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SPATIAL AVERAGES
OF
DIFFUSION COEFFICIENTS

by

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SPATIAL AVERAGES OF DIFFUSION COEFFICIENTS

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April 27, 1962

Spatial Averages of Diffusion Coefficients

Raymond L. Murray

Introduction

The method of forming the average macroscopic absorption cross section for a set of regions is unambiguous, using the criterion of equal total absorption for the system in its heterogeneous and homogeneous states. Thus

$$\bar{\Sigma}_a = \frac{\sum_i \int \phi_i \Sigma_{ai} dV_i}{\sum_i \int \phi_i dV_i} = \frac{V_1 \bar{\phi}_1 \Sigma_{a1} + V_2 \bar{\phi}_2 \Sigma_{a2} + \dots}{V_1 \bar{\phi}_1 + V_2 \bar{\phi}_2 + \dots}$$

The correct criterion for the case of transport cross section Σ_t or diffusion coefficient D is not obvious, since these parameters refer to neutron flow, not absorption. Analysis is presented for a simple geometry for which the answer may be found exactly, and various logical criteria are tested against the known result.

Formulation of Problem

A typical situation is a two region plane system, as sketched,

This configuration may be viewed in various ways:

- (a) A plane half-cell in a heterogeneous reactor
- (b) Half of core and reflector of a reactor
- (c) Two layers of a multiple reflector
- (d) Two layers of a radiation shield

The problem is to replace the layers by a single region with composite or average properties, as shown below.

The possible criteria that may be used to equate systems are listed.

1. Both in steady state
2. Total absorption is same
3. Total leakage is same
4. Total supply is same
5. Total neutrons in systems the same
6. External boundary conditions same

Items 2, 3, and 4 together imply 1.

Depending on the system, there are several ways neutrons are supplied. These are:

(a) Distributed sources, uniform or otherwise

(b) Surface sources

(c) Surface currents from adjacent media

Combinations of these are also possible.

Analysis of Simplest Arrangement

In order to have a standard for comparison, the simplest possible system was selected, with $S_0 = 0$, $S_1 = 0$, $k_0 = 0$, $k_1 = 0$, $\Sigma_{a0} = 0$, $\Sigma_{a1} = 0$. Assume an isotropic surface source at $z = 0$, injecting $S/2$ neutrons per second per cm^2 , with voids for $z < 0$ and $z > W$. Thus at $z = W$, the flux was taken to vanish.

The differential equations with zero source and absorption are

$$D_0 \phi_0'' = 0$$

$$D_1 \phi_1'' = 0$$

The solutions of which are

$$\phi_0 = A_0 + C_0 z$$

$$\phi_1 = A_1 + C_1 z$$

with four arbitrary constants present.

Four boundary conditions imposed are:

$$j_0(0) = S/2$$

$$\phi_0(W) = \phi_1(W)$$

$$j_0(w) = j_1(w)$$

$$\phi_1(W) = 0$$

Application of these and normalization to $S/2 = 1$, yields the arbitrary constants

$$A_0 = \frac{W - w}{D_1} + \frac{w}{D_0}$$

$$C_0 = -\frac{1}{D_0}$$

$$A_1 = \frac{W}{D_1}$$

$$C_1 = -\frac{1}{D_1}$$

A schematic plot of the flux distributions is given.

The uniform slab problem is considerably simpler, with solution as follows:

$$D\phi'' = 0$$

$$\phi = A + Cz$$

$$j(0) = S/2 = 1$$

$$\phi(W) = 0$$

Thus $A = \frac{W}{D}$

$$C = -\frac{1}{D}$$

The plot is

For each of the systems $j(W) = 1$, as readily verified. The steady state is guaranteed by the fact that the entering and escaping currents are both unity in a non-absorbing medium.

In order to be completely equivalent, the number of

neutrons in the systems should be equal, which is the same as saying that the total flux is the same.

$$\int_0^W \phi dz = \int_0^w \phi_0 dz + \int_w^W \phi_1 dz$$

Inserting

$$\phi_0 = \frac{W - w}{D_1} + \frac{w}{D_0} - \frac{z}{D_0}$$

$$\phi_1 = \frac{W - z}{D_1}$$

$$\phi = \frac{W - z}{D}$$

and integrating, we find the required value of D , appearing in

$$\frac{1}{D} = \frac{1 - (w/W)^2}{D_1} + \frac{(w/W)^2}{D_0}$$

Note that if $w \rightarrow 0$, $D = D_1$; if $w \rightarrow W$, $D = D_0$; if $D_1 = D_0$, $D = D_0$ or D_1 , all of which are correct limiting cases.

Let $D/D_1 \equiv y$; $w/W = g$, the fractional volume occupied by material 0, and $D_0/D_1 = x$, the ratio of diffusion coefficients of the two media. In this notation, the "correct" form is

$$y = \left(1 - g^2 + \frac{g^2}{x} \right)^{-1} \quad (C)$$

The limiting cases are: $g = 0$, $y = 1$; $g = 1$, $y = x$; $x = 1$, $y = 1$. We now consider several definitions of averages in

current use.

1. Flux and volume weighted transport cross section:

Let

$$\Sigma_t = \frac{\int \phi_0 \Sigma_{t0} dV_0 + \int \phi_1 \Sigma_{t1} dV_1}{\int \phi_0 dV_0 + \int \phi_1 dV_1}$$

or since $D_i = \frac{1}{\Sigma_{ti}}$

$$\frac{1}{D} = \frac{\frac{\bar{\phi}_0 V_0}{D_0} + \frac{\bar{\phi}_1 V_1}{D_1}}{\bar{\phi}_0 V_0 + \bar{\phi}_1 V_1}$$

The average fluxes are $\bar{\phi}_0 = \frac{W-w}{D_1} + \frac{w}{2D_0}$; $\bar{\phi}_1 = \frac{W-w}{2D_1}$ and with

$$D_0 = \frac{\frac{W^2 - w^2}{D_1} + \frac{w^2}{D_0}}{\left(\frac{W-w}{D_1} + \frac{w}{D_0}\right)^2}$$

$$V_0 = w,$$

$$V_1 = W - w,$$

or

$$y = \frac{1 - g^2 + \frac{g^2}{x}}{\left(1 - g + \frac{g}{x}\right)^2} \quad (1)$$

2. Flux and volume weighted diffusion coefficients:

$$D = \frac{\int \phi_0 D_0 dV_0 + \int \phi_1 D_1 dV_1}{\int \phi_0 dV_0 + \int \phi_1 dV_1}$$

or

$$D = \frac{D_0 \bar{\phi}_0 V_0 + D_1 \bar{\phi}_1 V_1}{\bar{\phi}_0 V_0 + \bar{\phi}_1 V_1}$$

Hence

$$D = \frac{2 \frac{D_0 w}{D_1} (W - w) + W^2 - 2Ww + 2w^2}{\frac{W^2 - w^2}{D_1} + \frac{w^2}{D_0}}$$

or

$$y = \frac{1 - 2g + 2g^2 + 2xg(1 - g)}{1 - g^2 + \frac{g^2}{x}} \quad (2)$$

3. Perturbation theory, $(\nabla\phi)^2$ weighting: two choices of flux are available.

(a) Let the reference flux be that for uniform mixture, $\phi = \frac{W}{D} - \frac{z}{D}$, with $\nabla\phi = -\frac{1}{D}$, $(\nabla\phi)^2 = \frac{1}{D^2}$. Let perturbations of diffusion coefficient from the value D be

$$\delta D_0 = D_0 - D, \quad \delta D_1 = D_1 - D$$

and require that the reactivity due to the change is zero

$$\int (\nabla\phi)^2 \delta D dV = 0$$

or

$$\int \delta D dV = 0$$

Inserting and simplifying,

$$D = \frac{W}{W} D_0 + \frac{W - w}{W} D_1$$

which is simple volume fraction weighting. Thus,

$$y = gx + 1 - g \quad (3a)$$

(b) Alternately, one may assume that the undisturbed flux is as in the two region system

$$(\nabla \phi_0)^2 = \frac{1}{D_0^2}, \quad (\nabla \phi_1)^2 = \frac{1}{D_1^2}$$

$$\int \frac{\delta D_0}{D_0^2} dV_0 + \int \frac{\delta D_1}{D_1^2} dV_1 = 0$$

where

$$\delta D_0 = D - D_0, \quad \delta D_1 = D - D_1$$

Inserting,

$$D = \frac{\frac{W}{D_0} + \frac{W - w}{D_1}}{\frac{W}{D_0^2} + \frac{W - w}{D_1^2}}$$

or

$$y = \frac{1 - g + \frac{g}{x}}{1 - g + \frac{g}{x^2}} \quad (3b)$$

Calculations.

The predictions of $D/D_1 = y$ as it depends on $w/W = g$ and $x = D_0/D_1$ by methods (1), (2), (3a), and (3b) are compared with the correct case (C). The results expressed as a fractional error $\frac{y}{y_C} - 1$ are shown in the accompanying figures. As must be the case, if $D_0 = D_1$, $x = 1$, then y is the correct value y_C , and the error $y/y_C - 1$ is zero.

The most surprising result is that none of the methods yields good results over the range of values of x and g .

An assesment of relative accuracy can be made for the physical situation of most probable interest, a cell with $w \ll W$, and composed of a metal-water mixture, where $D_0 > D_1$. For example, if the fuel plate is principally iron, $\sigma_s \simeq 11$ barns, $N = 0.085$, $\Sigma_t \simeq \Sigma_s = 0.93$, $D_0 = 1/\Sigma_t = 0.35$; with a water gap, $\lambda_t \simeq 0.5$, $D_1 \simeq 0.16$. Thus $x \simeq 2$. Suppose further that $w = 0.020$ in., $W = 0.040$ in., $g = 0.5$. The values of fractional error from the graphs are listed for the four cases.

Case	$\frac{y}{yC} - 1$
1	0.36
2	0.50
3a	0.32
3b	0.05

Although Case (3b) appears to be the best, it is seen to be accidental in view of the variations of graphs in that case. Generally speaking, it may be concluded that for g values in the range 0.25 to 4.0, that case (1), based on flux and volume weighted transport cross section, appears to be the best.

Extensions of this study should include systems with

absorption and internal sources. It must be noted, however, that the usual cell model is not a good vehicle for test, in view of the fact that the zero slope centerline boundary conditions admit no net current from the system, hence the diffusion coefficient is not meaningful. It would be necessary to set up a multi-layer system in a large region of the core through which a general gradient exists.

Case 1
Flux and Volume Weighted
Transport Cross Section

Case 2
Flux and Volume Weighted
Diffusion Coefficients

Case 3a
Perturbation Theory
Flow as in Mixture

Case 36
Perturbation Theory
Flux as in Two Regions

$\eta - 1$