



Chapter 5: The Multigroup Equations

4.1. Introduction

Now that we have computed the diffusion equation, and that you've seen how to apply it in some simple cases, we can go on to the multigroup equations.

What do I mean by "multigroup"? Ah, I see you're impatient to know! Well, you're in luck, I'm going to explain!

As you could have expected, we are going to start from the transport equation. Well, more precisely, the steady-state transport equation. We indeed consider that it doesn't change with time. That's false, but is an important approximation.

$$\hat{\Omega} \cdot \vec{\nabla} \Psi + \Sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega}) = \int_0^{\infty} dE' \int_{4\pi} d^2\Omega \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}, \hat{\Omega}') \Psi(\vec{r}, E', \hat{\Omega}') + s(\vec{r}, E, \hat{\Omega})$$

The corresponding diffusion equation is:

$$\vec{\nabla} \cdot D(\vec{r}) \vec{\nabla} \phi + \Sigma(\vec{r}, E) \phi(\vec{r}, E) = \int_0^{\infty} dE' \Sigma(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E') + s(\vec{r}, E)$$

One must remember that:

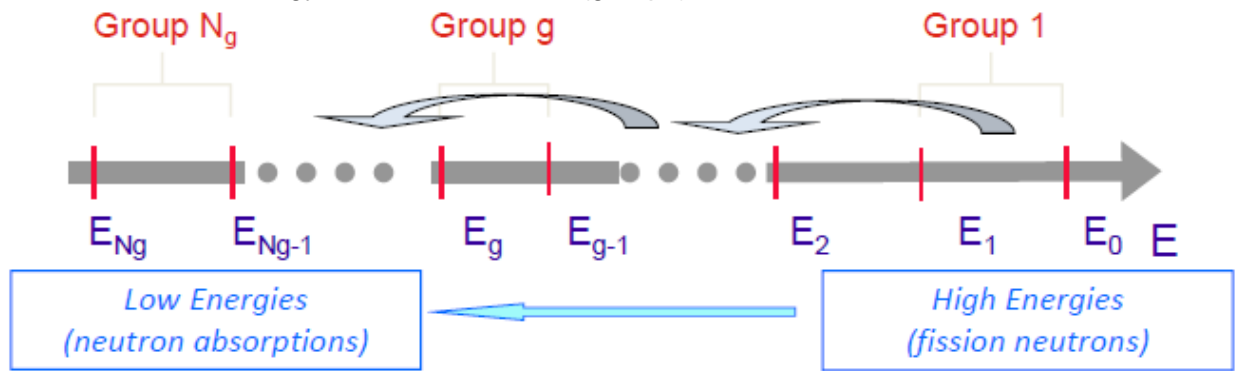
$$\phi(\vec{r}, E) = \int_{4\pi} d^2\Omega \Psi(\vec{r}, E, \hat{\Omega})$$

$$\vec{J} \cong -D \cdot \nabla \phi$$

4.2. The multigroup transport equations

What we want to do now is to discretize the energy variable E. Why, you ask? This way, we can separate the flux per energy *group* and gain information. The next questions will be: When does the cost overcome the gain?

So, we divide the energy domain in intervals (groups):



The neutrons starts off (on average) at the right of this scale (released by fission at an energy around 2.4 MeV) and go to the left, losing energy with scattering (collisions), finally being absorbed when the probability of that happening is high (“low” energy). For example, the group g represents the neutrons between the energy E_g and E_{g-1} .

So, each group is characterized by a value of the flux Ψ_g , the multigroup flux, which is the integral over the group g of the angular flux:

$$\Psi_g(\vec{r}, \hat{\Omega}) = \int_{E_g}^{E_{g-1}} dE \cdot \Psi(\vec{r}, E, \hat{\Omega})$$

In order to get an equation for Ψ_g , we integrate the transport equation over the group g :

$$\int_{E_g}^{E_{g-1}} dE \left[\hat{\Omega} \cdot \vec{\nabla} \Psi + \Sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega}) = \int_0^\infty dE' \int_{4\pi} d^2\Omega \cdot \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}, \hat{\Omega}') \Psi(\vec{r}, E', \hat{\Omega}') + s(\vec{r}, E, \hat{\Omega}) \right]$$

As in the previous lectures, we’re going to break down this equation and solve each part individually. And, as before, let’s start with the easy ones:

1 The displacement term:

We can interchange the integration in energy and the derivative in space, to get:

$$\int_{E_g}^{E_{g-1}} dE \cdot \hat{\Omega} \cdot \vec{\nabla} \Psi(\vec{r}, E, \hat{\Omega}) = \hat{\Omega} \cdot \vec{\nabla} \Psi_g(\vec{r}, \hat{\Omega})$$

4 The source term:

We integrate the known source over the group:

$$\int_{E_g}^{E_{g-1}} dE. s(\vec{r}, E, \hat{\Omega}) = s_g(\vec{r}, \hat{\Omega})$$

Now that the easy are done, we can tackle the more challenging terms.

2 The collision term:

This term can be rewritten in terms of Ψ_g as:

$$\int_{E_g}^{E_{g-1}} dE. \Sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega}) = \Sigma_g(\vec{r}) \Psi_g(\vec{r}, \hat{\Omega})$$

We've just introduced a new term here, the multigroup cross-section Σ_g .

$$\Sigma_g(\vec{r}) = \frac{1}{\Psi_g(\vec{r}, \hat{\Omega})} \int_{E_g}^{E_{g-1}} dE. \Sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega})$$

This cross-section represents a weighted average over the group. In particular, if Ψ doesn't depend much on energy (big variations of energy cause small variation of the flux), we can write:

$$\Sigma_g(\vec{r}) \cong \frac{1}{\Delta E} \int_{E_g}^{E_{g-1}} dE. \Sigma(\vec{r}, E) \stackrel{\text{def}}{=} \langle \Sigma \rangle$$

3 The scattering-in term:

We can replace the integral over energy as a sum of integrals over the groups:

$$\begin{aligned} \int_0^\infty dE' f(E') &= \sum_{g'=1}^{N_g} \int_{E_g}^{E_{g-1}} dE'. f(E') \\ \int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \int_{4\pi} d^2\Omega'. \Sigma_{s,g' \rightarrow g}(\vec{r}, E' \rightarrow E, \hat{\Omega}, \hat{\Omega}'). \Psi(\vec{r}, E', \hat{\Omega}') & \\ &= \sum_{g'=1}^{N_g} \int_{4\pi} d^2\Omega'. \Sigma_{s,g' \rightarrow g}(\vec{r}, \hat{\Omega}, \hat{\Omega}'). \Psi_{g'}(\vec{r}, \hat{\Omega}') \end{aligned}$$

How did we get there? Magic! No, what's important to see is the introduction of a new term, $\Sigma_{s,g' \rightarrow g}(\vec{r}, \hat{\Omega}, \hat{\Omega}')$. We'll call this term the multigroup transfer matrix.

$$\Sigma_{s,g' \rightarrow g}(\vec{r}, \hat{\Omega}, \hat{\Omega}') = \frac{1}{\Psi_{g'}(\vec{r}, \hat{\Omega})} \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \cdot \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}, \hat{\Omega}') \Psi(\vec{r}, E', \hat{\Omega}')$$

I trust that you'll do the math. If you do, and encounter a problem, let me know.

Question n°1 : ✪

Please demonstrate how we obtained the scattering-in term.

So, what can we make of all that? Well, we can write the **multigroup transport equation**:

$$\hat{\Omega} \cdot \vec{\nabla} \Psi_g(\vec{r}, \hat{\Omega}) + \Sigma_g(\vec{r}) \Psi_g(\vec{r}, \hat{\Omega}) = \sum_{g'=1}^{N_g} \int_{4\pi} d^2\Omega' \cdot \Sigma_{s,g' \rightarrow g}(\vec{r}, \hat{\Omega}, \hat{\Omega}') \cdot \Psi_{g'}(\vec{r}, \hat{\Omega}') + s_g(\vec{r}, \hat{\Omega})$$

This is a system of N_g coupled transport equations (g goes from 1 to N_g , the number of groups) for the N_g multigroup fluxes Ψ_g .

When the energy is between 20 MeV and 1 eV, we say that the neutron is in the slowing-down region. In this region, neutrons can only lose energy in a collision. Thus, neutrons can only go from a lower group to a higher group:

$$\Sigma_{s,g' \rightarrow g} = 0 \quad \text{si } g' > g$$

We face a triangular system, which can be solved by the forward substitution method, from $g = 1$ to $g = N_g$:

$$\hat{\Omega} \cdot \vec{\nabla} \Psi_1 + \Sigma_1 \Psi_1 = \int_{4\pi} d^2\Omega' \cdot \Sigma_{s,1 \rightarrow 1}(\hat{\Omega}, \hat{\Omega}') \cdot \Psi_1 + s_1$$

$$\hat{\Omega} \cdot \vec{\nabla} \Psi_2 + \Sigma_2 \Psi_2 = \int_{4\pi} d^2\Omega' \cdot \Sigma_{s,2 \rightarrow 2}(\hat{\Omega}, \hat{\Omega}') \cdot \Psi_2 + \int_{4\pi} d^2\Omega' \cdot \Sigma_{s,1 \rightarrow 2}(\hat{\Omega}, \hat{\Omega}') \cdot \Psi_1 + s_2$$

...

At the time of calculation, the known terms in the previous equations are highlighted in red. In the equation for the group g , we put all the contributions coming from the other groups with the external source. We thus get an equation which looks like a one-speed equation (see lecture 4), and which can be solved by the iterative scheme:

$$\hat{\Omega} \cdot \vec{\nabla} \Psi_g^n + \Sigma_g \Psi_g^n = \int_{4\pi} d^2\Omega' \cdot \Sigma_{s,g \rightarrow g} \cdot \Psi_g^n + q_g^n$$

In which:

$$q_g^n = s_g + \sum_{g' < g} \int_{4\pi} d^2\Omega' \cdot \Sigma_{s,g' \rightarrow g} \Psi_{g'}^n + \sum_{g' > g} \int_{4\pi} d^2\Omega' \Sigma_{s,g' \rightarrow g} \Psi_{g'}^{n-1} + \sum_i \frac{\chi_g^i}{4\pi} \sum_{g'=1}^{N_g} \nu_{g'}^i \cdot \Sigma_{g'}^i \phi_{g'}^{n-1}$$

So, if we know how to solve the one-speed equation, and we are supposed to, from the fourth lecture, we can solve the multigroup equations.

4.3. The multigroup cross-sections

Let's get back to the multigroup cross-section that we introduced earlier.

$$\Sigma_g(\vec{r}) = \frac{1}{\Psi_g(\vec{r}, \hat{\Omega})} \int_{E_g}^{E_{g-1}} dE \cdot \Sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega})$$

This cross-section depends on:

- The flux Ψ_g , which is the unknown of the multigroup equations
- The flux Ψ , which is the solution of the problem we were trying to avoid in the first place
- The space
- The angle (physical cross-sections do not depend on angle)

This cross-section is not a data. Its definition *contains* the solution of the problem.

In order to get a value for the multigroup cross-section, we replace the unknown flux Ψ with a weighting flux φ , which we hope is "close enough":

$$\Sigma_g(\vec{r}) = \frac{1}{\varphi_g(\vec{r}, E)} \int_{E_g}^{E_{g-1}} dE \cdot \Sigma(\vec{r}, E) \varphi(\vec{r}, E)$$

Many efforts go into the search of a good weighting flux, which will allow us to compute good reaction rates in the group. This is the problem of the resonant absorption and self-shielding, that we will tackle in later lectures.

The numerical solution of the transport equation is a two-step process.

1. Computing the multigroup cross-section from the microscopic cross-sections.
 - a. They are problem-dependent. They depend on the neutron spectrum, the temperature, the flux gradient, etc.
 - b. In order to obtain these cross-sections, we need to solve "local" (in space and/or energy) problems.
2. Solving the system of multigroup equations. This is more "standard" numerical analysis, but we still need to:

- Discretize the space (Finite elements, finite differences, finite volumes)
- Discretize the angle (S_N and P_N methods)
- Solve the resulting linear system (and it's a big one!)

4.4. The multigroup diffusion equations

Derivation of the multigroup diffusion equations is less rigorous than in the one-speed (one-energy) case, and it demands some more approximations. The whole demonstration (see lecture 4) is not necessary again here. In any event, one gets down to:

$$-\vec{\nabla} \cdot D_g \vec{\nabla} \phi_g + \Sigma_g(\vec{r}) \phi_g(\vec{r}) = \sum_{g' \neq g}^{N_g} \Sigma_{s,g' \rightarrow g}(\vec{r}) \phi_{g'}(\vec{r}) + s_g(\vec{r}) + \sum_i \chi_g^i \sum_{g'} \Sigma_{f,g'}^i(\vec{r}) \phi_{g'}(\vec{r})$$

In which:

$$\Sigma_g(\vec{r}) = \frac{1}{\phi_g(\vec{r}, E)} \int_{E_g}^{E_{g-1}} dE \cdot \Sigma(\vec{r}, E) \phi(\vec{r}, E)$$

$$\Sigma_{s,g' \rightarrow g}(\vec{r}) = \frac{1}{\phi_g(\vec{r})} \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \cdot \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E')$$

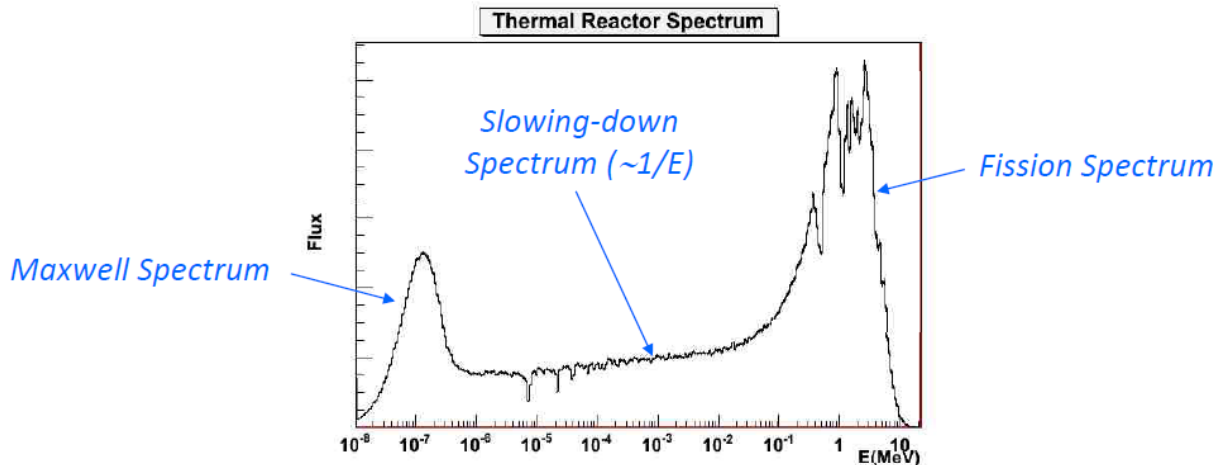
Multigroup diffusion should only be used with few groups ($N_g \leq 5$). Indeed, it takes a lot of collisions inside the group to have an almost isotropic flux. With narrow groups, the neutron will exit the group after only few (or even just one) collisions.

Industrial calculations of power reactor are based on the two group diffusion model with homogenized assemblies (and the results are quite satisfactory).

4.5. Weighting flux and energy meshes

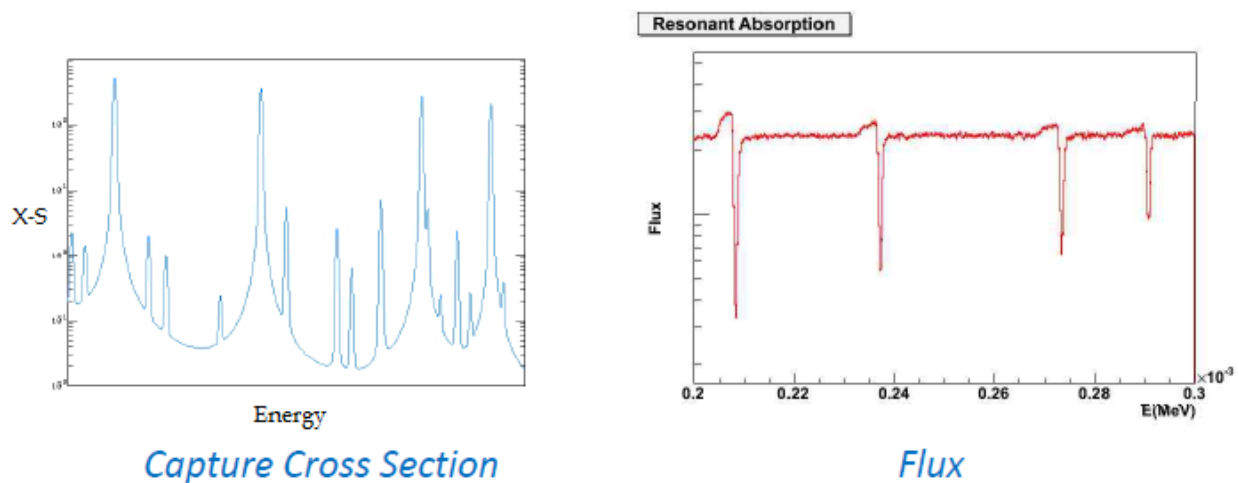
Everything in this paragraph will be detailed in later lectures.

I mentioned earlier the weighting flux. It comes from the reactor spectrum. For example, this is a typical PWR (pressurized water reactor) spectrum:



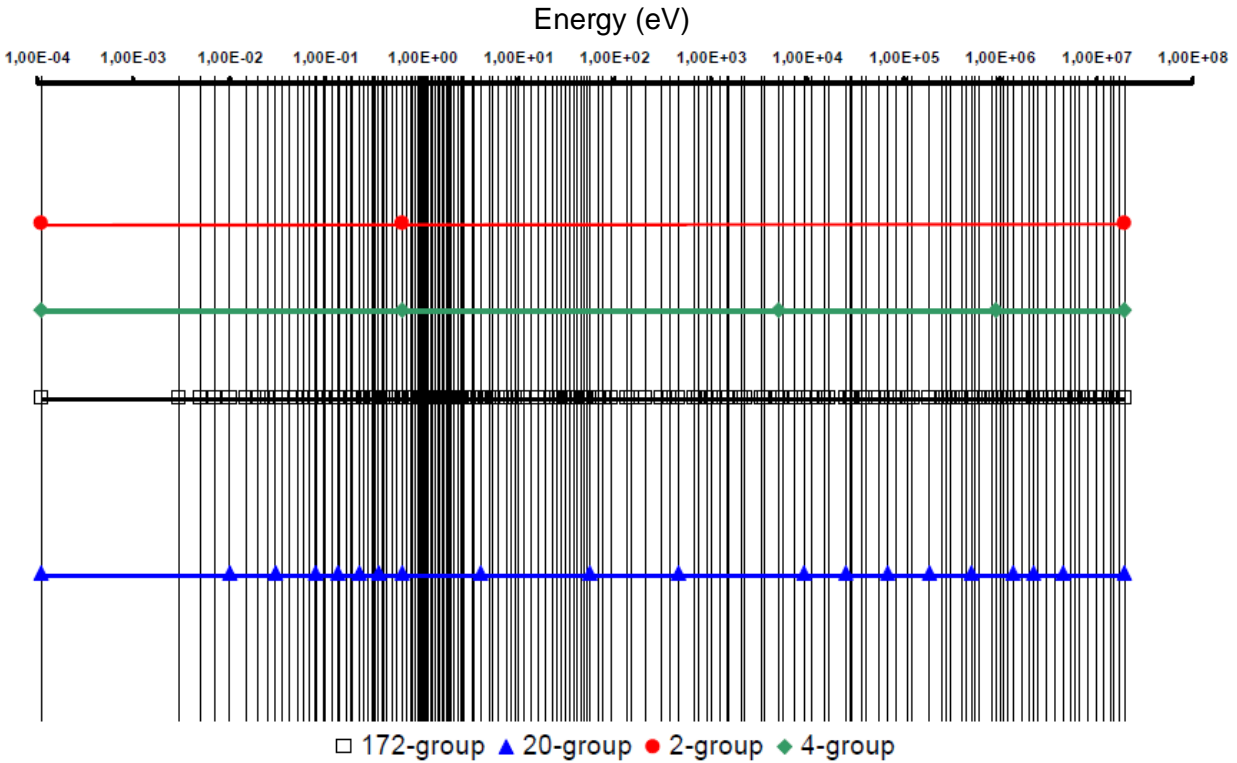
This works only outside the resonance version.

Indeed, within the resonances, we need a very good estimate of the weighting flux if we want to have a good value of the reaction rates.



We indeed see that over small regions of energy, cross-section and flux varies a lot (the ratio of the flux outside a resonance and inside can easily be a factor of more than 10), and the weighting flux would not be precise enough to take that into account. An energy group can contain several resonances.

The multigroup energy meshes are roughly (the exact values depend on the calculation codes you use) as follow:



Typically, we have (currently) three main energy meshes used.

- Reactor calculation (cycle length)
 - Two group diffusion
 - Homogenized assembly
- Assembly calculations (in order to homogenize)
 - 172 to 281 group transports
 - Resonances up to 100 eV are detailed (self-shielding model for $E > 100$ eV)
 - Exact 2D geometry
- Reference deterministic calculations
 - Around 12000 group transport
 - Cell or assembly calculations
 - Self-shielding models for ^{238}U and $E > 1$ keV
 - Probability tables for non-resolved resonances

4.6. An example: The two group diffusion

Let us now consider the two group diffusion equations, with the following simplifications:

1. All fissions are thermal (a fission is only triggered by a slow [low energy] neutron)
2. All fissions neutrons (neutrons released by fission) are fast [high energy]

The thermal neutrons are considered to have an energy up to around 1 eV, while the fast neutrons will be taken between 1 eV and 20 MeV.

The two group diffusion equations can be written:

$$\begin{aligned} -\vec{\nabla} \cdot D_1 \vec{\nabla} \phi_1 + (\Sigma_{a1} + \Sigma_{s,1 \rightarrow 2}) \phi_1 &= \nu \Sigma_{f2} \phi_2 \\ -\vec{\nabla} \cdot D_2 \vec{\nabla} \phi_2 + \Sigma_{a2} \phi_2 &= \Sigma_{s,1 \rightarrow 2} \phi_1 \end{aligned}$$

Let me explain this system again.

First equation:

The fast neutrons can leave the first group only by **being absorbed**, leaving the system (**streaming**), or being **scattered out** into the second group (thermal). That's what we write on the left side of the equation. On the right side, we write the gain in neutrons, which are the fast **neutrons coming from fissions** induced by thermal neutrons (ϕ_2).

Second equation:

The thermal neutrons can leave the second group only by **being absorbed** or leaving the system (**streaming**). Indeed, we have seen earlier that a neutron cannot gain energy in a collision in the slowing-down region (1eV – 20 MeV). So, a neutron in the group 2 cannot be lost by going back in the group 1. The neutrons gained, on the right hand side, are the neutrons **scattered in from the group 1** into the group 2.

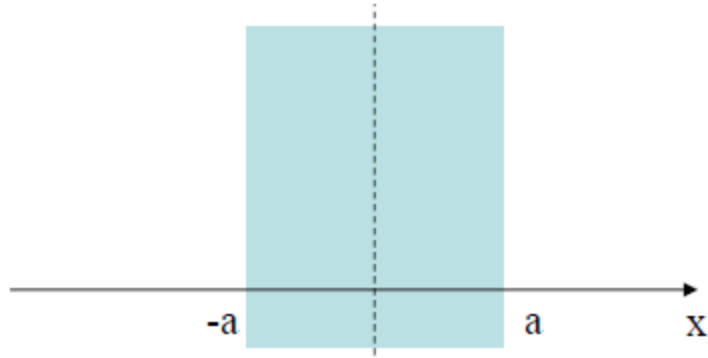
This is a coupled system of two differential equations for the two unknowns ϕ_1 and ϕ_2 . We can define the removal cross-section according to:

$$\Sigma_{r1} \stackrel{\text{def}}{=} \Sigma_{a1} + \Sigma_{s,1 \rightarrow 2}$$

We're now going to walk through an example of a 2-group diffusion problem. After that, you'll be able to tackle the homework problems on your own.

So!

Let us consider the same example than the one we saw during the last lecture, on the diffusion equation. We will consider an infinite (in y and z) slab of thickness $2a$.



We consider that:

$$\begin{aligned}\phi_1(a) &= \phi_2(a) = 0 \\ \phi_1(-a) &= \phi_2(-a) = 0\end{aligned}$$

We can write the two-group diffusion equations:

$$\begin{aligned}-D_1 \frac{d^2 \phi_1}{dx^2} + \Sigma_{r1} \phi_1 &= \nu \Sigma_{f2} \phi_2 \\ -D_2 \frac{d^2 \phi_2}{dx^2} + \Sigma_{a2} \phi_2 &= \nu \Sigma_{1 \rightarrow 2} \phi_1\end{aligned}$$

The solution (please refer to the fourth lecture) is a sum of exponentials. We set:

$$\begin{aligned}\phi_1(x) &= \varphi_1 e^{i\alpha x} \\ \phi_2(x) &= \varphi_2 e^{i\alpha x}\end{aligned}$$

From that, we get:

$$\begin{aligned}(D_1 \alpha^2 + \Sigma_{r1}) \varphi_1 - \nu \Sigma_{f2} \varphi_2 &= 0 \\ -\Sigma_{s,1 \rightarrow 2} \varphi_1 + (D_2 \alpha^2 + \Sigma_{a2}) \varphi_2 &= 0\end{aligned}$$

We know that the determinant of the system equals 0, which translates to:

$$(D_1 \alpha^2 + \Sigma_{r1})(D_2 \alpha^2 + \Sigma_{a2}) - \nu \Sigma_{f2} \Sigma_{s,1 \rightarrow 2} = 0$$

That's a fourth order algebraic equation (α^2), and has therefore four solutions. Let me tell you that:

$$k_\infty = \frac{\Sigma_{f2} \Sigma_{s,1 \rightarrow 2}}{\Sigma_{r1} \Sigma_{a2}}$$

You're going to have to trust me on that, 'till you work it through by yourself in the homework, that is.

We then can rewrite the previous equation as:

$$(1 + L_1^2 \alpha^2)(1 + L_2^2 \alpha^2) = k_\infty$$

In which we have:

$$L_1^2 = \frac{D_1}{\Sigma_{r1}} \quad \text{and} \quad L_2^2 = \frac{D_2}{\Sigma_{a2}}$$

One could develop the equation and rewrite it:

$$L_1^2 L_2^2 \alpha^4 + (L_1^2 + L_2^2) \alpha^2 - (k_\infty - 1) = 0$$

Okay, that looks tough. And, well, it kind of is. We need to solve for α .

What one can see is that the first two terms are always of the same signs (multiple-of-two powers). So eventually the way to solve it will depend on the infinite multiplication factor k_∞ .

$k_\infty > 1$:

We obtain in that case:

- A positive root $\alpha^2 = \chi^2$, which gives the two solutions $\cos(\chi x)$ and $\sin(\chi x)$ for the problem at hand
- A positive root $\alpha^2 = -\mu^2$, which gives the two solutions $\sinh(\mu x)$ and $\cosh(\mu x)$

$k_\infty < 1$:

We obtain in that case:

- Two negative root $\alpha^2 = -\mu_1^2$ or $-\mu_2^2$, which give the four solutions $\sinh(\mu_1 x)$, $\cosh(\mu_1 x)$, $\sinh(\mu_2 x)$, $\cosh(\mu_2 x)$

It might not seem very clear, so I highly recommend that you do the math. Trust me, even if it seems annoying with the results just being there, it helps tremendously to re-do things on a sheet of paper by yourself.

So, for each solution α_i , we have:

$$\varphi_2 = s_{\alpha_i} \varphi_1$$

In which:

$$s_{\alpha_i} = \frac{D_1 \alpha_i + \Sigma_{r,1}}{\nu \Sigma_{f,2}} = \frac{\Sigma_{s,1 \rightarrow 2}}{D_2 \alpha_i^2 + \Sigma_{a,2}}$$

We consider in the following the case $k_\infty > 1$. We can write:

$$\begin{aligned} \phi_1(x) &= A. \cos(\chi x) + B. \cosh(\mu x) + C. \sin(\chi x) + D. \sinh(\mu x) \\ \phi_2(x) &= A. s_\chi \cos(\chi x) + B. s_\mu \cosh(\mu x) + C. s_\chi \sin(\chi x) + D. s_\mu \sinh(\mu x) \end{aligned}$$

Given the symmetry of the problem at hand, we can eliminate the solutions \sin and \sinh . That leaves us with:

$$\begin{aligned} \phi_1(x) &= A. \cos(\chi x) + B. \cosh(\mu x) \\ \phi_2(x) &= A. s_\chi \cos(\chi x) + B. s_\mu \cosh(\mu x) \end{aligned}$$

That looks okay, but we can do better than that. We haven't yet considered the boundary conditions:

$$\phi_1(x = a) = \phi_2(x = a) = 0$$

These conditions are satisfied by $B = 0$ (we thus consider from now on $A \neq 0$. Indeed, if it is, we just got the obvious solution to the equation, the null function) and by:

$$\cos(\chi a) = 0$$

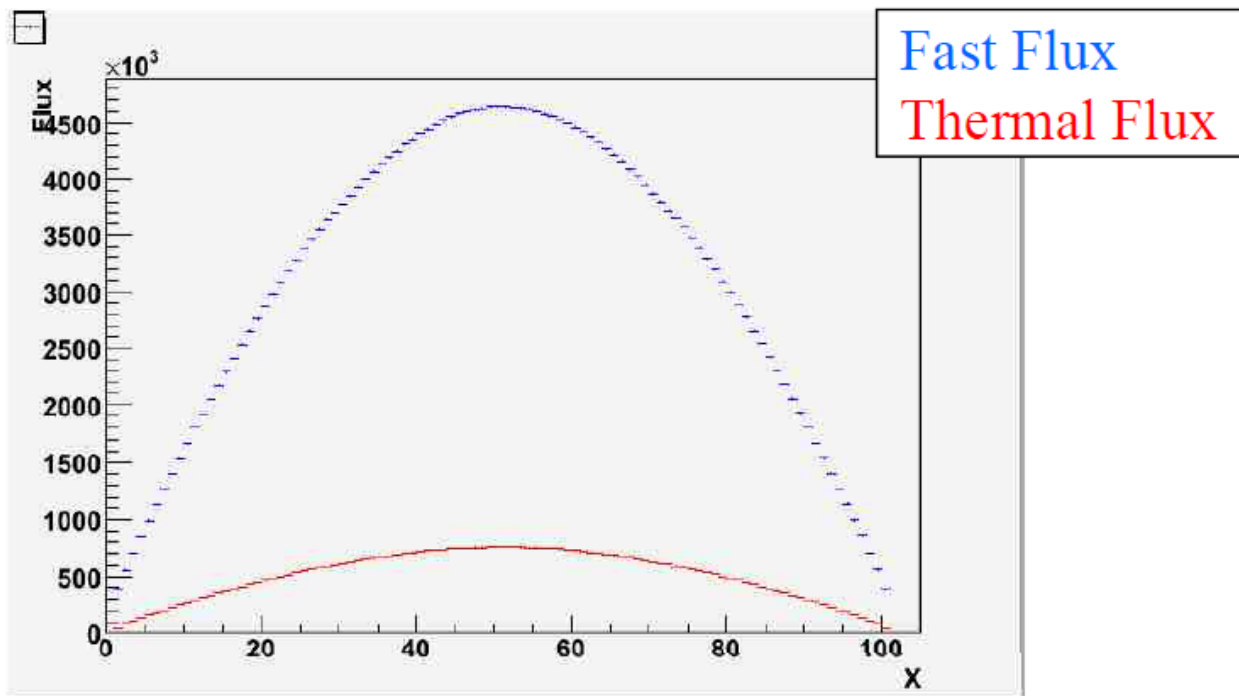
Since $\cos\left(\frac{\pi}{2}\right) = 0$, this condition is true if:

$$\chi = \frac{\pi}{2a}$$

We call this equation the "critical condition". It corresponds to the equality of the material buckling (χ) with the geometric buckling ($\frac{\pi}{2a}$).

So! We arrive at this quite nice looking set of equations:

$$\begin{aligned}\phi_1(x) &= A \cdot \cos(\chi x) \\ \phi_2(x) &= A \cdot s_\chi \cos(\chi x)\end{aligned}$$



(Graph from the CEA)

This is roughly what we obtain. ϕ_1 is the fast flux (blue curve).

Well, this ends the fifth 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 highly recommend that you actually do the math. I did not show every single step, and it would be very beneficial for you to take over the equations and make them yours, as it helps you clear things up. It also requires some effort, but that's the price of knowledge, isn't it?

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.