22.05 Reactor Physics – Part Nineteen

Extension of Group Theory to Reactors of Finite Size[1]

1. Background:

We reviewed group theory with the objective of being able to calculate $\phi(\mathbf{r}, E)$. Thus far, we have determined the energy behavior of the flux by applying the group method to an infinite homogeneous medium. We now extend the approach first to reactors of finite size and then to reactors of multiple regions. The former might be a bare (unreflected) slab. The latter might be a core with a moderator designed so that both sit in a tank that is surrounded by a reflector. Thus, our design is becoming realistic in terms of an actual operating reactor.

2. Review of Neutron Current:

The treatment of reactors of finite size requires treatment of neutron leakage. This is done by developing the concept of a neutron current and showing that leakage is given by the divergence of that current. See Parts 9 and 10 of these notes. We review the principal concepts here:

- The net current density $\mathbf{J}(\mathbf{r}, E)$ is the maximum over all orientations of a unit surface at **r** of the net number of neutrons with energies between E and E + dE crossing that unit surface per second, the direction of the vector being the direction of this maximum net flow

  $$\equiv \mathbf{J}(\mathbf{r}, E)dE$$

  The units of $\mathbf{J}(\mathbf{r}, E)$ are neutrons per unit energy per cm^2 per sec.

- Once $\mathbf{J}(\mathbf{r}, E)$, which is the net current through one particular unit surface (namely the one oriented so that this net flow is a maximum), is known, the net current through any surface at **r** can be obtained. Thus, if **r** is a vector normal to dS, we have

  Net current (neutrons per unit energy per sec) through **n** dS

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[1] Material in this section follows that of Henry, pp. 130-138. Portions that are verbatim are indicated by quotations.

$$= \mathbf{J}(\mathbf{r}, E) \cdot \mathbf{n}\ dS$$

- We then use Gauss's law to convert the surface integral to one over volume. Thus, the total rate at which neutrons are lost from a volume element dV per unit energy is:

  $$= \nabla \cdot \mathbf{J}(\mathbf{r}, E)\ dV\ dE$$

3. Fundamental Neutron Balance Condition:

"For a reactor in a steady-state critical condition the rate at which neutrons leak out of dV dE must equal the rate at which they are removed by interaction with the material in dV (i.e., by absorption and scattering-out). The physical statement that leakage equals production less removal then becomes:

$$\nabla \cdot \mathbf{J}(\mathbf{r},E)\ dV\ dE = \sum_j \chi^j(E) dV\, dE \int_0^\infty \nu^j \Sigma_f^j(\mathbf{r},E')\Phi(\mathbf{r},E')\ dE'$$

$$+\ dV\, dE \int_0^\infty \Sigma_s(\mathbf{r},E' \to E)\Phi(\mathbf{r},E')dE' - \Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E)\ dV\, dE$$

or

$$\nabla \cdot \mathbf{J}(\mathbf{r},E) + \Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E) = \int_0^\infty \left[\sum_j \chi^j(E) \nu^j \Sigma_f^j(\mathbf{r},E') + \Sigma_s(\mathbf{r},E' \to E) \right] \Phi(\mathbf{r},E')dE'$$

Where, for this general, heterogeneous, finite assembly, the cross sections, flux density, and current density are all expressed as functions of both energy and position. (Note: The summation over the lower case j is to cover all isotopes.) This equation is rigorous for the external-source-free, steady-state condition. We have made no approximations in deriving it other than those inherent in the basic expressions for reaction rates. Thus, if we could obtain $\Phi(\mathbf{r}, E)$ without approximation, it would be possible to compute the power level at all locations in a critical reactor with an accuracy limited only by the reliability of the nuclear data. Unfortunately, since the equation contains **J** as well as Φ, it cannot be solved for either of these functions without making use of some second equation relating them." (Henry, p. 120)

4. Fick's Law:

"As might be expected, the best that can 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 $\mathbf{J}(\mathbf{r}, \mathrm{E})$ to $\nabla\Phi(\mathbf{r}, \mathrm{E})$ by the equation:

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

Where $\mathrm{D}(\mathbf{r}, \mathrm{E})$ is called the diffusion constant." (Henry, p. 121) It is given by

$$\mathrm{D}(\mathbf{r}, \mathrm{E}) = \frac{1}{3\left[\Sigma_t(\mathbf{r}, \mathrm{E}) - \bar{\mu}_0\Sigma_s(\mathbf{r}, \mathrm{E})\right]}$$

Where $\bar{\mu}_0$ is the cosine of the scattering angle in the laboratory system. Fick's law is valid within weakly absorbing media. It fails at surfaces where material properties change abruptly and in the presence of strong absorbers."

5. Continuous Energy Diffusion Equation:

Substitution of the Fick's Law relation into the fundamental neutron balance equation yields an equation for $\Phi(\mathbf{r}, \mathrm{E})$, the scalar-flux density:

$$-\nabla \cdot \mathrm{D}(\mathbf{r}, \mathrm{E})\ \nabla\Phi(\mathbf{r}, \mathrm{E}) + \Sigma_t(\mathbf{r}, \mathrm{E})\Phi(\mathbf{r}, \mathrm{E})$$

$$= \int_0^\infty \left[\sum_j \chi^j(\mathrm{E})\nu^j\Sigma_f^j(\mathbf{r}, \mathrm{E}') + \Sigma_s(\mathbf{r}, \mathrm{E}' \to \mathrm{E})\right]\Phi(\mathbf{r}, \mathrm{E}')d\mathrm{E}'$$

It is this equation that we will now try to solve using group theory. The conditions imposed on the solution include that:

- $\Phi(\mathbf{r}, \mathrm{E})$ be real and non-negative.
- $\Phi(\mathbf{r}, \mathrm{E})$ be a continuous function of r within the reactor.
- The component $\mathrm{n} \cdot \mathbf{J}(\mathbf{r}, \mathrm{E})$ of the net current across an internal surface separating two different materials be continuous. (Note: D(**r**, E) is not continuous between two different media. Neither is $\nabla\Phi(\mathbf{r}, \mathrm{E})$. The requirement is on $(\mathrm{D}(\mathbf{r}, \mathrm{E}))\ (\mathrm{n} \cdot \nabla\Phi(\mathbf{r}, \mathrm{E}))$.)
- $\Phi(\mathbf{r}, \mathrm{E})$ go to zero at the extrapolation distance.

The solution of this equation requires that we simultaneously solve for both the energy and the spatial dependence of the flux. This is a major challenge and the approach taken is often iterative in that one solves for the energy dependence in an infinite media of the same composition as the actual reactor, defines group constants using that energy dependence, and then solves for the spatial dependence. The result is then checked to see if the assumed energy dependence was valid.

6. Solution of Diffusion Equation for a Bare, Homogeneous Core:

This is the simplest case that can be considered. It is also one that was addressed earlier using one-velocity theory where the neutrons were all assumed to be of a single uniform energy. Here, we explicitly retain the energy dependence.

Homogeneity implies that the concentrations of the materials are uniform. Thus, the material properties which are the macroscopic cross-sections and the diffusion constant are independent of r. Thus, the continuous energy diffusion equation becomes:

$$-D(E)\ \nabla^2\Phi(\mathbf{r},E)+\Sigma_t(E)\Phi(\mathbf{r},E)=\int_0^\infty\left[\frac{1}{\lambda}\chi(E)\nu\Sigma_f(E')+\Sigma_s(E'\to E)\right]\Phi(\mathbf{r},E')dE'$$

Next we assume that $\Phi(\mathbf{r},E)$ is separable and can be written as:

$$\Phi(\mathbf{r},E)=R(\mathbf{r})\Psi(E)$$

We can do this because the problem involves one region and hence can be described by a single spatial and a single energy function. This separability approach will not work for a multi-region reactor because then we would be requiring one energy function to be viable in multiple regions. To continue, substitute the above into the homogeneous diffusion equation and separate terms. Thus,

$$-D(E)\Psi(E)\ \frac{\nabla^2R(\mathbf{r})}{R(\mathbf{r})}+\Sigma_t(E)\Psi(E)=\int_0^\infty\left[\frac{1}{\lambda}\chi(E)\nu\Sigma_f(E')+\Sigma_s(E'\to E)\right]\Psi(E')dE'$$

or

$$-\frac{\nabla^2R(\mathbf{r})}{R(\mathbf{r})}=-\frac{\Sigma_t(E)}{D(E)}+\frac{1}{D(E)\Psi(E)}\int_0^\infty\left[\frac{1}{\lambda}\chi(E)\nu\Sigma_f(E')+\Sigma_s(E'\to E)\right]\Psi(E')dE'$$

"This result states that a function of **r** alone (the left side) equals a function of E alone (the right side), a situation which can be true only if both functions equal the same constant. We call this constant B_r^2 and expect, on physical grounds, that B_r^2 will be real (although it may be negative)." (Henry, p. 131) On physical terms, this equation states that geometrical considerations (left side) balance material conditions (right side). It follows that the separability assumption can be valid only if

$$\nabla^2 R(\mathbf{r}) = -B_r^2 R(\mathbf{r})$$

Let us apply this result to a bare slab that is infinite in the y and z directions and finite in the x direction. Thus,

$$\nabla^2 R(x) = -B_x^2 R(x)$$

The general solution for R(x) is:

$$R(x) = C_1 \sin\ B_x x + C_2 \cos\ B_x x$$

Where C_1 and C_2 are constants. Further assume that the slab extends in width from x=0 to x=L. Also assume that the extrapolation distance is small compared to L. Hence, $R(x) = 0$ at x=0 and at x=L. From this requirement we conclude that C_2=0.

The next requirement is that sin $B_x x$ equal zero at both x=0 and x=L for all values of B_x. Thus,

$$B_x \equiv B_{xn} = n\pi / L \quad \text{for } n = 0, \pm 1, \pm 2, \ldots$$

The only solution which is non-trivial and has no negative components is n=1. Thus, we obtain

$$R(x) = C_1 \sin\ B_{x1} x$$

$$= C_1 \sin\left(\frac{\pi x}{L}\right)$$

So, now we have the spatial component of the solution. We substitute this back into the original equation to obtain an equation in energy. Thus,

$$D(E)B_{x1}^2\ \Psi(E) + \Sigma_t(E)\Psi(E) = \int_0^\infty \left[\frac{1}{\lambda}\chi(E)\nu\Sigma_f(E') + \Sigma_s(E' \to E)\right]\Psi(E')dE'$$

This relation is identical in form to the infinite, homogeneous medium equation that was developed in Part 15 of these notes. The only difference is the presence of the $D(E)B_{x1}^2$ term. However, this term has the same behavior as $\Sigma_t(E)$. So, if we replace $\Sigma_t(E)$ by $\left(D(E)B_{x1}^2 + \Sigma_t(E)\right)$ we obtain the same result for $\Psi(E)$.

To solve the problem using the group theory approach, we define a group diffusion constant as:

$$D_g \equiv \frac{\int_{E_g}^{E_{g-1}} D(E)\Psi(E)dE}{\int_{E_g}^{E_{g-1}} \Psi(E)dE}$$

and obtain a group equation of the form:

$$\left(D_g B_{x1}^2 + \Sigma_{tg}\right)\Psi_g = \sum_{g'=1}^{G} \left[\frac{1}{\lambda}\chi'_g \nu\Sigma_{fg'} + \Sigma_{gg'}\right]\Psi_{g'} \quad (g = 1, 2, \ldots.G)$$

"Solution of these equations gives us an excellent approximation for the energy part $\Psi(E)$ of the solution $\Phi(\mathbf{r}, E) = R(\mathbf{r})\Psi(\mathbf{E})$. It also gives us the value of λ (the "eigenvalue") required if this solution is to be positive for all energy groups. If λ turns out to be unity, the theory is predicting that the particular slab reactor being analyzed will be critical. If λ is not unity, we can determine what must be done to make the system critical. For example, if solution of the critical determinant associated with the above equation yields a value of λ greater than unity, we know from our earlier discussion that the reactor will be supercritical. We may then search for the critical conditions by decreasing the fuel loading, increasing a control poison, or increasing the leakage out of the reactor (i.e., decreasing L_x and hence increase $D(E)B_{x1}^2$." (Henry p. 134)

The final solution is then:

$$\Phi(x, E) = C_1\Psi(E) \sin B_{x1}x = C_1\Psi(E) \sin \frac{\pi x}{L}$$

Where the constant C is found by specifying a power level and integrating over the core volume.

7. <u>Non-Leakage Probability:</u>

The above group equation can be summed over all groups and then solved for λ. The result is:

$$\lambda \equiv k_{eff} = \frac{\sum_{g=1}^{G} \nu\Sigma_{fg}\Psi_g}{\sum_{g=1}^{G}\left[D_g B_{x1}^2 + \Sigma_{ag}\right]\Psi_g}$$

$$= \frac{1}{1+\left[\sum_{g=1}^{G} D_g\Psi_g / \sum_{g=1}^{G}\Sigma_{ag}\Psi_g\right]B_{x1}^2}\ \frac{\sum_{g=1}^{G}\nu\Sigma_{fg}\Psi_g}{\sum_{g=1}^{G}\Sigma_{ag}\Psi_g}$$

The quantity on the right $\left(\nu\Sigma_{fg}\Psi_g / \Sigma_{ag}\Psi_g\right)$ is k_∞. Thus, we have

$$k_{eff} = (1 - P_L)k_\infty$$

where P_L is defined as the leakage probability and $(1\text{-}P_L)$ is the non-leakage probability. Thus, P_L for a slab is:

$$P_L \equiv \frac{\left[\int_0^\infty D(E)\Psi(E)dE / \int_0^\infty \Sigma_a(E)\Psi(E)dE\right]B_{x1}^2}{1+\left[\int_0^\infty D(E)\Psi(E)dE / \int_0^\infty \Sigma_a(E)\Psi(E)dE\right]B_{x1}^2}$$

"As would be expected, the leakage probability P_L increases as $B_{x1}(\equiv \pi / L)$ increases (i.e., as the core thickness L decreases). It also increases as $\Sigma_a(E)$ decreases and as D(E) increases (and thus as $\Sigma_{tr}(E)$ decreases). Decreases in either $\Sigma_a(E)$ or $\Sigma_{tr}(E)$ permit neutrons to move further between interactions, and this leads to a greater probability that they will leak out of the reactor before an interaction can occur." (Henry, p. 145)

8. Summary

"To sum up the situation for the finite homogeneous reactor: the solution the continuous-energy diffusion equation for a bare, homogeneous reactor is

$$\Phi(\mathbf{r}, E) = R(\mathbf{r})\Psi(E),$$

Where $R(\mathbf{r})$ is the one everywhere-positive solution of

$$\nabla^2 R(\mathbf{r}) = -B_{\mathbf{r}}^2 R(\mathbf{r})$$

$R(\mathbf{r})$ being the shape of the flux and $B_{\mathbf{r}}^2$, the geometrical buckling (often simply called the buckling), being a number that depends on the geometry and dimensions of the reactor, and where the spectrum function $\Psi(E)$ is the solution of

$$\left[D(E)B_r^2 + \Sigma_t(E)\right]\Psi(E) = \int_0^\infty \left[\frac{1}{\lambda}\chi(E)\nu\Sigma_f(E') + \Sigma_s(E' \to E)\right]\Psi(E')$$

A sequence of steps for calculating the criticality of a bare core is as follows:

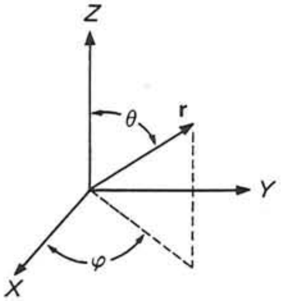
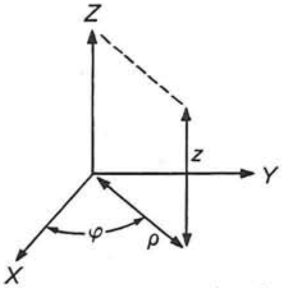
1. From the dimensions and geometry (assuming it is simple) obtain $B_{\mathbf{r}}^2$ and R(**r**) using the formulas given in the attached Table. (Note that for the bare core the spatial shape of the flux depends only on the geometry and not on the material constituents.)

2. Knowing $B_{\mathbf{r}}^2$, solve for λ and $\Psi(E)$.

3. If $\lambda \neq 1$, so that the reactor is not predicted to be critical, alter whatever parameter is adjustable (fuel loading, control-poison concentrations, size – i.e., $B_{\mathbf{r}}^2$) until λ=1.

For a large, bare, homogeneous reactor for which the leakage probability P_L is less than about 5 percent, the accuracy with which k_{eff} (i.e., λ) can be computed by this procedure (assuming cross-sections are known) is better than a few tenths of a percent. Thus, for the large, bare, homogeneous core, errors in predicting criticality due to nuclear data will almost always outweigh errors inherent in the use of the diffusion-theory approximations.” (Henry pp. 136-138)

Table 4.1 Expressions for the Laplacian, Flux Shape, and Geometrical Buckling of Bare, Homogeneous Reactors Having Simple Geometries

Geometry	∇^2	$R(\mathbf{r})$	$B_{\mathbf{r}}^2$
Rectangular parallelopiped of dimensions $L_x \times L_y \times L_z$	$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$	$C \sin \frac{\pi x}{L_x} \sin \frac{\pi y}{L_y} \sin \frac{\pi z}{L_z}$	$\left[\left(\frac{\pi}{L_x}\right)^2 + \left(\frac{\pi}{L_y}\right)^2 + \left(\frac{\pi}{L_z}\right)^2\right]$
Sphere of radius R 	$\frac{1}{r^2 \sin\theta}\left[\sin\theta \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2}{\partial \varphi^2}\right]$	$\frac{C \sin \frac{\pi r}{R}}{r}$	$\left(\frac{\pi}{R}\right)^2$
Cylinder of height L_z and radius R 	$\frac{1}{\rho}\left[\frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) + \frac{1}{\rho}\frac{\partial^2}{\partial \varphi^2} + \rho \frac{\partial^2}{\partial z^2}\right]$	$C J_0\left(\frac{2.405\,\rho}{R}\right) \sin \frac{\pi z}{L_z}$	$\left[\left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{L_z}\right)^2\right]$

From Henry, A. F. *Nuclear Reactor Analysis*. Cambridge, MA: MIT Press, 1975.
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