{in}(u)}{\xi \Sigma_t(u)} [f(u, u_{i-1}) - f(u, u_i)] du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi \Sigma_t(u)}} \quad (3.27)$$

$$\frac{1}{\Sigma_{tr}^i} = \frac{\int_{u_{i-1}}^{u_i} \frac{du}{\xi \Sigma_t(u) \Sigma_{tr}(u)}}{\int_{u_{i-1}}^{u_i} \frac{du}{\xi \Sigma_t(u)}} \quad (3.28)$$

Note that we average $1/\Sigma_{tr}$, rather than Σ_{tr} , in the same way as Σ_t, Σ_a , and Σ_{SH} .

$$K_{i1}^1 = \frac{1}{3\Sigma_{tr}^i} \quad (3.29)$$

$$K_{i1}^3 = \Sigma_a^i + \Sigma^{*i} + \frac{1}{f_i \int_{u_{i-}}^{u_{i+}} \frac{du}{\xi \Sigma_t(u)}} \quad (3.30)$$

$$K_{i1}^4 = \frac{1 - e^{-\Delta u_i}}{\Delta u_i} \Sigma_{SH}^i \quad (3.31)$$

$$K_{i2}^3 = \frac{1 + \frac{h_i}{f_i}}{\int_{u_{i-}}^{u_{i+}} \frac{du}{\xi \Sigma_t(u)}} \quad (3.32)$$

Note that K_{i1}^1 and K_{i1}^4 have the same form as for Option I.

Here

B = transverse buckling

Take $B = 0$ unless otherwise indicated

ξ = mean lethargy increase per collision

Σ_a = macroscopic absorption cross-section

Σ_t = macroscopic total cross-section for nonhydrogen

Σ_{SH} = macroscopic total cross-section for hydrogen

Σ_{in} = macroscopic inelastic scattering cross-section

$f(u, u')$ = probability that a neutron inelastically scattered at u goes to a lethargy greater than u' .

Σ_{tr} = macroscopic transport cross-section.

The K 's are region as well as lethargy-dependent.

K_{i1}^1 will be recognized as the diffusion coefficient.

K_{i1}^3 is evidently an effective cross-section for removal from the i^{th} group by anything but hydrogen collision and K_{i1}^4 is then an effective cross-section for removal by hydrogen scattering. K_{i2}^3 relates the slowing down densities at u_{i-1} and u_i to the average flux in the i^{th} group.

In the thermal group $i = I$, nothing gets scattered out. Further, the thermal flux is not a flux per unit lethargy, but an integral flux over the group.

$$\phi_I = \int_{u_{I-1}}^{\infty} \phi(u) du \quad . \quad (3.33)$$

To obtain the thermal flux correctly, one computes the kernels imposing the following values:

$$\frac{1}{f_I} = 0 \quad (3.34)$$

$$\Delta u_I = 1 \quad (3.35)$$

$$\sum_{SH}^I = 0 \quad (3.36)$$

$$e^{-\Delta u_I} = 0 \quad (3.37)$$

Thermal also poses some problems as far as cross-section averaging is concerned. In the first place, u_{I-1} is somewhat arbitrary. One may take it as corresponding to an energy 2.5 times thermal energy. For the thermal group, one may average the cross-sections over a Maxwellian distribution with velocities ranging from zero to infinity. This gives for a $1/v$ cross-section (microscopic) the average cross-section in the thermal group

$$\sigma_I = \frac{\sqrt{\pi}}{2} \sigma(kT) \approx 0.886 \sigma(kT),$$

where $\sigma(kT)$ is the value of the cross-section at thermal energy corresponding to temperature T .

This prescription is by no means unique and in certain cases might not be very good. However, it is about as good as one can do without going into properties of individual moderators.

C. Boundary Conditions

Consider the following boundary conditions

$$\text{I. } \phi(0) = 0 \quad (3.39a)$$

$$\text{II. } \phi'(0) = 0 \text{ (symmetric)} \quad (3.39b)$$

$$\text{III. } \phi(R) = 0 \quad (3.40a)$$

$$\text{IV. } \phi'(R) = -\gamma \phi(R) \quad (3.40b)$$

One condition (either I or II) is to be used at 0 and one (either III or IV) at R .

We take $n = 0, 1, \dots, N$, with $\phi(o) \rightarrow \phi_o \phi(R) \rightarrow \phi_N$.

$$\text{I. } \phi(o) = 0 \quad (3.39a)$$

We take

$$W_o = 0 \quad (3.41a)$$

$$Z_o = 0 \quad (3.41b)$$

$$\text{II. } \phi'_o(o) = 0 \text{ (symmetric)} \quad (3.39b)$$

In the symmetric case, $a_o = c_o$. Further, this situation can be represented by the relation

$$\phi_{-1} = \phi_1. \quad (3.42)$$

Then from eq. (3.2),

$$\phi_o = \frac{\phi_{-1} - W_{-1}}{Z_{-1}} = -\frac{W_{-1}}{Z_{-1}} + \frac{1}{Z_{-1}} \phi_{-1} = W_o + Z_o \phi_1 \quad (3.43)$$

Because of (3.42),

$$W_o = -\frac{W_{-1}}{Z_{-1}} \quad (3.44)$$

$$Z_o = \frac{1}{Z_{-1}} \quad (3.45)$$

Solving (3.44) and (3.45) for Z_{-1} and W_{-1} in terms of Z_o and W_o and inserting these values into (3.3) and (3.4) for $n = o$, one finds

$$Z_o = \frac{2a_o}{b_o} \quad (3.46)$$

$$W_o = \frac{Q_o}{b_o} \quad (3.47)$$

$$\text{III. } \phi(R) = 0 \quad (3.40a)$$

We take

$$\phi_N = 0 \quad (3.48)$$

$$\alpha_{i1}(n) = 0 \quad (\text{ef. eq. (3.9)}) \quad (3.49)$$

$$\text{IV. } \phi'(R) = -\gamma\phi(R) \quad (3.40b)$$

γ is then the reciprocal of the extrapolation distance. If we write

$$\gamma = \frac{\Gamma}{D}, \quad (3.50)$$

where D is the diffusion constant, then

$$\Gamma = \gamma D = \frac{1}{d} \frac{1}{3\Sigma_{tr}} = \frac{\Sigma_h}{M} \frac{1}{3\Sigma_{tr}} = \frac{1}{3M}. \quad (3.51)$$

Here

d = extrapolation length

Σ_{tr} = transport cross-section

M = geometrical constant (= 0.7104 for a slab)

This boundary condition is taken care of by the $\alpha_{i1}(n)$ in eq. (3.9). Under boundary condition IV,

$$\begin{aligned} \alpha_{i1}(n) &= \Gamma_i, & n &= N \\ &= 0, & n &< N \end{aligned} \quad (3.52)$$

$$\phi_N = W_N, \quad (3.53)$$

where in the computation of W_N , the terms

$$\sigma_{2N} a_{Ni} + \tau_{2N} \left[K_{i1}^4(N^+) + K_{i1}^3(N^+) \right] = 0 \quad (3.54)$$

in expression (3.9) for b_{ni} , for $n = N$.

In effect what the procedure does is to set up an $(N+1)^{st}$ mesh point a distance $1/\gamma$ beyond the N^{th} point, with void between, and take $\phi_{N+1} = 0$. The equations (3.37-39) incorporate the results of doing this.

D. Source and Initial Conditions

The sources for $u > u_0$ are given by contributions to the appropriate S_{ni} . For a fission source this is proportional to

$$f_1 = \int_{u_{i-1}}^{u_i} f(u) du, \quad (3.55)$$

where

$f(u)$ = number of fission neutrons per unit lethargy at u
per fission neutron.

The initial conditions are the slowing down densities at u_0 . These might be given by the FANTASIA-TRIPROD link. The conditions are

$\eta(n, u_0)$ = slowing down density at n and u_0 due to
scattering by hydrogen

$q(n, u_0)$ = slowing down density at n and u_0 due to
scattering by all elements but hydrogen

$$\tilde{\phi}_{n,1^-} = \frac{q(n,u_0)}{(\xi\Sigma_t)_{n1^-}} \quad (3.56)$$

where

$(\xi\Sigma_t)_{n1^-}$ = value of $\xi\Sigma_t$ at point n and lethargy u_0 .

Note that in spherical geometry the slowing down densities must be multiplied by r to give η and q .

E. Cross-Section and Nuclide Data

The required cross-section data for each element other than hydrogen are

σ_t = total cross-section

σ_s = elastic scattering cross-section

σ_a = absorption (non-neutron-producing) cross-section

$\sigma_{n'}$ = inelastic scattering (n,n') cross-section

σ_{2n} = $(n,2n)$ cross-section

σ_f = fission cross-section

These are given as microscopic cross-sections for a set of lethargy values u_α . Macroscopic cross-sections are denoted by replacing σ with Σ . The energy distribution of inelastically scattered neutrons is also required. In the continuum region (smaller initial lethargies) this is given by

$\sigma_{in}(u,E')$ = cross-section for inelastic scattering
from lethargy u to unit range of energies
about E' .

In the discrete region (higher initial lethargies) it is given by the excitation function

$f_{in}(u, Q_i)$ = cross-section for excitation of i^{th} level of the compound nucleus by inelastic scattering from lethargy u .

Q_i = excitation energy of i^{th} level.

In addition, the atomic weight A of each element must be given.

The transport cross-section is given by

$$\sigma_{tr} = \sigma_a + (1 - \bar{\mu}) \sigma_s, \quad (3.57)$$

where for isotropic center-of-mass elastic scattering, which we assume,

$$\bar{\mu} = \frac{2}{3A} \quad (3.58)$$

The cross-section data are given in the form described here in the NDA compilations.*

It is necessary to make sure that the inelastic differential energy cross-sections are used in a form that is consistent with the interpolation scheme of the TRIPROD program. As stated, the code takes inelastic cross-sections in two forms: either as the cross-section $\sigma_{in}(u', E)$ at u' per unit final energy about E , tabulated as a function of u' and E , or as an excitation cross-section $f_{in}(u', Q_i)$ tabulated as a function of u' and the excitation energy Q_i . In the available tabulated

* See, for example Ref.[2].

inelastic cross-section data $f_{in}(u', Q_i)$ may be available as interpolated in the initial lethargy directly from experiment*, for the lowest excitation levels Q_i . At higher incident energies one resorts to calculated cross-section in the form $\sigma_{in}(u', E)$.*

In general, $f_{in}(u', Q_i)$ may not sum precisely to the total observed inelastic cross-section at u' because of experimental inaccuracies. We therefore define the normalized excitation cross-section

$$g_i(u) = f_{in}(u, Q_i) \frac{1}{\sum_{\ell} f_{in}(u, Q_{\ell})} \quad (3.59)$$

g_i has the required property that

$$\sum_i g_i(u) = 1. \quad (3.60)$$

$\sigma_{in}(u)$ is the cross-section for neutron production by inelastic scattering. In terms of the (n, n') and $(n, 2n)$ cross-sections it is

$$\sigma_{in}(u) = \sigma_{n'}(u) + \sigma_{2n}(u) \quad (3.61)$$

This is because of the $(n, 2n)$ neutrons are included in $\sigma_{in}(u, E)$. In the discrete region, $\sigma_{2n}(u) = 0$.

Since $\sigma_{in}(u', E)$ is computed while $\sigma_{in}(u)$ is measured, integration of $\sigma_{in}(u, E)$ over E will not in general give $\sigma_{in}(u)$.

* See, for example Ref. [2].

Again we must impose a normalization. We assume that $\sigma_{in}(u', E)$ is linear in E between successive tabulated values. It is further assumed that if E takes on the values E_i and if there are P values of i in the tabulation, that

$$E_{P+1} = 0 \quad (3.62)$$

$$\sigma_{in}(u', 0) = 0 \quad (3.63)$$

$$E_{i+1} < E_i \quad (3.64)$$

$$\sigma_{in}(u', E) = 0 \quad E > E_1 \quad (3.65)$$

Then we can get a normalized cross-section

$$\sigma'_{in}(u', E) = \sigma_{in}(u', E) \frac{\sigma_{in}(u')}{\frac{1}{2} \sum_{i=1}^P \left\{ \sigma_{in}(u', E_i) + \sigma_{in}(u', E_{i+1}) \right\} (E_i - E_{i+1})} \quad (3.66)$$

In terms of g_i and σ'_{in} , the differential inelastic neutron cross-section is

$$\begin{aligned} \sigma'_{in}(u') f(u', u) &= E \sigma_{in}(u', E) \quad , \quad u' < u_{k_1} \\ &= \sum_i g_i(u') \delta(E' - E - Q_i) E, * \quad u' \geq u_{k_1} \end{aligned} \quad (3.67)$$

Here u_{k_1} is the smallest lethargy at which $f_{in}(u, Q_i)$ is given.

For $u_{k_2} < u' < u_{k_1}$, where u_{k_2} is the largest lethargy for which

we use the $\sigma_{in}(u', E)$ data, one takes

* Eq. (3.58) assumes that the excitation energy Q_i equals the neutron energy loss in the c.m. system. While not strictly true, this is an adequate approximation for our purposes.

$$\sigma_{in}'(u', E) = \sigma_{in}'(u_{k_2}, E) \quad . \quad (3.68)$$

Elsewhere we interpolate linearly in u' , for both $\sigma_{in}'(u', E)$ and $g_i(u')$.

In these equations, we have the usual relation between energy and lethargy

$$E' = E_0 e^{-u'} \quad . \quad (3.69)$$

Note that

$$Q_i < E_0 e^{-u} \quad . \quad (3.70)$$

In eq. (3.58), $f(u', u)$ is the number of neutrons inelastically scattered at u' that end up at u , per unit final lethargy. It is the quantity used in eqs. (3.23, 24, 26, and 27). For the discrete case,

$$f(u', u) = g_i(u') \delta(u' - u - \ln \frac{E_0}{Q_i}) \quad (3.71)$$

The mean lethargy loss per collision is given by

$$\xi = 1 - \frac{(A-1)^2}{2A} \ln \frac{A+1}{A-1} \quad (3.72)$$

So far all these have referred to a single element. To get the macroscopic quantities that go into the kernel computations, we denote each element by an index r . If

C_r = nuclear density of element r (nuclei per unit volume), then as functions of u ,

$$\Sigma_{tr} = \sum_r C_r (\sigma_{tr})_r \quad (3.73)$$

$$\Sigma_a = \sum_r C_r (\sigma_a)_r \quad (3.74)$$

$$\Sigma_{SH} = C_H (\sigma_{SH}) \quad (3.75)$$

$$\Sigma_{in}(u)f(u,u') = \sum_r C_r (\sigma_{in}(u))_r (f(u,u'))_r \quad (3.76)$$

$$\xi_{\Sigma_t} = \sum_r C_r \xi_r (\Sigma_t)_r \quad (3.77)$$

$$\Sigma_f = \sum_r C_r \sigma_f \quad (3.78)$$

Here C_H is the density of hydrogen atoms ($A=1$). The sum over r excludes hydrogen. In the computation of Σ_f only fissionable materials contribute.

F. Iteration Procedure-Fission

When TRIPROD is used in conjunction with FANTASIA, it starts below the energies of fission neutrons and there are no fission sources. When used as a reactor code, it covers all energies and a standard iteration procedure is used. One also needs to iterate in some way when uranium is present in a shield. We will discuss first TRIPROD operating as a unit.

One chooses a trial source distribution

$$S_{ni} = S_n f_i, \quad (3.79)$$

where f_i is the fission neutron distribution in lethargy, defined by (3.55).

Define

$$P_n = \sum_{i=1}^I \phi_{ni} \Sigma_f^i \Delta u_i \quad (3.80)$$

Let

- V = total sum of the thicknesses of all fuel regions,
- for a slab
- $= \frac{1}{2\pi}$ times total volume of all fuel regions divided by
- height, for a cylinder
- $= \frac{1}{4}$ times total volume of all fuel regions, for a sphere.
- $\gamma = 0$, slab
- $= 1$, cylinder or sphere.

Define

$$\nu_c = \frac{V}{\int_0^R r \gamma P_n dr} \quad (3.81)$$

For the next iteration, let

$$\nu_c P_n \rightarrow S_n$$

and repeat.

Ultimately the procedure should converge. Then let

$$k = \frac{\nu}{\nu_c} \quad (3.82)$$

ν is the number of neutrons produced per fission.

$k = 1$ is the criticality condition.

If the fissionable material is present in a shield, one can carry through similar procedure. In that case it is presumed that the effect of the fission is not the main effect, but a perturbation. Only part of the source is due to fission. One starts by assuming that that part vanishes. One solves the equation and finds P_n . The next estimate for the source due to fission is νP_n . One can iterate this procedure.

In fact, if the entire FANTASIA-TRIPROD scheme is used, the contribution due to fission will add sources to FANTASIA only, though the fissions may occur either fast, in FANTASIA, or thermal, in TRIPROD. In any case, one can iterate.

G. FANTASIA-TRIPROD Link

FANTASIA gives the number of neutrons slowing down past a cutoff energy E_0 (corresponding to $u = 0$ in TRIPROD) in each spatial interval. It also computes the slowing down density per unit length at the boundary points between intervals. The link picks up these values from FANTASIA and transforms them into point values at the spatial mesh points of TRIPROD.

The procedure, which is done separately for slowing down due to hydrogen and for that due to other elements but is identical for both, is to fit an exponential curve to the end point values of a FANTASIA interval. If the integrated slowing down density using this curve differs from the total number of neutrons computed by FANTASIA as slowing down in the interval by

less than the computed standard deviation of the latter quantity, the curve is used. If not, a quadratic form of curve is assumed. The three parameters are fit so that both the end point values and the integral over the region agree with the FANTASIA results.

The slowing down curve so obtained is continuous everywhere, agrees with the FANTASIA values at the boundaries of the intervals, and differs from the integrated FANTASIA value over each interval by less than the standard deviation in that interval.*

Thus consider the position interval $x_1 \leq x \leq x_2$. Let the slowing down density computed by FANTASIA be denoted by y , where

$$y_1 = y(x_1) \quad (3.83a)$$

$$y_2 = y(x_2) \quad (3.83b)$$

Let the total number of neutrons computed by FANTASIA to be slowed down in the interval be J .

We assume that in the interval

$$y = a e^{bx} . \quad (3.84)$$

Since the curve is to pass through (x_1, y_1) and (x_2, y_2) ,

$$b = \frac{1}{x_1 - x_2} \log \frac{y_1}{y_2} \quad (3.85)$$

$$a = y_1 e^{-bx_1} . \quad (3.86)$$

* If the fractional variance $\frac{\sigma^2}{J^2}$ is smaller than some prescribed value ϵ^2 , we use $J\epsilon$ rather than σ in the inequality (3.88). This is to eliminate a possible faulty criterion that could occur if the computed σ were accidentally small.

We compute the integral

$$K = \int_{x_1}^{x_2} y(x) dx = \frac{a}{b} (e^{bx_2} - e^{bx_1}) = \frac{y_2 - y_1}{b} \quad (3.87)$$

and compare it to J. If

$$|K - J| \leq \sigma, \quad (3.88)$$

where σ is the computed standard deviation for J, $y(x)$ is assumed to represent the slowing down density for $x_1 < x < x_2$.

If

$$|K - J| > \sigma, \quad (3.89)$$

$y(x)$ is obviously not a good representation. We then let

$$z(x) = A + Bx + Cx^2. \quad (3.90)$$

This is to be fit to y_1 , y_2 , and J. Then

$$C = \frac{3(y_2 + y_1)(x_2 - x_1) - 6J}{(x_2 - x_1)^3} \quad (3.91)$$

$$B = \frac{y_2 - y_1 - C(x_2^2 - x_1^2)}{x_2 - x_1} \quad (3.92)$$

$$A = y_1 - x_1(Cx_1 + B). \quad (3.93)$$

With these values for the parameters,

$$z(x_1) = y_1 \quad (3.94a)$$

$$z(x_2) = y_2 \quad (3.94b)$$

$$\int_{x_1}^{x_2} z(x) \, dx = J. \quad (3.95)$$

$z(x)$ is used in place of $y(x)$ in this case.

One expects the exponential fit to be valid except near material interfaces. The quadratic fit in those regions can take account of minima and maxima in the flux which may occur near interfaces.

REFERENCES

1. R. Aronson, J. Heitner, M.J. Kelly, and H. Steinberg, Neutron Dose and Thermal Flux Calculations with FANTASIA-TRIPROD, TRG-143-STR, (April 14, 1961).
2. E.S. Troubetzkoy, Fast Neutron Cross Sections of Iron, Silicon, Aluminum, and Oxygen, NDA 2111-3 Volume C, (November 1, 1959).
3. Herbert A. Steinberg, Generalized Quota Sampling, Nuclear Science and Engineering, Volume 15, No. 2, (February 1963).