

NE 250, F17
September 14, 2017

During the diffusion equation derivation we obtained two equations using the P_1 approximation: one for scalar flux and one for current. We then made a few simplifications / assumptions (full list of assumptions in the DE derivation):

- The angular flux can be represented by **linearly anisotropic** angular dependence (that is the P_1 expansion). The approximation is valid away from boundaries, away from neutron sources and sinks, and in media that are not highly absorbing.
- one speed (not essential to the derivation).
- isotropic source, azimuthally symmetric scattering, and scattering is at most linearly anisotropic.
- neutron current density changes slowly on a time scale compared to the mean collision time. Mathematically, this statement can be written as

$$\frac{1}{|\vec{J}(\vec{r}, t)|} \frac{\partial \vec{J}(\vec{r}, t)}{\partial t} \ll v\Sigma_t ;$$
$$\frac{1}{|\vec{J}(\vec{r}, t)|} \frac{\partial \vec{J}(\vec{r}, t)}{\partial t} \approx 0 .$$

The collision frequency $v\Sigma_t$ is typically on the order of 10^5 sec^{-1} or larger, so only an extremely rapid time variation of the current would invalidate this assumption (such rapid changes are very rarely encountered in reactor dynamics).

All of that got us to *Fick's law* and *the one-speed diffusion equation*.

$$\frac{1}{v} \frac{\partial \phi(\vec{r}, t)}{\partial t} = S(\vec{r}, t) - \Sigma_a(\vec{r})\phi(\vec{r}, t) + \nabla \cdot [D(\vec{r})\nabla \phi(\vec{r}, t)],$$

We talked about the boundary conditions necessary to solve this equation last time.

Now, let's revisit the the energy-dependent P_1 equations:

$$\begin{aligned}\frac{1}{v} \frac{\partial \phi(\vec{r}, E, t)}{\partial t} &= S(\vec{r}, E, t) + \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) - \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, t) \\ &\quad - \nabla \cdot \vec{J}(\vec{r}, E, t) \\ \frac{1}{v} \frac{\partial \vec{J}(\vec{r}, E, t)}{\partial t} &= S_1(\vec{r}, E, t) + \int_0^\infty dE' \bar{\mu}_0 \Sigma_s(\vec{r}, E' \rightarrow E) \vec{J}(\vec{r}, E', t) - \Sigma_t(\vec{r}, E) \vec{J}(\vec{r}, E, t) \\ &\quad - \frac{1}{3} \nabla \phi(\vec{r}, E, t)\end{aligned}$$

From the $\frac{1}{|\vec{J}(\vec{r}, t)|} \frac{\partial \vec{J}(\vec{r}, t)}{\partial t} \ll v \Sigma_t$ assumption, $\frac{1}{v} \frac{\partial \vec{J}(\vec{r}, t)}{\partial t} = 0$.

From the isotropic source assumption, $S_1(\vec{r}, E, t) = 0$.

The assumption of isotropic scattering would give $\Sigma_{s1}(E' \rightarrow E) = 0$, which results in

$$\vec{J}(\vec{r}, E, t) \approx -\frac{1}{3\Sigma_t(\vec{r}, E)} \nabla \phi(\vec{r}, E, t) .$$

However, the assumption of isotropic scattering is often too strong for most reactor calculations.

Instead, we can define an energy-dependent diffusion coefficient as

$$D(\vec{r}, E) = \frac{1}{3} \left[\Sigma_t(\vec{r}, E) - \frac{\int_0^\infty dE' \Sigma_{s1}(\vec{r}, E' \rightarrow E) J_i(\vec{r}, E', t)}{J_i(\vec{r}, E, t)} \right]^{-1} ,$$

which would automatically yield

$$\vec{J}(\vec{r}, E, t) = -D(\vec{r}, E) \nabla \phi(\vec{r}, E, t) .$$

[Note that $i = x, y, z$. We need to do each vector component separately since D is a scalar, and then recombine to get $\vec{J} = J_x \Omega_x + J_y \Omega_y + J_z \Omega_z$.]

This is artificial because D actually depends on \vec{J} .

One common way to avoid this issue is to neglect the anisotropic contribution to energy transfer in the scattering collision by saying

$$\Sigma_{s1}(\vec{r}, E' \rightarrow E) = \Sigma_{s1}(\vec{r}, E) \delta(E' - E)$$

such that

$$\int_0^\infty dE' \Sigma_{s1}(\vec{r}, E' \rightarrow E) J_i(\vec{r}, E', t) = \bar{\mu}_0 \Sigma_s(\vec{r}, E) J_i(\vec{r}, E, t) .$$

And all of that gives

$$D(\vec{r}, E) = \frac{1}{3} [\Sigma_t(\vec{r}, E) - \bar{\mu}_0 \Sigma_s(\vec{r}, E)]^{-1}.$$

Plugging this into the first P_1 equation gives

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi(\vec{r}, E, t)}{\partial t} = & S(\vec{r}, E, t) + \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) - \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, t) \\ & + \nabla \cdot [D(\vec{r}, E) \nabla \phi(\vec{r}, E, t)]. \end{aligned}$$

Now, let's make the *one-group* (not one-speed) assumption. This means that we will integrate the entire equation over all energy space $[\int_0^\infty dE(\cdot)]$; we will often weight this integration with the flux (more discussion on this later).

“Group constants” are defined as follows (note that subscripts are now group number, not expansion coefficient or anything else):

$$\begin{aligned} \Sigma_{t,1}(\vec{r}) &= \frac{\int_0^\infty dE \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, t)}{\int_0^\infty dE \phi(\vec{r}, E, t)} = \text{effective group cross section} \\ \phi_1(\vec{r}, t) &= \int_0^\infty dE \phi(\vec{r}, E, t) = \text{group flux} \end{aligned}$$

Thus, $\int_0^\infty dE \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, t) = \Sigma_{t,1}(\vec{r}) \phi_1(\vec{r}, t)$.

We can use the same process for the other terms:

$$\begin{aligned} \int_0^\infty dE \frac{1}{v} \frac{\partial \phi(\vec{r}, E, t)}{\partial t} &= \frac{1}{v_1} \frac{\partial \phi_1(\vec{r}, t)}{\partial t}, \\ \text{where } \frac{1}{v_1} &= \frac{\int_0^\infty dE \frac{1}{v} \phi(\vec{r}, E, t)}{\phi_1(\vec{r}, t)} \end{aligned}$$

$$\int_0^\infty dE S(\vec{r}, E, t) = S_1(\vec{r}, t)$$

$$\int_0^\infty dE \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) = \int_0^\infty dE' \Sigma_s(\vec{r}, E') \phi(\vec{r}, E', t) = \Sigma_{s,1} \phi_1$$

$$\int_0^\infty dE \nabla \cdot [D(\vec{r}, E) \nabla \phi(\vec{r}, E, t)] = \nabla \cdot [D_1(\vec{r}) \nabla \phi_1(\vec{r}, t)]$$

Note again that although the subscripts used here for the one-group approximation look the same as those used in the P_1 approximation derivation, the quantities are not the same (group index vs. Legendre series expansion index). Combining all of the above terms, we have

$$\frac{1}{v_1} \frac{\partial \phi_1(\vec{r}, t)}{\partial t} = S_1(\vec{r}, t) - \Sigma_{a,1}(\vec{r}) \phi_1(\vec{r}, t) + \nabla \cdot [D_1(\vec{r}) \nabla \phi_1(\vec{r}, t)] ,$$

which is the *one-group* diffusion equation.

We were talking about currents and boundary conditions at the end of last class, so let's quickly revisit that.

For the TE, the one-group vacuum boundary condition is $\psi_1(\vec{r}_s, \hat{\Omega}, t) = 0$ for $\hat{\Omega} \cdot d\vec{S} < 0, \forall \vec{r}_s$ on \vec{S} .

We will seek to satisfy this in an integral sense for the diffusion equation, remembering that

$$J_{\pm,1} = \int_{2\pi^\pm} d\hat{\Omega} \hat{\Omega} \cdot \hat{e}_s \psi_1(\vec{r}, E, \hat{\Omega}, t) .$$

Therefore, $J_{-,1}(\vec{r}_s, t) = 0$.

Using the P_1 approximation for this, then

$$J_{-,1} = \int_{2\pi^-} d\hat{\Omega} \hat{\Omega} \cdot \hat{e}_s \psi_1(\vec{r}, E, \hat{\Omega}, t) \approx \frac{1}{4} \phi_1(\vec{r}, t) + \frac{D_1(\vec{r})}{2} \hat{e}_s \cdot \nabla \phi_1(\vec{r}, t) = 0 .$$

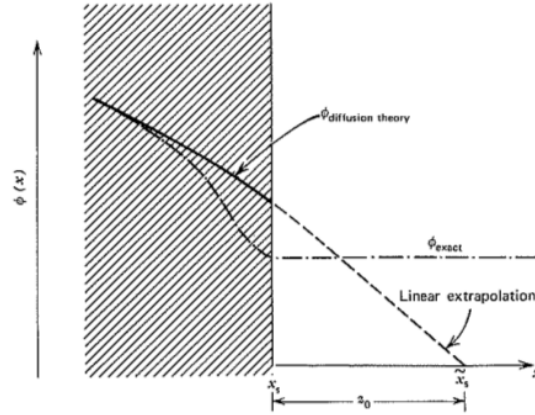
In 1D,

$$J_{-,1}(z_s, t) = \frac{1}{4} \phi_1(z_s, t) + \frac{D_1(z_s)}{2} \frac{d\phi_1(z_s, t)}{dz} \Big|_{z_s} = 0$$

$$\frac{d\phi_1(z_s, t)}{dz} \Big|_{z_s} = \frac{-\phi_1(z_s, t)}{2D_1(z_s)}$$

In order to use the diffusion approximation, we must accept that the above solution at the vacuum is wrong, necessitating the introduction of an extrapolation distance:

$$\tilde{z}_s = z_s + 2D_1(z_s)$$



We therefore typically use the boundary condition $\phi(\tilde{z}_s) = 0$. Note again that a more accurate extrapolation distance that is obtained from transport theory is $\tilde{z}_s = z_s + z_0$; $z_0 = 0.7104\lambda_{tr}$.

There are a few other types of conditions we might encounter or apply (the same as before; taking the P_1 approach more explicitly combined with the one-group assumption doesn't change the conditions):

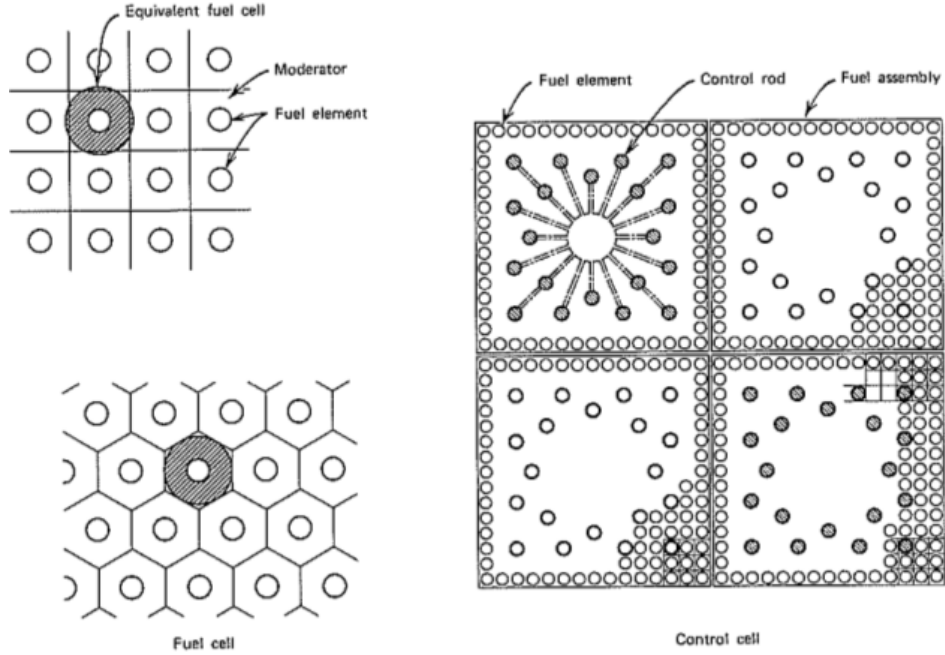
- We know that the flux must be nonnegative, finite, and real.
- Symmetry often lets us eliminate solutions that don't make physical sense (e.g. at the centerline of a slab we know that $\phi(-x) \neq -\phi(x)$).
- We use *unit cells* or *control cells* that are repeated in a regular fashion. One can argue that there should be no net transfer of neutrons between cells, so $\vec{J}(\vec{r})$ vanishes on those boundaries.
- When these cells are near strong absorbers, we usually end up doing a transport correction to get more accurate boundary conditions. (Note that within the derivation of the DE, we used transport corrections in some occasions to make it more accurate.)

A quick one-speed diffusion summary:

$$\frac{1}{v} \frac{\partial \phi}{\partial t} = S(\vec{r}, t) + \Sigma_a(\vec{r})\phi(\vec{r}, t) + \nabla \cdot D(\vec{r})\nabla \phi(\vec{r}, t) ,$$

where

- $\phi(\vec{r}, 0) = \phi_0(\vec{r}) \forall \vec{r}$
- $\phi(\tilde{r}_s, t) = 0$ or $J_-(\vec{r}_s, t) = 0$; (free surface)



- ϕ and the normal component of \vec{J} are continuous across surfaces
- $0 \leq \phi(\vec{r}, t) < \infty$ (except near localized sources).
- $D = \lambda_{tr}/3 = [3(\Sigma_{tr} - \bar{\mu}_0 \Sigma_s)]^{-1}$
- $\vec{r}_0 = 0.7104 \lambda_{tr}$.

This equation is **parabolic**. Equations of this form apply to heat conduction, gas diffusion, the wave function, etc.

If we are in a situation where the materials are homogeneous, we drop \vec{r} dependence in all of the coefficients (we can then bring the ∇ inside the D). We also frequently neglect time dependence. In this case:

$$\begin{aligned}
 -D \nabla^2 \phi(\vec{r}) + \Sigma_a \phi(\vec{r}) &= S(\vec{r}) \\
 \nabla^2 \phi(\vec{r}) - \frac{1}{L^2} \phi(\vec{r}) &= \frac{S(\vec{r})}{D}
 \end{aligned}$$

this second equation is in *Helmholtz form*; which we use to take advantage of common mathematical solution techniques. Note that L is the neutron diffusion length

$$L \equiv \sqrt{\frac{D}{\Sigma_a}},$$

which is a measure of how far neutrons diffuse before they are absorbed.