22.05 Reactor Physics - Part Twenty

Extension of Group Theory to Reactors of Multiple Regions
One Energy Group[*]

1. Background:

The objective remains to determine $\Phi(\mathbf{r}, \mathrm{E})$ for reactors of finite size. The first such case that we examined was a bare homogeneous core. The major steps in the solution were to:

- Modify the continuous energy diffusion equation, in which cross-section and flux were functions of **r** and E for a homogeneous medium. Hence, cross-sections become functions of E alone. Flux remains a function of **r** and E.
- Assume separability of the energy and spatial functions of the flux. That is $\Phi(\mathbf{r}, \mathrm{E}) = \mathrm{R}(\mathbf{r})\Psi(\mathbf{E})$.
- Substitute the separability assumption into the homogenized diffusion equation and separate terms so that a function of position equals a function of energy. This is only possible if both functions equal a constant. This constant is called the buckling, $\mathrm{B}_{\mathbf{r}}^2$.
- Solve for the spatial solution.
- Substitute the spatial solution into the homogenized diffusion equation.
- Define group constants within each energy group.
- Solve for the energy dependence of the flux.

This sequence is unique to a bare (unreflected) core and is **NOT** the general case. Specifically, for cores of multiple regions (fuel/moderator and reflector), the separability assumption does not hold. As a result, the sequence for obtaining a solution for $\Phi(\mathbf{r}, \mathrm{E})$ changes. In particular, the energy dependence is obtained before the spatial dependence.

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[*] Material in this section follows that of Henry pp 144-150. Portions that are verbatim are indicated by quotations.

The problem is considered here for a two region reactor with one energy group being assumed. In the next section of these notes, we consider a two region reactor with two energy groups. Finally, we extend the idea to multiple region reactors with multiple energy groups.

2. <u>One Energy Group:</u>

The term "one-group theory" is used to describe several different methods of solution in reactor physics. Earlier (Section 10 of these notes) we derived a one-velocity model and used it to solve for the spatial flux in bare cores. That approach is often called "one-group theory" because the single velocity corresponds to a single energy group. But, a distinction should be made between that derivation and what we will do next because, even though the result is the same, the method of derivation employed here is far more rigorous.

The starting point is the continuous energy diffusion equation which we restate below:

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

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

For a homogeneous medium, this becomes:

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

We wish to apply this equation to a two region reactor subject to the assumption that each region is homogeneous. Thus, we modify the above equation by adding a superscript k to each parameter (D, Σ_t, Σ_s, Σ_f, etc.). A given value of this superscript corresponds to a particular region. For example, k=1 might be core/moderator; k=2 might be reflector, k=3 might be shielding, etc. The equation becomes:

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

$$(k = 1, 2, 3, \ldots, K) \qquad \text{(A)}$$

For the case at hand, k = 2 because there are two physical regions. (<u>Note</u>: The "one" in one-group theory refers to the number of energy groups and hence there is one energy function $\Psi(\mathrm{E})$ that will apply to each region.) We can now see why the separability assumption (Φ (r,E)=R(r)ψ(E)) that was used for the homogeneous bare core (k=1) will not work for a multi-region reactor (k≥2). Each region has its own set of material properties (i.e., D^k, Σ^k, etc.) A single function $\psi(E)$ cannot satisfy k different sets of properties.

A preferred approach, and one that is viable, is to recognize that after a few collisions, neutron behavior is independent of neutron origin. Thus, the neutron energy spectrum in a given region should be characteristic of only the homogenized materials that are present in that region. Thus, we assume separability within each region. Here the word "within" implies a few mean paths inside a given region. Thus, we assume:

$$\Phi(\mathbf{r},E) \cong R^k(\mathbf{r})\Psi^k(E) \qquad \text{(B)}$$

Where $\Psi^k(E)$ is an energy spectrum function for region k.

This is the essential assumption of one-group diffusion theory. As a result of making it, we can further assume that, within a given region, the type of analysis done for the bare homogeneous reactor remains relevant. Thus, "the essential strategy of one-group diffusion theory is: 1) assume that separabilty (equation B above) is valid within each region k; 2) find an appropriate spectrum function $\psi^k(E)$ for each region; and 3) connect the spatial function $R^k(r)$ for each region to the corresponding spatial functions of neighboring regions." (Henry, p. 146).

Given the above strategy, we expect that the leakage term can be approximated as:

$$-\nabla \cdot D^k(E)\,\nabla\Phi(\mathbf{r},E) = D^k(E)\left(B_m^k\right)^2 \Phi(\mathbf{r},E)$$

Where $\left(B_m^k\right)^2$ is a number and is called the materials buckling. For the single region reactor, we encountered a similar quantity, B_r^2, which depended on the geometry of the reactor and was termed the "geometric buckling." The materials buckling is different. Specifically, $\left(B_m^k\right)^2$ has nothing to do with either the geometry of the reactor or of an individual region. It is found by recognizing that each region k is part of a critical reactor for which λ is unity. Hence, $\left(B_m^k\right)^2$ is found by writing the homogeneous diffusion equation for each region as:

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

for $\mathbf{r}$ in the interior of region k, and selecting $\left(B_m^k\right)^2$ as the eigenvalue that yields an everywhere positive solution for the flux. It is important to understand the physical meaning of this number and we quote from Henry (p. 146):

"The number $\left(B_m^k\right)^2$ is characteristic of the mixture of materials making up region k and, for that reason, is called the materials buckling. Mathematically it is an eigenvalue of the homogeneous equation. As can be seen from that equation, its effect on neutron balance is to regulate the leakage rate so that the portion of the reactor in the interior of region k behaves in a sustained, critical fashion. If the k_∞ of that region exceeds unity, the number of neutrons removed from dE dV per second by out-leakage, scattering, and absorption will equal the number introduced into dE dV by fissioning and scattering from other energies; while, if the k_∞ is less than unity, the number removed by scattering and absorption will equal the number introduced by fissioning, scattering, and leakage into the region. Thus, if the k_∞ for region-k material is less than unity, $\left(B_m^k\right)^2$ will be a negative number so that the extra neutrons needed for overall balance will be supplied by negative leakage, i.e., by net leakage into dV. In reflector material, for which $\nu\Sigma_f(E) = 0$, $\left(B_m^k\right)^2$ will always be negative." (Henry, pp. 146-147)

We now substitute $\Phi(\mathbf{r}, E) = R^k(\mathbf{r})\Psi^k(E)$ into the modified homogeneous diffusion equation for region k, eliminate the spatial function, and obtain:

$$D^k(E)\left(B_m^k\right)^2\Psi^k(E) + \Sigma_t^k(E)\Psi^k(E) = \int_0^\infty \left[\chi^k(E)\nu\Sigma_f^k(E') + \Sigma_s^k(E' \to E)\right]\Psi^k(E')dE' \tag{C}$$

This relation can be solved using the methods developed earlier (Section 16 of these notes) to find $\Psi(E)$. It will be recalled that the approach is to divide the energy range (0-10 MeV) into G groups where G might be as large as 3000. The width of each group, ΔE_g, is selected so that cross-section properties will be constant over that group. This allows a further assumption that the flux $\Psi(E)$ will be constant over each group. Group constants can now be defined. These are of the form:

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

$$\Sigma_{tg} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(E)\Psi(E)dE}{\Psi_g}$$

Note that these group constants are defined: 1) for an assumed flux shape, $\Psi(E)$ and 2) a narrow energy range, ΔE_g. This will be in contrast to a different set of group constants that we will define later when we solve for spatial flux shape. Use of the above group constants allows us to rewrite Equation (C) as a set of algebraic relations, which are readily solvable numerically.

So, at this point we can obtain $\Psi(\mathrm{E})$. The objective therefore becomes to obtain the spatial flux shape. Thus far the derivation has been rigorous. But a problem now arises in that we have to treat the interfaces between regions. The preferred boundary conditions are the standard ones that flux and the normal component of the current be continuous at all energies. However, this isn't possible because the $\Psi(\mathrm{E})$ differ for each region. To quote Henry (p. 147), "The basic problem is that the separable forms $\mathrm{R}^{\mathrm{k}}(\mathbf{r})\Psi^{\mathrm{k}}(\mathrm{E})$ (k=1,2,…K,), which are good approximations to $\Phi(\mathbf{r},\mathrm{E})$ in the interior portions of the regions, *cannot* be valid near interfaces between regions, since, if superscripts k and *l* designate two adjacent regions of different composition so that $\Psi^{\mathrm{k}}(\mathrm{E})$ and $\Psi^{l}(\mathrm{E})$ are different functions of E, then, if $\mathbf{r}_c$ is any point on the interface between these regions, $\mathrm{R}^{\mathrm{k}}(\mathbf{r}_{\mathrm{c}})\Psi^{\mathrm{k}}(\mathrm{E})$ cannot equal $\mathrm{R}^{1}(\mathbf{r}_{\mathrm{c}})\Psi^{1}(\mathrm{E})$ for all energies. (If it did, then $\Psi^{\mathrm{k}}(\mathrm{E})$ would have to have the same energy shape $\Psi^{1}(\mathrm{E})$. Thus, assuming that the separable form $\mathrm{R}^{\mathrm{k}}(\mathbf{r})\Psi^{\mathrm{k}}(\mathrm{E})$ is valid throughout each region k makes it impossible to meet the continuity-of-flux boundary condition at the interface between regions." The best one can do is to adopt "the much weaker boundary condition that the integrals over all energies of $\Phi(\mathbf{r},\mathrm{E})$ and $\mathbf{n}\cdot\nabla\Phi(\mathbf{r},\mathrm{E})$ be continuous. This boundary condition is entirely consistent with the continuity of $\Phi(\mathbf{r},\mathrm{E})$ and $\mathbf{n}\cdot \mathrm{D}\nabla\Phi(\mathbf{r},\mathrm{E})$ at all energies since, if there were continuity at each energy, the integrals over all energies would certainly be continuous. (The reverse implication cannot, of course, be drawn.)

To be specific, one-group theory is based on the following assumptions:

1. $\Phi(\mathbf{r},\mathrm{E}) = \mathrm{R}^{\mathrm{k}}(\mathrm{r})\Psi^{\mathrm{k}}(\mathrm{E})$ throughout each composition k, $\Psi^{\mathrm{k}}(\mathrm{E})$ being found by solving Equation C as described above.

2. If k and *l* indicate any two adjacent compositions and $\mathbf{r}_c$ is a point on the interface, we require that

   $$\int_0^\infty \mathrm{dE}\ \mathrm{R}^{\mathrm{k}}(\mathbf{r}_{\mathrm{c}})\Psi^{\mathrm{k}}(\mathrm{E}) = \int_0^\infty \mathrm{dE}\ \mathrm{R}^{1}(\mathbf{r}_{\mathrm{c}})\Psi^{1}(\mathrm{E})$$

   and

   $$\int_0^\infty \mathrm{dE}\ \mathbf{n}_{\mathrm{k}}\cdot \mathrm{D}^{\mathrm{k}}(\mathrm{E})\nabla\left[\mathrm{R}^{\mathrm{k}}(\mathbf{r}_{\mathrm{c}})\Psi^{\mathrm{k}}(\mathrm{E})\right] = \int_0^\infty \mathrm{dE}\,\mathbf{n}_{\mathrm{k}}\cdot \mathrm{D}^{1}(\mathrm{E})\nabla\left[\mathrm{R}^{1}(\mathbf{r}_{\mathrm{c}})\Psi^{1}(\mathrm{E})\right]$$

   Note: If $\Psi(\mathrm{E})$ is normalized so that $\int_0^\infty \Psi(\mathrm{E})\mathrm{dE} = 1$, then these conditions become:

$$R^k(\mathbf{r}_c) = R^1(\mathbf{r}_c)$$

and

$$\left[\int_0^\infty D^k(E)\Psi^k(E)dE\right]\mathbf{n}_k \cdot \nabla R^k(\mathbf{r}_c) = \left[\int_0^\infty D^1(E)\Psi^1(E)dE\right]\mathbf{n}_k \cdot \nabla R^1(\mathbf{r}_c)$$

We now substitute the separability relation (equation labeled as B above) into the homogenized diffusion equation for each region (equation labeled as (A) above) and integrate over all energies so as to comply with the boundary conditions. The result is:

$$-\nabla \cdot \left[\int_0^\infty D^k(E)\Psi^k(E)dE\right]\nabla R^k(\mathbf{r}) + \left[\int_0^\infty \Sigma_t^k(E)\Psi^k(E)dE\right]R^k(\mathbf{r})$$

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

$$= \frac{1}{\lambda}\left[\int_0^\infty \nu\Sigma_f^k(E')\Psi^k(E')dE'\right]R^k(\mathbf{r}) + \left[\int_0^\infty \Sigma_s^k(E')\Psi^k(E')dE'\right]R^k(\mathbf{r})$$

(D)

Next, we define a set of one-group cross-sections:

$$D^k \equiv \int_0^\infty D^k(E')\Psi^k(E)dE$$

$$\Sigma_t^k \equiv \int_0^\infty \Sigma_t^k(E')\Psi^k(E)dE$$

$$\nu\Sigma_t^k \equiv \int_0^\infty \nu\Sigma_t^k(E')\Psi^k(E)dE$$

$$\Sigma_s^k \equiv \int_0^\infty \Sigma_s^k(E')\Psi^k(E)dE$$

$$\Sigma^k \equiv \Sigma_t^k - \Sigma_s^k = \Sigma_a^k$$

These numbers are independent of both space and energy. They may be computed for any region k once we have determined the nuclear concentrations n^j and the microscopic cross-section $\sigma^j(E)$ of the material in region k and have obtained the spectrum functions $\Psi^k(E)$.” (Henry, pp. 144-149)

It is important to recognize the differences between these group constants that are used to obtain the spatial flux shape from the ones defined earlier to obtain the energy flux shape. First, the current group constants (spatial calculations) are integrated over a very wide energy range. Here, that range is 0 to ∞. The more common ranges and the ones that we use later on are thermal, epithermal, and fast. Second, the shape of $\Psi^k(E)$ is known. This is what allows evaluation of the integration over such wide ranges.

One other clarification is appropriate. The word "group" as used here refers to the number of energy ranges over which the above integrations are performed. For the present set of lecture notes, there is one range (0 to ∞) and hence one group. The more common approach, as is already noted, is for three ranges (thermal, epithermal, and fast) and hence three groups.

"Upon substitution of those one-group cross-sections, we obtain:

$$-\nabla \cdot D^k \nabla R^k(\mathbf{r}) + \Sigma^k R^k(\mathbf{r}) = \frac{1}{\lambda} \nu \Sigma_f^k R^k(\mathbf{r})$$

With boundary conditions:

$$R^k(\mathbf{r}_c) = R^1(\mathbf{r}_c)$$

$$\mathbf{n}_k \cdot D^k \nabla R^k(\mathbf{r}_c) = \mathbf{n}_k \cdot D^1 \nabla R^1(\mathbf{r}_c)$$

The condition that the flux is to vanish on the external surface of the reactor is met by requiring that the appropriate $R^k(\mathbf{r})$ vanish for any $\mathbf{r}$ on that surface.

Finally, since $R^k(\mathbf{r})$ is everywhere continuous throughout the reactor, the superscript k is redundant. The point $\mathbf{r}$ automatically specifies the region k. Accordingly, we shall replace all the $R^k(\mathbf{r})$ by the single function $\Phi(\mathbf{r})$, the one-group scalar flux. (Note that $\Phi(\mathbf{r})$ is not a flux per unit energy; its units are (speed) x (neutrons/cc) = neutrons per square cm per sec.)

With this change in notation the one-group diffusion equation for a reactor composed of several homogeneous regions becomes

$$-\nabla \cdot D^k \nabla \Phi(\mathbf{r}) + \Sigma^k \Phi(\mathbf{r}) = \frac{1}{\lambda} \nu \Sigma_f^k \Phi(\mathbf{r})$$

With the following boundary conditions:

1. $\Phi(r)$ and the normal component $n \cdot D \nabla \Phi(\mathbf{r})$ are continuous across interfaces between different compositions;

2. $\Phi(\mathbf{r}) = 0$ on the outer boundary of the reactor.

The above equation is sometimes called the one-velocity diffusion equation since it can also be derived by assuming that all the neutrons are traveling at a single speed. The trouble with that approach is that it provides no systematic procedure for finding the one-group constants D^k, Σ^k, and $\nu\Sigma_f^k$, and makes it hard to account for such effects as fast fission, resonance capture, and fast-neutron leakage. It also makes one-group theory appear much cruder than it actually is. According to the view we have adopted, the one-group theory actually provides a very detailed energy-dependent flux, namely, $\Psi^k(E)\Phi(\mathbf{r})$, in each region. The essential approximation consists of a very crude treatment of the "transition zones" between the different material compositions. In these zones the true scalar flux density $\Phi(\mathbf{r},E)$ actually changes gradually from the $\Psi^k(E)$ appropriate to the interior parts of one region to that appropriate to the interior parts of the next. We replace this gradual change by an abrupt one and in so doing make an error in the net leakage rate from one region to the next." (Henry, pp. 149-150)

It is important to recognize that for this multi-region reactor example, the spectral (or energy) functions are identified before the spatial solution is obtained. The latter is done numerically using finite difference equations.

3. Summary

1. Consider the reactor that is to be analyzed and the desired accuracy of the solution. Determine:

    a) The number of distinct regions into which the reactors will be divided (i.e., fuel/moderator; reflector; shield)

    b) The number of energy groups that will be used when obtaining the shape of the spatial flux. (Note: The number used to determine the shape of the energy flux is normally several thousand.)

2. Write out the continuous energy diffusion equation for each region. Assume homogeneity within each region.

3. Assume separability of the flux (i.e., $\Phi(\mathbf{r},E) \cong R(\mathbf{r})\Psi(E)$) within each region.

4. Approximate the leakage term via the relation:

$$-\nabla \cdot D^k(E)\,\nabla\Phi(\mathbf{r},E) = D^k(E)\left(B_m^k\right)^2 \Phi(\mathbf{r},E)$$

This is obtained by analogy with the bare homogeneous case where we were able to solve directly for the spatial part.

5. Substitute separability (step 3) into the equation step (4) and eliminate R(**r**). Solve the resulting equation for $\Psi(E)$ by dividing the full energy range into several thousand groups, taking the flux shape as constant over each group, and defining group constants over each ΔE_g.

6. Select boundary conditions in an integral sense. The range(s) of integration on the boundary conditions is the same as the range(s) chosen for the number of energy groups used to compute the spatial flux.

7. Combine the separability relation, the solution for $\Psi(E)$, and the definitions of the boundary conditions to obtain the equation labeled as "D" in the notes.

8. Define a set of group cross-sections that are to be integrated over the energy range(s) selected for the spatial flux determination. Evaluate these group constants – this is possible because $\Psi(E)$ is now known.

9. Rewrite the integral equation labeled as "D" as a set of algebraic ones. Solve, numerically.

10. Readjust fuel concentrations, etc., and repeat the calculations until a design for which $\lambda=1$ is obtained. When designing an actual reactor, it is common practice to do steps (1) – (5) of the above sequence only once. It is then assumed that $\Psi(E)$ is insensitive to small changes in material concentrations and/or geometry. Steps (6) – (10) are then done many times until a critical configuration is identified. This approach reduces computer time because Step 5 which involves thousands of groups is only done once.