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NEUTRON DIFFUSION FORMULAE FOR HOMOGENEOUS, AXIALLY SYMMETRIC, ANISOTROPIC MEDIA, FOR MONTE CARLO APPLICATIONS

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ABSTRACT

Probability distributions and mean values relating to the diffusion of monoenergetic neutrons in a homogeneous but anisotropic medium are derived, as a basis for studies of Monte Carlo calculations of radial and axial diffusion coefficients in heterogeneous systems. The generalization of diffusion theory for application to anisotropic media is also discussed.

CONTENTS

1. INTRODUCTION

Axial gas coolant channels in a reactor core introduce neutron streaming problems. In an approximately axially symmetric configuration, the usual procedure is to replace the actual core, for macroscopic analysis, by an equivalent homogeneous medium with different radial and axial diffusion coefficients in each neutron energy group. Unless simplifying assumptions are made and the gas channels are of comparatively simple shape, the calculation of the effective diffusion coefficients by neutron transport theory is difficult.

An alternative method is to use a Monte Carlo calculation, as a probabilistic model already exists in the formulation of a neutron's collision history in terms of mean free paths, scattering cross-sections, etc. It is sufficient to consider monoenergetic neutrons, so that collision mechanics are greatly simplified. To formulate a Monte Carlo approach, it is necessary to have the appropriate relations between diffusion coefficients and various statistics relating to a neutron's flight path in a homogeneous, axially symmetric, anisotropic medium. It is also natural to enquire into the formulation of diffusion theory in such a medium, e.g., the relation between diffusion coefficient and the angular distribution of the mean path lengths in various directions. This subject is considered first to establish the concept of a homogeneous anisotropic medium for neutron diffusion.

2. DIFFUSION THEORY AND ANISOTROPIC MEDIA

In axially symmetric geometries, the radial and axial diffusion coefficients D_R and D_Z are defined by Fick's Law for neutron currents,

$$J_R = -D_R \frac{\partial \Phi}{\partial R} \quad ; \quad J_Z = -D_Z \frac{\partial \Phi}{\partial z} \tag{1}$$

In spherical co-ordinates r, θ, φ, the neutron current in the r direction is therefore

$$\begin{aligned} J_r &= -D_R \frac{\partial \Phi}{\partial R} \sin\theta - D_Z \frac{\partial \Phi}{\partial z} \cos\theta \\ &= -\frac{\partial \Phi}{\partial r}\{D_R \sin^2\theta + D_Z \cos^2\theta\} - \frac{1}{r}\frac{\partial \Phi}{\partial \theta}\{D_R - D_Z\}\sin\theta\cos\theta \end{aligned} \tag{2}$$

It follows that Fick's Law is valid only for the symmetry axes.

For (1) to hold in a homogeneous medium, the mean free paths for neutrons travelling in the R and Z directions must be different. In general, $l(\Omega)$, the mean free path for neutrons travelling in the Ω direction, must be a continuous function of Ω. With the particular symmetry here considered,

$$l(\bar{\Omega}) = l(\theta) = l(\pi - \theta) = l(\pi + \theta) \tag{3}$$

Mean free path is now a vector quantity, and the scalar mean free path, which corresponds to the unambiguous "mean free path" in an isotropic medium, is

$$\bar{l} = \frac{1}{4\pi}\int_{\Omega} l(\Omega)\, d(\Omega) = \int_0^{\frac{\pi}{2}} l(\theta)\sin\theta\, d\theta \tag{4}$$

To proceed further requires consideration of the vector neutron flux $\varphi(\bar{r}, \bar{\Omega}) = v\, n(\bar{r}, \bar{\Omega})$ at point $\bar{r}$.

2.1 Isotropic Scattering

In a purely scattering medium, the scattering rate per unit volume, $\Phi \Sigma_s$, defines the cross–section Σ_s. For spherically symmetric scattering, the emission density $Q(\bar{r})$ is

$$Q(\bar{r}) = \frac{1}{4\pi} \Sigma_s \, \Phi(\bar{r}) \tag{5}$$

The basic equation for $\varphi(\bar{r}, \bar{\Omega})$ is

$$\varphi(\bar{r}, \bar{\Omega}) = \int_0^\infty Q(\bar{r} - R\bar{\Omega}) \exp(-R/l_s(\theta)) \, dR \tag{6}$$

Diffusion theory corresponds to taking the Taylor's expansion.

$$\Phi(\bar{r} - R\bar{\Omega}) = \Phi(\bar{r}) - R \sin\theta \cos\varphi \frac{\partial \Phi(r)}{\partial r} - R \sin\theta \sin\varphi \frac{\partial \Phi(\bar{r})}{\partial y} - R \cos\theta \frac{\partial \Phi(r)}{\partial z} \tag{7}$$

in equation (6). Thus the vector neutron flux is

$$\varphi(\bar{r}, \bar{\Omega}) = \frac{\Sigma_s}{4\pi} \left[l_s(\theta) \Phi(\bar{r}) - l_s^2(\theta) \left\{ \sin\theta \cos\varphi \frac{\partial \Phi(\bar{r})}{\partial x} + \sin\theta \sin\varphi \frac{\partial \Phi(\bar{r})}{\partial y} + \cos\theta \frac{\partial \Phi(\bar{r})}{\partial z} \right\} \right] \tag{8}$$

In the absence of flux gradients, the angular flux distribution is not uniform unless $l_s(\theta)$ is constant.

Since

$$\Phi(\bar{r}) = \int_0^{2\pi} \int_0^{\pi} \varphi(\bar{r}, \theta, \varphi) \sin\theta \, d\theta \, d\varphi \tag{9}$$

equation (8) gives, as might be expected,

$$\Sigma_s = 1/\bar{l}_s \tag{10}$$

The neutron currents in the R and Z directions are

$$J_Z(\bar{r}) = \int_0^{2\pi} \int_0^{\pi} \varphi(\bar{r}, \theta, \varphi) \cos\theta \sin\theta \, d\theta \, d\varphi = -\frac{\Sigma_s}{2} \frac{\partial \Phi}{\partial z} \int_0^{\pi} l_s^2(\theta) \sin\theta \cos^2\theta \, d\theta \tag{11}$$

$$J_R(\bar{r}) = \int_0^{2\pi} \int_0^{\pi} \varphi(\bar{r}, \theta, \varphi) \sin^2\theta \sin\varphi \, d\theta \, d\varphi = -\frac{\Sigma_s}{4} \frac{\partial \Phi}{\partial R} \int_0^{\pi} l_s^2(\theta) \sin^3\theta \, d\theta \tag{12}$$

The radial and axial diffusion coefficients are therefore

$$D_R = \frac{\Sigma_s}{2} \int_0^{\frac{\pi}{2}} l_s^2(\theta) \sin^3\theta \, d\theta \tag{13}$$

$$D_Z = \Sigma_s \int_0^{\frac{\pi}{2}} l_s^2(\theta) \sin\theta \cos^2\theta \, d\theta \tag{14}$$

2.2 Anisotropic Scattering and Capture

Assume that $l_a(\theta)/l_s(\theta)$ is independent of θ.

If $\Sigma = \Sigma_a + \Sigma_s = 1/\bar{l}$

let

$$\alpha = \Sigma_a/\Sigma, \quad \beta = \Sigma_s/\Sigma \tag{15}$$

The transport equation for a source free medium can be written now as

$$\bar{\Omega} \cdot \text{grad}\, \varphi(\bar{r}, \bar{\Omega}) + (\alpha + \beta)\, \varphi(\bar{r}, \bar{\Omega})/l(\bar{\Omega})$$

$$= \int_{\Omega'} \frac{\beta}{l(\bar{\Omega}')} \, p(\bar{\Omega}' \to \bar{\Omega}) \, \varphi(\bar{r}, \bar{\Omega}') \, d\Omega' \tag{16}$$

where $p(\bar{\Omega}' \to \bar{\Omega})\, d\Omega$ is the probability of a neutron being scattered from direction $\bar{\Omega}'$ to $d\Omega$ about $\bar{\Omega}$.

From (8) the form of the vector flux must be

$$\varphi(\bar{r}, \bar{\Omega}) = A(\bar{r})\, l(\theta) + l^2(\theta) \{ B(\bar{r}) \sin\theta\cos\varphi + C(\bar{r}) \sin\theta \sin\varphi + E(\bar{r}) \cos\theta \} \tag{17}$$

i.e.,

$$\left.\begin{aligned} \Phi(\bar{r}) &= 4\pi\, \bar{l}\, A(\bar{r}) \\ J_x(\bar{r}) &= \pi B(\bar{r}) \int_0^{\pi} l^2(\theta) \sin^3\theta \, d\theta \\ J_y(\bar{r}) &= \pi C(\bar{r}) \int_0^{\pi} l^2(\theta) \sin^3\theta \, d\theta \\ J_z(\bar{r}) &= 2\pi D(\bar{r}) \int_0^{\pi} l^2(\theta) \sin\theta\cos^2\theta \, d\theta \end{aligned}\right\} \tag{18}$$

Integration of (16) over the unit sphere gives

$$4\pi A \alpha + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = 0 \tag{19}$$

Assuming that

$$p(\bar{\Omega}' \to \bar{\Omega}) = \frac{1}{4\pi}(1 + 3\bar{\mu}(\bar{\Omega}' . \bar{\Omega})) \tag{20}$$

where $\bar{\mu}$ is the mean cosine of the scattering angle, substituting into (16), multiplying by the direction cosines of the unit vector $\bar{\Omega}$ and integrating over the unit sphere gives

$$\frac{dA}{d(x,y,z)} = -(B, C, E)\,[\alpha + \beta(1-\bar{\mu})] \tag{21}$$

The diffusion coefficients are therefore

$$\left.\begin{aligned} Dx = Dy &= -\Sigma^2 \int_0^{\frac{\pi}{2}} 1^2(\theta)\sin^3\theta\, d\theta \,/\, 2(\Sigma - \bar{\mu}\Sigma_s) \\ D_Z &= -\Sigma^2 \int_0^{\frac{\pi}{2}} 1^2(\theta)\sin\theta\cos^2\theta\, d\theta \,/\, (\Sigma - \bar{\mu}\Sigma_s) \end{aligned}\right\} \tag{22}$$

These relations and the particular examples in (13) and (14), represent the slight generalization of elementary diffusion theory to allow for anisotropy.

3. DIFFUSION OF MONOENERGETIC NEUTRONS FROM A POINT SOURCE

The time dependent equation for neutron density,

$$v D_R \frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial n}{\partial R}\right) + v D_Z \frac{\partial^2 n}{\partial z^2} - v\Sigma_a n = \frac{\partial n}{\partial t} \tag{23}$$

has the solution

$$n(R,z,t) = \frac{N_o (D_R/D_Z)^{\frac{1}{2}}}{(4\pi D_R vt)^{\frac{3}{2}}} \exp\left\{-\Sigma_a vt - \frac{R^2}{4D_R vt} - \frac{z^2}{4D_Z vt}\right\} \tag{24}$$

corresponding to the release of N_o neutrons at the origin at $t = o$. Hence the probability $P(R, |z| \, t)\, dR\, d|z|$ that a neutron released at the origin will be in the volume element $2\pi R\, dR\, d|z|$ at time t is

$$P(R, |z|, t = \frac{4\pi R (D_R/D_Z)^{\frac{1}{2}}}{(4\pi D_R vt)^{\frac{3}{2}}} \exp\left\{-\Sigma_a vt - \frac{R^2}{4D_R vt} - \frac{z^2}{4D_Z vt}\right\} \tag{25}$$

The probability distribution of the radial distance travelled in time t is

$$P(R, t) = \int_0^\infty P(R, |z|, t)\, d\,|z|$$

$$= \frac{R}{2 D_R vt} \exp \{ -\Sigma_a vt - \frac{R^2}{4 D_R vt} \} \tag{26}$$

The mean radial distance travelled in time t is

$$\overline{R}(t) = \int_0^\infty R\,P(R,t)\,dR = e^{-\Sigma_a vt} (\pi D_R vt)^{\frac{1}{2}} \tag{27}$$

and the mean square radial distance is

$$\overline{R^2(t)} = \int_0^\infty R^2 P(R, t)\,dR = 4 D_R vt\ e^{-\Sigma_a vt} \tag{28}$$

In a similar way the probability distribution for the axial distance travelled in time t is

$$P(|z|,t) = (\pi D_Z vt)^{-\frac{1}{2}} \exp \{ -\Sigma_a vt - \frac{z^2}{4 D_Z vt} \} \tag{29}$$

so

$$\overline{|z|(t)} = 2 (D_Z vt/\pi)^{\frac{1}{2}}\ e^{-\Sigma_a vt} \tag{30}$$

$$\overline{z^2(t)} = 2 D_Z vt\ e^{-\Sigma_a vt} \tag{31}$$

The mean square distance travelled from the origin in time t is

$$\overline{r^2(t)} = \int_0^\infty \int_0^\infty (R^2 + z^2)\, P(R, |z|, t)\; dR\, d(z)$$

$$= \overline{R^2(t)} + \overline{z^2(t)}$$

$$= 2\, vt\, (D_Z + 2 D_R)\ e^{-\Sigma_a vt} \tag{32}$$

Also

$$\overline{r(t)} = \int_0^\infty \int_0^\infty (R^2 + z^2)^{\frac{1}{2}}\, P(R, |z|, t)\; dR\, d\,|z|$$

but this integration is best perfomed using spherical co-ordinates ($\theta = 0$ corresponding to the axis of symmetry Z).

The probability $P(r, \theta, t)\, d r\, d\theta$ that a neutron will be in the annulus $2\pi r^2 \sin\theta\, d\theta\, dr$ at time t is from (24)

$$P(r,\theta, t) = \frac{2\pi r^2 (D_R/D_Z)^{\frac{1}{2}}}{(4\pi D_R vt)^{\frac{3}{2}}} \sin\theta \exp\left\{-\Sigma_a vt - \frac{r^2 \sin^2\theta}{4 D_R vt} - \frac{r^2\cos^2\theta}{4 D_R vt}\right\} dr\, d\theta \qquad (33)$$

Integrating over all angles gives the probability of a neutron being in dr at r, t as

$$P(r, t) = r \exp\left\{-\Sigma_a vt - \frac{r^2}{4 D_R vt}\right\} \operatorname{erf}\left\{\frac{r\sqrt{\frac{D_R}{D_Z} - 1}}{\sqrt{4 vt D_R}}\right\} / 2 vt (D_R^2 - D_R D_Z)^{\frac{1}{2}} \qquad (34)$$

Thus

$$\overline{r(t)} = 2 \left(\frac{D_R^2 vt / D_Z \pi}{\frac{D_R}{D_Z} - 1}\right)^{\frac{1}{2}} e^{-\Sigma_a vt} \left\{\tan^{-1}\left(\sqrt{\frac{D_R}{D_Z} - 1}\right) + \frac{D_Z}{D_R}\sqrt{\frac{D_R}{D_Z} - 1}\right\} \qquad (35)$$

For $D_R = D_Z = D$

$$\overline{r(t)} = 4 (D\, vt)/\pi)^{\frac{1}{2}} e^{-\Sigma_a vt} \qquad (36)$$

The probability that a neutron will be captured in $2\pi R\, dR\, d|z|$ at R, $|z|$ is

$$P_c(R, |z|)\, dR\, d|z| = \Sigma_a v \int_0^\infty P(R, |z|, t)\, dt$$

From (25)

$$P_c(R, |z|) = \Sigma_a R \exp\left\{-\Sigma_a\left(\frac{R^2}{D_R} + \frac{z^2}{D_Z}\right)\right\} / (R^2 D_R D_Z + z^2 D_R^2)^{\frac{1}{2}} \qquad (37)$$

from which it follows that

$$P_c(R) = \frac{\Sigma_a}{D_R} R K_o (R\sqrt{\Sigma_a/D_R}) \qquad (38)$$

involving a modified Bessel function of the second kind, and

$$P_c(|z|) = (\Sigma_a/D_Z)^{\frac{1}{2}} \exp(-z\sqrt{\Sigma_a/D_Z}) \qquad (39)$$

The mean distances and mean square distances to capture can be obtained by the use of these distributions, but use can also be made of the following relation. If X is a measure of location and

$$P_c(X, t) = \Sigma_a v P(X, t)$$

then by integration

$$\overline{X_c^m} = \int_0^\infty \int_0^\infty \Sigma_a v \; X^m \; P(X,t) \, dX \, dt$$

$$\text{i.e.,} \quad \overline{X_c^m} = \Sigma_a v \int_0^\infty \overline{X^m(t)} \; dt \tag{40}$$

Using (40)

$$\overline{R_c} = \Sigma_a v \int_0^\infty \overline{R(t)} \, dt = \frac{\pi}{2} \sqrt{D_R/\Sigma_a} \tag{41}$$

etc. In this way, it is found that

$$\overline{R_c^2} = 4 \, D_R / \Sigma_a \tag{42}$$

$$\overline{|z_c|} = \sqrt{D_Z/\Sigma_a} \tag{43}$$

$$\overline{z_c^2} = 2 \, D_Z/\Sigma_a \tag{44}$$

$$\overline{r_c} = \left(\frac{D_R^2}{\Sigma_a (D_R - D_Z)} \right)^{\frac{1}{2}} \left\{ \tan^{-1} \sqrt{\frac{D_R}{D_Z} - 1} + \frac{D_Z}{D_R} \sqrt{\frac{D_R}{D_Z} - 1} \right\} \tag{45}$$

$$\overline{r_c^2} = 2(D_Z + 2 D_R) / \Sigma_a \tag{46}$$

Formulae (42) (44) and (46) give the usual interpretation of radial and axial diffusion lengths in terms of the mean square distances to capture.

4. CONCLUSION

This collection of formulae is intended to provide a fairly complete coverage of the implications of the anisotropic diffusion equation for homogeneous media. By following neutrons through heterogeneous media and estimating statistics of the flight path, these formulae should enable the validity and magnitude of equivalent axial and radial diffusion coefficients to be determined.

5. NOTATION

D	Diffusion coefficient
J	Neutron current
l	A mean free path
n	Neutron density
$P(x_i, x_j, t)\, dx_i\, dx_j$	The probability that a neutron released at the origin of co–ordinates ($x_i = x_j = 0$) at time $t = 0$ will be in $dx_i\, dx_j$ at x_i, x_j and time t
$P_c(x_i, x_j)\, dx_i\, dx_j$	The probability that a neutron will be captured in $dx_i\, dx_j$ at x_i, x_j.
$Q(\bar{r})$	Emission density – neutrons per unit solid angle
$\bar{r}$	Position vector
r, θ, φ	Spherical co–ordinates
R, z	Cylindrical co–ordinates
x, y, z	Cartesian co–ordinates
v	Neutron velocity
$\overline{x_i^m(t)}$	The mean value of the m'th moment of the distance travelled by a neutron in the x_i direction in time t
$\overline{x_{iC}^m}$	The mean value of the m'th moment of the distance travelled to capture in the x_i direction
Σ	Macroscopic cross–section
$\bar{\Omega}$	Unit directional vector
$d\Omega$	Solid angle about $\bar{\Omega}$
$\varphi(\bar{r}, \bar{\Omega})$	Vector neutron flux
$\Phi(\bar{r})$	Scalar neutron flux

Suffixes

a	Absorption
s	Scattering
c	Capture
R	Radial (R) direction
Z	Axial (z) direction