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On the role of the adjoint Boltzmann equation in the calculation of energy deposition

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Abstract. The adjoint Boltzmann equation is used to develop a formalism for calculating energy deposition in moderators. Examples of the technique are given and include a point source of fast neutrons in an infinite medium and a uniform source in a sphere of finite radius. Using elastic scattering to describe the slowing down process we calculate the heating rates in moderators with mass numbers 1, 2, 3, 4, 5, 10, 16 and 50. Our results are compared with some recent Monte Carlo calculations on compressed pellets of deuterium and tritium and good agreement is found.

1. Introduction

The rate of energy deposited by fast particles as they slow down in a host medium is of considerable practical importance. In nuclear reactors, for example, fission fragments dissipate their energy in the surrounding fuel material, thereby heating it and also damaging it. The damage is generally calculated from the number of atoms displaced from their equilibrium positions and the amount of energy that goes into nuclear scattering (Chadderton 1965). In addition, the fast neutrons, acting over a much larger volume, also cause damage as they slow down. Moreover, in a graphite reactor, the neutrons lead to significant heating of the moderator and consequent effects on the kinetic behaviour of the system. More recently, from studies of the heating of laser-compressed deuterium–tritium spheres (Beynon and Constantine 1977) it has emerged that neutron heating can contribute significantly to the so-called 'bootstrap' effect. It is clear therefore that accurate methods for calculating the energy dissipation rate of neutrons as they slow down are desirable.

The purpose of the present paper is to show that the adjoint Boltzmann equation is ideally suited for calculating energy deposition. This is done by considering the physical meaning of the adjoint function and then averaging it over the appropriate region in phase space. In this way the adjoint equation can be reduced to a simple form which is amenable to the usual methods of solving the transport equation. In many cases, however, it is superior to the normal Boltzmann equation since the adjoint slowing down operator has some very powerful properties. To illustrate our method, we consider the heating which results from a point source of 14 MeV neutrons in an infinite medium. We calculate the spatial variation of the energy deposition and also the total energy deposited within a sphere of radius R centred on the source. We also consider a finite sphere with a uniformly distributed source and calculate the total energy deposited within it. Elastic scattering is assumed, isotropic in the centre of mass system. To obtain analytical solutions it is necessary to assume that the total cross-section is independent of energy. This assumption leads to a remarkable simplification of the equation, since it then reduces to a pseudo-one-speed form and is therefore amenable to solution by many methods (Davison 1957). For the point source problem we assume linearly anisotropic scattering in the laboratory system and are able to solve the equation by Fourier transform. In the case of the finite sphere, we use a variational method which in itself contains some novel features. Extensive tables are given of the heating rates and these are compared graphically with the work of Beynon and Constantine (1977). Finally, to obtain some ideas on the effect of an energy-dependent cross-section we solve, for some special cases, the equations governing the mean square energy deposition length, i.e. a measure of the mean distance from the source which the particles have travelled in giving up their energy. This is compared with the conventional slowing down length to zero energy.

2. The adjoint equation

It is known that the Green's function of the linear Boltzmann equation

$$\left(\frac{\partial}{\partial t}+v\mathbf{\Omega}.\nabla_r+v\Sigma(E)\right) G(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E,\mathbf{\Omega},\boldsymbol{r},t)$$
$$=\iint \mathrm{d}\mathbf{\Omega}'\,\mathrm{d}E'\Sigma(E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega})\,v'G(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E',\mathbf{\Omega}',\boldsymbol{r},t)$$
$$+\delta(t-t_0)\,\delta(\boldsymbol{r}-\boldsymbol{r}_0)\,\delta(\mathbf{\Omega}-\mathbf{\Omega}_0)\,\delta(E-E_0) \tag{1}$$

is related to the solution of the adjoint equation $G^\dagger(\ldots)$ by (Bell and Glasstone 1970)

$$G^\dagger(E,\mathbf{\Omega},\boldsymbol{r},t\rightarrow E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0)=G(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E,\mathbf{\Omega},\boldsymbol{r},t) \tag{2}$$

where $t>t_0$.

Now the physical interpretation of $G(\ldots)\,\mathrm{d}\boldsymbol{r}\,\mathrm{d}E\,\mathrm{d}\mathbf{\Omega}$ is the average number of particles with energy between E and $(E+\mathrm{d}E)$ travelling in the solid angle $\mathrm{d}\mathbf{\Omega}$ about $\mathbf{\Omega}$ in the volume element $\mathrm{d}\boldsymbol{r}$ at time t due to one particle with energy E_0 and direction $\mathbf{\Omega}_0$ at position $\boldsymbol{r}_0$ at time t_0. If, therefore, we are interested in the average energy deposited per unit time in the volume V at time t by a particle with energy E_0 and direction $\mathbf{\Omega}_0$ injected at $\boldsymbol{r}_0$ at an earlier time t_0, this can be defined as

$$\bar{\nu}(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow t)=\int_V \mathrm{d}\boldsymbol{r}\int_0^{E_0}\mathrm{d}ET(E)v\Sigma(E)\int \mathrm{d}\mathbf{\Omega}G(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E,\mathbf{\Omega},\boldsymbol{r},t) \tag{3}$$

or in terms of the adjoint function

$$\bar{\nu}(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow t)=\int_V \mathrm{d}\boldsymbol{r}\int_0^{E_0}\mathrm{d}ET(E)v\Sigma(E)\int \mathrm{d}\mathbf{\Omega}G^\dagger(E,\mathbf{\Omega},\boldsymbol{r},t\rightarrow E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0) \tag{4}$$

where $T(E)$ is the average amount of energy transferred in a collision. But the adjoint equation is

$$\left(-\frac{\partial}{\partial t}-v\,.\nabla\mathbf{\Omega}_r+v\Sigma(E)\right) G^\dagger(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E,\mathbf{\Omega},\boldsymbol{r},t)$$
$$=v\iint \mathrm{d}\mathbf{\Omega}'\,\mathrm{d}E'\Sigma(E,\mathbf{\Omega}\rightarrow E',\mathbf{\Omega}')\,G^\dagger(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E',\mathbf{\Omega}',\boldsymbol{r},t) \tag{5}$$

where

$$G^\dagger(E_0,\mathbf{\Omega}_0,\boldsymbol{r}_0,t_0\rightarrow E,\mathbf{\Omega},\boldsymbol{r},t_0)=\delta(E-E_0)\,\delta(\mathbf{\Omega}-\mathbf{\Omega}_0)\,\delta(\boldsymbol{r}-\boldsymbol{r}_0). \tag{6}$$

Following Lewins (1965) we may regard the condition at $t=t_0$ as the response function of a detector in contrast to the source which appears in equation (1).

Using equation (2), multiplying equation (5) by $v_0\Sigma(E_0)T(E_0)$ and integrating over E_0 and $\boldsymbol{r}_0$, we find

$$\left(-\frac{\partial}{\partial t}-v\boldsymbol{\Omega}.\nabla_r+v\Sigma(E)\right)\bar{\nu}(E,\boldsymbol{\Omega},\boldsymbol{r},t\to t_0)$$
$$=v\iint \mathrm{d}\boldsymbol{\Omega}'\,\mathrm{d}E'\,\Sigma(E,\boldsymbol{\Omega}\to E',\boldsymbol{\Omega}')\,\bar{\nu}(E',\boldsymbol{\Omega}',\boldsymbol{r},t\to t_0) \tag{7}$$

subject to

$$\bar{\nu}(E,\boldsymbol{\Omega},\boldsymbol{r},t_0\to t_0)=v\Sigma(E)T(E)\int_{v_0}\mathrm{d}\boldsymbol{r}_0\,\delta(\boldsymbol{r}-\boldsymbol{r}_0). \tag{8}$$

We observe, therefore, that the energy deposition can be calculated directly from an adjoint equation, thereby obviating the need to calculate the flux and perform separately the necessary averaging operations.

At a free surface, the boundary condition on $\bar{\nu}(\ldots)$ follows from the definition of the adjoint, namely

$$\bar{\nu}(E,\boldsymbol{\Omega},\boldsymbol{r}_s,t\to t_0)=0;\qquad \boldsymbol{n}.\boldsymbol{\Omega}<0 \tag{9}$$

where $\boldsymbol{n}$ is an inward pointing normal to the surface at $\boldsymbol{r}_s$.

In the case of the steady state, where a source is continuously emitting particles, the energy flux is defined as

$$\bar{H}(E,\boldsymbol{\Omega},\boldsymbol{r})=\int_{-\infty}^{t_0}\mathrm{d}t\qquad \bar{\nu}(E,\boldsymbol{\Omega},\boldsymbol{r},t\to t_0) \tag{10}$$

and therefore from equations (5) and (6) we find

$$[-\boldsymbol{\Omega}.\nabla_r+\Sigma(E)]\,\bar{H}(E,\boldsymbol{\Omega},\boldsymbol{r})$$
$$=\iint \mathrm{d}E'\,\mathrm{d}\boldsymbol{\Omega}'\,\Sigma(E,\boldsymbol{\Omega}\to E',\boldsymbol{\Omega}')\,\bar{H}(E',\boldsymbol{\Omega}',\boldsymbol{r})+T(E)\Sigma(E)\,U(\boldsymbol{r}) \tag{11}$$

where

$$U(\boldsymbol{r})=\int_{v_0}\mathrm{d}\boldsymbol{r}_0\,\delta(\boldsymbol{r}-\boldsymbol{r}_0). \tag{12}$$

Equation (11) is the basic equation for study, however an alternative measure of the energy deposition, which is useful when the fraction of energy passing through a surface is required is given by

$$\mathrm{H}_s(E_0,\boldsymbol{\Omega}_0,\boldsymbol{r}_0\to\boldsymbol{r})=\int_{-\infty}^{t}\mathrm{d}t_0\int_0^{E_0}\mathrm{d}E v\Sigma(E)T(E)\int_{\boldsymbol{n}.\boldsymbol{\Omega}>0}\mathrm{d}\boldsymbol{\Omega}\boldsymbol{n}.\boldsymbol{\Omega}G(E_0,\boldsymbol{\Omega}_0,\boldsymbol{r}_0,t_0\to E,\boldsymbol{\Omega},\boldsymbol{r},t)$$

then the source term in equation (11) becomes

$$T(E)\,\Sigma(E)\,U(\boldsymbol{r})\,\boldsymbol{n}.\boldsymbol{\Omega}.$$

If we denote the right-hand side of equation (11) by $q(E,\boldsymbol{\Omega},\boldsymbol{r})$ then it may be changed to the following integral form (Case and Zweifel 1967)

$$\bar{H}(E,-\boldsymbol{\Omega},\boldsymbol{r})=\int_v\frac{\mathrm{d}\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\exp\left[-\Sigma(E)|\boldsymbol{r}-\boldsymbol{r}'|\right]q\left(E,\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|},\boldsymbol{r}'\right)\delta_2\left(\boldsymbol{\Omega}.\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\right) \tag{13}$$

which can be further reduced to a set of equations for the angular moments $\bar{H}_{lm}(E,\boldsymbol{r})$ defined by

$$\bar{H}(E,-\boldsymbol{\Omega},\boldsymbol{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\frac{2l+1}{4\pi}\right)^{1/2}\bar{H}_{lm}(E,\boldsymbol{r})\,Y_{lm}(\boldsymbol{\Omega}) \tag{14}$$

where $Y_{lm}(\mathbf{\Omega})$ are the generalized spherical harmonics (Case and Zweifel 1967). These equations are (Williams 1971)

$$\left(\frac{2l+1}{4\pi}\right)^{1/2} \bar{H}_{lm}(E, \boldsymbol{r})$$
$$= \int_v \frac{\mathrm{d}\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^2} \exp\left[-\Sigma(E)|\boldsymbol{r}-\boldsymbol{r}'|\right] Y_{lm}^*(\mathbf{\Omega}_{\mathrm{R}}) \sum_{l'm'} \left(\frac{2l'+1}{4\pi}\right)^{1/2} [4\pi T(E)\Sigma(E)$$
$$\times U(\boldsymbol{r}')\, \delta_{l'0}\, \delta_{mm'} + \int \mathrm{d}E'\, \Sigma_{l'}(E \to E')\, \bar{H}_{l'm'}(E', \boldsymbol{r}')]\, Y_{l'm'}(\mathbf{\Omega}_{\mathrm{R}}) \qquad (15)$$

with

$$\mathbf{\Omega}_{\mathrm{R}} = \frac{(\boldsymbol{r}-\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

and $\Sigma_l(E \to E')$ defined by the expansion

$$\Sigma(E, \mathbf{\Omega} \to E', \mathbf{\Omega}') = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi}\, \Sigma_l(E \to E')\, P_l(\mathbf{\Omega}'.\mathbf{\Omega}). \qquad (16)$$

Thus, for example, in the case of isotropic scattering we have a single equation for $\bar{H}_{0,0}(E, \boldsymbol{r})$ and, for linearly anisotropic scattering, four equations for $\bar{H}_{0,0}$, $\bar{H}_{1,0}$, $H_{1,1}$, $\bar{H}_{1,-1}$. $\bar{H}(E, \mathbf{\Omega}, \boldsymbol{r})$ can then be reconstructed from equation (14). Note, however, that if we are interested in the amount of energy deposited in V_0 by an isotropic source situated at the point $\boldsymbol{r}$, then this is given directly by $\bar{H}_{0,0}(E, \boldsymbol{r})/4\pi$. Equations (15) will prove to be of some value in practical applications of the theory. With minor variations in the interpretation of $G^\dagger$, the method described in this section has been used in radiation damage calculations for the evaluation of deposited energy (Sigmund *et al* 1971). This method has, however, not been used before in neutron transport theory and therefore we shall consider a number of problems of practical interest.

3. Energy deposition by neutrons slowing down in an homogeneous, infinite medium

Consider a source of neutrons in an infinite, homogeneous medium. If the scattering is taken to be elastic and we ignore absorption, equation (11) can be written

$$[-\mathbf{\Omega}.\nabla + \Sigma(E)]\, \bar{H}(E, \mathbf{\Omega}, \boldsymbol{r}) = \frac{2}{1-\alpha} \int_\alpha^1 \mathrm{d}x\, \Sigma[E, \theta(x)]$$
$$\times \int \mathrm{d}\mathbf{\Omega}'\delta[\mu_0 - f(x)]\, \bar{H}(Ex, \mathbf{\Omega}', \boldsymbol{r}) + T(E)\Sigma(E)\, U(\boldsymbol{r}). \qquad (17)$$

The elastic scattering slowing down kernel has been used such that (Williams 1966)

$$\Sigma(E, \mathbf{\Omega} \to E', \mathbf{\Omega}') = \frac{2}{1-\alpha}\frac{1}{E}\, \Sigma[E, \theta(E'/E)]\, \delta(\mathbf{\Omega}.\mathbf{\Omega}' - f(E'/E)), \quad \alpha E < E' < E \qquad (18)$$

where

$$\alpha = [(A-1)/(A+1)]^2$$

and A is the ratio of scatterer to neutron mass. θ is the scattering angle in the centre of mass system and f is the cosine of the scattering angle in the laboratory system. θ and f are related to $x = E'/E$ by

$$\cos\theta(x) = \frac{2}{1-\alpha}\, x - \frac{1+\alpha}{1-\alpha} \qquad (19)$$

$$f(x)=\frac{A+1}{2}x^{1/2}-\frac{A-1}{2}x^{-1/2}. \tag{20}$$

Clearly, for this kernel $\Sigma(E)T(E)=\frac{1}{2}(1-\alpha)E\Sigma_{\mathrm{tr}}(E)$ (see appendix).

As an example, we shall consider the solution of equation (17) in plane symmetry and we shall solve it by introducing the Fourier transform

$$\tilde{\bar{H}}(E, \mu, k)=\int_{-\infty}^{\infty}\mathrm{d}z \exp(-\mathrm{i}kz)\,\bar{H}(E, \mu, z) \tag{21}$$

where $\bar{H}(E, \mu, z)$ is the energy deposited in a slab of material due to a neutron with energy E travelling in the direction μ from the plane z. Applying the transform to equation (17) we obtain

$$[\mathrm{i}\mu k+\Sigma(E)]\,\tilde{\bar{H}}(E, \mu, k)=\frac{2}{1-\alpha}\int_{\alpha}^{1}\mathrm{d}x\,\Sigma[E, \theta(x)]$$
$$\times\int \mathrm{d}\mathbf{\Omega}'\delta[\mu_0-f(x)]\,\tilde{\bar{H}}(Ex, \mathbf{\Omega}', k)+\frac{1-\alpha}{2}E\bar{U}(k)\,\Sigma_{\mathrm{tr}}(E). \tag{22}$$

Expanding $\tilde{\bar{H}}$ in spherical harmonics and introducing the moments

$$\tilde{\bar{H}}_l(E, k)=\int_{-1}^{1}\mathrm{d}\mu\,P_l(\mu)\,\tilde{\bar{H}}(E, \mu, k), \tag{23}$$

equation (22) becomes

$$\tilde{\bar{H}}_m(E, k)=\sum_{l=0}^{\infty}\frac{2l+1}{2}\int_{-1}^{1}\frac{\mathrm{d}\mu P_m(\mu)P_l(\mu)}{\Sigma(E)+\mathrm{i}k\mu}\,\frac{4\pi}{1-\alpha}\int_{\alpha}^{1}\mathrm{d}x\Sigma[E, \theta(x)]P_l(f(x))\,\tilde{\bar{H}}_l(Ex, k)$$
$$+\bar{U}(k)\frac{(1-\alpha)}{2}E\Sigma_{\mathrm{tr}}(E)\int_{-1}^{1}\frac{\mathrm{d}\mu P_m(\mu)}{\Sigma(E)+\mathrm{i}k\mu}. \tag{24}$$

To find the angular distribution we simply return to equation (22) and write it as

$$\tilde{\bar{H}}(E, \mu, k)=\frac{1}{\Sigma(E)+\mathrm{i}\mu k}\Bigg(\frac{1-\alpha}{2}E\Sigma_{\mathrm{tr}}(E)\,\bar{U}(k)$$
$$+\sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu)\,\frac{4\pi}{1-\alpha}\int_{\alpha}^{1}\mathrm{d}x\Sigma[E, \theta(x)]P_l[f(x)]\,\tilde{\bar{H}}_l(Ex, k)\Bigg). \tag{25}$$

Knowing the $\tilde{\bar{H}}_l$ from (20) we can obtain $\tilde{\bar{H}}$ and by inversion $\bar{H}(E, \mu, z)$.

3.1. Energy deposition spatial moments

The coupled set of equations given by (24) is truncated according to the degree of accuracy required in the scattering kernel. In general, even the case of isotropic scattering cannot be solved exactly without further approximation. However, a useful measure of the rate of energy deposition as a function of position can be obtained from the 'mean square energy deposition depth' which we define as

$$\overline{z^2}(E)=\frac{\int_{-\infty}^{\infty}\mathrm{d}z\,z^2\bar{H}_0(E, z)}{\int_{-\infty}^{\infty}\mathrm{d}z\,\bar{H}_0(E, z)} \tag{26}$$

where $\bar{U}(k)$ is set equal to unity thus expressing the deposition of all initial energy.

In terms of the Fourier transform we may write equation (26) in the following more convenient form:

$$\overline{z^2}(E) = -\frac{1}{\tilde{\bar{H}}_0(E,k)} \frac{\mathrm{d}^2}{\mathrm{d}k^2} \tilde{\bar{H}}_0(E,k) \bigg|_{k=0}. \tag{27}$$

If we then expand $\tilde{\bar{H}}_m(E,k)$ as follows:

$$\tilde{\bar{H}}_m(E,k) = H_m^{(0)}(E) + \mathrm{i}kH_m^{(1)}(E) - \frac{k^2}{2} H_m^{(2)}(E) + \dots \tag{28}$$

then it is easily seen that

$$\overline{z^2}(E) = H_0^{(2)}(E)/H_0^{(0)}(E). \tag{29}$$

Expanding equation (24), and collecting up coefficients of k^n, we find the following equations for the moments:

$$\Sigma(E)H_0^{(0)}(E) = \frac{4\pi}{1-\alpha}\int_\alpha^1 \mathrm{d}x\Sigma[E,\theta(x)]H_0^{(0)}(Ex) + (1-\alpha)E\Sigma_{\mathrm{tr}}(E) \tag{30}$$

$$\Sigma(E)H_1^{(1)}(E) = \frac{4\pi}{1-\alpha}\int_\alpha^1 \mathrm{d}x\Sigma[E,\theta(x)]f(x)H_1^{(1)}(Ex) + \tfrac{1}{3}H_0^{(0)}(E) \tag{31}$$

$$\Sigma(E)H_0^{(2)}(E) = \frac{4\pi}{1-\alpha}\int_\alpha^1 \mathrm{d}x\Sigma[E,\theta(x)]H_0^{(2)}(Ex) + 2H_1^{(1)}(E) \tag{32}$$

and hence $\overline{z^2}(E)$.

These equations are also valid for inelastic scattering provided the appropriate forms for the scattering kernels are used. The extension to mixtures is also straightforward.

In the special case where $\Sigma(E,\theta) = \Sigma(E)g(\theta)/4\pi$ and $\Sigma(E) \propto E^{-k}$, we can solve equations (30)–(32) exactly. The value of $\overline{z^2}$ is then

$$\overline{z^2}(E) = \frac{2}{3\Sigma(E)\Sigma_{\mathrm{tr}}(E)} \frac{1}{Z_1(k,\alpha)Z_2(k,\alpha)} \tag{33}$$

where

$$Z_1(k,\alpha) = 1 - \frac{1}{1-\alpha}\int_\alpha^1 \mathrm{d}x\, g(x)x^{2k+1} \tag{34}$$

$$Z_2(k,\alpha) = 1 - \frac{1}{1-\alpha}\int_\alpha^1 \mathrm{d}x\, g(x)f(x)x^{k+1}. \tag{35}$$

For isotropic scattering in the centre of mass system, i.e. $g=1$, these integrals are readily performed. We note that the energy dependence of $\overline{z^2}(E)$ follows that of the cross-section at the initial energy of the neutron.

It is interesting to compare the energy deposition distances with the mean square stopping distance. We can show by the usual procedures that this quantity is given by

$$\overline{z_s^2}(0) = \frac{2}{3\Sigma(E)\Sigma_{\mathrm{tr}}(E)} \frac{1}{Z_1(k-\frac{1}{2},\alpha)Z_2(k-1,\alpha)}. \tag{36}$$

In table 1 values of $\overline{z^2}(E)$ and $\overline{z_s^2}(0)$ are given for $k=0, \frac{1}{2}, 1$ and a range of values of A. We note that $\overline{z_s^2}(0)$ is infinite for $k=0$ since, if the cross-section is constant, particles never actually stop. An important consequence of the comparison is that in all cases

$\overline{z^2}(E) < \overline{z_s{}^2}(0)$. Thus the bulk of the particle's energy is deposited much closer to the source than the actual distribution of slowed down particles would suggest. For example, for $A=2$ and $k=\frac{1}{2}$, the energy deposition length is about 30% less than the slowing down length. A further observation is that $\overline{z^2}$ passes through a minimum as a function of A (generally $A \simeq 2$) and suggests that a maximum rate of energy deposition exists for this value of A. This phenomenon arises from the interaction between the competing processes of energy transfer and angle of deflection. An approximate solution based on isotropic scattering in the laboratory system would therefore not detect this effect.

Table 1. Mean square energy deposition length and mean square stopping distance in units of the mean free path at the initial energy. The upper figure denotes $\Sigma^2(E)\, \overline{z^2}(E)$ and the lower one $\Sigma^2(E)\, \overline{z_s{}^2}(0)$.

A	k = 0	k = $\frac{1}{2}$	k = 1
1	2·222	1·500	1·244
	∞	2·667	1·667
2	2·177	1·488	1·250
	∞	2·250	1·547
3	2·388	1·580	1·312
	∞	2·370	1·592
4	2·657	1·701	1·388
	∞	2·604	1·689
5	2·951	1·835	1·472
	∞	2·880	1·811
10	4·534	2·593	1·955
	∞	4·437	2·548
16	6·501	3·560	2·587
	∞	6·397	3·510
50	17·80	9·187	6·320
	∞	17·69	9·132

3.2. *The spatial variation of the energy deposition*

Although the energy deposition length is a useful measure of the way in which energy is transferred from the particles to the host medium, it is desirable to have a more complete picture of the variation of energy transfer with position. Therefore we return to equation (24) and make the assumption of a cross-section which is independent of energy. Then it is found that $\tilde{\bar{H}}_m(E, k)$ can be written

$$\tilde{\bar{H}}_m(E, k) = \frac{1-\alpha}{2} E\bar{F}_m(k) \tag{37}$$

where the $\bar{F}_m(k)$ are obtained from

$$\bar{F}_m(k) = \sum_{l=0}^{\infty} \frac{2l+1}{2} \int_{-1}^{1} \frac{\mathrm{d}\mu P_m(\mu) P_l(\mu)}{\Sigma(E)+\mathrm{i}k\mu} \frac{\Sigma}{1-\alpha} \int_{\alpha}^{1} \mathrm{d}x\, g(x) P_l(f(x))\, x \bar{F}_l(k)$$
$$+ \Sigma_{\mathrm{tr}} \bar{U}(k) \int_{-1}^{1} \frac{\mathrm{d}\mu P_m(\mu)}{\Sigma(E)+\mathrm{i}k\mu} \tag{38}$$

where we have additionally assumed that $\Sigma(E, \theta) = \Sigma g(x)/4\pi$. Equations (38) are equivalent to a one-speed approximation and therefore amenable to exact solution.

Let us cast the equations into a neater form by defining

$$c_l(\alpha)=\frac{1}{1-\alpha}\int_\alpha^1 \mathrm{d}x\, xg(x)\, P_l(f(x)) \tag{39}$$

and

$$\Delta_{ml}(k)=\Sigma\int_{-1}^1 \frac{\mathrm{d}\mu P_m(\mu)P_l(\mu)}{\Sigma(E)+\mathrm{i}k\mu} \tag{40}$$

when equations (38) become

$$\bar{F}_m(k)=\sum_{l=0}^{\infty}\frac{2l+1}{2}\,\Delta_{ml}(k)\,c_l(\alpha)\,\bar{F}_l(k)+(\Sigma_{\mathrm{tr}}/\Sigma)\,\Delta_{m0}(k)\,\bar{U}(k). \tag{41}$$

To obtain an estimate of the energy deposition, we shall assume that $c_l=0$ for $l>1$. This corresponds to allowing linearly anisotropic scattering; an approximation which is generally acceptable even for neutron–proton slowing down. In that case only two equations, involving $\bar{F}_0$ and $\bar{F}_1$ arise; namely

$$\bar{F}_0(k)=\tfrac{1}{2}c_0\Delta_{00}(k)\bar{F}_0(k)+\tfrac{3}{2}c_1\Delta_{01}(k)\bar{F}_1(k)+(\Sigma_{\mathrm{tr}}/\Sigma)\Delta_{00}(k)\,\bar{U}(k) \tag{42}$$

and

$$\bar{F}_1(k)=\tfrac{1}{2}c_0\Delta_{10}(k)\bar{F}_0(k)+\tfrac{3}{2}c_1\Delta_{11}(k)\bar{F}_1(k)+(\Sigma_{\mathrm{tr}}/\Sigma)\Delta_{10}(k)\,\bar{U}(k). \tag{43}$$

Solving for $\bar{F}_0(k)$ we find

$$\tfrac{1}{2}\bar{F}_0(k)=\frac{\Sigma_{\mathrm{tr}}}{\Sigma}\,\bar{U}(k)\left[\left(1+\frac{3\Sigma^2c_0\bar{\mu}}{k^2}\right)\frac{\Sigma}{k}\tan^{-1}\left(\frac{k}{\Sigma}\right)-\frac{3\bar{\mu}c_0\Sigma^2}{k^2}\right]$$
$$\times\left[1-\frac{3\bar{\mu}c_0(1-c_0)\Sigma^2}{k^2}-\left(c_0-\frac{3\bar{\mu}c_0(1-c_0)\Sigma^2}{k^2}\right)\frac{\Sigma}{k}\tan^{-1}\left(\frac{k}{\Sigma}\right)\right]^{-1} \tag{44}$$

where we have defined $\bar{\mu}$ by $c_1=\bar{\mu}c_0$. From the physical point of view $\bar{\mu}$ is the effective mean cosine of scattering for energy transfer in a collision; it differs from the normal definition of $\bar{\mu}$ as can be seen from the definition of c_l given by equation (39). For isotropic scattering in the centre of mass system, i.e. $g=1$, it is readily seen that

$$c_0(\alpha)=\frac{1+\alpha}{2}=\frac{A^2+1}{(A+1)^2} \tag{45}$$

$$c_1(\alpha)=\frac{4(5A^2+1)}{15A(A+1)^2}=\bar{\mu}c_0(\alpha). \tag{46}$$

To find $F_0(z)$ we must invert the transform given by equation (44), which requires a knowledge of the singularities. Clearly there are branch points at $k=\pm\mathrm{i}\Sigma$ and poles at the zeroes of the denominator. Davison (1946) shows that provided $3\bar{\mu}(c_0-1)<1$, then there are two purely imaginary roots. This condition is obeyed by our values of c_l and we shall designate the roots by $\pm\mathrm{i}\nu$. That is, $\pm\nu$ are the roots of

$$G(\nu)=1+\frac{3\bar{\mu}c_0(1-c_0)}{\nu^2}-\left(1+\frac{3\bar{\mu}(1-c_0)}{\nu^2}\right)\frac{c_0}{2\nu}\ln\left(\frac{1+\nu}{1-\nu}\right) \tag{47}$$

where we have scaled ν in units of Σ.

Following the normal rules of complex integration (Davison 1957, Williams 1971) we can write

$$\tfrac{1}{2}F_0(z)=\int_{-\infty}^{\infty}\mathrm{d}z'\,f(|z-z'|)\,U(z') \tag{48}$$

where

$$f(z)=\Sigma A(c_0,\bar{\mu})\exp(-\nu|z|)+\frac{\Sigma}{2}\int_0^1\frac{d\mu}{\mu}g(c_0,\bar{\mu},\mu)\exp(-\Sigma|z|/\mu). \tag{49}$$

We have defined

$$A(c_0,\bar{\mu})=\frac{\nu(1-\nu^2)}{c_0\{\nu^2-1+c_0+3\bar{\mu}(1-c_0)[3-c_0-3(1-c_0)(1-\bar{\mu}c_0)/\nu^2]\}} \tag{50}$$

and

$$\frac{1}{g(c_0,\bar{\mu},\mu)}=\left(\frac{\pi c_0\mu}{2}[1+3\bar{\mu}(1-c_0)\mu^2]\right)^2$$
$$+\left[1+3\bar{\mu}c_0(1-c_0)\mu^2-[1+3\bar{\mu}(1-c_0)\mu^2]\frac{c_0}{2}\mu\ln\left(\frac{1+\mu}{1-\mu}\right)\right]^2. \tag{51}$$

Using the point-to-plane transformation (Weinberg and Wigner 1958)

$$f(r)=-\frac{1}{2\pi r}\left.\frac{df(z)}{dz}\right|_{z=r} \tag{52}$$

we find

$$\tfrac{1}{2}F_0(0)=4\pi\int_0^\infty dr r^2\,U(r)f(r) \tag{53}$$

where

$$f(r)=\frac{\nu\Sigma}{2\pi r}A(c_0,\bar{\mu})\exp(-\nu r)+\frac{\Sigma^2}{4\pi r}\int_0^1\frac{d\mu}{\mu^2}g(c_0,\bar{\mu},\mu)\exp(-\Sigma r/\mu)$$

and we have taken the source to be at the origin.

In table 2 we show values of ν versus the mass number of the struck nucleus. Also shown is the value of ν for $\bar{\mu}=0$, i.e. assuming isotropic scattering in the laboratory system. It is clear from this table that the value of ν is close to unity for the light elements and this indicates a rapid deposition of energy with position; notice also that ν has a maximum for $A=2$, a fact on which we shall comment further below. Since c_0 acts as a fictitious ratio of scattering to total cross-section its small value places the solution well into the transport regime. Thus it is most unlikely that a diffusion approximation would be of any value for assessing the behaviour of $f(z)$. We shall present further evidence for this assertion below.

Equations (52) and (54) enable us to write an expression for the rate of energy deposition from an isotropic point source in an infinite medium, viz:

$$\tfrac{1}{2}\bar{H}_0(E,r)=\frac{1-\alpha}{2}Ef(r). \tag{54}$$

Table 2. Values of ν versus the mass number of the struck nucleus. ν is the root of equation (47). c_0 and $\bar{\mu}$ are defined by equations (45) and (46).

A	c_0	$\bar{\mu}$	ν	$\nu(\bar{\mu}=0)$
1	0·5	0·8	0·77607	0·95750
2	$0{\cdot}5\dot{5}$	0·56	0·79675	0·93272
3	0·625	$0{\cdot}40\dot{8}$	0·78123	0·89064
4	0·68	0·31764706	0·75743	0·84707
5	$0{\cdot}72\dot{2}$	0·25846154	0·73171	0·80634
10	0·83471074	0·13227723	0·61968	0·65625
16	0·88927336	0·08307393	0·52978	0·55033
50	0·96155325	0·02665814	0·33005	0·33436

Now it is of considerable interest to calculate the fraction of energy given up in the sphere of radius R surrounding the source since this has some bearing on the neutron heating of laser-compressed deuterium–tritium spheres (Beynon and Constantine 1977). Thus we define the energy deposited per source neutron from equation (53) by

$$D(E, R)=\frac{1-\alpha}{2} E 4\pi \int_0^R \mathrm{d}r\, r^2 f(r) \tag{55}$$

where $U(r)=0$ for $r>R$.

Performing the integrations over r leads to

$$D(E, R)=\frac{1-\alpha}{2} E\left(\frac{2A(c_0, \bar{\mu})}{\nu}[1-(1+\nu R)\exp(-\nu R)]\right.$$
$$\left.+\int_0^1 \mathrm{d}\mu\, g(c_0, \bar{\mu}, \mu)\{1-(\Sigma R/\mu)\exp(-\Sigma R/\mu)\}\right) \tag{56}$$

which we write as

$$D(E, R)=D(E, R)_{\mathrm{asy}}+D(E, R)_{\mathrm{trans}}. \tag{57}$$

The subscripts 'asy' and 'trans' denote the contributions to the total energy deposited from the asymptotic and integral transient components of the solution, respectively. We should emphasize at this point that our values for $D(E, R)$ will differ from those of Beynon and Constantine for three reasons: (i) we have not considered a mixture of scattering species, (ii) we have not included inelastic scattering events and (iii) our 'sphere' is not bare but embedded in an infinite medium. None of these restrictions is likely to have a significant effect on the results and we shall eliminate restriction (iii) entirely in the next section.

To conform to the notation of Beynon and Constantine we choose $\Sigma R=0{\cdot}2203\ \rho R$ and evaluate $D(E, R)$ for $E=14$ MeV and a range of values of ρR. The results are shown in tables 3 and 4. It is particularly important to note the ratio of D_{asy}/D; thus for $\rho R<2$,

Table 3. Deposited energy in spherical region of radius R, density ρ, with units of MeV/source neutron; ρR is in g cm^{-2}.

		$A=1$					$A=2$		
ρR	D_{asy}	D_{tr}	D	D_{asy}/D	ρR	D_{asy}	D_{tr}	D	D_{asy}/D
0·2	0·004861	0·2958	0·3007	0·0162	0·2	0·005265	0·2667	0·2720	0·0194
0·4	0·01901	0·5753	0·5943	0·0320	0·4	0·02058	0·5159	0·5365	0·0384
0·6	0·04181	0·8354	0·8772	0·0477	0·6	0·04523	0·7519	0·7971	0·0565
0·8	0·07267	1·080	1·152	0·0631	0·8	0·07857	0·9748	1·0533	0·0746
1·0	0·1110	1·309	1·420	0·0782	1·0	0·1200	1·185	1·305	0·0920
1·2	0·1563	1·525	1·681	0·0930	1·2	0·1688	1·385	1·554	0·109
1·4	0·2081	1·728	1·936	0·107	1·4	0·2246	1·574	1·798	0·125
1·6	0·2658	1·920	2·186	0·122	1·6	0·2867	1·753	2·039	0·141
1·8	0·3290	2·101	2·430	0·135	1·8	0·3547	1·922	2·277	0·156
2	0·3972	2·272	2·669	0·149	2	0·4280	2·083	2·511	0·170
3	0·8008	2·998	3·799	0·211	3	0·8604	2·772	3·633	0·237
4	1·278	3·552	4·830	0·265	4	1·369	3·306	4·675	0·293
5	1·795	3·977	5·772	0·311	5	1·919	3·722	5·641	0·340
6	2·328	4·307	6·635	0·351	6	2·482	4·047	6·529	0·380
7	2·860	4·562	7·422	0·385	7	3·042	4·302	7·344	0·414
8	3·377	4·762	8·139	0·415	8	3·583	4·501	8·084	0·443
9	3·871	4·918	8·789	0·440	9	4·098	4·659	8·757	0·468
10	4·336	5·040	9·376	0·462	10	4·581	4·783	9·364	0·489

Table 3 *continued*

		$A=3$					$A=4$		
ρR	D_{asy}	D_{tr}	D	D_{asy}/D	ρR	D_{asy}	D_{tr}	D	D_{asy}/D
0·2	0·005441	0·2257	0·2311	0·0234	0·2	0·005452	0·1928	0·1982	0·0272
0·4	0·02127	0·4375	0·4587	0·0458	0·4	0·02133	0·3742	0·3955	0·0539
0·6	0·04679	0·6388	0·6856	0·0682	0·6	0·04694	0·5469	0·5940	0·0790
0·8	0·08131	0·8297	0·9110	0·0892	0·8	0·08164	0·7109	0·7925	0·103
1·0	0·1242	1·011	1·135	0·109	1·0	0·1248	0·8666	0·9914	0·126
1·2	0·1749	1·182	1·357	0·129	1·2	0·1758	1·015	1·015	0·148
1·4	0·2327	1·346	1·578	0·147	1·4	0·2341	1·155	1·389	0·169
1·6	0·2972	1·500	1·798	0·165	1·6	0·2992	1·289	1·588	0·188
1·8	0·3678	1·648	2·015	0·183	1·8	0·3705	1·416	1·786	0·207
2	0·4441	1·787	2·231	0·199	2	0·4477	1·537	1·985	0·226
3	0·8946	2·390	3·285	0·272	3	0·9048	2·059	2·964	0·305
4	1·427	2·860	4·287	0·333	4	1·447	2·468	3·915	0·370
5	2·003	3·228	5·231	0·383	5	2·038	2·789	4·827	0·422
6	2·596	3·517	6·113	0·425	6	2·650	3·041	5·690	0·466
7	3·187	3·744	6·931	0·460	7	3·261	3·239	6·500	0·502
8	3·761	3·923	7·684	0·489	8	3·859	3·395	7·254	0·532
9	4·308	4·065	8·373	0·514	9	4·432	3·519	7·951	0·557
10	4·824	4·176	9·000	0·536	10	4·975	3·617	8·592	0·579

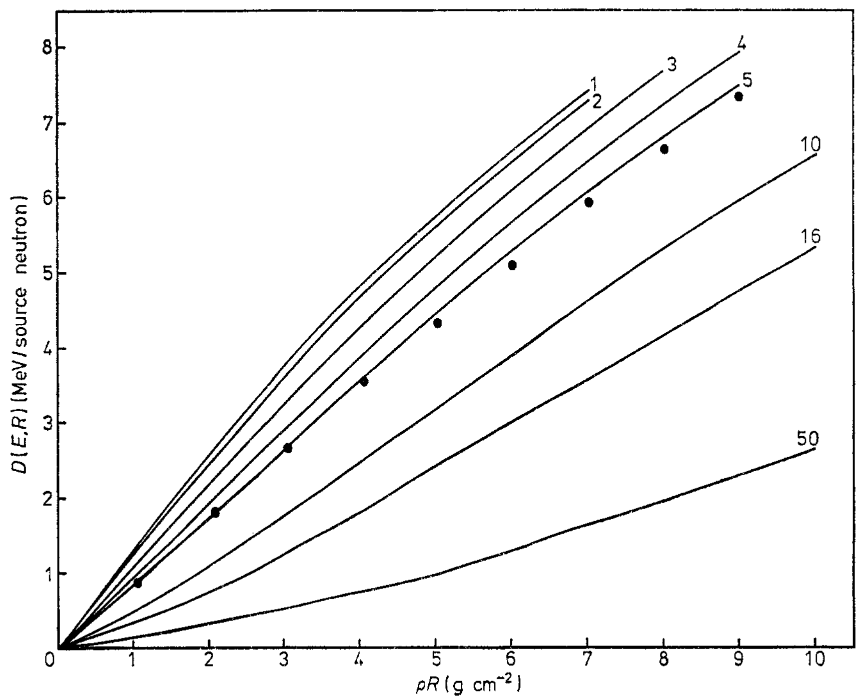

Figure 1. Energy deposition (MeV/source neutron) in a sphere of radius R, density ρ resulting from an isotropic point source of 14 MeV neutrons at the origin. The number on each curve denotes the mass number of the moderator. ●, results of Beynon and Constantine (1977) for deuterium–tritium spheres.

Table 4. Deposited energy in spherical region of radius R, density ρ, with units of MeV/source neutron; ρR is in g cm^{-2}.

		$A=5$					$A=10$		
ρR	D_{asy}	D_{tr}	D	D_{asy}/D	ρR	D_{asy}	D_{tr}	D	D_{asy}/D
0·2	0·005352	0·1674	0·1728	0·0289	0·2	0·004380	0·09957	0·1039	0·0421
0·4	0·02095	0·3251	0·3460	0·0607	0·4	0·01721	0·1932	0·2104	0·0818
0·6	0·04615	0·4753	0·5215	0·0885	0·6	0·03802	0·3031	0·3411	0·111
0·8	0·08031	0·6180	0·6983	0·115	0·8	0·06638	0·3669	0·4332	0·153
1	0·1229	0·7536	0·8765	0·140	1	0·1019	0·4471	0·5490	0·186
1·2	0·1732	0·8825	1·056	0·164	1·2	0·1441	0·5233	0·6674	0·216
1·4	0·2308	1·005	1·236	0·187	1·4	0·1926	0·5956	0·7882	0·244
1·6	0·2952	1·122	1·417	0·208	1·6	0·2471	0·6643	0·9114	0·271
1·8	0·3659	1·232	1·598	0·229	1·8	0·3072	0·7296	1·037	0·296
2	0·4423	1·338	1·780	0·249	2	0·3726	0·7917	1·164	0·320
3	0·8971	1·794	2·691	0·333	3	0·7675	1·059	1·827	0·420
4	1·440	2·150	3·590	0·401	4	1·250	1·268	2·518	0·496
5	2·034	2·430	4·464	0·456	5	1·792	1·431	3·223	0·556
6	2·653	2·650	5·303	0·500	6	2·371	1·558	3·929	0·603
7	3·276	2·824	6·100	0·537	7	2·967	1·659	4·626	0·641
8	3·887	2·961	6·848	0·568	8	3·567	1·737	5·304	0·672
9	4·477	3·069	7·546	0·593	9	4·161	1·799	5·960	0·698
10	5·039	3·154	8·193	0·615	10	4·740	1·848	6·588	0·719

		$A=16$					$A=50$		
ρR	D_{asy}	D_{tr}	D	D_{asy}/D	ρR	D_{asy}	D_{tr}	D	D_{asy}/D
0·2	0·003398	0·06661	0·0700	0·0485	0·2	0·001420	0·02307	0·02449	0·0580
0·4	0·01338	0·1291	0·1425	0·0939	0·4	0·005624	0·04462	0·05024	0·112
0·6	0·02965	0·1885	0·2181	0·136	0·6	0·01253	0·06500	0·07753	0·162
0·8	0·05191	0·2447	0·2966	0·175	0·8	0·02207	0·08424	0·1060	0·208
1	0·07986	0·2979	0·3778	0·211	1	0·03415	0·1024	0·1366	0·2501
1·2	0·1132	0·3484	0·4616	0·245	1·2	0·04870	0·1196	0·1683	0·289
1·4	0·1518	0·3963	0·5481	0·277	1·4	0·06565	0·1358	0·2014	0·326
1·6	0·1952	0·4417	0·6369	0·306	1·6	0·08493	0·1511	0·2361	0·360
1·8	0·2433	0·4848	0·7281	0·334	1·8	0·1065	0·1657	0·2722	0·391
2	0·2959	0·5257	0·8216	0·360	2	0·1302	0·1794	0·3096	0·420
3	0·6171	0·7013	1·318	0·468	3	0·2793	0·2382	0·5175	0·540
4	1·018	0·8375	1·856	0·549	4	0·4735	0·2833	0·7568	0·626
5	1·476	0·9435	2·420	0·610	5	0·7057	0·3182	1·024	0·689
6	1·975	1·026	3·001	0·658	6	0·9700	0·3452	1·315	0·738
7	2·500	1·091	3·591	0·696	7	1·260	0·3662	1·626	0·775
8	3·039	1·142	4·181	0·727	8	1·571	0·3826	1·954	0·804
9	3·583	1·182	4·765	0·752	9	1·900	0·3954	2·295	0·828
10	4·123	1·213	5·336	0·773	10	2·241	0·4054	2·646	0·847

the asymptotic part of the solution is less than 15% of the total. This is a clear indication of the failure of diffusion theory and suggests the mandatory use of transport theoretic methods for solving these problems. In figure 1 we compare some of our results with those obtained by Beynon and Constantine for a point source in a finite sphere (their figure 2). While the results are not directly comparable on a one-to-one basis, the general agreement is encouraging and indicates that our basic assumptions are sound.

Table 5. Deposited energy in spherical region of radius R, density ρ in the isotropic approximation. Units are MeV/source neutron and ρR is in g cm^{-2}.

ρR	A 1	2	3	4	5	10	16	50
0·2	0·3107	0·2769	0·2344	0·2008	0·1747	0·1047	0·0703	0·0245
0·4	0·6205	0·6539	0·4717	0·4051	0·3533	0·2130	0·1436	0·0504
0·6	0·9318	0·8356	0·7130	0·6141	0·5370	0·3261	0·2207	0·0779
0·8	1·242	1·117	0·9567	0·8265	0·7244	0·4431	0·3012	0·1069
1	1·551	1·399	1·202	1·0416	0·9152	0·5638	0·3848	0·1375
1·2	1·858	1·679	1·449	1·259	1·109	0·6879	0·4714	0·1696
1·4	2·161	1·959	1·696	1·478	1·305	0·8151	0·5609	0·2031
1·6	2·463	2·238	1·943	1·698	1·502	0·9454	0·6532	0·2383
1·8	2·760	2·514	2·189	1·919	1·702	1·078	0·7482	0·2749
2	3·054	2·787	2·436	2·140	1·902	1·214	0·8456	0·3130
3	4·454	4·109	3·643	3·242	2·912	1·921	1·366	0·5244
4	5·729	5·335	4·791	4·312	3·911	2·661	1·929	0·7683
5	6·872	6·452	5·861	5·329	4·876	3·413	2·521	1·041
6	7·883	7·456	6·843	6·280	5·791	4·164	3·130	1·337
7	8·771	8·349	7·733	7·157	6·649	4·901	3·745	1·654
8	9·545	9·138	8·534	7·959	7·443	5·614	4·358	1·988
9	10·21	9·829	9·248	8·685	8·172	6·298	4·963	2·335
10	10·79	10·43	9·881	9·338	8·837	6·948	5·553	2·692

In table 5, for completeness, we give the values of $D(E, R)$ in the case of $\bar{\mu}=0$, i.e. isotropic scattering in the laboratory system. Clearly, this approximation is not to be relied upon for energy deposition problems, there being errors of the order of 100% for low mass numbers.

4. Energy deposition from a uniform source in a finite sphere

In order to consider the effect of a finite medium on the energy deposition, it is necessary to include the appropriate boundary conditions into the problem. Thus we return to the set of integral equations (15). For simplicity, we assume a spherical body of radius R in which $U(\boldsymbol{r})$, the deposition region, is a function of the radial coordinate only, i.e. $U(\boldsymbol{r})=U(r)$. It can then be shown that the integral equations reduce to

$$r\bar{H}_l(E, r)=\sum_{l'=0}^{\infty}\frac{2l'+1}{2}\int_0^R \mathrm{d}r'r'\, K_{ll'}(r, r', E)\left(\int_0^\infty \mathrm{d}E'\Sigma_{l'}(E\rightarrow E')\bar{H}_{l'}(E', r')\right.$$
$$\left.+\frac{1-\alpha}{2}E\Sigma_{\mathrm{tr}}(E)\, U(r')\,\delta_{l',0}\right) \tag{58}$$

where

$$K_{ll'}(r, r', E)=\int_{|r-r'|}^{r+r'}\frac{\mathrm{d}t}{t}\exp\left(-\Sigma(E)t\right)P_l\left(\frac{r^2+t^2-r'^2}{2rt}\right)P_{l'}\left(\frac{r^2-t^2-r'^2}{2r't}\right) \tag{59}$$

If now we use the elastic scattering kernel with constant cross-section, we can write equation (58) in the following one-speed form:

$$rF_l(r)=\sum_{l'=0}^{\infty}\frac{2l'+1}{2}\int_0^R \mathrm{d}r'r'\, K_{ll'}(r, r')\left[c_{l'}(\alpha)F_{l'}(r')+2U(r')\,\delta_{l',0}\right] \tag{60}$$

where distances are measured in units of Σ^{-1}.

Clearly, the energy deposited in the region defined by U, by an isotropic, spherically symmetric shell source of radius r, will be

$$\frac{\Sigma_{\mathrm{tr}}}{\Sigma}\frac{1-\alpha}{2}E\tfrac{1}{2}F_0(r).$$

If the source is uniformly distributed over the volume R then the total energy deposited will be

$$D(E,R)=\frac{1-\alpha}{2}E\frac{\Sigma_{\mathrm{tr}}}{\Sigma}2\pi\int_0^R \mathrm{d}r\,r^2 F_0(r). \tag{61}$$

We shall further assume that we are interested in the energy deposited in the complete body, therefore $U=1$.

In order to obtain an estimate of the value of $D(E, R)$ we shall solve equation (60) by a variational method. However, to be consistent with the work in the previous section the scattering will be taken to be linearly anisotropic in the laboratory system and isotropic in the centre-of-mass system.

After some algebra, we can write equation (60) as follows.

$$G_0(r)=\tfrac{1}{2}\int_{-R}^{R}\mathrm{d}r'\,[c_0G_0(r')+2r']\,M_{00}(r,r')+\frac{3c_1}{2}\int_{-R}^{R}\mathrm{d}r'G_1(r')M_{01}(r,r') \tag{62}$$

$$G_1(r)=\frac{3c_1}{2}\int_{-R}^{R}\mathrm{d}r'G_1(r')M_{11}(r,r')+\tfrac{1}{2}\int_{-R}^{R}\mathrm{d}r'\,[c_0G_0(r')+2r']M_{10}(r,r') \tag{63}$$

where $G_n(r)=rF_n(r)$ and $M_{ij}(r, r')$ are related to the kernels $K_{ij}(r, r')$. We have, in fact, used a transformation which reduces the spherical problem in $(0, R)$ to an equivalent slab one in $(-R, R)$, thereby reducing the complexities of the kernels. However, it should be stressed that the equations (62) and (63) are not simply related to the real slab problem as they are for isotropic scattering (Davison 1957). We have merely introduced a convenient mathematical artifice to aid the calculation. The kernels M_{ij} are given by

$$M_{00}(r,r')=E_1(|r-r'|) \tag{64}$$

$$M_{01}(r,r')=-M_{10}(r,r')=\frac{|r-r'|}{(r-r')}E_2(|r-r'|)-\frac{E_3(|r-r'|)}{r'} \tag{65}$$

$$M_{11}(r,r')=\frac{1}{4rr'}\,[(r+r')^2E_3(|r-r'|)-(1+|r-r'|)\exp(-|r-r'|)]. \tag{66}$$

Equations (62) and (63) are further changed in form by writing

$$H_{ij}(r,r')=\tfrac{1}{2}c_0M_{ij}(r,r') \tag{67}$$

$$f_0(r)=c_0^{-1/2}\,[c_0G_0(r)+2r] \tag{68}$$

$$f_1(r)=c_0^{1/2}\,G_1(r) \tag{69}$$

$$Q(r)=2r/c_0^{1/2} \tag{70}$$

when we can write

$$f_0(r)=\int_{-R}^{R}\mathrm{d}r'f_0(r')H_{00}(r,r')+\beta\int_{-R}^{R}\mathrm{d}r'f_1(r')H_{01}(r,r')+Q(r) \tag{71}$$

$$f_1(r)=\beta\int_{-R}^{R}\mathrm{d}r'f_1(r')H_{11}(r,r')+\int_{-R}^{R}\mathrm{d}r'f_0(r')H_{10}(r,r') \tag{72}$$

where $\beta=3c_1/2c_0=3\bar{\mu}/2$.

Now it is readily shown that the functional

$$\mathscr{F}[\tilde{f},\tilde{f}^{\dagger}]=(\tilde{f}^{\dagger},Q)+(Q^{\dagger},\tilde{f})-(\tilde{f}^{\dagger},H\tilde{f}) \tag{73}$$

is stationary about

$$F_{st}=(Q^{\dagger},f)=\int_{-R}^{R}\mathrm{d}r\ Q^{\dagger}(r)f_0(r). \tag{74}$$

In writing the functional we have introduced a matrix operator notation such that f is the column vector of f_0, f_1.

Also equations (71) and (72) are written

$$Hf=Q \tag{75}$$

and $f^{\dagger}$ is the solution of the equation adjoint to (75). Now if we take $Q^{\dagger}(r)=2r/c_0^{1/2}$, the stationary value of the functional is related to $D(E, R)$ as follows

$$D(E,R)=\frac{1-\alpha}{4}\pi\left(F_{st}-\frac{8R^3}{3c_0}\right). \tag{76}$$

Moreover, examination of the adjoint equation shows that $f_0^{\dagger}=f_0$ and $f_1^{\dagger}=-\beta f_1$. Therefore it is not necessary to guess an adjoint trial function.

Multiplying out the functional (73) we obtain

$$F=4/c_0^{1/2}(r,f_0)-(f_0,\overline{1-H_{00}}f_0)-2\beta(f_1,H_{10}f_0)+\beta(f_1,\overline{1-\beta H_{11}}f_1). \tag{77}$$

Let us now choose trial functions

$$\tilde{f}_0(r)=Br \tag{78}$$

$$I_1(r)=Cr^2 \tag{79}$$

and optimize F by setting $\partial F/\partial B=\partial F/\partial C=0$. After some algebra we can write

$$D(E,R)=\frac{1-\alpha}{2}EV\left(\frac{M_0-\bar{\mu}\Delta}{1-c_0(M_0-\bar{\mu}\Delta)}\right) \tag{80}$$

where $V=4\pi R^3/3$ and

$$\Delta=\frac{45}{128}\frac{c_0M_1^2}{1-\bar{\mu}c_0M_2}. \tag{81}$$

The integrals M_i are given by

$$M_0=\frac{3}{4R^3}\int_{-R}^{R}\mathrm{d}r\ r\int_{-R}^{R}\mathrm{d}r'r'\ M_{00}(r,r') \tag{82}$$

$$M_1=\frac{2}{R^4}\int_{-R}^{R}\mathrm{d}r\ r^2\int_{-R}^{R}\mathrm{d}r'r'\ M_{10}(r,r') \tag{83}$$

$$M_2=\frac{15}{8R^5}\int_{-R}^{R}\mathrm{d}r\ r^2\int_{-R}^{R}\mathrm{d}r'r'^2\ M_{11}(r,r'). \tag{84}$$

Using equations (64), (65) and (66) for $M_{ij}(r,r')$ we can evaluate the M_i to find the following results

$$M_0=1-\frac{3}{8R^3}[2R^2-1+(1+2R)\exp(-2R)] \tag{85}$$

$$M_1=\frac{4}{3R}\left(1-\frac{3}{2R^3}\left[R^2-1+(R+1)^2\exp(-2R)\right]\right). \tag{86}$$

$$M_2=\tfrac{1}{2}\left(1-\frac{15}{4R^5}\left[\tfrac{1}{2}R^4-R^2+\tfrac{9}{4}-(R+\tfrac{3}{2})(R^2+2R+\tfrac{3}{2})\exp(-2R)\right]\right). \tag{87}$$

Since $\Delta>0$ for all R and α we may conclude that D(anisotropic) < D(isotropic): a physically reasonable result. In the special case of isotropic scattering where $\bar{\mu}=0$, we can write D as

$$D(E,R)=\frac{1-\alpha}{2}EV\frac{M_0}{1-c_0M_0} \tag{88}$$

where M_0 is the well-known collision probability for a sphere. In table 6 we present values of $D(E,R)/V$ for isotropic scattering for a range of mass numbers. In table 7, the same quantity is given using the more exact equation (80) which includes linearly anisotropic scattering. Table 8 is the result of using the so-called transport approximation in which the isotropic formalism of equation (88) is employed but with a modified value

Table 6. Total heating in MeV per source neutron in sphere of radius R, density ρ in the isotropic approximation with uniformly distributed source. Units of ρR are g cm^{-2}.

	A							
ρR	1	2	3	4	5	10	16	50
0·5	0·568	0·507	0·430	0·369	0·321	0·193	0·130	0·0454
1	1·114	0·999	0·853	0·734	0·642	0·389	0·263	0·0925
1·5	1·639	1·476	1·266	1·095	0·960	0·588	0·399	0·141
2	2·140	1·935	1·669	1·449	1·275	0·788	0·538	0·192
2·5	2·618	2·376	2·060	1·796	1·586	0·989	0·678	0·243
3	3·073	2·800	2·438	2·135	1·892	1·191	0·821	0·296
3·5	3·505	3·205	2·804	2·466	2·191	1·392	0·964	0·351
4	3·915	3·592	3·157	2·786	2·484	1·592	1·108	0·406
4·5	4·304	3·961	3·500	3·097	2·769	1·791	1·253	0·462
5	4·672	4·313	3·823	3·398	3·047	1·989	1·398	0·519
5·5	5·020	4·647	4·136	3·689	3·318	2·184	1·542	0·577
6	5·349	4·966	4·435	3·969	3·580	2·376	1·686	0·635

Table 7. Total heating in MeV/source neutron in a sphere of radius R, density ρ for linearly anisotropic scattering with uniformly distributed source. Units of ρR are g cm^{-2}.

	A							
ρR	1	2	3	4	5	10	16	50
0·5	0·565	0·505	0·429	0·368	0·321	0·193	0·130	0·0454
1	1·103	0·992	0·847	0·730	0·639	0·388	0·263	0·0925
1·5	1·616	1·460	1·255	1·086	0·954	0·585	0·398	0·141
2	2·104	1·909	1·650	1·435	1·265	0·784	0·536	0·192
2·5	2·567	2·340	2·033	1·776	1·571	0·983	0·676	0·243
3	3·007	2·752	2·403	2·109	1·871	1·183	0·817	0·296
3·5	3·425	3·146	2·761	2·432	2·165	1·382	0·959	0·350
4	3·821	3·523	3·105	2·746	2·452	1·580	1·102	0·405
4·5	4·196	3·882	3·437	3·051	2·733	1·776	1·246	0·461
5	4·552	4·224	3·755	3·346	3·005	1·971	1·389	0·518
5·5	4·889	4·550	4·061	3·631	3·271	2·164	1·532	0·576
6	5·209	4·861	4·355	3·906	3·528	2·354	1·675	0·634

of c_0 given by

$$c_0' = \frac{(1-\bar{\mu})c_0}{1-\bar{\mu}c_0}. \tag{89}$$

Comparison of tables 7 and 8 shows that, for this type of problem, the use of c_0' results in severe underestimates of the energy deposition. Indeed, comparing tables 6 and 7 we note that the effect of anisotropic scattering on D is relatively small, leading to around a 2% correction. This is in marked contrast to the point source problem of the previous section where the errors were much larger. The reason for this behaviour is due to the flat spatial neutron distribution in the finite sphere thus causing leakage to have a smaller effect. This can be seen more clearly from table 9 where we give the 'collision probability' $M_0 - \bar{\mu}\Delta$ for various values of A and compare it with the case for $\bar{\mu}=0$ ($A=\infty$). The value of $\bar{\mu}\Delta$ is always very small, being of the order of 2% of M_0. It appears therefore to be acceptable to use the isotropic scattering approximation for calculations of this type. Figure 2 compares our results with those of Beynon and Constantine (1977) which, considering the differences in scattering model, can be considered as satisfactory agreement.

Table 8. Total heating in MeV/ source neutron in sphere of radius R, density ρ with modified isotropic scattering and uniformly distributed source. Units of ρR are g cm^{-2}.

ρR	A 1	2	3	4	5	10	16	50
0·5	0·553	0·499	0·426	0·366	0·320	0·193	0·130	0·0454
1	1·058	0·968	0·835	0·724	0·635	0·388	0·263	0·0925
1·5	1·520	1·409	1·228	1·072	0·945	0·585	0·398	0·141
2	1·942	1·821	1·603	1·409	1·249	0·783	0·536	0·191
2·5	2·328	2·207	1·961	1·735	1·546	0·981	0·676	0·243
3	2·681	2·568	2·301	2·049	1·835	1·178	0·817	0·296
3·5	3·004	2·905	2·624	2·351	2·115	1·375	0·959	0·350
4	3·300	3·219	2·930	2·641	2·387	1·570	1·101	0·406
4·5	3·572	3·512	3·221	2·919	2·649	1·763	1·244	0·462
5	3·822	3·786	3·495	3·185	2·902	1·954	1·387	0·519
5·5	4·051	4·041	3·755	3·439	3·146	2·142	1·529	0·576
6	4·263	4·280	4·000	3·682	3·381	2·327	1·670	0·635

Table 9. The effective collision probability of a sphere of radius R, density ρ for various degrees of anisotropy. $A=\infty$ corresponds to the isotropic case M_0.

ρR	A 1	2	3	4	5	10	16	50	∞
0·5	0·077569	0·077659	0·077715	0·077755	0·077785	0·077862	0·077899	0·077948	0·077974
1	0·14611	0·14641	0·14660	0·14673	0·14683	0·14709	0·14722	0·14738	0·14747
1·5	0·20698	0·20755	0·20791	0·20816	0·20835	0·20884	0·20908	0·20939	0·20955
2	0·26127	0·26214	0·26268	0·26306	0·26335	0·26409	0·26444	0·26490	0·26515
2·5	0·30991	0·31106	0·31178	0·31229	0·31267	0·31365	0·31412	0·31473	0·31506
3	0·35364	0·35505	0·35595	0·35657	0·35704	0·35824	0·35881	0·35957	0·35996
3·5	0·39309	0·39476	0·39579	0·39652	0·39707	0·39846	0·39913	0·40000	0·40047
4	0·42881	0·43068	0·43184	0·43267	0·43327	0·43484	0·43559	0·43657	0·43709
4·5	0·46123	0·46328	0·46456	0·46546	0·46612	0·46783	0·46864	0·46971	0·47028
5	0·49074	0·49295	0·49431	0·49528	0·49599	0·49781	0·49868	0·49982	0·50042
5·5	0·51769	0·52002	0·52145	0·52247	0·52331	0·52513	0·52604	0·52723	0·52786
6	0·54234	0·54478	0·54627	0·54732	0·54809	0·55008	0·55102	0·55225	0·55290

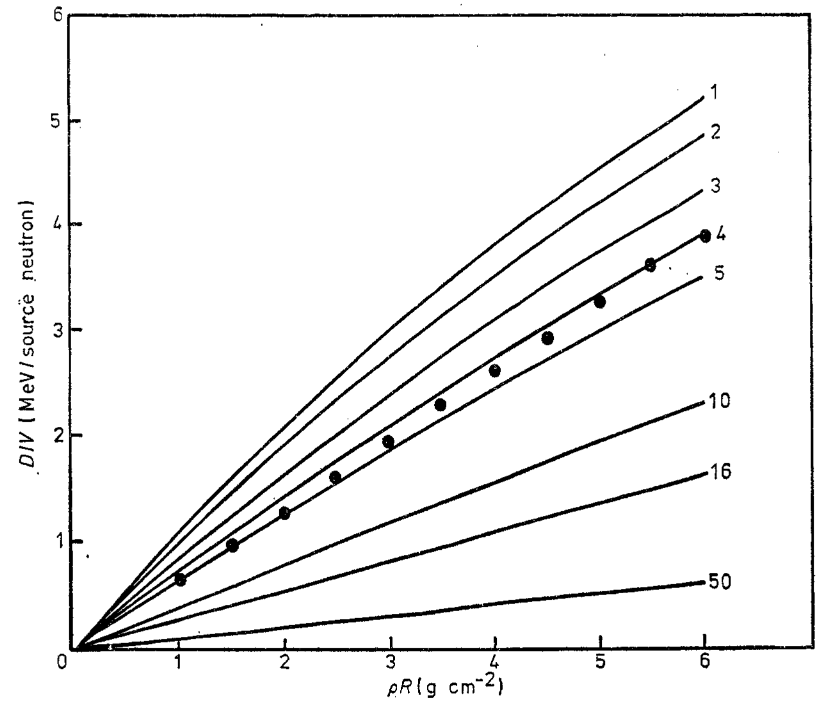

Figure 2. Energy deposition (MeV/source neutron) in a sphere of radius R, density ρ resulting from a uniformly distributed source of 14 MeV neutrons. The number on each curve denotes the mass number of the moderator. ●, results of Beynon and Constantine (1977) for deuterium–tritium spheres.

5. Summary and conclusions

The role of the adjoint Boltzmann equation has been explored in some detail and from it we have shown how the energy deposition rate in a volume of moderating material can be calculated directly. The adjoint equation has been converted to a set of coupled integral equations, a form which is convenient for analytical and numerical solution. For the purpose of exposition we take the scattering to be elastic, although this is by no means essential. Then, considering an infinite, homogeneous medium we employ Fourier transforms to solve the integral equations. Without further approximation to the scattering cross-section a complete inversion of the Fourier transform cannot be obtained. However, a set of exact coupled equations can be deduced from which the mean square energy deposition length $\overline{z^2}(E)$ can be obtained for arbitrary variation of cross-section. For a cross-section that behaves as E^{-k} we obtain solutions and tabulate $\overline{z^2}$. This is compared with the mean square distance for a neutron to reach zero energy $\overline{z_s{}^2}(0)$ and it is noted that $\overline{z^2}(E) < \overline{z_s{}^1}(0)$ for all k and A, thereby indicating that the energy is deposited much nearer to the source than the distribution of number density would suggest.

To demonstrate the spatial variation of the energy deposition, we assume a cross-section independent of energy and linearly anisotropic scattering. This enables the Fourier inversion to be performed and hence we obtain the amount of energy deposited in a shell of radius r and thickness dr due to a point 14 MeV source at the origin. By integration we calculate the energy deposited in a sphere of radius R about the source.

It is particularly instructive to study the analytical form of the expression for the deposited energy since it is composed of two parts: that due to the asymptotic solution and that due to the integral transient. In all practical cases considered the contribution from the integral transient is of the same order, or very much greater than that due to the asymptotic term. This result implies that the use of diffusion theory for such problems is not to be recommended. In addition, we also see that the assumption of isotropic scattering leads to substantial errors of the order of 100% in the deposited energy for low mass number moderators $A \leqslant 5$. For the thermonuclear problem this is clearly a significant factor to be borne in mind.

A further problem is examined, namely that of a uniformly distributed source of 14 MeV neutrons in a finite sphere of radius R. Linear anisotropy is assumed and the resulting integral equations are cast into variational form. It is shown that the extremum of this functional is directly related to the heating rate. After introducing trial functions for the flux and current we can cast the heating rate into a form which involves collision probabilities. These are rather more general than the usual collision probabilities since they account for anisotropy. However, numerical calculations show that the effect of anisotropy in this problem is small, being of the order of 2%. In this problem and in that of the point source, we have compared our results with those of Beynon and Constantine (1977). Agreement is not perfect for a number of reasons: first, we have assumed a single species medium, and secondly, we have neglected the variation of cross-section with energy and the inelastic scattering. However, the inclusion of inelastic events has the result of effectively increasing the mass number of the scattering medium, and, indeed, we note that the results of Beynon and Constantine can be explained on the basis of a medium with a mass number of between 4 and 5. Our equations can, of course, be integrated numerically with the appropriate scattering data but these simple calculations indicate the usefulness of preliminary analytical study.

Appendix

To calculate the average energy lost by a particle in a collision, we note that the amount of energy deposited by particles of energy E_0, which have slowed down to energy E, is (Williams 1976)

$$W(E)=\int_E^{E_0} \mathrm{d}E'\phi(E') \int_0^{E'} \Sigma(E' \to E'')(E'-E'')\,\mathrm{d}E'' \tag{A1}$$

where $\phi(E)$ is the particle flux. We see therefore that the cross-section for energy transfer $\Sigma(E)T(E)$ is given by

$$\Sigma(E)T(E)=\int_0^E \Sigma(E \to E')(E-E')\,\mathrm{d}E'. \tag{A2}$$

Using the cross-section

$$\Sigma(E \to E')=\frac{4\pi\Sigma(E, \theta(E'/E))}{E'(1-\alpha)}; \quad \alpha E < E' < E \tag{A3}$$

where

$$\cos\theta\left(\frac{E'}{E}\right)=\frac{2}{1-\alpha}\frac{E'}{E}-\frac{1+\alpha}{1-\alpha} \tag{A4}$$

we readily find that

$$\Sigma(E)T(E)=\frac{1-\alpha}{2}E\Sigma_{\mathrm{tr}}(E) \tag{A5}$$

where the transport cross-section in the CM system is defined by

$$\Sigma_{\mathrm{tr}}(E)=2\pi\int_0^\pi \Sigma(E,\,\theta)\,(1-\cos\,\theta)\,\sin\,\theta\,\mathrm{d}\theta. \tag{A6}$$

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