22.211 Lecture 8

Heterogeneous Resonance Absorption

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Outline

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Objectives

- Resonance escape probability
- Heterogeneous resonance absorption
- Equivalence model
- Fuel escape probability

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Homogeneous Slowing Down

In the resonance region we can neglect the direct contributions from fission. We will also assume that the source is exclusively made up of elastic down scattering.

$$\begin{aligned}(\Sigma_{t1}(u)+\Sigma_{t0}(u))\phi(u) &= \int_{u-\epsilon_0}^{u} \frac{e^{-(u-u')}}{1-\alpha_0}\Sigma_{s0}(u')\phi(u')du' \\ &+ \int_{u-\epsilon_1}^{u} \frac{e^{-(u-u')}}{1-\alpha_1}\Sigma_{s1}(u')\phi(u')du' \\ &= R_0\left[\phi(u)\right] + R_1\left[\phi(u)\right]\end{aligned}$$

0 is the resonant nuclide and 1 is the moderator

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After Factorization

We factorize the flux into two components

$$\phi(u) = \psi(u)\varphi(u)$$

The flux outside of the resonance (where there is no significant absorption, $\psi(u)$, can be approximated by (for H-1)

$$\psi(u) = \frac{R_1\big[\phi(u)\big]}{\Sigma_{t1}}$$

We can thus cancel $\psi(u)$ everywhere to get

$$(\Sigma_{t1} + \Sigma_{t0}(u))\varphi(u) = R_0\big[\varphi(u)\big] + \Sigma_{t1}$$

We then divide by N_0 to obtain (with $\sigma_d = \Sigma_{t1}/N_0$)

$$(\sigma_d + \sigma_{t0}(u))\varphi(u) = r_0\big[\varphi(u)\big] + \sigma_d$$

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Intermediate Resonance Model

Resonances are neither wide or narrow and can be better represented as a mixture of both models.

$$r_{0,IR}\left[\varphi(u)\right] = \lambda_g \sigma_{p0} + (1-\lambda_g)\sigma_{s0}(u)\varphi(u)$$

The λ_g parameter is group dependent and will also depend on dilution.

$$\varphi_{IR}(u) = \frac{\lambda_g \sigma_{p0} + \sigma_d}{\sigma_{a0}(u) + \lambda_g \sigma_{s0}(u) + \sigma_d}$$

$$\sigma_d = \frac{\sum_{i=1}^{N} \lambda_i N_i \sigma_{pi}}{N_0}$$

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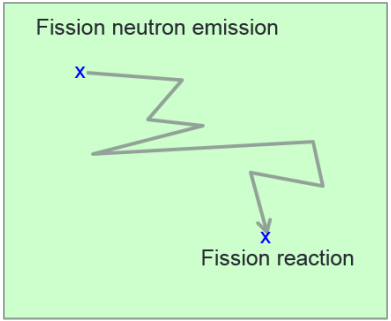
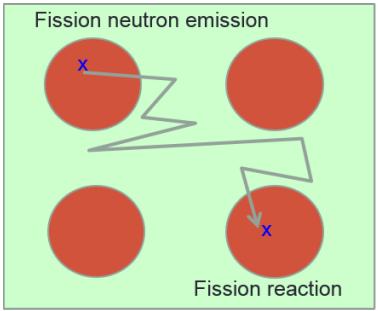
Homogeneous vs Heterogeneous

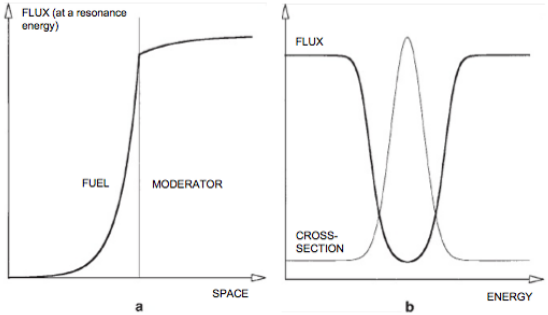


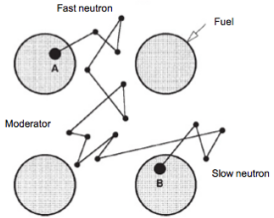
Homogeneous Reactor



Heterogeneous Reactor

Flux shape in fuel pin





Heterogeneous Slowing Down

Goal: Identify a problem that is equivalent to the homogeneous equation so that we can solve cross-sections in the homogeneous system as a function of dilution and establish an equivalence to the heterogeneous system.
2 region problem, balance of neutrons

$$V_f R_f\left[\phi_f(u)\right] P_{f\to f} + V_m R_m\left[\phi_m(u)\right] P_{m\to f} = V_f \Sigma_{tf} \phi_f(u)$$

$$V_f R_f\left[\phi_f(u)\right] P_{f\to m} + V_m R_m\left[\phi_m(u)\right] P_{m\to m} = V_m \Sigma_{tm} \phi_m(u)$$

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Collision probabilities

Probability of going from an isotropic source at point A and making a first collision at B

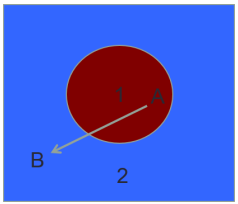
$$\frac{e^{-\tau}}{4\pi R^2}\Sigma_{tm} \quad where \;\; \tau = \int_0^R \Sigma_t(s)ds$$

Probability of going to any point in region 2

$$\int \frac{e^{-\tau}}{4\pi R^2}\Sigma_{tm} dV_m$$

If A is arbitrary and we want the average probability per unit volume in region 1, we get

$$P_{f\to m} = \frac{\Sigma_{tm}}{V_f}\int\int \frac{e^{-\tau}}{4\pi R^2} dV_m dV_f$$



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Reciprocity relation

Likewise, we can define

$$P_{m\to f} = \frac{\Sigma_{tf}}{V_m}\int\int \frac{e^{-\tau}}{4\pi R^2} dV_f\, dV_m$$

The integrals are symmetric, thus

$$P_{f\to m}\frac{V_f}{\Sigma_{tm}} = P_{m\to f}\frac{V_m}{\Sigma_{tf}}$$

which we can express

$$P_{f\to m} V_f \Sigma_{tf} = P_{m\to f} V_m \Sigma_{tm}$$

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Using same process as the homogeneous case

$$\phi(u) = \varphi(u)\psi(u)$$

$$\psi(u) = \frac{R_m\left[\phi_m\right]}{\Sigma_{tm}}$$

$$R_f\left[\phi_f(u)\right] = \psi(u)R_f\left[\varphi(u)\right]$$

And the reciprocity relation

$$V_m\Sigma_{tm}P_{m\to f} = V_f\Sigma_{tf}P_{f\to m}$$

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In the fuel

$$R_f\left[\varphi(u)\right]P_{f\to f}(u) + \Sigma_{tf}(u)(1 - P_{f\to f}(u)) = \Sigma_{tf}(u)\varphi(u)$$

Divide by $P_{f\to f}$ and N_f

$$r_f\left[\varphi(u)\right] + \frac{\sigma_{tf}(u)(1 - P_{f\to f}(u))}{P_{f\to f}(u)} = \frac{\sigma_{tf}(u)\varphi(u)}{P_{f\to f}(u)}$$

where we can define

$$\sigma_e(u) = \frac{\sigma_{tf}(u)(1 - P_{f\to f}(u))}{P_{f\to f}(u)} = \frac{\sigma_{tf}(u)P_{f\to m}(u)}{1 - P_{f\to m}(u)}$$

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Equivalence

We get the same equation as the homogeneous model, except for the energy/lethargy dependence of the dilution

$$r_f\left[\varphi(u)\right] + \sigma_e(u) = (\sigma_e(u) + \sigma_{tf}(u))\varphi(u)$$

Equivalence with homogeneous model will exist if we can set $\sigma_e(u)$ to a constant

$$\sigma_e(u) = \frac{\sigma_{tf}(u)P_{f\to m}(u)}{1 - P_{f\to m}(u)} = c_1$$

which implies

$$P_{f\to m}(u) = \frac{c_2}{\Sigma_{tf}(u) + c_2} \quad \Longrightarrow \quad c_1 = \frac{c_2}{N_f}$$

This is the basis of most self-shielding models used today!

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Multiple Nuclides in the Fuel

For multiple nuclides in the fuel, we treat them one resonant nuclide at the time assuming the other nuclides provide dilution (like in the homogeneous case).

$$R_f\left[\varphi(u)\right] = R_{f,0}\left[\varphi(u)\right] + \sum_{i=1}^{N} R_{f,i}\left[\varphi(u)\right] = R_{f,0}\left[\varphi(u)\right] + \sum_{i=1}^{N} \Sigma_{t,f,i}$$

thus making

$$r_{f,0}\left[\varphi(u)\right] + \sigma_b = (\sigma_b + \sigma_{tf0}(u))\varphi(u)$$

with

$$\sigma_b = \sigma_{d,fuel} + \sigma_e = \frac{\sum_{i=1}^{N} \lambda_i N_{i,f} \sigma_{pi,f}}{N_0} + \sigma_e$$

where λ_i is the intermediate resonance factor that measures the efficacy of a nuclide in comparison to H-1, $N_{i,f}$ is the nuclide density of nuclides in the fuel other then the nuclide of interest, N_0 is the nuclide density of the nuclide of interest in the fuel.

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Escape Probability

$P_{f\to m}$ in an isolated system is the probability that a neutron will escape the fuel region and make it's first flight collision in the moderator, this is also called the escape probability P_e.

$$P_e(E,\Omega) = \frac{1}{V_f}\int_S (\vec{n}\cdot\Omega)dS\int_0^l e^{-\Sigma_{tf}(E)s}ds$$

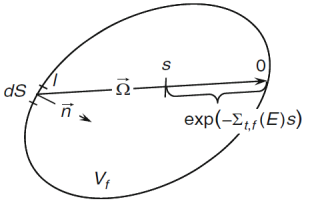

Figure 16
Calculation of escape probability

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Historical Approximations

- Wigner approximation

$$P_e(E) = \frac{1}{\Sigma_{tf}(E)\bar{l} + 1} \quad \Longrightarrow \quad \sigma_e = \frac{1}{\bar{l}N_0}$$

- Bell-Wigner approximation

$$P_e(E) = \frac{b}{\Sigma_{tf}(E)\bar{l} + b} \quad \Longrightarrow \quad \sigma_{e,b} = \frac{b}{\bar{l}N_0} = b\sigma_e$$

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N-term Rational Approximation

The rational form can also be used as a sum of multiple terms since each of them is equal to a constant. This allows for improved accuracy over the single term.

$$P_e(E) = \sum_{n=1}^{N} \beta_i \frac{\alpha_i \Sigma_e}{\Sigma_{tf}(E) + \alpha_i \Sigma_e}$$

which implies that

$$P_e(E) = \sum_{n=1}^{N} \beta_i P_{e,i}(E)$$

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Slowing down equation

recall

$$r_f\left[\varphi(u)\right] + \sigma_e(u) = (\sigma_e(u) + \sigma_{tf}(u))\varphi(u)$$

with

$$\sigma_e(u) = \frac{\sigma_{tf}(u)P_{f\to m}(u)}{1 - P_{f\to m}(u)} = c$$

which we can rewrite as

$$\Big(\sum_{i=1}^{N}\beta_i - \sum_{i=1}^{N}\beta_i P_{e,i}(u)\Big) r_f\left[\varphi(u)\right] + \sigma_{tf}(u)\sum_{i=1}^{N}\beta_i P_{e,i}(u)$$
$$= \sigma_{tf}(u)\sum_{i=1}^{N}\beta_i P_{e,i}(u)\varphi(u) + \Big(\sum_{i=1}^{N}\beta_i - \sum_{i=1}^{N}\beta_i P_{e,i}(u)\Big)\sigma_{tf}(u)\varphi(u)$$

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where we imposed

$$\sum_{i=1}^{N} \beta_i = 1$$

Pulling out the sum, we get

$$\sum_{i=1}^{N} \beta_i \Bigg[(1 - P_{e,i}(u)) r_f \left[\varphi(u)\right] + \sigma_{tf}(u) P_{e,i}(u) \\ = \sigma_{tf}(u) P_{e,i}(u) \varphi(u) + (1 - P_{e,i}(u)) \sigma_{tf}(u) \varphi(u) \Bigg]$$

which corresponds to N slowing down equations

2-term approximation

If we use a 2-term approximation defined

$$P_e(u) = \beta_1 \frac{\alpha_1}{\Sigma_{tf}(u)\bar{l} + \alpha_1} + \beta_2 \frac{\alpha_2}{\Sigma_{tf}(u)\bar{l} + \alpha_2}$$

which can be written

$$P_e(u) = \beta \frac{\alpha_1}{\Sigma_{tf}(u)\bar{l} + \alpha_1} + (1-\beta) \frac{\alpha_2}{\Sigma_{tf}(u)\bar{l} + \alpha_2}$$

Note that for the escape probability, we can write it as a function of lethargy (u) or energy (E), simply by changing the dependency of Σ_{tf} accordingly.

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Carlvik approximation - Infinite cylinder

Carlvik derived a 2-term rational approximation that matches the limits (0 and ∞) of the escape probability and the derivatives as we approach these limits.

$$P_e(E) = 2\frac{2}{\Sigma_{tf}(E)\bar{l}+2} - \frac{3}{\Sigma_{tf}(E)\bar{l}+3}$$

This yields two equivalent cross-sections

$$\sigma_{e1} = \frac{\alpha_1}{\bar{l}N_0} = \alpha_1\sigma_e \qquad \sigma_{e2} = \frac{\alpha_2}{\bar{l}N_0} = \alpha_2\sigma_e$$

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How to use it

The two-term expansion allows to evaluate the contribution from each term separately from the lookup tables. The resonance integral term becomes:

$$RI_{eff} = 2RI\left(\frac{\sum_{i=1}^{N}\lambda_i N_{i,f}\sigma_{pi,f}}{N_0} + 2\sigma_e\right) - RI\left(\frac{\sum_{i=1}^{N}\lambda_i N_{i,f}\sigma_{pi,f}}{N_0} + 3\sigma_e\right)$$

where RI is the resonance integral table from which we lookup, λ_i is the intermediate resonance factor that measures the efficacy of a nuclide in comparison to H-1, $N_{i,f}$ is the nuclide density of nuclides in the fuel other then the nuclide of interest, N_0 is the nuclide density of the nuclide of interest in the fuel.

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Process

- Generate resonance integral table for resonant isotope as a function of hydrogen
- Compute $\sigma_e = \frac{1}{lN_0}$
- Compute potential x.s. of non-resonant isotope in fuel
- Find RI_1 from interpolation table for $\sigma_b = \frac{\sum_{i=1}^{N} \lambda_i N_{i,f} \sigma_{pi,f}}{N_0} + \alpha_1 \sigma_e$
- Find RI_2 from interpolation table for $\sigma_b = \frac{\sum_{i=1}^{N} \lambda_i N_{i,f} \sigma_{pi,f}}{N_0} + \alpha_2 \sigma_e$
- Compute effective xs using

$$\sigma_{eff} = \frac{\beta RI_1 + (1-\beta) RI_2}{\beta \phi_1 + (1-\beta)\phi_2}$$

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Dancoff Effect

- Dancoff (Oppenheimer student) and Gainsburg identified this effect during the Manhattan project
- Escape probability assumes fuel is isolated in infinite moderator (i.e. first collision of neutron leaving fuel is always with moderator)
- In reality, neighboring fuel pins shadow a portion of the solid angle of neutron emitted from fuel pin of interest
- Dancoff introduced the following correction

$$C = \frac{I_0 - I}{I_0}$$

where I_0 is the number of neutrons entering the fuel region in an isolated system, while I is the number of neutrons entering the fuel as part of a lattice. It defines the probability of crossing moderator and reaching the next fuel rod.

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Fuel to moderator probability

When pins are placed in a lattice, the escape probability is not sufficient. A correction is needed to account for the probability that a neutron leaving the fuel will cross the moderator and collide in a neighboring fuel pin. The closer the pins, the higher that probability becomes (and larger the correction needs to be). Defining the thickness of the moderator by l, the uncollided probability between fuel regions is given by $e^{-\Sigma_{tm} l}$. This distance l will depend on the direction of travel, thus we can define the Dancoff correction factor (C) has

$$C = \frac{\int_{(\vec{n}\cdot\Omega)>0} (\vec{n}\cdot\Omega) d\Omega \int_S (\vec{n}\cdot\Omega) dS e^{-\Sigma_{tm} l}}{\int_{(\vec{n}\cdot\Omega)>0} (\vec{n}\cdot\Omega) d\Omega \int_S (\vec{n}\cdot\Omega) dS}$$

For an isolated geometry, $e^{-\Sigma_{tm} l}$ is equal to zero, thus the Dancoff correction is zero.

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Historical Perspective

We can insert the Dancoff correction in the Wigner, Bell-Wigner and Carlvik approximation. Here are the equations for the Wigner and the Bell-Wigner approximations.

- Wigner approximation

$$P_{f\to M}(E) = \frac{1-C}{\Sigma_{tf}(E)\bar{l}+1} \quad \Longrightarrow \quad \sigma_e = \frac{1-C}{\bar{l}N_0}$$

- Bell-Wigner approximation

$$P_{f\to M}(E) = \frac{b^+}{\Sigma_{tf}(E)\bar{l}+b^+} \quad \Longrightarrow \quad \sigma_{e,b^+} = \frac{b^+}{\bar{l}N_0} \qquad b^+ = \frac{(1-C)b}{1-C+Cb}$$

where $P_{f\to M}$ is the probability of leaving a fuel pin and colliding with the moderator. In the case of an isolated fuel pin, $C = 0$ and the equations revert to what we had previously.

Historical Perspective

We can insert the Dancoff correction in the Wigner, Bell-Wigner and Carlvik approximation. Here are the equations for Carlvik with the Dancoff correction.

$$P_{f\to M}(E) = \beta\frac{\alpha_1}{\Sigma_f(E)\bar{l}+\alpha_1} + (1-\beta)\frac{\alpha_2}{\Sigma_f(E)\bar{l}+\alpha_2}$$

with

$$\alpha_{1,2} = \frac{(5A+6) \mp \sqrt{A^2+36A+36}}{2(A+1)}$$

and

$$\beta = \frac{\frac{4A+6}{A+1}-\alpha_1}{\alpha_2-\alpha_1} \quad A = \frac{1-C}{C}$$

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Optimal Two-Term Rational Approximation

The current state-of-the-art has gone away from these analytical formulations and relies instead on a numerical procedure. The fuel-to-fuel (or fuel-to-moderator) collision probabilities are computed for a representative geometry and the parameters for the 2-term rational approximation are found through an error minimization problem.

- Search for optimal $\{\beta, \alpha_1, \alpha_2\}$ parameters
- Use a set of P reference values $P^{ref}_{f\leftarrow f}$
- Minimize RMS between two-term $P_{f\leftarrow f}$ and $P^{ref}_{f\leftarrow f}$

$$RMS = \sqrt{\frac{\sum_{p=1}^{P}\left(P_{f\leftarrow f}(\Sigma_{f,p}, \bar{l}) - P^{ref}_{f\leftarrow f,p}\right)^2}{P}}$$

with

$$P_{f\leftarrow f} = \beta\frac{\Sigma_f(E)}{\alpha_1\Sigma_e + \Sigma_f(E)} + (1-\beta)\frac{\Sigma_f(E)}{\alpha_2\Sigma_e + \Sigma_f(E)}$$

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- Reference probabilities can be generated from fixed source calculations
- Typically, they are generated for an infinite pin cell, which includes the infinite lattice Dancoff correction (C)
- Actual Dancoff corrections are then computed for each pin in the core or assembly, and partial cross-section for group g computed as

$$\sigma_{k,g} = \sigma_g \frac{RI_g\left(\frac{\sum_{i=1}^{N}\lambda_i N_{i,f}\sigma_{pi,f}}{N_0} + D_k\sigma_e\right)}{RI_g\left(\frac{\sum_{i=1}^{N}\lambda_i N_{i,f}\sigma_{pi,f}}{N_0} + D_\infty\sigma_e\right)}$$

where RI_g is the resonance integral at a given dilution and $D_k = 1 - C_k$ is the Dancoff factor for pin k.

Reference

- Read Chapter 9, section 3.5

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