

# 22.211 Lecture 15

## Bare Homogeneous Reactors

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April 3, 2023

# Outline

- 1 Objectives
- 2 Multigroup Discretization
- 3 Bare Homogeneous Reactors
  - 2 groups

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# Objectives

- Derive multigroup form of Diffusion equation
- Bare homogeneous reactors in 1 group
- Bare homogeneous reactors in 2 groups

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# Diffusion Equation

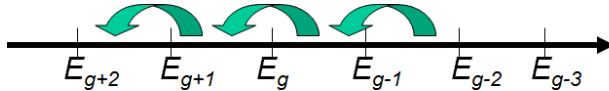
General form of the steady-state diffusion equation

$$\begin{aligned} -\nabla \cdot D(\vec{r}, E) \nabla \phi(\vec{r}, E) + \Sigma_t(\vec{r}, E) \phi(\vec{r}, E) = & \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E') \\ & + \chi(E) \int_0^\infty \nu \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') + S(\vec{r}, E) \end{aligned}$$

It represents a balance of neutrons in a volume element.

# Energy discretization

As you've seen previously, the energy dependency of nuclear data is quite complicated. We can approximate the flux shape for simple homogeneous problems, but not when the spatial dependency becomes complicated. You've learned approximations that can be made in the fast range, resonance range, thermal range. We can use these approximations to simplify the diffusion equation over a few non-overlapping groups.



# Conservation of Reaction Rates

Define the group average flux

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

Integrate the diffusion equation over each energy group. To preserve the reaction rate, we must define the multigroup cross-sections

$$\Sigma_{t,g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E) \phi(\vec{r}, E) dE}{\int_{E_g}^{E_{g-1}} \phi(\vec{r}, E) dE}$$

How can we define the multigroup constants if we need the continuous energy flux?



## Other multigroup constants

The diffusion coefficient should be weighted by gradient of the flux

$$D_g(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} D(\vec{r}, E) \nabla \phi(\vec{r}, E) dE}{\int_{E_g}^{E_{g-1}} \nabla \phi(\vec{r}, E) dE} \approx \frac{\int_{E_g}^{E_{g-1}} D(\vec{r}, E) \phi(\vec{r}, E) dE}{\int_{E_g}^{E_{g-1}} \phi(\vec{r}, E) dE}$$

The fission spectrum is expressed as

$$\chi_g = \int_{E_g}^{E_{g-1}} \chi(E)$$

However, if you have many isotopes and/or trying to compute an effective  $\chi$ , you need to weight  $\chi$  by the fission rates.

# Multigroup Diffusion Equation

$$\begin{aligned} -\nabla \cdot D_g(\vec{r}) \nabla \phi_g(\vec{r}) + \Sigma_{t,g}(\vec{r}) \phi_g(\vec{r}) &= \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}(\vec{r}) \phi_{g'}(\vec{r}) \\ &+ \chi_g \sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) \phi_{g'}(\vec{r}) + S_g(\vec{r}) \end{aligned}$$

$$J^{\pm}(\mathbf{r}_s, E) = \frac{1}{4}\phi(\mathbf{r}_s, E) \mp \frac{D}{2}\nabla\phi(\mathbf{r}_s, E)$$

# Derivation in 1D, 1 group

On the left boundary

$$J^+(x) = \int_0^1 \mu \psi(x, \mu) d\mu$$

$$J^+(x) = \int_0^1 \left( \frac{\mu}{2} \phi(x) + \frac{3}{2} \mu^2 J(x) \right) d\mu$$

$$J^+(x) = \frac{1}{4} \phi(x) + \frac{1}{2} J(x) = \frac{1}{4} \phi(x) - \frac{D}{2} \nabla \phi(x)$$

Repeating the same process for the right boundary yields a similar expression that changes the sign of the second term.

# Boundary Conditions

- ① Vacuum  $J^{\pm} = 0$
- ② Vacuum - Extrapolated distance  $\phi(x_s + 2D) = 0$
- ③ Reflective  $J^{+} = J^{-}$
- ④ Albedo

$$\alpha = \frac{J^{\mp}}{J^{\pm}}$$

# Extrapolated Distance

Instead of setting a partial current to zero at the boundary to represent the vacuum BC, you can instead set the scalar flux to zero at an extrapolated distance.

$$J^-(x_s) = \frac{1}{4}\phi(x_s) + \frac{D}{2} \frac{d\phi(x_s)}{dx} \Big|_{x=x_s} = 0$$

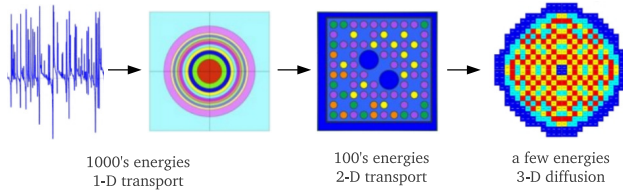
$$\frac{1}{\phi(x_s)} \frac{d\phi(x_s)}{dx} = \frac{-1}{2D}$$

approximate the derivative

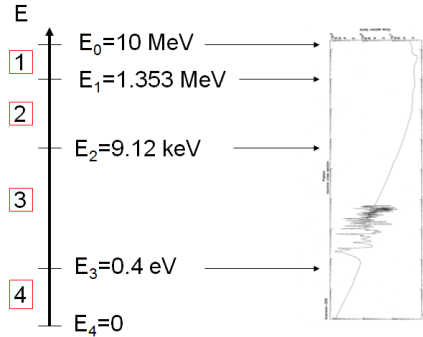
$$\frac{d\phi(x_s)}{dx} = \frac{\phi(x_s + x_{\text{ext}}) - \phi(x_s)}{x_s + x_{\text{ext}} - x_s} = \frac{-\phi(x_s)}{x_{\text{ext}}}$$

after substitution, we find that  $x_{\text{ext}} = 2D$ .

# Big Picture Condensation Process



# How do we pick groups?



This is only an example ... group structures are selected to isolate certain physical phenomena such as resonances, thermal neutron scattering ...



## 2 group equation

Group 1 (Fast group)

$$\begin{aligned} -\nabla \cdot D_1(\vec{r}) \nabla \phi_1(\vec{r}) + \Sigma_{t,1}(\vec{r}) \phi_1(\vec{r}) &= \Sigma_{s,1 \rightarrow 1}(\vec{r}) \phi_1(\vec{r}) + \Sigma_{s,2 \rightarrow 1}(\vec{r}) \phi_2(\vec{r}) \\ &+ \chi_1 \nu \Sigma_{f,1}(\vec{r}) \phi_1(\vec{r}) + \chi_1 \nu \Sigma_{f,2}(\vec{r}) \phi_2(\vec{r}) + S_1(\vec{r}) \end{aligned}$$

Group 2 (Thermal group)

$$\begin{aligned} -\nabla \cdot D_2(\vec{r}) \nabla \phi_2(\vec{r}) + \Sigma_{t,2}(\vec{r}) \phi_2(\vec{r}) &= \Sigma_{s,1 \rightarrow 2}(\vec{r}) \phi_1(\vec{r}) + \Sigma_{s,2 \rightarrow 2}(\vec{r}) \phi_2(\vec{r}) \\ &+ \chi_2 \nu \Sigma_{f,1}(\vec{r}) \phi_1(\vec{r}) + \chi_2 \nu \Sigma_{f,2}(\vec{r}) \phi_2(\vec{r}) + S_2(\vec{r}) \end{aligned}$$

We can simplify further by defining the group removal cross-section

$$\Sigma_{r,g} = \Sigma_{t,g} - \Sigma_{s,g \rightarrow g}$$

# Upscattering Correction

To simplify the equations we commonly remove the up-scattering cross section by defining an effective down scattering cross section.

$$\Sigma_{s,1\rightarrow 2,eff} = \frac{\Sigma_{s,1\rightarrow 2}(\vec{r})\phi_1(\vec{r}) - \Sigma_{s,2\rightarrow 1}(\vec{r})\phi_2(\vec{r})}{\phi_1(\vec{r})}$$

# Thermal Reactor Considerations

Typically, the group boundary is set around 1eV. This implies that  $\chi_1 \approx 1$  and  $\chi_2 \approx 0$ .

Group 1 (Fast group)

$$-\nabla \cdot D_1(\vec{r}) \nabla \phi_1(\vec{r}) + \Sigma_{r,1}(\vec{r}) \phi_1(\vec{r}) = \\ \chi_1 (\nu \Sigma_{f,1}(\vec{r}) \phi_1(\vec{r}) + \nu \Sigma_{f,2}(\vec{r}) \phi_2(\vec{r})) + S_1(\vec{r})$$

Group 2 (Thermal group)

$$-\nabla \cdot D_2(\vec{r}) \nabla \phi_2(\vec{r}) + \Sigma_{a,2}(\vec{r}) \phi_2(\vec{r}) = \Sigma_{s,1 \rightarrow 2}(\vec{r}) \phi_1(\vec{r}) + S_2(\vec{r})$$

Verify the given data before making these assumptions!

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$$-D\nabla^2\phi(\vec{r}) + \Sigma_a\phi(\vec{r}) = \frac{1}{k}\nu\Sigma_f\phi(\vec{r})$$

or if we re-arrange

$$\nabla^2\phi(\vec{r}) + B_m^2\phi(\vec{r}) = 0$$

where we define the material buckling

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

# Fundamental Mode

In a bare homogeneous reactor, we know the spatial solution is the solution to Helmholtz equation

$$\nabla^2 \Phi(\vec{r}) + B_g^2 \Phi(\vec{r}) = 0$$

with  $\Phi(\vec{r}_s) = 0$ . We can thus write

$$\phi(\vec{r}) = \phi \Phi(\vec{r})$$

and isolate the geometrical buckling to get

$$-B_g^2 = \frac{\nabla^2 \Phi(\vec{r})}{\Phi(\vec{r})}$$

# Criticality in 1 group

In 1 group, criticality can be easily expressed by

$$B_m = B_g$$

or

$$k = \frac{\nu \Sigma_f}{DB_g^2 + \Sigma_a}$$

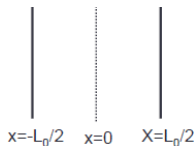
How to we get the geometrical buckling?

# Slab example

General solution is of the form

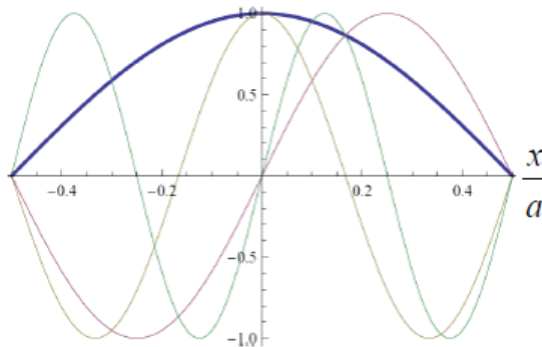
$$\phi(x) = C_1 \sin(B_g x) + C_2 \cos(B_g x)$$

$$B_n = \frac{n\pi}{L}, \quad \phi(x) = \begin{cases} A_n \cos(B_n x) & \text{for } n = 1, 3, 5, \dots \\ A_n \sin(B_n x) & \text{for } n = 2, 4, 6, \dots \end{cases}$$





# Modes of slab problem



Geometrical buckling is the term that corresponds to the fundamental mode. Thus for the slab  $B_g = \frac{\pi}{L}$

# General solution

$$\frac{d^2 y(x)}{dx^2} - b^2 y(x) = S(x)$$

$$y(x) = y_{hom}(x) + y_p(x)$$




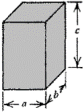

$$y_{hom}(x) = C_1 e^{bx} + C_2 e^{-bx}$$

$$\frac{d^2 y(x)}{dx^2} + a^2 y(x) = S(x)$$

$$y(x) = y_{hom}(x) + y_p(x)$$

$$y_{hom}(x) = C_1 \sin(ax) + C_2 \cos(ax)$$

# Buckling for simple geometries

		Geometric Buckling $B_g^2$	Flux profile
Slab		$\left(\frac{\pi}{a}\right)^2$	$\cos \frac{\pi x}{a}$
Infinite Cylinder		$\left(\frac{\nu_0}{R}\right)^2$	$J_0\left(\frac{\nu_0 r}{R}\right)$
Sphere		$\left(\frac{\pi}{R}\right)^2$	$r^{-1} \sin\left(\frac{\pi r}{R}\right)$
Rectangular Parallelepiped		$\left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2$	$\cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi y}{b}\right) \cos\left(\frac{\pi z}{c}\right)$
Finite Cylinder		$\left(\frac{\nu_0}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$	$J_0\left(\frac{\nu_0 r}{R}\right) \cos\left(\frac{\pi z}{H}\right)$

# Cylindrical Reactor

Starting from the fundamental mode equation

$$\nabla^2 \Phi(r, z) + B_g^2 \Phi(r, z) = 0$$

we expand for a cylinder as

$$\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} \Phi(r, z) + \frac{\partial^2}{\partial z^2} \Phi(r, z) + B_g^2 \Phi(r, z) = 0$$

assuming separation of variables

$$\Phi(r, z) = \psi(r)\chi(z)$$

# Separation of Variables

After substitution, we get

$$\frac{1}{r\psi(r)} \frac{d}{dr} r \frac{d}{dr} \psi(r) + \frac{1}{\chi(z)} \frac{d^2}{dz^2} \chi(z) + B_g^2 = 0$$

Each term depends only on a single variable and must thus each equal a constant such that

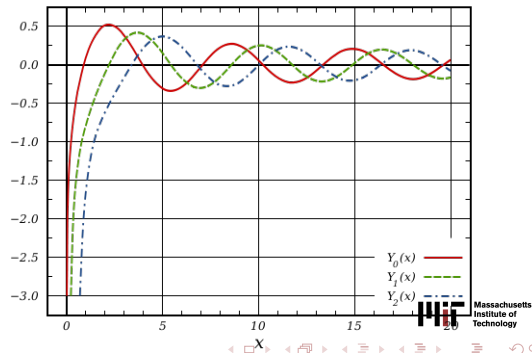
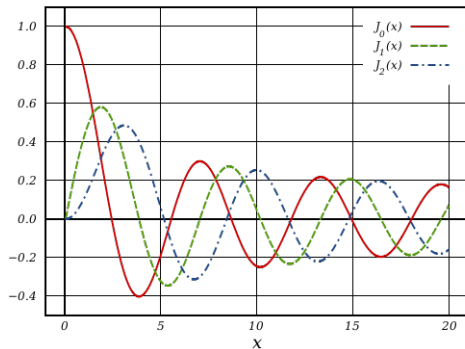
$$B_g^2 = B_z^2 + B_r^2$$

In the  $z$  direction, the buckling will yield the same solution as in the slab,  $B_z = \frac{\pi}{H}$ .

# Radial direction

General form of the solution is

$$\psi(r) = C_3 J_0(B_r r) + C_4 Y_0(B_r r)$$

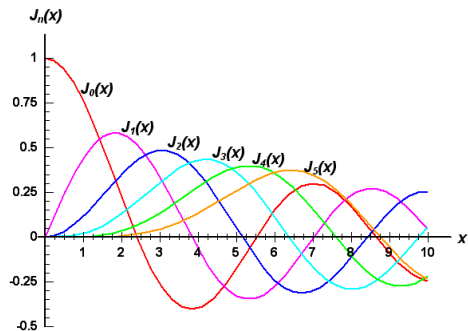


$$\frac{d^2\phi}{dr^2} + \frac{1}{r} \frac{d\phi}{dr} + \left( B_r^2 - \frac{n^2}{r^2} \right) \phi = 0$$

the solution is

$$\phi(r) = C_1 J_n(B_r r) + C_2 Y_n(B_r r)$$

In our case,  $n = 0$ ,  $C_2$  becomes 0 to maintain a finite flux at the center, and the fundamental mode is  $J_0$  with a first zero at 2.405.



# Axial Flux peaking - Neglecting extrapolation distances

We can calculate the peaking factor of the flux (or power) by taking the ratio of the maximum value of the flux to the average. The simplest way is to normalize the volume average to 1.

$$\overline{\phi(z)} = \frac{1}{V} \int_{-H/2}^{H/2} \phi(z) dV = 1$$

Replacing flux shape and volume element

$$\frac{C_z}{H} \int_{-H/2}^{H/2} \cos\left(\frac{\pi z}{H}\right) dz = 1$$

which yields  $C_z = 1.57$  which also corresponds to the peak of the axial flux.



# Radial Flux peaking - Neglecting extrapolation distances

We can calculate the peaking factor of the flux (or power) by taking the ratio of the maximum value of the flux to the average. The simplest way is to normalize the volume average to 1.

$$\overline{\phi(r)} = \frac{1}{V} \int_0^R \phi(r) dV = 1$$

Replacing flux shape and volume element

$$\frac{C_r}{R^2} \int_0^R r J_0\left(\frac{2.405r}{R}\right) dr = 1$$

which yields  $C_r = 2.32$  which also corresponds to the peak of the radial flux.

## 2 groups

Group 1 (Fast group)

$$-D_1 \nabla^2 \phi_1(\vec{r}) + \Sigma_{r,1} \phi_1(\vec{r}) = \frac{\chi_1}{k} (\nu \Sigma_{f,1} \phi_1(\vec{r}) + \nu \Sigma_{f,2} \phi_2(\vec{r}))$$

Group 2 (Thermal group)

$$-D_2 \nabla^2 \phi_2(\vec{r}) + \Sigma_{a,2} \phi_2(\vec{r}) = \Sigma_{s,1 \rightarrow 2} \phi_1(\vec{r})$$

The source free steady-state diffusion equation is an eigenvalue problem. Eigenvalue is placed on the fission source.

# Fundamental Mode

We assume that each group will have the same solution corresponding to the fundamental mode.

$$\nabla^2 \Phi(\vec{r}) + B_g^2 \Phi(\vec{r}) = 0$$

with  $\Phi(\vec{r}_s) = 0$ . Please note that the extrapolated distance boundary condition would be different for each group making the solutions slightly different. For this derivation we will assume that the extrapolation distance is zero and we will discuss this implication later. Thus the solutions for the 2 group system becomes

$$\phi_1(\vec{r}) = \phi_1 \Phi(\vec{r}) \quad \phi_2(\vec{r}) = \phi_2 \Phi(\vec{r})$$

Both fluxes have the same shape, just different magnitudes. Using the previous equation, we can isolate the geometrical buckling

$$-B_g^2 = \frac{\nabla^2 \Phi(\vec{r})}{\Phi(\vec{r})}$$

replacing in our 2 group equations and dividing by the flux shape everywhere, we get

$$D_1 B_g^2 \phi_1 + \Sigma_{r1} \phi_1 = \frac{1}{k} \left( \chi_1 \nu \Sigma_{f1} \phi_1 + \chi_1 \nu \Sigma_{f2} \phi_2 \right)$$

$$D_2 B_g^2 \phi_2 + \Sigma_{a2} \phi_2 = \Sigma_{s1 \rightarrow 2} \phi_1$$

We now have a simple system that we can represent in matrix form

$$\begin{bmatrix} D_1 B_g^2 + \Sigma_{r1} - \frac{1}{k} \nu \Sigma_{f1} & -\frac{1}{k} \nu \Sigma_{f2} \\ -\Sigma_{s1 \rightarrow 2} & D_2 B_g^2 + \Sigma_{a2} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

We can solve for  $k$  by setting the determinant of the matrix to 0

$$(D_1 B_g^2 + \Sigma_{r1} - \frac{1}{k} \nu \Sigma_{f1})(D_2 B_g^2 + \Sigma_{a2}) - \Sigma_{s1 \rightarrow 2} \frac{1}{k} \nu \Sigma_{f2} = 0$$

and isolating  $k$

$$k = \frac{\nu \Sigma_{f1}}{\Sigma_{r1} + D_1 B_g^2} + \frac{\Sigma_{s1 \rightarrow 2}}{\Sigma_{r1} + D_1 B_g^2} \frac{\nu \Sigma_{f2}}{\Sigma_{a2} + D_2 B_g^2}$$

# Example

Using the following 2 group x.s., find the critical bare homogeneous cylinder with height to diameter ratio of 1.

- $D_1 = 1.0$
- $\nu\Sigma_{f,1} = 0.02$
- $\Sigma_{r,1} = 0.08$
- $\Sigma_{s,1\rightarrow 2} = 0.058$
- $D_2 = 1.0$
- $\Sigma_{a,2} = 0.25$
- $\nu\Sigma_{f,2} = 0.5$

Geometrical buckling of the cylinder is given by (where  $H = 2R$ )

$$B_g^2 = \left( \frac{2.405}{H/2 + 2D} \right)^2 + \left( \frac{\pi}{H + 4D} \right)^2$$

# Example

Set  $k = 1$ , replace  $y = B_g^2$  and solve for  $y$

$$y^2 + 0.31y - 0.014 = 0$$

and find the roots  $y_1 = 0.1475$  and  $y_2 = -0.4575$ . Only positive root is valid. Negative root implies that an external current of neutrons would be needed to make core critical. Replace  $y_1$  in  $B_g^2$  equation and solve for  $H$ , and we once again find 2 roots,  $H_1 = 10.96\text{cm}$  and  $H_2 = -18.5\text{cm}$ , with once again only the positive root being valid.

# Eigenvector and Reactor Power

The solution of the eigenvalue problem provides a flux shape for the fundamental mode, but does not provide any idea of the flux magnitude.

- Flux must be normalized to reactor power
- Each fission produces  $\approx 200\text{MeV}$  per fission
- Detailed simulations must account for actual energy produce by each isotope as well as the deposition of the energy (in fuel, water or structure), it must also account for energy from capture.

$$Power = \int_V \kappa \Sigma_f \phi dV$$