

## “CHAPTER 5” DIFFUSION THEORY

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### ABSTRACT

In many nuclear reactor physics texts (excluding Elmer Lewis’s recent text however), “Chapter 5” is dedicated to diffusion theory; hence, the title of this submission. Here, we will investigate analytical solutions to the most basic form of the monoenergetic 1D stationary diffusion equation. The intuitive approach taken radically departs from the usual method of solving the diffusion equation. In particular, we consider a general setting such that the method accommodates *all* solutions to the monoenergetic diffusion equations in 1D plane and curvilinear geometries. This is not your father’s diffusion theory and, for this reason, we anticipate it will eventually become the classroom standard.

**KEYWORDS:** Neutron diffusion equation, Monoenergetic analytical solutions, Consistency, Curvilinear geometries

### 1. INTRODUCTION

With titles of

*The Diffusion of Neutrons*  
*Diffusion Theory: The Homogeneous One-velocity Reactor*  
*The Diffusion of Neutrons*  
*The One-Speed Diffusion Theory Model,*

Chapters 5 in such well-known reactor physics texts of Edlund [1], Meghreblian and Holmes [2], Larmarsh [3] and Duderstadt and Hamilton [4] have been the primary source of our analytical solutions to the neutron diffusion equation since the 1950s. Little has changed since then, until recently. Our aim is to demonstrate a new paradigm where the monoenergetic neutron diffusion equations in 1D plane homogeneous and heterogeneous media as well as in curvilinear geometries and the multigroup approximation have a common origin enabling straightforwardly intuitive analytical representation. Here, we solidify the mathematics required to resolve the monoenergetic diffusion equation applied to classical 1D nuclear reactors. We derive a consistent theory for monoenergetic plane geometry for both multiplying and non-multiplying media alike. Multigroup solutions in heterogeneous media and in curvilinear geometries then immediately follow the pattern of 1D plane monoenergetic theory, but will not be considered here. The concept is simply to enable the independent solutions of the homogeneous diffusion equation to include boundary conditions to form the general solution. Once one knows the independent solutions then any particular solution follows through the method of Variation of Parameters (VoP). From matching of current at interfaces and specifying

the flux and current at free surfaces, a three term recurrence results for the interfacial fluxes. Thus, we find the analytical solution as simply as the finite difference or finite element numerical solution but avoiding discretization error altogether. Our method provides nuclear engineering students with reinforcement of their study of second order ODEs including Wronskians, independent solutions to the homogeneous diffusion equation, particular solutions and solving 3- term recurrence. Arguably, our approach is the most efficient and consistent way of solving the neutron diffusion equation in 1D and, we therefore hope, will eventually become the educational standard adopted in all “Chapters 5” of future reactor physics texts.

## 2. SOLUTION TO THE 1-D- MONENERGETIC DIFFUSION EQUATION IN A HOMOGENEOUS MEDIUM

In the following, we consider the one-group characterization of a homogeneous reactor of width  $\Delta$

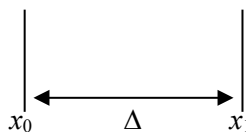


Fig. 1. Homogeneous diffusing medium.

shown in Fig. 1. The neutron diffusion equation is

$$D \frac{d^2 \phi(x)}{dx^2} + (v\Sigma_f - \Sigma_a) \phi(x) = -Q(x), \quad (0a)$$

where a spatially dependent source is included for generality. With buckling

$$B^2 \equiv \frac{v\Sigma_f - \Sigma_a}{D}, \quad (0b)$$

the diffusion equation becomes

$$\frac{d^2 \phi(x)}{dx^2} + B^2 \phi(x) = -\frac{Q(x)}{D}. \quad (1)$$

We leave the boundary conditions unspecified for the moment other than to assume they exist.

The general solution to Eq(1), written as the sum of the solutions to the homogeneous equation and a particular solution, is

$$\phi(x) = \phi_h(x) + \phi_p(x), \quad (2a)$$

where

$$\frac{d^2 \phi_h(x)}{dx^2} + B^2 \phi_h(x) = 0 \quad (2b)$$

and

$$\frac{d^2 \phi_p(x)}{dx^2} + B^2 \phi_p(x) = q(x) \equiv -\frac{Q(x)}{D}. \quad (2c)$$

One uniformly observes, essentially in all reactor physics texts as well as in ODE math classes, the choice of two linearly independent exponentials for the solution to the homogeneous equation

$$\phi_h(x) = ae^{iBx} + be^{-iBx}. \quad (3a)$$

Introducing the known boundary conditions at  $x_0$  and  $x_1$  gives the following set of equations for the unknown coefficients  $a, b$ :

$$\begin{aligned} \phi_h(x_0) &= ae_0^+ + be_0^-; & e_0^+ &\equiv e^{iBx_0}, & e_0^- &\equiv e^{-iBx_0} \\ \phi_h(x_1) &= ae_1^+ + be_1^-; & e_1^+ &\equiv e^{iBx_1}, & e_1^- &\equiv e^{-iBx_1}, \end{aligned} \quad (3b)$$

to yield by Cramer's rule

$$\begin{aligned} a &= \frac{\begin{vmatrix} \phi_h(x_0) & e_0^- \\ \phi_h(x_1) & e_1^- \end{vmatrix}}{\begin{vmatrix} e_0^+ & e_0^- \\ e_1^+ & e_1^- \end{vmatrix}} = -\frac{e_1^- \phi_h(x_0) - e_0^- \phi_h(x_1)}{2i \sin(B\Delta)} \\ b &= \frac{\begin{vmatrix} e_0^+ & \phi_h(x_0) \\ e_1^+ & \phi_h(x_1) \end{vmatrix}}{\begin{vmatrix} e_0^+ & e_0^- \\ e_1^+ & e_1^- \end{vmatrix}} = -\frac{e_0^+ \phi_h(x_1) - e_1^+ \phi_h(x_0)}{2i \sin(B\Delta)}. \end{aligned} \quad (3c,d)$$

The simple re-arrangement,

$$\phi_h(x) = \frac{\left[ e^{iB(x_1-x)} - e^{-iB(x_1-x)} \right]}{2i \sin(B\Delta)} \phi_h(x_0) + \frac{\left[ e^{iB(x-x_0)} - e^{-iB(x-x_0)} \right]}{2i \sin(B\Delta)} \phi_h(x_1) \quad (3e)$$

gives

$$\phi_h(x) = h(x_1 - x) \phi_h(x_0) + h(x - x_0) \phi_h(x_1), \quad (3f)$$

where the new independent solution is

$$h(x) \equiv \frac{\sin(Bx)}{\sin(B\Delta)}; \quad (3g)$$

with the property

$$h(0) = 0, \quad h(\Delta) = 1. \quad (3h)$$

Thus, the solution automatically satisfies the boundary conditions, at least for the homogeneous ODE.

Once we have the solutions to the homogeneous ODE, VoP then provides the particular solution as

$$\phi_p(x) \equiv -\frac{1}{D} \left[ h(x-x_0) \int_x^{x_1} dx' h(x_1-x') W^{-1}(x') Q(x') + h(x_1-x) \int_{x_0}^x dx' h(x'-x_0) W^{-1}(x') Q(x') \right]. \quad (4a)$$

Note

$$\phi_p(x_0) = 0, \quad \phi_p(x_1) = 0, \quad (4b)$$

where the Wronskian is

$$W(x) \equiv \begin{vmatrix} h(x-x_0) & h_j(x_1-x) \\ h'(x-x_0) & h'(x_1-x) \end{vmatrix} = -\frac{B}{\sin(B\Delta)}. \quad (4c)$$

and is non-zero for all buckling. Since

$$\phi_h(x) = \phi(x) - \phi_p(x), \quad (5a)$$

the general solution becomes

$$\phi(x) = h(x_1-x)[\phi_0 - \phi_p(x_0)] + h(x-x_0)[\phi_1 - \phi_p(x_1)] + \phi_p(x), \quad (5b)$$

where

$$\phi_0 \equiv \phi_0(x_0), \quad \phi_1 \equiv \phi_1(x_1). \quad (5c)$$

We could also write the solution as

$$\phi(x) = h(x_1-x)\phi_0 + h(x-x_0)\phi_1 + \tilde{\phi}_p(x), \quad (6a)$$

where

$$\tilde{\phi}_p(x) = \phi_p(x) - h(x_1-x)\phi_p(x_0) - h(x-x_0)\phi_p(x_1), \quad (6b)$$

which is an alternative of many possible particular solutions.

Several principles of solving ODEs are in play here. Specifically, when solving an ODE, one has many practical choices for the two linearly independent solutions with some more convenient than others. As demonstrated, it is convenient to choose functions that automatically satisfy the boundary conditions as identities. Moreover, we choose the particular solution in the same way according to Eqs(4a) and (6b).

The advantage of Eq(5b), called the customized solution, is clear for the homogeneous medium and will become clearer for the heterogeneous medium. To solve any 1D problem in plane geometry, one need only assume Eq(5b) rather than the exponential solution, thus avoid solving for the coefficients  $a$  and  $b$  in the complementary solution, Eq(3a). No matrix algebra is necessary for the single medium with the solution entirely transparent. In addition, note that nothing was said about whether the medium was fissioning or not. The procedure as presented thus far should be equally applicable. If fissioning or not, the sign of  $B^2$  can be either negative or positive. The case presented tacitly assumed  $B^2$  was positive. If however,  $B^2$  is negative, the *sine* switches branches and becomes the hyperbolic *sine* (*sinh*) and we write

$$h^\pm(x) \equiv \frac{\chi^\pm(x)}{\chi^\pm(\Delta)} \quad (7a)$$

with

$$\chi^\pm(x) \equiv \begin{cases} \sinh(Bx), B^2 < 0 \\ \sin(Bx), B^2 > 0, \end{cases} \quad (7b)$$

where  $B_j \equiv |B_j|$  and Eq(5b) becomes

$$\phi(x) = h^\pm(x_1 - x)[\phi(x_0) - \phi_p(x_0)] + h^\pm(x - x_0)[\phi(x_1) - \phi_p(x_1)] + \phi_p(x); B_j^2 \leq 0. \quad (7c)$$

### 3. SOLUTION TO THE 1-D- ONE-GROUP DIFFUSION EQUATION IN A HETEROGENEOUS MEDIUM

We now consider the one-group characterization of the heterogeneous reactor configuration of  $n$  slabs as shown here

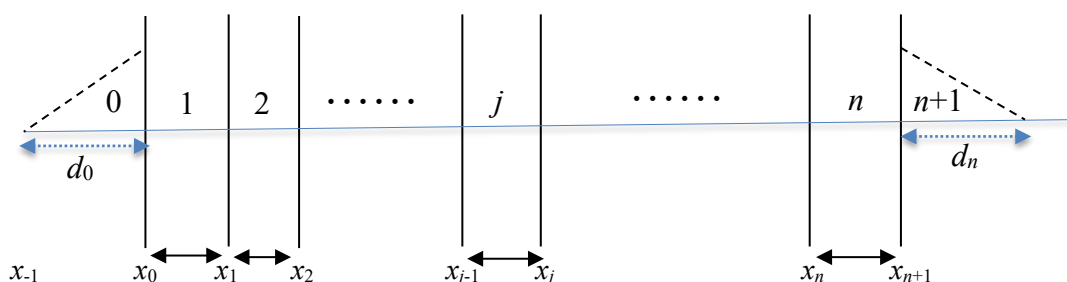


Fig.2. Heterogeneous diffusing medium.

Now the diffusion equation becomes

$$\frac{d^2\phi_j(x)}{dx^2} + B_j^2\phi_j(x) = -\frac{Q_j(x)}{D_j} \quad (8a)$$

with

$$B_j^2 \equiv \frac{\nu\Sigma_{fj} - \Sigma_{aj}}{D_j}. \quad (8b)$$

We also require flux and current continuity at the interior slab interfaces

$$\begin{aligned} \phi_{j-1}(x_{j-1}) &= \phi_j(x_{j-1}) \\ -D_{j-1} \left. \frac{d\phi_{j-1}(x)}{dx} \right|_{x_{j-1}} &= -D_j \left. \frac{d\phi_j(x)}{dx} \right|_{x_{j-1}} \end{aligned} \quad (8c,d)$$

The analysis begins with the development of the region wise solution to Eqs(8) in slab  $j$

$$\phi_j(x) = h_j^\pm(x_j - x)[\phi_{j-1} - \phi_{p,j}(x_{j-1})] + h_j^\pm(x - x_{j-1})[\phi_j - \phi_{p,j}(x_j)] + \phi_{p,j}(x); B_j^2 \leq 0, \quad (9a)$$

where the interfacial fluxes are

$$\phi_{j-1} = \phi_j(x_{j-1}), \quad \phi_j \equiv \phi_j(x_j). \quad (9b)$$

$h_j^\pm(x)$  is now region wise

$$h_j^\pm(x) \equiv \frac{\chi_j^\pm(x)}{\chi_j^\pm(\Delta)}, \quad (9c)$$

where for the two branches of the *sine* function are

$$\chi_j^\pm(x) \equiv \begin{cases} \sinh(B_j x), B_j^2 < 0 \\ \sin(B_j x), B_j^2 > 0. \end{cases} \quad (9d)$$

As above, the first two terms of Eq(9a) are the homogenous solutions and the third is the particular solution. The solution automatically satisfies flux continuity at slab interfaces since

$$h_j^\pm(0) = 0, \quad h_j^\pm(\Delta_j) = 1. \quad (10)$$

Again, when we apply VoP, the following particular solution emerges:

$$\phi_{p,j}(x) = -\frac{\chi_j^\pm}{D_j B_j} \left[ h_j^\pm(x - x_{j-1}) \int_x^{x_j} dx' h_j^\pm(x_j - x') Q_j(x') + h_j^\pm(x_j - x) \int_{x_{j-1}}^x dx' h_j^\pm(x' - x_{j-1}) Q_j(x') \right]. \quad (11)$$

The advantage of the customized form of the solution is apparent when we satisfy the interfacial conditions of Eqs(8c,d) to give the following three-term recurrence relation for the coupling coefficients between two adjacent regions:

$$\phi_j + b_j \phi_{j-1} + \gamma_j \phi_{j-2} = f_j, \quad 2 \leq j \leq n \quad (12a)$$

with

$$f_j \equiv -[g_{p,j}^{a\pm} + \gamma_j g_{p,j}^{b\pm}] \quad (12b)$$

$$g_{p,j}^{a\pm} \equiv \frac{\chi_j^\pm}{D_j B_j} \int_{x_{j-1}}^{x_j} dx' h_j^\pm(x' - x_{j-1}) Q_j(x') \quad (12c,d)$$

$$g_{p,j}^{b\pm} \equiv \frac{\chi_j^\pm}{D_j B_j} \int_{x_{j-1}}^{x_j} dx' h_j^\pm(x_j - x') Q_j(x')$$

and

$$\gamma_j^\pm \equiv \left[ \frac{D_{j-1} B_{j-1}}{\chi_{j-1}^\pm} \right] \left[ \frac{\chi_j^\pm}{D_j B_j} \right] \quad (12e,f)$$

$$b_j^\pm \equiv -(Y_j^\pm + \gamma_j^\pm Y_{j-1}^\pm)$$

$$Y_j^\pm \equiv \begin{cases} \cosh(B_j \Delta_j), B_j^2 < 0 \\ \cos(B_j \Delta_j), B_j^2 > 0. \end{cases} \quad (12g)$$

### 3.1. Including Boundary Conditions

Assume vacuum on the boundaries, which is defined as no incoming partial current, or [3]

$$J_+(x_0) = \frac{\phi_0}{4} - \frac{D_1}{2} \frac{d\phi_1(x)}{dx} \Big|_{x_0} = 0, \quad J_-(x_n) = \frac{\phi_n}{4} + \frac{D_n}{2} \frac{d\phi_n(x)}{dx} \Big|_{x_n} = 0. \quad (13a,b)$$

Assuming no sources in the first and last slabs using Eq(9a) with  $j=1$  and  $n$  gives

$$\phi_0 - \frac{2D_1B_1}{\chi_1} [1 + 2D_1B_1Y_1]^{-1} \phi_1 = 0 \quad (14a)$$

$$\phi_n + \frac{2D_nB_n}{\chi_n} [1 + 2D_nB_nY_n]^{-1} \phi_{n-1} = 0 \quad (14b)$$

relating the boundary fluxes of the first and last slabs. Equations (14a,b) completes the recurrence of Eq(12a).

For vacuum boundary conditions at the extrapolated distances  $d_0$  and  $d_n$  shown in Fig. 2, one can extend the medium out in both directions and ask that the flux at the ends of the extensions  $x_{-1}$  and  $x_{n+1}$ ,  $\phi_{-1}, \phi_{n+1}$ , to vanish. In this case,

$$\begin{aligned} \phi_0(x) &= h_0(x_0 - x)\phi_{-1} + h(x - x_{-1})\phi_0 \\ \phi_{n+1}(x) &= h_{n+1}(x_{n+1} - x)\phi_n + h(x - x_n)\phi_{n+1} \end{aligned} \quad (15a,b)$$

and

$$\begin{aligned} \frac{d\phi_0(x)}{dx} \Big|_{x_0} &= \frac{B_1Y_1}{\chi_1} \phi_0 = \frac{\phi_0 - \phi_{-1}}{d_0} \Rightarrow d_0 = \frac{\tanh(B_1d_0)}{B_1} \\ \frac{d\phi_{n+1}(x)}{dx} \Big|_{x_n} &= \frac{B_{n+1}Y_{n+1}}{\chi_{n+1}} \phi_n = \frac{\phi_{n+1} - \phi_n}{d_n} \Rightarrow d_n = \frac{\tanh(B_nd_n)}{B_n}. \end{aligned} \quad (15c,d)$$

Thus, the extrapolation distance, to be determined iteratively, can be different at each surface. The physical boundaries now become  $x_0 - d_0$  and  $x_n + d_n$ , where the flux vanishes.

#### 4. AN EXAMPLE: ENTERING CURRENT AT $x = 0, x_n$

Partial currents  $J_+$  and  $J_-$  enter a heterogeneous slab, devoid of sources, at the left and right boundaries. The incoming currents at the boundaries are from Eqs(13a,b)

$$J_+(x_0) = \frac{\phi_0}{4} - \frac{D_1}{2} \frac{d\phi_1(x)}{dx} \Big|_{x_0}, \quad J_-(x_n) = \frac{\phi_n}{4} + \frac{D_n}{2} \frac{d\phi_n(x)}{dx} \Big|_{x_n}. \quad (16a,b)$$

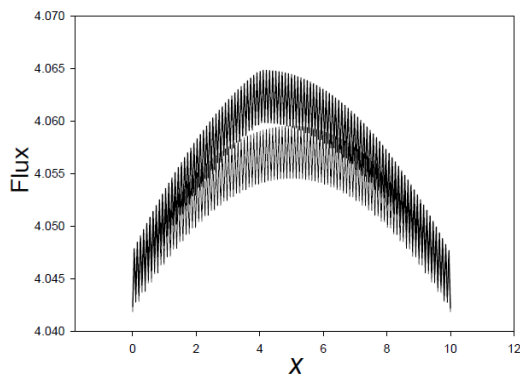
As above, using Eq(9a) with  $j = 1$  and  $n$  at  $x_0$  and  $x_n$  respectively gives

$$\phi_0 - \frac{2D_1B_1}{\chi_1} \left[ 1 + 2D_1B_1 \frac{Y_1}{\chi_1} \right]^{-1} \phi_1 = 4J_+(x_0) \left[ 1 + 2D_1B_1 \frac{Y_1}{\chi_1} \right]^{-1} \quad (17c)$$

$$\phi_n - \frac{2D_n B_n}{\chi_n} \left[ 1 + 2D_n B_n \frac{Y_n}{\chi_n} \right]^{-1} \phi_{n-1} = 4J_-(x_n) \left[ 1 + 2D_n B_n \frac{Y_n}{\chi_n} \right]^{-1}. \quad (17d)$$

to be solved along with Eq(12a) using several possible methods-- including transformation of the boundary value recurrence into two initial value recurrences, tridiagonal matrix inversion by the Thompson algorithm, matrix diagonalization. As a demonstration, a 101 slab heterogeneous medium, with  $J_+, J_- = 1$ , of alternating

Fig. 3. Random medium of fissioning and non-fissioning material.



fissioning and non-fissioning regions with the bucklings of  $\pm 0.1$  respectively and diffusion coefficient of unity is shown in Fig. 3. The oscillatory behavior is clear. In addition, we increase the buckling at slab 41 by 1% resulting in the dark curve. The perturbation indicates that the analytical solutions reflects small changes.

On a final note, for a homogeneous medium assuming medium width  $h$  is small, the coefficients of the recurrence relation can be expanded in a Taylor series to give for Eq(12a)

$$\phi_j - (2 + B^2 h^2) \phi_{j-1} + \phi_{j-2} = -\frac{h^2}{2D} [Q_j + Q_{j+1}], \quad (18)$$

which is the finite difference (FD) form of recurrence.

It is interesting to observe that both the analytical solution and FD approximation derive from the same recurrence relation and therefore represent essentially identical numerical effort. The question is therefore - Why would one use finite difference when the analytical is as easily obtained?

## 5. CONCLUSIONS

We have presented a new approach to analytically solving the 1D neutron diffusion equation. The power of the new approach is the two-slab connection between multiple slabs in a heterogeneous medium to give a readily solvable tridiagonal matrix for interfacial fluxes.

Unfortunately, space limitation precludes discussion of straightforward extensions to curvilinear and multigroup diffusion theory other than to write the following:

+ **For curvilinear geometries:** From the plane/point transformation, spherical geometry follows the identical form presented in plane geometry. Cylindrical geometry follows using Bessel functions as the independent solutions, but since Bessel functions do not combine like sines and cosines of different argument, an additional step forcing the linearly independent solutions to give the appropriate boundary conditions must be included.

+ **For Multigroup Diffusion theory:** The multigroup diffusion equations, when put in vector form, resemble the one group equation. The solution in plane geometry then gives a matrix function corresponding to  $h_j^\pm(x)$  leading to solutions in curvilinear geometries and multigroup approximation.

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