MIE407 Nuclear Reactor Theory & Design

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Nuclear Stability:

- Stability of nucleus is the result of the balance between the strong nuclear force and the electromagnetic force.
- Range of the strong nuclear force is about $1\,\mathrm{fm}$ (femtometre, $10^{-13}\,\mathrm{cm}$)
- The strong nuclear force acts equally between protons and neutrons, but neutrons also reduce repulsions between protons by pushing them further apart from each other.
- Fermi approx: $r = R_0 A^{1/3}$ where $R_0 = 1.2\,\mathrm{fm}$
- The strong nuclear force is repulsive at very small distances, which contributes to the incompressibility of the nucleus.
- The strong nuclear force is insignificant at larger than around 4 proton diameters.

Nuclear Binding Energy:

- The binding energy of a nucleus can be found by calculating the mass defect of the nucleus compared to the mass of the unbound nucleons.

$$E_B = [Zm_p + (A - Z)m_n - m]c^2 \equiv \Delta M \times c^2 \tag{1}$$

- The binding energy is usually expressed as the average binding energy per nucleon $\varepsilon = E_B/A$.
- $1\,\mathrm{u}{=}931.5\,\mathrm{MeV/c^2}$

Compound nucleus decay modes:

- Neutron capture (n, γ): Nucleus decays to a lower energy state by emitting some gamma rays. $n +^A X \to^{A+1} X^* \to^{A+1} X + \gamma$
- Elastic scattering (n, n'): Neutron is re-emitted after leaving the nucleus in the ground state.
- Inelastic scattering $(n, n'\gamma)$: Neutron (usually high energy) is re-emitted at a lower energy, leaving the nucleus in an excited state. Then, the nucleus emits some gamma rays to return to the ground state.
- Fission (n, f): Nucleus splits into two fragments with approx. $2 : 3$ mass ratio.
- Particle emission $(n, \alpha), (n, p), (n, kn)$: A particle other than a neutron, or multiple neutrons are emitted. Only occurs with very high energy neutrons. Hence, only a small number of $(n, 2n)$ reactions occur in nuclear reactors.

Nuclear Fission

- When a thermal neutron ($\leq 1\,\mathrm{eV}$) is absorbed by a U-235 nucleus, it forms a compound nucleus that fissions with $\approx 84\%$ probability.
- Fission is a threshold reaction. In cases for U-235, the threshold energy is lower than the energy gained by binding the extra neutron. Hence, fissions may occur by neutrons with any energy. However, for U-238, the threshold energy is about 1 MeV greater than the energy gained by binding the extra neutron. Hence, fissions only occur by neutrons with kinetic energy greater than 1 MeV, which rarely occurs in even a fast reactor.
- Under thermal conditions ($0.0253\,\mathrm{eV}$ or $2200\,\mathrm{m/s}$) the distribution of fission products is a strong bimodal distribution (Peaks at $A = 96, 135$).
- Most neutrons (prompt neutrons) emitted in fission are released at the instant of fission.
- A small number of fission fragments also emit neutrons (delayed neutrons). These compose of $< 1\%$ of the total neutrons, but they are significant in the transient behavior of the reactor.
- Delayed neutrons result from high nuclear excitation of the daughter (when the excess energy exceed the nuclear binding energy of the neutron)
- Between 0 to 7 prompt neutrons may be emitted by fission, on average around 2.4. This is very important.
- The fission neutron spectrum is approximately $\chi(E) = 0.484 \sinh\left(\sqrt{2E}\right) e^{-E} \mathrm{MeV}^{-1}$. Integrate this over a interval of E to obtain the probability of energy in that interval. (Average $2\,\mathrm{MeV}$)
- Delayed neutrons are much lower energy ($400\,\mathrm{keV}$)
- Reaction Rate stuff
  - Intensity $I = nv$ $(1/\mathrm{cm}^2\mathrm{s})$
  - Flux ϕ $(1/\mathrm{cm}^2\mathrm{s})$
  - Number density $N = \frac{\rho N_A}{M}$ $(1/\mathrm{cm}^3)$
  - Microscopic cross section σ $(1/\mathrm{cm}^2)$
  - Macroscopic cross section $\Sigma = N\sigma$ $(1/\mathrm{cm})$
  - Reaction rate $R = \Sigma\phi$ $(1/\mathrm{cm}^3\mathrm{s})$
- *Passive* or non-multiplying media are characterized by the scattering (σ_s) and capture (σ_c) cross sections.
- *Multiplying* media contain at least one fissile or fissionable (fissile at high energy only) isotope and are further characterized by fission cross-section σ_f and ν.

1 Propogation of Neutrons in a Passive Medium

- Due to interactions with the medium, the initial intensity I_0 decreases to $I(x)$ at depth x.
- The rate of decrease is the reaction rate $I' = -R = \Sigma I$, with solution $I(x) = I_0 e^{-\Sigma x}$. Σ is the total cross-section.
- Understood in probability terms, $e^{-\Sigma x}$ is the probability that a neutron survive to depth x. Also, for very small Δx, $\Sigma \Delta x$ is the probability that a neutron will interact in Δx.
- Finally, $\Sigma e^{-\Sigma x} \Delta x$ is the probability that a neutron will interact between distance x and $x + \Delta x$.
- The **mean free path** is defined as the average distance a neutron travels before interacting

  $$\lambda = \int_0^\infty x p(x) \mathrm{d}x = \int_0^\infty x \Sigma e^{-\Sigma x} \mathrm{d}x = \frac{1}{\Sigma} \tag{2}$$

  Note that the mean free path can be used for a single reaction type also, e.g. $\lambda_s, \lambda_c, \lambda_f$.
- Point neutron source. The intensity of the source is $\dot{S}$.

- In empty space, $\phi(r) = \frac{\dot{S}}{4\pi r^2}$.
- In medium, $\phi(r) = \frac{\dot{S}}{4\pi r^2} e^{-\Sigma r}$
- If there is scattering, these equations will underestimate the flux.

2 Neutron Flux and Current

- In analyzing a nuclear reactor, we are interested in the neutron population at any position/time, and the rates of all nuclear reaction at any position/time.
- The neutron density is $n(\mathbf{r}, \mathbf{v}, t)$. It is useful to express the velocity vector as the speed v and the unit direction $\mathbf{\Omega}$. We also use kinetic energy (which contains the same information as the speed $E = \frac{1}{2}mv^2$) i,e, $n(\mathbf{r}, E, \mathbf{\Omega}, t)$.
- $n(\mathbf{r}, E, \mathbf{\Omega}, t)$ is a density function with units $1/\mathrm{cm}^3\mathrm{eVsr}$. $n(\mathbf{r}, E, \mathbf{\Omega}, t)\mathrm{d}V\mathrm{d}E\mathrm{d}\Omega$.
- With $\mu := \cos\theta$, we have $\mathrm{d}\Omega = -\mathrm{d}\varphi\mathrm{d}\mu/4\pi$, when we integrate over the all solid angles, we can integrate φ from 0 to 2π and μ from 1 to -1.
- Here, we define $\mathrm{d}\Omega = \mathrm{d}S/4\pi = -\mathrm{d}\varphi\,\mathrm{d}(\cos\theta)/4\pi$. Note that $\int_{4\pi}\mathrm{d}\Omega = \frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}\mu = 1$
- The **angular neutron density** $n(\mathbf{r}, E, \mathbf{\Omega})$ is an important reactor parameter used in the definition of neutron flux and current.
- The integral of the angular neutron density over all solid angles is the **neutron density** in $\mathrm{cm}^{-3}\mathrm{eV}^{-1}$

$$n(\mathbf{r}, E) = \int_{4\pi} n(\mathbf{r}, E, \mathbf{\Omega})\mathrm{d}\Omega. \tag{3}$$

- If some quantity q with density ρ can flow by a velocity field $\mathbf{v}$, we can define the **vector flux**

$$\mathbf{j} = \rho\mathbf{v}. \tag{4}$$

  We can define the **neutron flux density** as

$$\phi(\mathbf{r}, E, \mathbf{\Omega}) = n(\mathbf{r}, E, \mathbf{\Omega})\mathbf{v}(\mathbf{r}, E, \mathbf{\Omega}). \tag{5}$$

- The magnitude of vector flux density is the combined distance traveled by these neutrons (**this is important for determining reaction rate**) is defined as the **scalar neutron flux**,

$$\Phi(\mathbf{r}, E) = \int_{4\pi} \phi(\mathbf{r}, E, \mathbf{\Omega})\mathrm{d}\Omega = v\int_{4\pi} n(\mathbf{r}, E, \mathbf{\Omega})\mathrm{d}\Omega. \tag{6}$$

- The **neutron (net) current density** (**this is important for determining neutron transport**) is

$$\mathbf{J}(\mathbf{r}, E) = \int_{4\pi} \mathbf{v}n(\mathbf{r}, E, \mathbf{\Omega})\mathrm{d}\Omega = v\int_{4\pi} \hat{\mathbf{\Omega}}\, n(\mathbf{r}, E, \mathbf{\Omega})\mathrm{d}\Omega \tag{7}$$

- Since the integral in (7) is performed over all direction, which yields a vector that points in a particular direction. The direction of $\mathbf{J}$ represents the direction of **net** neutron flow.
- We can specify a unit vector $\hat{n}$ that is normal to $\mathrm{d}A$, then $\mathbf{J}\cdot\hat{n}\mathrm{d}A$ is the net number of neutrons crossing the surface $\mathrm{d}A$ per unit energy and unit time.

3 Neutron Diffusion Equation

- We will first try to understand how neutrons flows through an volume element $\Delta V = \Delta x \Delta y \Delta z$ within a passive medium. In a passive medium, there are two types of interactions (absorption and scattering).
- For sake of simplicity, we will assume a partial current $\mathbf{J} = J_x \hat{x}$. Due to interactions, we have

$$\frac{J_x(x+\Delta x, y, z) - J_x(x, y, z)}{\Delta x} \rightarrow \frac{\partial J_x}{\partial x} \mathrm{d}V \tag{8}$$

  We can repeat this for the J_y and J_z to obtain the **leakage** form

$$\mathrm{d}\mathcal{L} = \operatorname{div} \mathbf{J} \mathrm{d}V. \tag{9}$$

- At steady state, the net leakage (9) represents a mismatch between neutron gain and loss.
- The overall neutron balance in $\mathrm{d}V$ becomes

$$\mathrm{d}\mathcal{L} = (Q - R_a)\mathrm{d}V \tag{10}$$

  where Q is the source density in $\mathrm{cm}^{-3}\mathrm{s}^{-1}$ and $R_a = \Sigma_a \phi$ is the rate of absorption per unit volume.

$$\operatorname{div} \mathbf{J} + \Sigma_a \Phi = Q. \tag{11}$$

  equation (11) is the **neutron balance equation**.
- We need an equation to relate $\mathbf{J}$ and Φ. The most common approximation is the **diffusion approximation**, which assumes the neutron flux (**not neutron density**) behaves like a fluid

$$\mathbf{J}(\mathbf{r}) = -\mathbf{D}(\mathbf{r}) \nabla \Phi(\mathbf{r}) \tag{12}$$

- Here, the diffusion coefficient $\mathbf{D}$ has the dimensions of length. This depends on spatial position because the material in the reactor is not homogeneous. The diffusion coefficient is related to the cross-sections of the medium

$$D = \frac{\lambda_{tr}}{3} = \frac{1}{\Sigma_{tr}}, \tag{13}$$

  where λ_{tr} is the transport mean free path in cm.

3.1 Transport Cross-Section

- The macroscopic transport cross-section is determined by the density of the medium,

$$\Sigma_{tr} = N \sigma_{tr} \tag{14}$$

- The microscopic transport cross-section accounts for both absorption and inelastic scattering

$$\sigma_{tr} = \sigma_a + (1 - \bar{\mu})\sigma_s, \tag{15}$$

  where $\bar{\mu} \approx \frac{2}{3A}$ is the average cosine of the scattering angle θ.
- In the center of mass frame, the scattering is isotropic, but in the lab frame it is not due to conservation of momentum. $0 \leq \theta < 180°$ or $0 \leq \bar{\theta} < 90°$. As $\mu = \cos\theta, 1 \geq \mu > 0$.
- Typically, $\bar{\mu} << 1$ for heavier atoms $A >> 1$, so $\sigma_{tr} = \sigma_a + \sigma_s = \sigma_t$. In this course, **make this approximation unless otherwise told**.

3.2 Limitations of the Diffusion Approximation

- Underlying diffusion theory is an approximation that expresses the scattering kernel as an expression in Legendre polynomials, in which the first order term are used

$$\Sigma_s(z, \mathbf{\Omega} \to \mathbf{\Omega}') = \Sigma_s(z, \Omega \cdot \Omega') = \frac{1}{2\pi} \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \Sigma_s(z) \tag{16}$$

where $\mu = \cos(\mathbf{\Omega} \cdot \mathbf{\Omega}')$ and P_l is the Legendre polynomial of order l.

- This approximation is good **except**:
  - Near a strong source or absorber
  - At the boundary between two media with dissimilar neutron diffusion characteristics

3.3 Equation and Boundary Conditions

- Combining the diffusion approximation with the neutron balance equation, we obtain the **neutron diffusion equation**

$$(\mathrm{div}(D\nabla) + \Sigma_a)\Phi = Q \tag{17}$$

- A reactor core is modelled composed of numerous homogeneous regions in which this dependence on $\mathbf{D}$ vanishes. Then, this reduces to

$$(-D\Delta + \Sigma_a)\Phi = Q \tag{18}$$

- The net current at a plane $x = b$ inside a homogeneous material region in a slab reactor consists of two contributions

$$J_+(b) = \frac{\Phi(b)}{4} - \frac{D}{2}\frac{\mathrm{d}\Phi}{\mathrm{d}x} \tag{19}$$

$$J_-(b) = \frac{\Phi(b)}{4} + \frac{D}{2}\frac{\mathrm{d}\Phi}{\mathrm{d}x} \tag{20}$$

- These equations yield the net current at $x = b$ which agrees with Fick's law.
- Since neutrons leaving one region must enter the other, the additional boundary conditions are

$$J_+^A(b) = J_+^B(b) \tag{21}$$

$$J_-^A(b) = J_-^B(b) \tag{22}$$

Then substituting the values for J, we obtain

$$\frac{\Phi_A(b)}{4} - \frac{D_A}{2}\frac{\mathrm{d}\Phi_A}{\mathrm{d}x} = \frac{\Phi_B(b)}{4} - \frac{D_B}{2}\frac{\mathrm{d}\Phi_B}{\mathrm{d}x} \tag{23}$$

$$\frac{\Phi_A(b)}{4} + \frac{D_A}{2}\frac{\mathrm{d}\Phi_A}{\mathrm{d}x} = \frac{\Phi_B(b)}{4} + \frac{D_B}{2}\frac{\mathrm{d}\Phi_B}{\mathrm{d}x} \tag{24}$$

We can add and subtract these equations and obtain

$$\Phi_A(b) = \Phi_B(b) \tag{25}$$

$$D_A\frac{\mathrm{d}\Phi_A}{\mathrm{d}x} = D_B\frac{\mathrm{d}\Phi_B}{\mathrm{d}x} \tag{26}$$

Thus, we know from Fick's law that

$$J_A(b) = J_B(b) \tag{27}$$

$$\tag{28}$$

- When region B is vacuum, there is no return current. Hence,

$$0 = J_-^A(b) = \frac{\Phi_A(b)}{4} + \frac{D_A}{2}\frac{\mathrm{d}\Phi_A}{\mathrm{d}x} \tag{29}$$

$$\frac{\mathrm{d}\Phi_A}{\mathrm{d}x} = -\frac{1}{2D_A}\Phi_A(b) = -\frac{3}{2}\frac{\mathrm{d}\Phi_A}{\mathrm{d}\lambda_{tr}^A} \tag{30}$$

- We approximate beyond the boundary the neutron current is linear thus,

$$\delta_{ex} = -\frac{\Delta_A(b)}{\frac{\mathrm{d}\Phi_A}{\mathrm{d}x}} = \frac{2}{3}\frac{\lambda_{tr}^A}{\Phi_A(b)}\Phi_A(b) = \frac{2}{3}\lambda_{tr}^A \tag{31}$$

  With neutron transport theory, we get a better approximation for $\delta_{ex} = 0.71\lambda_{tr}^A$. This value δ_{ex} is called the **extrapolation length**.

3.4 Solution of the Neutron Diffusion Equation

- Consider a point isotropic source $\dot{S}$ in an infinite homogeneous and isotropic medium. The problem has spherical symmetry and has no source apart from $r = 0$, so the neutron diffusion equation reduces to

$$-D\Delta\Phi + \Sigma_a\Phi = 0 \tag{32}$$

$$-\frac{D}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\Phi}{\mathrm{d}r}\right) + \Sigma_a\Phi = 0 \tag{33}$$

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\Phi}{\mathrm{d}r}\right) - \frac{\Sigma_a}{D}\Phi = 0 \tag{34}$$

  We will define the **diffusion area** as

$$L^2 = \frac{D}{\Sigma_a} = \frac{1}{3\Sigma_{tr}\Sigma_a} \tag{35}$$

  Therefore,

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\Phi}{\mathrm{d}r}\right) - \frac{\Phi}{L^2} = 0 \tag{36}$$

- We can think of the diffusion area as
- Using the substitution $\Phi(r) = R(r)/r$, the differential equation becomes

$$\frac{\mathrm{d}^2R}{\mathrm{d}r^2} - \frac{R}{L^2} = 0 \tag{37}$$

  So the general solution is

$$R(r) = Ae^{-r/L} + Be^{r/L}. \tag{38}$$

- We can determine A and B using the boundary conditions at $r = 0$ and $r = \infty$. With the condition $\Phi(\infty) = \lim_{r\to\infty} R(r)/r = 0$, we have $B = 0$. For the boundary condition at $r = 0$, we have $\Phi(0) = \dot{S} = A/r$

4 Neutron Interaction with Matter

- Most of the neutron interactions are elastic scattering as it takes a very high energy neutron to excite a nucleus.

- In the lab frame, the nucleus is stationary and the neutron is moving. As momentum is conserved, the initial velocity of the neutron and the final velocity of the neutron and nucleus are on a plane, so we can solve this as a 2D problem.
- In the center of mass frame, the observer will see the two particle approach it, collide, and leave the center of mass at a different angle.
- Let the nucleus be at the origin. Then, the center of mass will be

$$x_0 = \frac{m_n x}{m_n + M} = \frac{x}{1 + M/m_n} \approx \frac{1}{1+A} \tag{39}$$

$$v_{cm} = \frac{\mathrm{d}x_0}{\mathrm{d}t} = \frac{v}{1 + M/m_n} \approx \frac{1}{1+A} v \tag{40}$$

- In the center of mass frame, the total momentum is zero. The speeds are

$$\text{neutron} \qquad v_c = v - v_{cm} = v - \frac{1}{1+A} v = \frac{A}{1+A} v \tag{41}$$

$$\text{nucleus} \qquad V_c = V + v_{cm} = 0 + \frac{1}{1+A} v = -\frac{1}{1+A} v \tag{42}$$

- From conservation of momentum we know that the velocities after collision can be related with

$$v_c' = -\frac{M}{m} V_c' \tag{43}$$

- As kinetic energy is also conserved in elastic collisions, so in the center of mass frame, the speed is unchanged. Hence, only the angle rotates by the angle of scattering Θ.
- We suppose the center of mass is moving in the z direction. Then, the xy component of the final velocity is the same in the lab and center of mass frames, so

$$v' \sin\theta = v_c' \sin\Theta \tag{44}$$

$$v' \cos\theta = v_{cm} + v_c' \cos\Theta \tag{45}$$

  Then, we can divide the two equations

$$\cot\theta = \frac{v_{cm} + v_c' \cos\Theta}{v_c' \sin\Theta} \tag{46}$$

$$= \cot\Theta + \frac{1}{A\sin\Theta} \tag{47}$$