Chapter 4: The Diffusion Equation

4.1. Introduction

We have seen that the transport equation is exact, but difficult to solve. Moreover, we only really need the scalar flux $\phi(\vec{r}, E, t)$, since we really want to compute reaction rates $\Sigma.\phi$. In order to obtain that, we must then use the diffusion equation. This is, numerically and mathematically speaking, well known. The diffusion equation is an approximation of the transport equation. It gives good results for diffusive problems (neutrons undergoing a lot of collisions), far from heterogeneities. Thermal reactors are currently computed with two group diffusion.

4.2. The Diffusion Equation

The angular flux introduced during the first lecture is actually more than we usually need. In most cases we are happy with just the scalar flux $\phi(\vec{r})$.
Recall that:

$$\phi(\vec{r}, E, t) = \int_{4\pi} d^2\,\Omega.\Psi(\vec{r}, E, \hat{\Omega}, t)$$

In order to derive an equation $\phi(\vec{r})$, we integrate the transport equation over all angles:

$$\int_{4\pi} d^2\,\Omega.\boldsymbol{B}.\Psi(\vec{r}, E, \hat{\Omega}, t)$$

where **B** is the Boltzmann equation.

$$\int_{4\pi} d^2\,\vec{\Omega}\left(\vec{\Omega}.\vec{\nabla}\Psi + \Sigma(\vec{r})\Psi(\vec{r},\vec{\Omega}) = \int_{4\pi} d^2\vec{\Omega}.\Sigma_s\left(\vec{r},\vec{\Omega}.\vec{\Omega'}\right)\Psi\left(\vec{r},\vec{\Omega'}\right) + s(\vec{r},\vec{\Omega})\right)$$

1 2 3 4

1 $$\int_{4\pi} d^2\Omega\,\hat{\Omega}\cdot\bar{\nabla}\psi(\bar{r},\hat{\Omega}) = \bar{\nabla}\cdot\bar{J}(\bar{r})$$

2 $$\int_{4\pi} d^2\Omega\,\Sigma(\bar{r})\psi(\bar{r},\hat{\Omega}) = \Sigma(\bar{r})\phi(\bar{r})$$

3 $$\int_{4\pi} d^2\Omega \int_{4\pi} d^2\Omega'\,\Sigma_s(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')\psi(\bar{r},\hat{\Omega}') = \int_{4\pi} d^2\Omega'\,\psi(\bar{r},\hat{\Omega}') \int_{4\pi} d^2\Omega\,\Sigma_s(\bar{r},\hat{\Omega}\cdot\hat{\Omega}') = \Sigma_s(\bar{r})\phi(\bar{r})$$

4 $$\int_{4\pi} d^2\bar{\Omega}\,s(\bar{r},\bar{\Omega}) = S(\bar{r})$$

Thus, we obtain:

$$\bar{\nabla}\cdot\bar{J} + \Sigma_a(\bar{r})\phi(\bar{r}) = S(\bar{r})$$

Note that in this equation, $\Sigma_a = \Sigma - \Sigma_s$

We can see that the final result has two unknowns, J and ϕ. We now need an equation for the current J. Let's multiply the transport equation by Ω, and then integrate over all angles:

$$\int_{4\pi} d^2\Omega\,\hat{\Omega}\left(\hat{\Omega}\cdot\bar{\nabla}\psi + \Sigma(\bar{r})\psi(\bar{r},\hat{\Omega}) = \int_{4\pi} d^2\Omega'\,\Sigma_s(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')\psi(\bar{r},\hat{\Omega}') + s(\bar{r},\hat{\Omega})\right)$$

That yields to:

1 $$\int_{4\pi} d^2\Omega\,\hat{\Omega}\hat{\Omega}\cdot\bar{\nabla}\psi(\bar{r},\hat{\Omega}) = \bar{\nabla}\cdot\mathbf{\Pi}(\bar{r})$$

2 $$\int_{4\pi} d^2\Omega\,\hat{\Omega}\Sigma(\bar{r})\psi(\bar{r},\hat{\Omega}) = \Sigma(\bar{r})\bar{J}(\bar{r})$$

3 $$\int_{4\pi} d^2\Omega\,\hat{\Omega} \int_{4\pi} d^2\Omega'\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\psi(\bar{r},\hat{\Omega}') = \int_{4\pi} d^2\Omega'\psi(\bar{r},\hat{\Omega}') \int_{4\pi} d^2\Omega\,\hat{\Omega}\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) = \int_{4\pi} d^2\Omega'\psi(\bar{r},\hat{\Omega}')\bar{\mu}_0\Sigma_s\hat{\Omega}'$$

$$= \bar{\mu}_0\Sigma_s\bar{J}(\bar{r})$$

4. $$\int_{4\pi} d^2\Omega \hat{\Omega} s(\bar{r},\hat{\Omega}) = \bar{S}_1(\bar{r})$$

Thus, we obtain:

$$\bar{\nabla} \cdot \mathbf{\Pi} + \Sigma(\bar{r})\bar{J}(\bar{r}) = \overline{\mu}_0 \Sigma_s(\bar{r})\bar{J}(\bar{r}) + \bar{S}_1(\bar{r})$$

Some definitions are needed here:

$$\overline{\mu}_0 = \left\langle \hat{\Omega} \cdot \hat{\Omega}' \right\rangle$$

This is the average cosine of the neutron deflection angle in a collision.

$$\mathbf{\Pi}(\bar{r}) = \int_{4\pi} d^2\Omega \hat{\Omega}\hat{\Omega} \psi(\bar{r},\hat{\Omega})$$ ⟵ *new unknown*

Matrix 3×3 ⟶ $$(\Pi)_{ij} = \int_{4\pi} d^2\Omega \Omega_i \Omega_j \psi(\bar{r},\hat{\Omega})$$

For each new moment of the transport equation we take, a new unknown appears… We then need a closure relation: the flux dependence on angle is weak.

$$\psi(\bar{r},\hat{\Omega}) \approx A(\bar{r}) + \bar{B}(\bar{r}) \cdot \hat{\Omega}$$ ⟵ *Linear dependence on* $\boldsymbol{\Omega}$

We will be able to use those results:

$$\int_{4\pi} d^2\Omega = 4\pi \qquad \int_{4\pi} d^2\Omega \hat{\Omega} = \bar{0} \qquad \int_{4\pi} d^2\Omega \hat{\Omega}\hat{\Omega} = \frac{4\pi}{3}\mathbf{Id}_3$$

Identity matrix 3×3

We then obtain:

$$\psi(\bar{r},\hat{\Omega}) \approx \frac{1}{4\pi}\phi(\bar{r}) + \frac{3}{4\pi}\bar{J}(\bar{r}) \cdot \hat{\Omega}$$

$$\bar{\nabla} \cdot \mathbf{\Pi}(\bar{r}) \approx \frac{1}{3}\bar{\nabla}\phi(\bar{r})$$

We have now computed what is known as the P_1 equations:

$$\begin{cases} \bar{\nabla} \cdot \bar{J} + \Sigma_a \phi(\bar{r}) = S(\bar{r}) \\ \frac{1}{3} \bar{\nabla} \phi + \Sigma_{tr} \bar{J}(\bar{r}) = \bar{S}_1(\bar{r}) \end{cases}$$

where we have defined the transport cross-section as:

$$\Sigma_{tr} = \Sigma - \overline{\mu}_0 \Sigma_s$$

If now we consider that we have isotropic sources, then $S_1 = 0$, and we can solve the second equation for $\vec{J}$:

$$\bar{J} = -\frac{1}{3\Sigma_{tr}} \bar{\nabla} \phi = -D \bar{\nabla} \phi$$

Diffusion coefficient

This is known as the Fick's law, from this good fellow on the right.
This allows us to finally derive the diffusion equation:

Adolf Eugen Fick
(1829-1901)

$$-\bar{\nabla} \cdot D(\bar{r}) \bar{\nabla} \phi + \Sigma_a(\bar{r}) \phi(\bar{r}) = S(\bar{r})$$

where $D = \frac{1}{3\Sigma_{tr}} = \frac{1}{3(\Sigma_t - \overline{\mu}_0 \Sigma_s)}$

So, here we are, with the diffusion equation. I hope you remember the second lecture, and the quite ugly transport equation. This is much better, isn't it? This equation is a differential equation of the second order, in a 3-dimensional phase space. Plus, the scientific community has a very large experience in the numerical resolution of this equation.

One must however know that if you approximate the transport equation, you have to lose some precision and to limit the applicability field. In the case of the diffusion equation, we used the Fick's law. This is valid for a diffusive medium. That means that the neutrons need to have a lot of collisions in order for the flux to be almost isotropic. We then need two things:

- $\Sigma_a \ll \Sigma_s$
- Not much leakage

The diffusion is not a very good approximation where the flux gradient is big:

$$\left.\begin{aligned}\phi(\bar{r}) &= \int_{4\pi} d^2\Omega\,\psi(\bar{r},\hat{\Omega}) \\ \bar{J}(\bar{r}) &= \int_{4\pi} d^2\Omega\,\hat{\Omega}\,\psi(\bar{r},\hat{\Omega})\end{aligned}\right\} \Rightarrow \left|\bar{J}\right| \le \phi \quad \left(\text{Fick} : \left|\bar{J}\right| = D\left|\bar{\nabla}\phi\right|\right)$$

Some variants of the diffusion equation exist which are flux-limited: in this case, the diffusion coefficient depends on the flux and its gradient.

The solution to the diffusion equation approaches the asymptotic mode of the solution to the transport equation, but it neglects the boundary layers. That means that the diffusion is good far from material interfaces and from localized sources.

Overall, the diffusion is a robust approximation. It can be fairly accurate, and even when it is not that great, it never is totally off. Most reactors are simulated in 3-dimensional, 2 groups diffusion.

4.3. The Boundary Conditions

In addition to the diffusion equation itself, we need the boundary conditions to show that this equation has one and only one solution. In practice, the boundary conditions consist of a relationship to be satisfied involving the flux and its derivative.

We can write the void boundary condition:

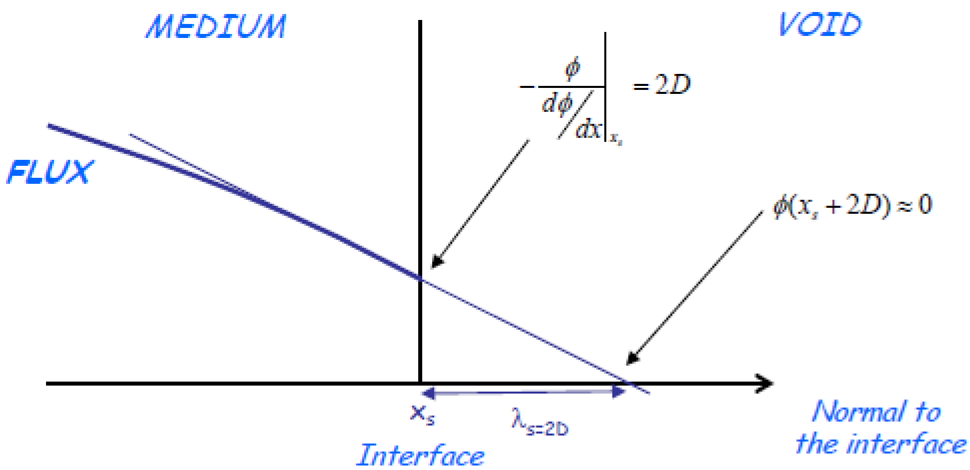
$$\psi(\bar{r}_s,\hat{\Omega}) = 0 \qquad \hat{n}\cdot\hat{\Omega} < 0$$

In diffusion, we require that the incoming partial current vanishes. Recall that the incoming partial current is the J^- that we saw in a previous lecture. This translates into:

$$J^-(x_s) \equiv \int_{\hat{n}\cdot\hat{\Omega}<0} d^2\Omega\left|\hat{n}\cdot\hat{\Omega}\right|\psi(x_s,\hat{\Omega}) \cong \frac{\phi(x_s)}{4} + \frac{D}{2}\left.\frac{d\phi}{dx}\right|_{x_s} = 0$$

This can also be written as:

$$\left.\frac{d\phi/dx}{\phi}\right|_{x_s} = -\frac{1}{2D}$$



The boundary conditions can be approximated by:

$$\phi(x_s + 2D) \approx 0$$

Thus, we have an extrapolation distance, which tells us where the flux vanishes.

$$\tilde{x}_s = x_s + \frac{2}{3\Sigma_{tr}}$$

Nota bene: A “better” value of this extrapolation distance would be: $\tilde{x}_s = x_s + 0.7104\frac{1}{\Sigma_{tr}}$

At the interface between two regions, the angular flux is continuous. Of course, a discontinuous flux would not be physical.

$$\psi^+(\bar{r}_s, \hat{\Omega}) = \psi^-(\bar{r}_s, \hat{\Omega}) \quad \forall \hat{\Omega}$$

We can recall that one can write the angular flux as a function of the scalar flux and the current. This implies that we require both the scalar flux and the current to be continuous.

$$\psi(\bar{r}, \hat{\Omega}) \approx \frac{1}{4\pi}\phi(\bar{r}) + \frac{3}{4\pi}\bar{J}(\bar{r}) \cdot \hat{\Omega} \quad \Longrightarrow \quad \begin{aligned} \phi^+(\bar{r}_s) &= \phi^-(\bar{r}_s) \\ J^+(\bar{r}_s) &= J^-(\bar{r}_s) \\ D^+\nabla\phi\big|_{r_s^+} &= D^-\nabla\phi\big|_{r_s^-} \end{aligned}$$

4.4. An example: The source problems

Well, I think it's time for us to go over an example. That will illustrate the lecture and make it more meaningful. Hopefully.
So, let's consider that we are given the geometry, the materials, and the sources. We want to obtain the scalar flux ϕ, solution of the diffusion equation:

$$-\bar{\nabla}\cdot D(\bar{r})\bar{\nabla}\phi(\bar{r})+\Sigma_a(\bar{r})\phi(\bar{r})=S(\bar{r})$$

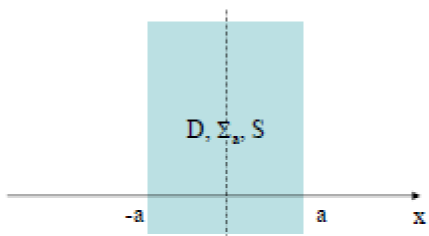
For homogeneous media, we know that the cross-sections are independent of space, thus:

$$-D\nabla^2\phi+\Sigma_a\phi(\bar{r})=S(\bar{r})$$

Laplacian

Finally, we have the boundary conditions. At the interface between two media, we have the continuity of the flux and of the current.

Let's be practical here and take a concrete example. We will consider an infinite (in y and z) slab of thickness $2a$, with an external source of neutrons:



We can write the diffusion equation and the boundary condition. a is the extrapolated distance.

Diffusion Equation

$$-D\frac{d^2\phi}{dx^2}+\Sigma_a\phi=S$$

Boundary Condition

$$\phi(a)=\phi(-a)=0$$

A particular solution of the diffusion equation is :

$$\phi_p(x)=\frac{S}{\Sigma_a}$$

Indeed, it is easy to see that a derivative of a constant (derivated twice within the Laplacian actually) yields zero, so the term $-D\frac{d^2\phi}{dx^2}$ disappears when the flux is taken constant. We are then left with:

$$\Sigma_a\phi=S$$

It is then trivial to obtain the particular solution of the diffusion equation.

Then, it gets a little trickier. One can solve this problem by good ol' means, that is, solving a differential equation. Not that complicated when you have the method. However, there is something nice with the Laplacian equations. We already have the solution. Then, it's only a matter of reading a table.

First, we have the Laplacian. Some problems, like the one we're considering now, use the Cartesian coordinates. Some require the cylindrical or spherical coordinates. Here is the translation of a Laplacian ($\nabla^2 f$) in those different coordinates systems:

- Cartesian coordinates

$$\nabla^2 f = \underbrace{\frac{\partial^2 f}{\partial x^2}}_{1D} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

- Cylindrical coordinates

$$\nabla^2 f = \underbrace{\frac{\partial^2 f}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial f}{\partial \rho}}_{1D} + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2}$$

- Spherical coordinates

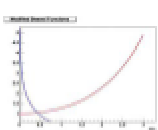
$$\nabla^2 f = \underbrace{\frac{\partial^2 f}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial f}{\partial \rho}}_{1D} + \frac{1}{\rho^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{\rho^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}$$

As you can see, the Laplacian in Spherical coordinate is not that pretty…
Now, the interesting part: its solutions!

The only thing one has to do is transform the diffusion equation in what is known as the Helmholtz equation. It looks like:

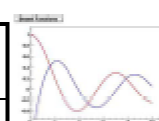
$$\nabla^2 f + B^2 f = 0$$

Once you have something that looks like that, it's only a matter of reading the following table:



Modified Bessel functions

Geometry	$B^2<0$ $(1/L^2=-B^2)$	$B^2>0$ $(\chi^2=B^2)$
Cartesian	sinh(x/L) cosh(x/L)	sin(χx) cos(χx)
Cylindrical	$I_0(\rho/L)$ $K_0(\rho/L)$	$J_0(\chi\rho)$ $Y_0(\chi\rho)$
Spherical	sinh(r/L)/r cosh(r/L)/r	sin(χr)/r cos(χr)/r



Bessel functions

Friedrich Wilhelm Bessel (1784-1846)

Pretty neat, isn't it? The only problem is that it only works for one-dimensional geometries. Sorry guys and gals, if you have a two or three-dimensional problems, you'll have to solve the differential equation.

An example of how to use this table. Let's consider we have the following equation:

$$-D\nabla^2\phi + \Sigma_a\phi(\bar{r}) = \nu\Sigma_f\phi(\bar{r})$$

The sources are the fission neutrons. If we consider that it is a one-dimensional problem, we can use the Cartesian coordinates, $\vec{r}$ becomes x for example.
We can re-write it:

$$\nabla^2\phi + \frac{\nu\Sigma_f - \Sigma_a}{D}\phi = 0$$

We can get from that:

$$B^2 = \frac{\nu\Sigma_f - \Sigma_a}{D}$$

Then, it all depends on whether B^2 is greater than 0 or not to select the appropriate column.

So, let us come back to the problem we had. We had gotten a particular solution and were about to solve the homogeneous equation:

$$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi = 0, \qquad L^2 = \frac{D}{\Sigma_a} \qquad \text{(L^2: migration area)}$$

We define $\frac{D}{\Sigma_a}$ as being the migration area. That's more for notation than understanding of physical effect.

Now, if we write the Helmholtz equation from this homogeneous equation, we obtain:

$$B^2 = -\frac{\Sigma_a}{D}$$

It is to note that Σ_a and D are always positive by definition. Thus the squared value of L being the ratio (squared value is always positive). Hence, B^2 here is negative. Reading the corresponding column in the table we've seen, we can write the solution to the homogeneous equation:

$$\phi_h(x) = A'\cosh(x/L) + B'\sinh(x/L)$$

Therefore, the scalar flux can easily be obtained now, by adding the homogeneous and particular solution:

$$\phi(x) = A'\cosh(x/L) + B'\sinh(x/L) + \frac{S}{\Sigma_a}$$

We can now use the boundary condition to solve for A' and B'.

$$\phi(a) = \phi(-a) = 0$$

We know, from our trigonometry classes (might be a while, I'll give you that), that:

$$\cosh(x) = \cosh(-x)$$
$$\sinh(x) = -\sinh(-x)$$

So:

$$\phi(a) = A' \cosh(a/L) + B' \sinh(a/L) + \frac{S}{\Sigma_a}$$
$$\phi(-a) = A' \cosh(a/L) - B' \sinh(a/L) + \frac{S}{\Sigma_a}$$

Hence, by subtracting one equation to the other:

$$2B' \sinh(a/L) = 0$$

So, $B' = 0$

If we add the two equations, we get:

$$2A' \cosh(a/L) = \frac{2S}{\Sigma_a}$$

So:

$$A' = \frac{S}{\Sigma_a} . \frac{1}{\cosh(a/L)}$$

And finally, we write the solution of our 1-D slab :

$$\phi(x) = \frac{S}{\Sigma_a}\left[1 - \frac{\cosh(x/L)}{\cosh(a/L)}\right]$$

Isn't that great? I'm available for any question you may have. You'll be able to practice more on this subject in the next set of homework.

Well, this ends the fourth lecture. If you have any question, please let me know directly or post a thread in the dedicated subreddit. Do not forget, and I can't stress this enough: if you have a question, then someone else in the class is wondering the same thing, or should be. Therefore, asking it will help you and others.

I noticed the formula-to-text ratio is higher in this lecture than in the previous ones. If you feel like it needs more explanation of the steps, that you cannot find the origin of a simplification or development in the previous lectures, let me know and I will see what I can do to improve the way I tackled this chapter.

Once again, there is another thing that I should repeat. If you do not understand something, do not feel like it's your fault, and do not give up. It merely means that my explanations were not good enough. I will gladly upgrade the class by taking into account your suggestions and remarks.

On a last note, I'm sorry about some of the equations quality in this lecture. This time I did not feel like rewriting all of the equations and copied them from an old presentation I had written. It is readable though, which is the most important. Looked great in the word document!