22.05 Reactor Physics - Part Ten

Neutron Diffusion Theory: One Velocity Model

1. Background:

We now have sufficient tools to begin a study of the second method for the determination of neutron flux as a function of position and energy. This method is, diffusion theory. Both diffusion theory and Monte Carlo methods are currently in use as reactor design tools. Both are actually quite similar in terms of set up because, for each, a detailed model of the reactor is essential and the accuracy of the result is largely a function of the quality of the model. Once the model is developed, the two differ in the method of solution.

The model that is needed for diffusion theory has the following inputs:

- A list of the mathematical constraints on the model. Is the core symmetric and hence only half is modeled with the other half being taken as a mirror image? What boundary conditions are to be imposed? What geometry (x, y, z; or r, θ z,) for example, is to be used?
- A list of the materials that will be present. These typically include: light water, U-235, U-238, Zircalloy, steel, boron, etc.
- For each material, the cross-section is specified. These are usually a function of neutron energy.
- A geometric description of the reactor. Where is the fuel, the moderator, the control devices?
- For each geometric location, what material composition is present?

Details of model construction can be found in the description of any of the computer codes that are used to calculate flux. The point to be made here is that the assembly of the model is non-trivial and this has a bearing on how we approach the study of diffusion theory.

In the introductory lecture, we noted that the goal of reactor physics analysis is to calculate the neutron population at any given time and at every point r as a function of energy and angle of travel. Thus, we could attempt to use diffusion theory to solve for $\phi(r, E, \mathbf{\Omega}, t)$. Such an approach is feasible but it is rather daunting. Accordingly, we will first apply diffusion theory for the solution of $\phi(r, t)$ or perhaps only $\phi(r)$. Such an approach is called “one velocity theory” because we are treating all neutrons as having one speed or energy.

2. Value of One Velocity Theory:

The one velocity model is formally obtained by integrating over both E and $\boldsymbol{\Omega}$. Thus,

$$\phi(r,t) = \int_E \int_{\boldsymbol{\Omega}} \phi(r,E,\boldsymbol{\Omega},t)\,dE,d\boldsymbol{\Omega}$$

Is it of value? We saw from the life cycle analysis that energy dependence is essential. The various factors each pertained to a particular energy range. So, we do not expect a one velocity model to provide useful results for situations where changes of neutron energy are important. For example, it could not describe a thermal reactor because, in that case, neutrons are born at fast energies and slow down to be absorbed by U-235. But, the one velocity model could describe a fast reactor where neutron slowing down is not as important. In fact, it has been used for this purpose. In particular, it is of use for bare (unreflected) cores.

3. Equation of Continuity:

The object is to write a relation that will allow the calculation of $\phi(r,t)$. This is sometimes called a neutron balance equation or a neutron conservation equation. The starting point is the word definition of the core multiplication factor:

$$K = \frac{\text{Neutrons Produced from Fission}}{\text{Neutrons Absorbed} + \text{Neutrons Leaked Out}}$$

Thus, it follows that:

$$\text{Change} = \text{Production} - \text{Absorption} - \text{Leakage}$$

or

$$\begin{bmatrix}\text{Time rate of change of}\\ \text{Neutrons in dV at r at}\\ \text{time t}\end{bmatrix} = \begin{bmatrix}\text{Number neutrons produced in}\\ \text{dV at r at t per second}\end{bmatrix} - \begin{bmatrix}\text{Number neutrons absorbed in}\\ \text{dV at r at t per second}\end{bmatrix} - \begin{bmatrix}\text{Net number of neutrons that}\\ \text{leak out of dV at r and t}\\ \text{per second}\end{bmatrix}$$

Let n(r,t) be the number of neutrons at r and t per unit volume. Thus,

$$\frac{\partial}{\partial t}[n(r,t)dV] = S(r,t)dV - A(r,t)dV - L(r,t)dV$$

Where S, A, and L are the source, absorption, and leakage terms, respectively. The above may be rewritten as:

$$\frac{\partial}{\partial t} n(r,t) = S(r,t) - A(r,t) - L(r,t)$$

The definition of neutron flux is that $\phi = nv$. Thus, the term on the left may be written as:

$$\frac{\partial}{\partial t} n(r,t) = \frac{1}{v}\frac{\partial}{\partial t}\left(\phi(r,t)\right)$$

The source term, S, is simply the product of the fission reaction rate and the number of neutrons per fission. Thus,

$$S(r,t) = \nu\bar{\Sigma}_f\phi(r,t)$$

Where $\bar{\Sigma}_f$ is the macroscopic fission cross-section averaged over all energies.

The absorption term is the absorption reaction rate. Thus,

$$A(r,t) = \bar{\Sigma}_a\phi(r,t)$$

Where $\bar{\Sigma}_a$ is the macroscopic absorption cross-section averaged over all energies.

This leaves the leakage term to be evaluated. To repeat from the previous section: let **J** be the neutron current density vector on the surface of V and let **n** in a unit normal pointing outward from the surface. Thus, the leakage of neutrons from diffusion through the surface A of volume V is:

$$\begin{aligned} L(r,t) &= \int_A J(r,t) \bullet \mathbf{n}\,dA \\ &= \int_v \nabla \bullet J(r,t)\,dV \end{aligned}$$

Where we have used Gauss's Theorem to transform the surface to a volume integral. Thus, the equation of continuity (one velocity model) becomes

$$\frac{1}{v}\frac{\partial\phi(r,t)}{\partial t} = \nu\bar{\Sigma}_F\phi(r,t) - \bar{\Sigma}_a\phi(r,t) - \nabla \bullet J(r,t)$$

If the flux is not a function of time (reactor exactly critical), then, we obtain

$$0 = \nu\bar{\Sigma}_F\phi(r) - \bar{\Sigma}_a\phi(r) - \nabla \bullet J(r)$$

4. **Fick's Law**:

The continuity equation cannot be evaluated as written because it contains both $\phi(r,t)$ and $\mathbf{J}(r,t)$. We need to rewrite the current density in terms of the flux. This is done through the application of Fick's Law which arises from the study of chemical diffusion. We again quote from Henry's Nuclear Reactor Analysis (p. 121):

"As might be expected, the best that can be done to relate **J** to Φ without actually finding a solution for N(**r**, Ω,E) is an approximation. Fortunately there turns out to be a rather accurate approximation that is quite satisfactory for many reactor-design calculations. It is called Fick's Law, and it relates J(**r**,E) to $\nabla\phi(\mathbf{r},E)$, by the equation

$$\mathbf{J}(\mathbf{r}, E) = -D(\mathbf{r},E)\ \nabla\phi(\mathbf{r},E)$$

Where D(**r**,E) is called the diffusion constant.

This relationship between the net current and the gradient of the scalar flux seems plausible if we recall that $\phi(\mathbf{r},E)$ is $v(E)\ n(\mathbf{r},E)$, where $n(\mathbf{r},E)\,dE$ is the number of neutrons in dE per unit volume. Thus Fick's Law states that the net current across a surface of neutrons with energies in dE is proportional to the rate of decrease of the density of neutrons in dE across that surface. Moreover the direction of the net current is the direction in which n(r, E) is decreasing at its maximum rate. (Recall that, mathematically, the gradient of a function is a vector pointing in the direction of the maximum rate of increase of that function; thus $-\nabla n(\mathbf{r},E)$ points in the direction of the maximum rate of decrease of n(**r**,E).) The neutron population thus tends to drift from a region of high concentration to one of low concentration, like gas diffusing through a porous plug, and this drift gives rise to a net current."

5. Validity of Fick's Law:

Fick's law is valid provided that there are roughly equal number of neutrons moving in all directions at all energies. Consider two material compositions.

a) Core Interior: Here there is a repeated pattern of fuel, clad, coolant/moderator. Neutrons are moving isotropically.

b) Absorber: Here there is a flow of neutrons into the absorber and no flow from the absorber.

Fick's Law can model the first situation but not the second. In general, Fick's law is not valid whenever there are abrupt changes in the scatter and absorption cross-

sections such that the net flow of neutrons is in one direction only. Thus, it is expected to:

a) Be valid whenever more than a few mean free paths from a surface.

b) Be invalid at absorber surfaces or near core-moderator surfaces. (In the latter case, high energy neutrons leave the core and enter the moderator where they are thermalized. Low energy neutrons leave the moderator and enter the core.) So, this situation becomes an issue when we study the energy dependence of the flux.)

Lamarsh (p. 194) puts it more bluntly: "Fick's Law is invalid:

a) in a medium that strongly absorbs neutrons;

b) within three mean free paths of either a neutron source or the surface of a material; and

c) when neutron scattering is strongly anisotropic."

6. **<u>Evaluation of the Diffusion Constant</u>**: The parameter D in Fick's Law is called the diffusion constant. Its units are those of length. Its value is given approximately by the relation:

$$D = \frac{\lambda_{tr}}{3} = \frac{1}{3\Sigma_{tr}}$$

and

$$\lambda_{tr} = 1/\Sigma_{tr} = \frac{1}{\left[\Sigma_t - \overline{\mu}_0\Sigma_s\right]} \cong \frac{1}{\Sigma_s\left(1-\overline{\mu}_0\right)}$$

$$\Sigma_t = \Sigma_a + \Sigma_s$$

$$\overline{\mu}_0 = \frac{2}{3A}$$

Where A is the atomic mass of the medium through which the diffusion occurs. Other symbols are:

λ_{tr} is the transport mean free path (cm),

Σ_{tr} is the macroscopic transport cross-section,

Σ_s is the macroscopic scattering cross-section,

Σ_t is the macroscopic total removal cross-section, and

$\bar{\mu}_0$ is the average value of the cosine of the angle at which neutrons are scattered (Lab System).

Note: The above expression for D and the theoretical basis for Fick's Law can be obtained from the study of the transport equation.

7. **Neutron Diffusion Equation**: The leakage term in the continuity equation can now be written as:

$$\nabla \bullet \mathbf{J}(r,t) = \nabla \bullet (-D\nabla\phi(r,t))$$

Where we have dropped the position and energy dependence of D.

or,

$$\nabla \bullet J(r) = -D\nabla^2\phi(r)$$

Hence, the continuity equation becomes:

$$\frac{1}{v}\frac{\partial\phi(r,t)}{\partial t} = \nu\bar{\Sigma}_F\phi(r,t) - \bar{\Sigma}_a\phi(r,t) + D\nabla^2\phi(r,t)$$

or, for steady state:

$$0 = \nu\bar{\Sigma}_F\phi(r) - \bar{\Sigma}_a\phi(r) + D\nabla^2\phi(r,t)$$

8. **Boundary Conditions**: The continuity and diffusion equations are similar to equations that arise in heat transport, physics, and other fields. What makes each solution unique is the boundary conditions. For problems involving reactor flux, some of the more common boundary conditions include:

a) Limits on Flux:

— Flux (ϕ) must be real and non-negative,

— Flux must be finite.

b) Interface Conditions: Interfaces are surfaces where two different material compositions meet. Examples include the boundary between the core/moderator region and a reflector. Both the neutron flux and the component of neutron current normal to the surface are continuous across the boundary. Thus, for materials A and B, we require that

$$\phi_A = \phi_B$$

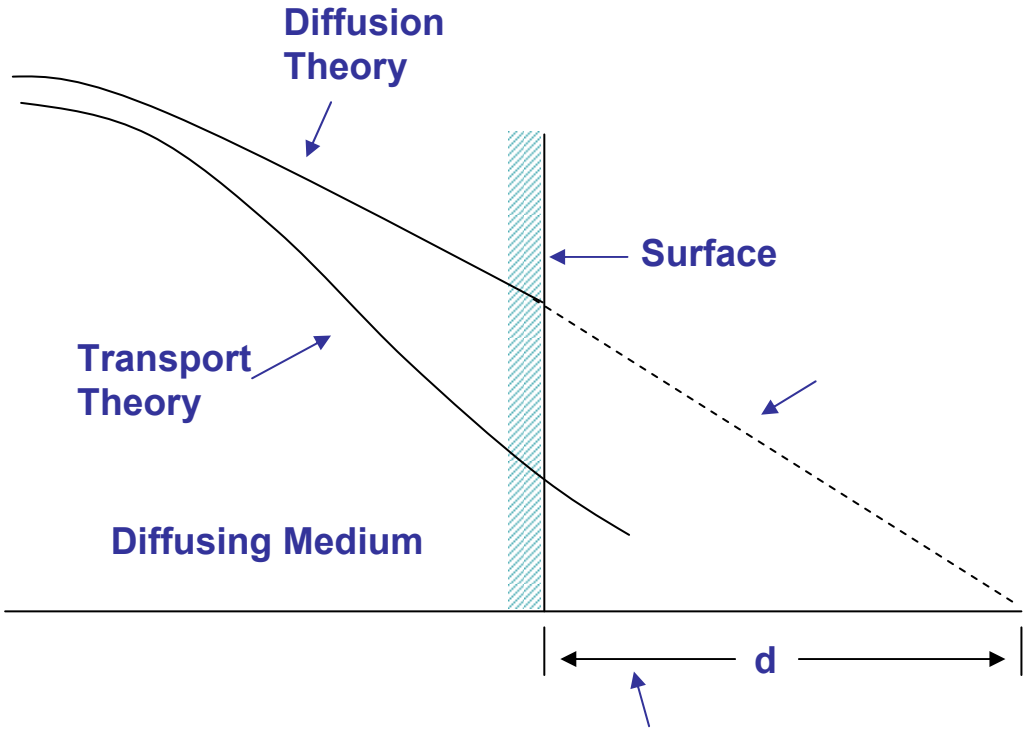
$$(\mathbf{J}_A)_n = (\mathbf{J}_B)_n$$

Where ϕ_A and ϕ_B are the neutron fluxes in A and B respectively and $(\mathbf{J}_A)_n$ and $(\mathbf{J}_B)_n$ are the normal components of the neutron currents both evaluated at the interface. Note that the gradient of the flux $(d\phi/dx)$ is **NOT** continuous across the boundary. That is:

$$\mathbf{J} = -Dd\phi/dx$$

If J and ϕ are continuous, then $d\phi/dx$ will change abruptly because the value of D, the diffusion constant, is different for each medium. Hence, there will be a change in the slope of the flux at the interface.

c) Extrapolation Distance: Fick's Law is not valid at surfaces and hence neither is the diffusion equation. However, transport theory is valid. Comparisons of transport (exact) and diffusion (valid only 3 mean paths from surface) calculations show that if the flux, as calculated from diffusion theory, is assumed to go to zero at some distance d beyond the surface, then the diffusion theory prediction in the interior of the medium will be accurate. The following figure illustrates the idea.



The value of the extrapolation distance d is found to be 0.71 λ_{tr} and because the diffusion constant equals $\lambda_{tr}/3$.

$$d = 2.13D$$

Most values of d are a few cm or less. For large reactors where d << actual size, d can be set to zero.

CAUTION: The extrapolated flux is not a physically real quantity. Radiation levels associated with both neutrons and photons are not zero at distance d from a reactor surface. They remain very high, often well above lethal.

9. Illustration of the Success/Limitations of Diffusion Theory:

The MIT Research Reactor (MITR) is a hexagonal core that contains three rings of fuel. The inner or A-Ring has three elements, the middle or B-Ring has nine, and the outermost or C-Ring has fifteen. (See following figure.) Light water, which serves as both coolant and moderator, flows through the fuel elements that form each ring. In addition, there are plenums of light water both above and below the core. As one moves radially outward from the C-Ring, one encounters a region of light water, the control blades (borated stainless steel), the aluminum core tank, and the heavy water reflector.

The MITR was designed using a diffusion theory code. Experiments were then done to verify the accuracy and to develop flux correlation factors for regions where the diffusion theory prediction was inaccurate. One would expect diffusion theory to fail at the fuel water interfaces which are the plenums that are above and below the core and the region of light water that surrounds the C-Ring.

Measurements of the neutron flux (thermal) were made as a function of axial position (height) within each ring. These were compared to the diffusion theory prediction and a "correction factor" defined as:

$$\text{Correction Factor} = \frac{\text{Measured Value}}{\text{Predicted Value}}$$

The attached figure shows the axial correction factors for the A and C-Rings. As expected, the value of the factor is near unity (excellent agreement) for the interior portion of the A-Ring. It deviates from unity (poor agreement) at both the lower and upper regions because of the presence of the water plenums. Fast neutrons are traveling into those plenums; thermal neutrons are returning. So, Fick's Law does not hold. The agreement is marginal for all of the C-Ring which forms a surface with the control blades (strong absorbers) or the light water moderator. So, we conclude that our understanding of the capabilities and limitations of diffusion theory is correct.