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**NEW ANALYTICAL RESULTS FROM SLOWING-DOWN
THEORY, AND THEIR APPLICATION TO A CHECK OUT
OF THE RBU SLOWING-DOWN ROUTINE**

D. H. THOMSEN AND A. G. GIBBS

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THE RBU SLOWING-DOWN ROUTINE

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D. H. Thomsen and A. G. Gibbs

INTRODUCTION

The purpose of this paper is twofold: to present some new analytical results from neutron slowing-down theory, and to use these results as a check on the Monte Carlo slowing-down routine presently used in the RBU burnup code.⁽¹⁾

Both the analysis and the calculations presented herein concern the simplest possible model of the slowing-down process: the case of a purely scattering medium, whose cross section does not depend on energy and whose constituent atoms scatter neutrons isotropically in the center-of-mass system.

SUMMARY

The analytical results are compared to Monte Carlo calculations done using the RBU slowing-down routine. The comparison indicates that the routine is working properly.

ANALYTICAL RESULTS

Many analytical results are well-known for the simple model of slowing-down. For example, in a medium whose atoms have mass A , the mean logarithmic energy decrement ξ , and $\bar{\mu}$, the average cosine of the laboratory scattering angle, are given by

$$\xi = 1 + \frac{\alpha \ln \alpha}{1 - \alpha}$$

and

$$\bar{\mu} = \frac{2}{3A},$$

where

$$\alpha = \left(\frac{A - 1}{A + 1} \right)^2.$$

To supplement these and other known results, we have derived analytical expressions for four other quantities characteristic of this model. These quantities are

- The mean square distance, $\langle R_n^2 \rangle$, between the starting point of a neutron and the point where it makes its n^{th} collision
- The probability p_n that a neutron with initial energy E_0 slows through energy αE_0 on its n^{th} collision
- An approximate expression for the neutron age
- The mean square displacement, $\langle R_2^2(\alpha E_0) \rangle$ of those neutrons which slow through energy αE_0 on their second collision.

We first derive an expression for $\langle R_n^2 \rangle$. Since

$$\underline{R}_n = \sum_{j=1}^n \underline{r}_j, \quad (1)$$

where $\underline{r}_j$ is the vector length of the j^{th} flight,

$$\langle R_n^2 \rangle = \langle \underline{R}_n \cdot \underline{R}_n \rangle = \sum_{j,k=1}^n \langle \underline{r}_j \cdot \underline{r}_k \rangle. \quad (2)$$

Since the cross section is assumed to be constant (σ) for this model, the length of any one flight does not depend on its orientation relative to previous flights. Thus,

$$\begin{aligned} \langle r_j \rangle &= 1/\sigma \equiv \lambda \\ \text{and} \\ \langle r_j^2 \rangle &= 2/\sigma^2 \end{aligned} \quad (3)$$

In addition, it is easily shown that the average cosine of the angle between the j^{th} and k^{th} flights is given by

$$\langle \cos \theta_{jk} \rangle = \bar{\mu} |j-k| \quad (4)$$

Thus, Equation (2) can be rewritten as

$$\langle R_n^2 \rangle = \frac{2n}{\sigma^2} + \frac{1}{\sigma^2} \sum_{j \neq k=1}^n \bar{\mu} |j-k| \quad (5)$$

The double sum in Equation (5) can be carried out by doing the $j < k$ and $j > k$ parts separately and by using the known result for the partial sum of a geometric series. By using some algebra, we find that

$$\begin{aligned} \langle R_n^2 \rangle &= \frac{2}{\sigma^2 (1 - \bar{\mu})^2} [(1 - \bar{\mu})n \\ &\quad - \bar{\mu}(1 - \bar{\mu}^n)] \end{aligned} \quad (6)$$

Next, we derive an expression for p_n , the probability that a neutron slows past energy αE_0 on its n^{th} collision. The expression for p_n will be used below to derive an approximate expression for the neutron age at energy αE_0 . To find p_n , we use the well-known expression for the slowing-down kernel and integrate over all possible events $E_0 \geq E_1 \geq E_2 \dots \geq E_{n-1} > \alpha E_0 > E_n$ which can lead to the passing

of the neutron through energy αE_0 on its n^{th} collision. Since the calculation is quite straightforward, although lengthy, we give only the result, which is

$$p_n = \frac{\alpha}{y^n} \left[\frac{x^{n-1}}{(n-1)!} - \alpha \sum_{i=n-1}^{\infty} \frac{x^i}{i!} \right] \quad (7)$$

where

$$x = \ln \frac{1}{\alpha}$$

and

$$y = (1 - \alpha) \quad .$$

An approximate expression for the neutron age is given by Glasstone and Edlund:⁽²⁾

$$\tau(E) = \int_0^t D v dt' \quad , \quad (8)$$

where t is the time when the neutron passes through energy E , and $v = \sqrt{2E/m}$.

For the present model, D is a constant,

$$D = 1/[3\sigma(1 - \bar{\mu})] \quad , \quad (9)$$

so that Equation (8) reduces to

$$\frac{\tau(E)}{D} = \int_0^t v dt' \quad . \quad (10)$$

The integral is easily recognized as the total path length travelled by the neutron from its starting point to the point where it slows through energy E . Therefore, Equation (10) can also be written as

$$\frac{\tau(E)}{D} = \left\langle \sum_{j=1}^n r_j \right\rangle \quad (11)$$

where $r_j = |\underline{r}_j|$ and n indicates the index of the collision where the neutron slows through energy E . Using Equation (3) and considering $E = \alpha E_0$, we can rewrite Equation (11) as

$$\frac{\tau(\alpha E_0)}{D} = \frac{1}{\sigma} \sum_{n=1}^{\infty} n p_n \quad (12)$$

The sum can be carried out by using Equation (7) for p_n . The order of the n and i summations is interchanged, and the known results for exponential and geometric series are used. The result is simply

$$\frac{\tau(\alpha E_0)}{D} = \frac{1}{\sigma} \left(e^{x/y} - \frac{y}{\alpha} \right) \quad (13)$$

It should be emphasized that while this is an approximate expression for the neutron age, it can be used as a precise check on numerical computation, because Equation (11) can also be evaluated by Monte Carlo techniques.

An expression for the actual neutron age has not been derived because of the complexities introduced into the analysis by the coupling between the scattering angle and energy loss of a neutron during a collision. We have, however, derived an expression for the mean square displacement $\langle R_2^2(\alpha E_0) \rangle$ of those neutrons which slow through energy αE_0 on their second collision. We first recall⁽²⁾ in deriving the expression that in the slowing-down range the energies of a neutron before and after the n^{th} collision are related by

$$\frac{E_n}{E_{n+1}} = \frac{A^2 + 2A\eta_n + 1}{(A + 1)^2} \quad (14)$$

where η_n is the cosine of the n^{th} scattering angle in the center-of-mass system (CM). From Equation (14), we find that

$$\begin{aligned} \frac{E_2}{E_0} &= \frac{E_2}{E_1} \cdot \frac{E_1}{E_0} \\ &= \frac{(A^2 + 2A\eta_2 + 1)(A^2 + 2A\eta_1 + 1)}{(A + 1)^4} \quad (15) \end{aligned}$$

Suppose now that we consider a particular value of η_1 and ask: for what values of η_2 will the second scattering result in $E_2 < \alpha E_0$? From Equation (15) we find that $E_2 < \alpha E_0$ provided that

$$\eta_2 < \hat{\eta}_2 \equiv - \frac{2A + (A^2 + 1)\eta_1}{(A^2 + 2A\eta_1 + 1)} \quad (16)$$

Since scattering is isotropic in the CM, the probability that Equation (16) is satisfied for a given η_1 ; hence, that $E_2 < \alpha E_0$ is

$$\begin{aligned} P(E_2 < \alpha E_0 | \eta_1) &= \int_0^{\hat{\eta}_2} \frac{1}{2} d\eta_2 \\ &= \frac{1}{2}(\hat{\eta}_2 + 1) \quad (17) \end{aligned}$$

To calculate $\langle R_2^2(\alpha E_0) \rangle$, we will need the transposed distribution, the probability that η_1 occurred given that $E_2 < \alpha E_0$. We denote this probability by $P(\eta_1 | E_2 < \alpha E_0)$, and obtain it from

$$\begin{aligned} P(\eta_1 | E_2 < \alpha E_0) &= \frac{P(\eta_1)}{P(E_2 < \alpha E_0)} \\ &\quad \cdot P(E_2 < \alpha E_0 | \eta_1) \quad (18) \end{aligned}$$

Here $P(\eta_1)$ and $P(E_2 < \alpha E_0)$ denote the respective probability distributions for scattering with CM cosine η_1 and for finding $E_2 < \alpha E_0$. From Equation (17), the definition of p_2 , and the isotropy of η_1 , it follows that

$$P(\eta_1 | E_2 < \alpha E_0) = \frac{1}{4p_2} (\hat{\eta}_2 + 1) \quad (19)$$

The distance R_2 between the starting point of a neutron and the point where it makes its second collision is related to the lengths of the first two flights (r_1 and r_2) and to η_1 by

$$R_2^2 = r_1^2 + r_2^2 + 2r_1r_2 \cdot \frac{(1 + A\eta_1)}{(A^2 + 2A\eta_1 + 1)^{1/2}} \quad (20)$$

The average of this quantity over the lengths r_1 and r_2 , and over η_1 [using the distribution Equation (19)] is $\langle R_2^2(\alpha E_0) \rangle$, the desired quantity. By using Equations (3) and (19) and by performing the necessary integration, we find

$$\langle R_2^2(\alpha E_0) \rangle = \frac{(A - 1)^2}{\sigma^2 p_2} \cdot \left[\frac{(A + 1)^2}{4A^2} \log \frac{1}{\alpha} - \frac{1}{3A^2} - \frac{1}{A} \right] \quad (21)$$

This completes the derivation of new analytical results. In Table I we show numerical values for a medium with $\sigma = 1.0 \text{ cm}^{-1}$ and $A = 19.277588$. In the following section, these are compared to the results of Monte Carlo calculations for the same medium.

CHECKOUT OF THE RBU SLOWING DOWN ROUTINE

The purpose of this study was to check the RBU Monte Carlo slowing down routine and the spherical boundary routine. Three RBU calculations were made (Run 1-3). Runs 1 and 2 were a check of both the elastic scattering and the boundary routine, while Run 3

TABLE I. Analytical Values of Parameters for a Medium with $\sigma = 1.0 \text{ cm}^{-1}$, $A = 19.277588$

$\lambda = 1/\sigma$	1.000000 cm
$\alpha = (A-1)^2/(A+1)^2$	0.8124660
$x = \ln 1/\alpha$	0.2076813
$y = (1-\alpha)$	0.1875340
$\bar{\mu} = 2/3A$	0.03458247
$D = \frac{1}{3\sigma(1-\bar{\mu})}$	0.3452737 cm
$\xi = 1 + \frac{\alpha \ln \alpha}{1-\alpha}$	0.1002489
$\frac{\tau(\alpha E_0)}{D}$ (Eq. 13)	2.795756 cm ²
P_2	0.4654361
$\langle R_1^2 \rangle$	2.000000 cm ²
$\langle R_2^2 \rangle$	4.06916 cm ²
$\langle R_3^2 \rangle$	6.14072 cm ²
$\langle R_4^2 \rangle$	8.21236 cm ²
$\langle R_5^2 \rangle$	10.2840 cm ²
$\langle R_2^2(\alpha E_0) \rangle$	3.35620 cm ²

was only a check of the elastic scattering routine. Run 1 was made without using any internal boundaries while Run 2 used 20 internal boundaries in the form of concentric spheres about the origin. The results of Runs 1 and 2 were compared and no change was observed that could not be explained by statistical fluctuations. Thus, it is concluded that the spherical boundaries are treated properly.

A point, isotropic, 10 MeV monoenergetic source at the point $x = y = z = 0$ was assumed for all three calculations.

The medium was taken to be a pure scatterer with a constant mean free path of 1.0 cm and a mass per atom of 19.277588 neutron masses. The neutrons were allowed to slow down below some minimum input energy and then dropped. For Run 3, the minimum energy was αE_0 (8.12466 MeV).

If the neutron had not suffered five collisions when it crossed αE_0 , it was not dropped until after the fifth collision. The input parameters used in each run are listed in Table II. The quantities obtained in the Monte Carlo calculation can be divided into

TABLE II. Monte Carlo Input Parameters

Parameters that were the same for all runs

Source energy	10 MeV
Source spacial distribution	Point at $x=y=z=0$
Source angular distribution	Isotropic
Mean free path	1 cm (constant in energy)
Cross section types	Pure elastic scatterer
Atomic weight	19.277588 neutron masses
Scattering angle distribution	Isotropic in center of mass

Parameters differing for each run

<u>Parameter</u>	<u>RUN 1</u>	<u>RUN 3</u>	<u>RUN 3</u>
Minimum energy (eV)	961.12	8.6517×10^4	8.12466×10^6
Number of spherical boundaries (centered at origin)	1	20	1
Number of initial neutrons	1600	3000	15000

Region boundaries for Run 2

<u>Region</u>	<u>Radius(cm)</u>	<u>Region</u>	<u>Radius(cm)</u>
1	5	11	10
2	1	12	12
3	2	13	14
4	3	14	16
5	4	15	18
6	5	16	20
7	6	17	25
8	7	18	30
9	8	19	50
10	9	20	1000

Outside boundary for Runs 1 and 3

1000 cm

two types. The first type consists of quantities tallied for each collision which include the mean free path λ , the average logarithmic energy decrement ξ , and the average cosine of the scattering angle $\bar{\mu}$ in the laboratory system. The above values were calculated from the equations

$$\begin{aligned}\lambda &= \frac{1}{N} \sum_{i=1}^N |\vec{r}_i - \vec{r}_{i-1}| \\ &= \frac{1}{N} \sum_{i=1}^N \left[(x_i - x_{i-1})^2 \right. \\ &\quad \left. + (y_i - y_{i-1})^2 + (z_i - z_{i-1})^2 \right]^{1/2} \\ \xi &= \frac{1}{N} \sum_{i=1}^N \ln \frac{E_{i-1}}{E_i} \\ \bar{\mu} &= \frac{1}{N} \sum_{i=1}^N \frac{|\vec{v}_1 - \vec{v}_{1+1}|}{|\vec{v}_i| |\vec{v}_{i+1}|} \\ &= \frac{1}{N} \sum_{i=1}^N (\alpha_i \alpha_{i+1} + \beta_i \beta_{i+1} + \gamma_i \gamma_{i+1}).\end{aligned}$$

The second type of quantities calculated were those depending on a series of collisions. Quantities of this type include the flux, the collision density, the age, etc. The collision density as a function of energy was tallied by counting the number of collisions in each micro-energy group. Of greatest importance were the ages of the neutrons at different energies.

The age of a neutron with energy E was defined as the age the neutron had when it suffered a collision which reduced its energy below energy E . Age

can be defined in two ways. The two ages will be designated as

$$\tau_{v_i} = \int_0^t D v_i dt = D \sum_{j=1}^k v_j \Delta t_j$$

$$\text{and as } \tau_{r_i} = \frac{1}{\sigma} r_k^2$$

where k is the index of the collision at which the energy of the neutron becomes less than E . The average values of the ages then becomes

$$\tau_v(E) = \frac{1}{N} \sum_{i=1}^N \tau_{v_i} \quad \text{and} \quad \tau_r(E) = \frac{1}{N} \sum_{i=1}^N \tau_{r_i}.$$

It should be noted that τ_v is dependent only on the path lengths when D is a constant, while τ_r depends on both the path lengths and the scattering angles.

RESULTS FOR THE ENERGY RANGE BETWEEN E_0 AND αE_0

The results for the energy range between E_0 and αE_0 for the three calculations are shown in Table III along with the analytical results. As noted above, the analytical result for $\tau_r(\alpha E_0)$ was not obtained, but a comparison value was calculated by using the 05R Monte Carlo.⁽³⁾ The 05R calculated value is used in Table III. The value of the collision density, $F(u)$, as a function of lethargy for Run 3 is shown in Figure 1. The analytical values for $F(u) \Delta u_i$ were calculated by using

the formula

$$F(u) \Delta u_i = q/\alpha \left[\exp\left(\frac{\alpha u_{i+1}}{1-\alpha}\right) - \exp\left(\frac{\alpha u_i}{1-\alpha}\right) \right]$$

TABLE III. Comparison of Analytical and Monte Carlo Calculated Parameters

Parameter Number IV Particles	Analytical	Run 1 1600	Run 2 3000	Run 3 15,000
λ (cm), Mean free path	1.00000000	0.9988 $\pm$.0020	1.0001 $\pm$.0020	
ξ , Average logarithmic energy decrement	0.1002489	0.1000 $\pm$.00020	0.10036 $\pm$.00020	
$\bar{\mu}$ Average cosine of the scattering angle	0.03458247	0.0348 $\pm$.0020	0.0340 $\pm$.0020	
$\tau_V(\alpha E_0) = \langle D \sum_i v_i \Delta t_i \rangle_{\alpha E_0}$	0.9653013 cm ²	1.0019 $\pm$.0170	0.9731 $\pm$.0140	0.9699 $\pm$.0050
$\tau_T(\alpha E_0) = \langle 1/6R^2(\alpha E_0) \rangle$	1.0938 $\pm$.0180 cm ² *	1.1090 $\pm$.0360	1.0964 $\pm$.0360	1.0883 $\pm$.0150
$\langle R_2^2(\alpha E_0) \rangle$	3.35620 cm ²			3.4232 $\pm$.060
$\langle R_1^2 \rangle$	2.00000 cm ²			2.0460 $\pm$.0330
$\langle R_2^2 \rangle$	4.06916 cm ²			4.1373 $\pm$.0680
$\langle R_3^2 \rangle$	6.14072 cm ²			6.1504 $\pm$.0970
$\langle R_4^2 \rangle$	8.21236 cm ²			8.1306 $\pm$.1060
$\langle R_5^2 \rangle$	10.28400 cm ²			10.2050 $\pm$.1080
P_2	0.465436 cm ²			0.46387 $\pm$.0040

* Comparison value from an OSR Monte Carlo⁽³⁾ run with 10,000 histories.

where q is the number of source neutrons. For each of the three calculations, some of the values of $F(u)$ were outside the one standard deviation error bars. This is expected since only 68% of the points need be within the error bars for statistical agreement with the analytical value. Since all the values calculated are within statistical agreement, the elastic scattering portion of RBU appears to be working correctly.

RESULTS IN THE ENERGY RANGE BELOW αE_0

The values of interest below αE_0 are the neutron age as a function of energy, and the flux as a function of energy and radius. Neither of these quantities was obtained analytically, but the Monte Carlo results still provide useful information for checking

out both the Monte Carlo elastic scattering routine and the boundary routine.

The fluxes as a function of energy and space were obtained for Run 2. There were no analytical results to compare with directly, but the spatial shape was as expected from age theory for a point source. The flux shape appeared to be in error for some of the low energies near the center, but by following more histories, these errors were proven statistical.

The most appropriate quantity for checking both the effect of the boundaries and elastic scattering routine is the neutron age as a function of energy. An approximate value for age as a function of energy can be obtained from the equation

$$\tau(E) = \int_E^{\alpha E_0} \frac{D}{\xi \Sigma_s} \frac{dE}{E} + C$$

FIGURE 1. Collision Density Versus Lethargy (Run 3)

where C is a first flight correction factor. The value of C was obtained by requiring the above expression to agree with the analytical value of $\tau_v(\alpha E_0)$. The results obtained for Run 2 is shown in Figure 2. The values of $\tau_v(E)$ were so close to $\tau(E)$ that the theory line almost always contains the Monte Carlo

calculated value. The values of $\tau_r(E)$ do not fall on the line, as expected, because $\tau_r(\alpha E_0)$ is not equal to $\tau_v(\alpha E_0)$. The values of $\tau_r(E)$ do fall close enough to the line to make any large error in the Monte Carlo value for $\tau_r(E)$ readily apparent.

FIGURE 2. Age Versus Lethargy (Run 2, 3000 Source Neutrons)

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