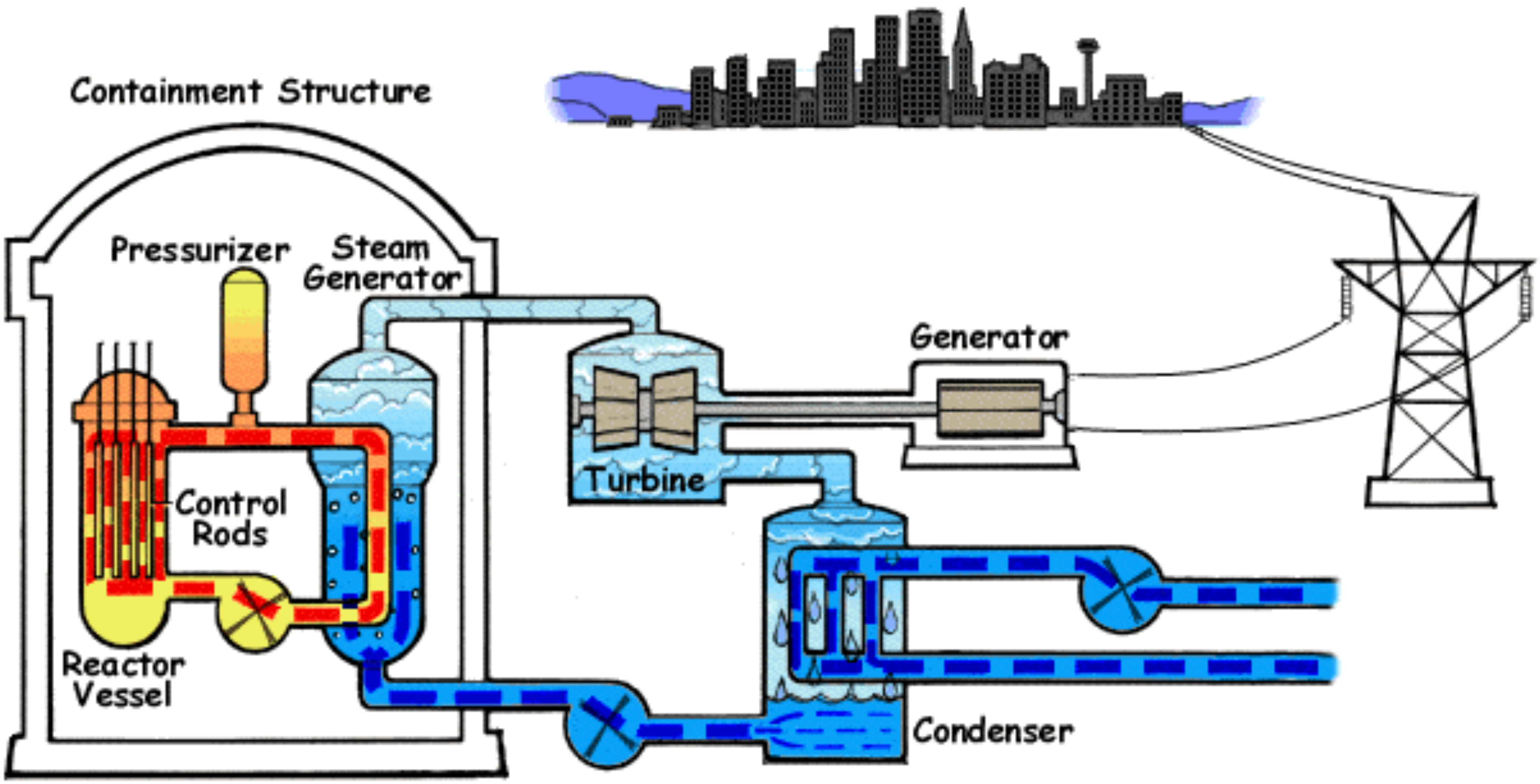
Pressurized Water Reactor (PWR)



Models:

- Involve neutron transport, thermal-hydraulics, chemistry
- Inherently multi-scale, multi-physics

CRUD Measurements: Consist of low resolution images at limited number of locations.

Pressurized Water Reactor (PWR)

3-D Neutron Transport Equations:

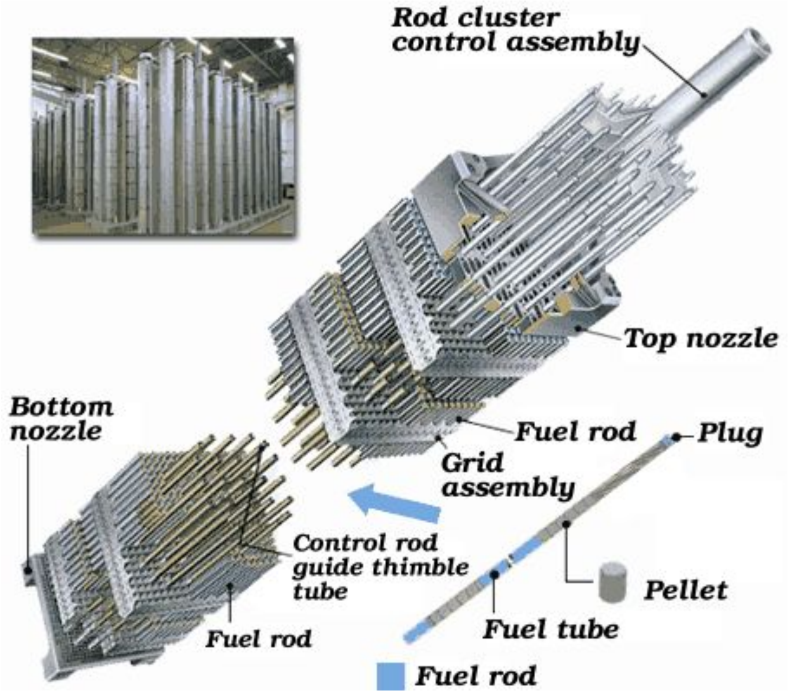
$$\frac{1}{|v|}\frac{\partial \varphi}{\partial t} + \Omega \cdot \nabla \varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t)$$
$$= \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(E' \to E, \Omega' \to \Omega)\varphi(r,E',\Omega',t)$$
$$+ \frac{\chi(E)}{4\pi}\int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E')\Sigma_f(E')\varphi(r,E',\Omega',t)$$

Challenges:

- Linear in the state but function of 7 independent variables:

  $$r = x, y, z; E; \Omega = \theta, \phi; t$$

- Very large number of inputs or parameters; e.g., 100,000; Parameter selection critical.
- ORNL Code: Denovo
- Codes can take hours to days to run.



Pressurized Water Reactor (PWR)

Thermo-Hydraulic Model: Mass, momentum and energy balance for fluid

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \nabla \cdot (\alpha_f \rho_f v_f) = -\Gamma$$

$$\alpha_f \rho_f \frac{\partial v_f}{\partial t} + \alpha_f \rho_f v_f \cdot \nabla v_f + \nabla \cdot \sigma_f^R + \alpha_f \nabla \cdot \sigma + \alpha_f \nabla p_f$$
$$= -F^R - F + \Gamma(v_f - v_g)/2 + \alpha_f \rho_f g$$

$$\frac{\partial}{\partial t}(\alpha_f \rho_f e_f) + \nabla \cdot (\alpha_f \rho_f e_f v_f + Th) = (T_g - T_f)H + T_f \Delta_f$$
$$-T_g(H - \alpha_g \nabla \cdot h) + h \cdot \nabla T - \Gamma[e_f + T_f(s^* - s_f)]$$
$$-p_f\left(\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f v_f) + \frac{\Gamma}{\rho_f}\right)$$

Note: Similar equations for gas

Challenges:

- Nonlinear coupled PDE with nonphysical parameters due to closure relations;
- CASL code: COBRA (CTF)
- COBRA is a sub-channel code, which cannot be resolved between pins.
- Codes can take minutes to days to run.

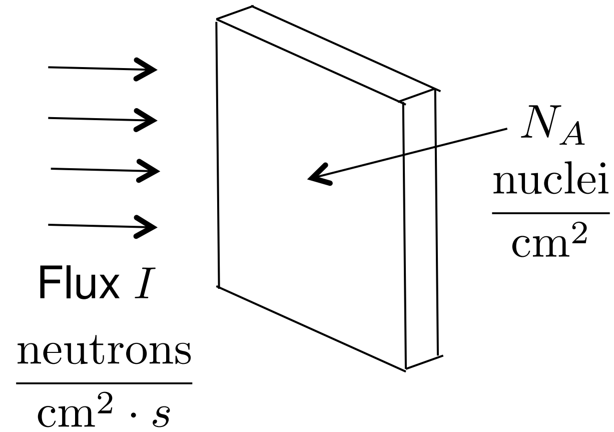
Microscopic Cross-Sections

Cross-Sections: Probability that a neutron-nuclei reaction will occur is characterized by nuclear cross-sections.

- Assume target is sufficiently thin so no shielding.
- Rate of Reactions:

$$R = \sigma I N_A$$

Note: σ is microscopic cross-section (cm^2)



- Microscopic Cross-Sections: Related to types of reactions.

σ_f: Fission

σ_s: Scatter

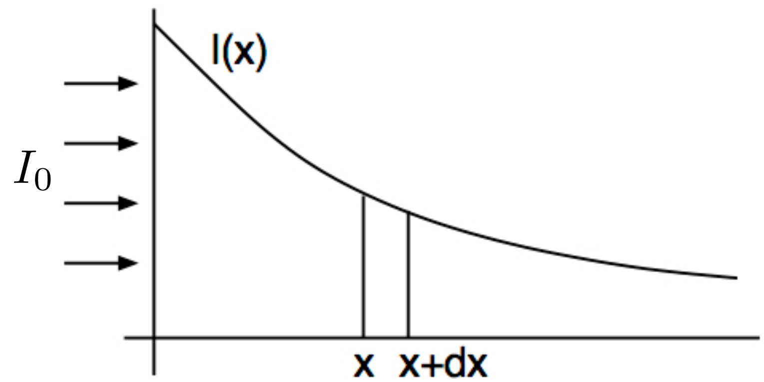
σ_t: Total

Reference: J.J. Duderstadt and L.J. Hamilton, *Nuclear Reactor Analysis,* John Wiley and Sons, 1976.

Macroscopic Cross-Sections

Macroscopic Cross-Sections: Accounts for shielding

Total Reaction Rate per Unit Area:



$$dR = \sigma_t I dN_A$$
$$= \sigma_t I N dx$$

Strategy: Equate reaction rate to decrease in intensity

$$-dI(x) = -[I(x+dx) - I(x)]$$
$$= \sigma_t I N dx$$
$$\Rightarrow \frac{dI}{dx} = -N\sigma_t I(x)$$
$$\Rightarrow I(x) = I_0 e^{-N\sigma_t x}$$

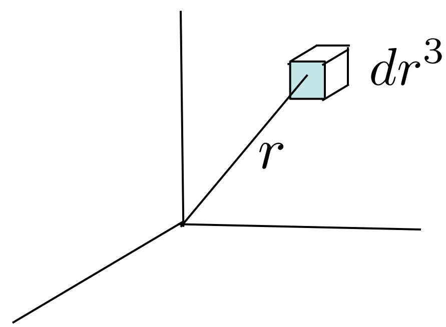
Total Macroscopic Cross-Section: $\Sigma_t \equiv N\sigma_t$

Frequency: With which reactions occur $v\Sigma_t$ $\quad \frac{cm}{s}\frac{1}{cm} = \frac{1}{s}$

Neutron Flux in Reactor

Neutron Density: $N(r,t)$

- $N(r,t)dr^3$: Expected number of neutrons in dr^3 about r at time t
- $N(r,E,t)dr^3dE$: Expected number neutrons in dr^3 with energies E in dE



Reaction Rate Density: Interaction frequency $v\Sigma$ where v is neutron speed

$$F(r,E,t)dr^3 = v\Sigma N(r,E,t)dEdr^3$$

Angular Neutron Density:

- $n(r,E,\hat{\Omega},t)dr^3dEd\hat{\Omega}$: Expected number of neutrons in dr^3 about r with energy E about dE, moving in direction $\hat{\Omega}$ in solid angle $\hat{\Omega}$ at time t

Angular Neutron Flux: $\varphi(r,E,\hat{\Omega},t) = vn(r,E,\hat{\Omega},t)$

Neutron Transport Equation

Conservation Law:

$$\frac{\partial}{\partial t}\left[\int_V n(r, E, \hat{\Omega}, t) dr^3\right] = \text{gain in } V - \text{loss in } V$$

Gain Mechanisms:

(1) Neutron sources (fission)

(2) Neutrons entering V

(3) Neutrons of different $E', \hat{\Omega}'$ that change to $E, \hat{\Omega}$ due to scattering collision

Loss Mechanisms:

(4) Neutrons leaving V

(5) Neutrons suffering a collision

Neutron Transport Equation

Terms:

(1) $\int_V S(r, E, \hat{\Omega}, t) dr^3 dE d\hat{\Omega}$ where S is a source term

(5) Rate at which neutrons collide at point r is

$$f_t = v\Sigma_t(r, E) n(r, E, \hat{\Omega}, t)$$

$\Rightarrow$ (5) = $\left[\int_V v \sum_t (r, E) n(r, E, \hat{\Omega}, t) dr^3\right] dE d\hat{\Omega}$

(2), (4) Consider the rate at which neutrons leak out of surface

$$j(r, E, \hat{\Omega}, t) \cdot dS = v\hat{\Omega} n(r, E, \hat{\Omega}, t) \cdot dS$$

so leakage is

$$\text{(4) - (2)} = \left[\int_S dS \cdot v\hat{\Omega} n(r, E, \hat{\Omega}, t)\right] dE d\hat{\Omega}$$

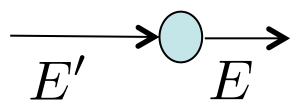
$$= \left[\int_V \nabla \cdot v\hat{\Omega} n(r, E, \hat{\Omega}, t) dr^3\right] dE d\hat{\Omega}$$

$$= \left[\int_V v\hat{\Omega} \cdot \nabla n(r, E, \hat{\Omega}, t) dr^3\right] dE d\hat{\Omega}$$

Neutron Transport Equation

Terms: Scattering cross-sections

- Consider first a beam of neutrons of incident intensity I, all of energy E', hitting a thin target of surface atomic density N_A



Note: Microscopic differential scattering cross-section is proportionality constant

$$\frac{\text{Rate}}{\text{cm}^2} = \sigma_s(E' \rightarrow E) I N_A dE$$

when neutron scatters from energy E' to final energy E in range E to $E + dE$

Microscopic scattering cross-section:

$$\sigma_s(E') = \int_0^\infty dE \sigma_s(E' \rightarrow E)$$

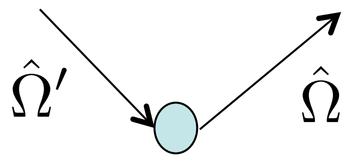
Macroscopic scattering cross-section:

$$\Sigma_s(E' \rightarrow E) \equiv N \sigma_s(E' \rightarrow E)$$

Neutron Transport Equation

Terms: Scattering cross-sections

- Consider how change in direction



$$\sigma_s(\hat{\Omega}') = \int_{4\pi} d\hat{\Omega}\sigma_s(\hat{\Omega}' \to \hat{\Omega})$$

(3) Rate at which neutrons scatter from $E', \hat{\Omega}'$ to $E, \hat{\Omega}$ is

$$\left[\int_V v'\Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega})n(r, E', \hat{\Omega}', t)dr^3\right] dEd\hat{\Omega}$$

To incorporate contributions from any $E', \hat{\Omega}'$, we integrate to obtain

$$(3) = \left[\int_V dr^3 \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' v'\Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega})n(r, E', \hat{\Omega}', t)\right] dEd\hat{\Omega}$$

Neutron Transport Equation

Conservation Law:

$$0 = \int_V \left[\frac{\partial n}{\partial t} + v\hat{\Omega} \cdot \nabla n + v\Sigma_t n(r, E, \hat{\Omega}, t) \right.$$
$$\left. - \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' v' \Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega}) n(r, E', \hat{\Omega}', t) - S(r, E, \hat{\Omega}, t) \right] dr^3 dE d\hat{\Omega}$$

Since this must hold for any control volume, it follows that

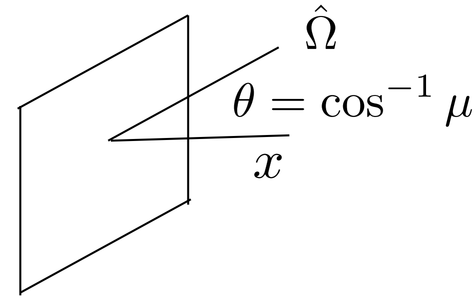
$$\frac{\partial n}{\partial t} + v\hat{\Omega} \cdot \nabla n + v\Sigma_t n(r, E, \hat{\Omega}, t)$$
$$= \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' v' \Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega}) n(r, E', \hat{\Omega}', t) + S(r, E, \hat{\Omega}, t)$$

Angular Flux: $\varphi(r, E, \hat{\Omega}, t) = vn(r, E, \hat{\omega}, t)$

$$\frac{1}{v}\frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_t(r, E)\varphi(r, E, \hat{\Omega}, t)$$
$$= \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \Sigma_s(E' \to E, \hat{\Omega}' \to \hat{\Omega}) \varphi(r, E', \hat{\Omega}', t) + S(r, E, \hat{\Omega}, t)$$

Neutron Transport Equation

Plane Symmetry: Flux depends only on x



- $\Omega_x = \cos\theta$
- $\int_{4\pi} d\hat{\Omega}' = \int_0^{\pi} d\theta' \sin\theta'$

Then

$$\hat{\Omega}\cdot\nabla\varphi = \Omega_x \frac{\partial\varphi}{\partial x} = \cos\theta\frac{\partial\varphi}{\partial x}$$

so

$$\frac{1}{v}\frac{\partial\varphi}{\partial t} + \cos\theta\frac{\partial\varphi}{\partial x} + \Sigma_t\varphi(x,E,\theta,t)$$
$$= \int_0^{\pi} d\theta'\sin\theta' \int_0^{\infty} dE'\Sigma_s(E'\to E,\theta'\to\theta)\varphi(x,E',\theta',t) + S(x,E,\theta,t)$$

1-D Neutron Transport Equation:

$$\frac{1}{v}\frac{\partial\varphi}{\partial t} + \mu\frac{\partial\varphi}{\partial x} + \Sigma_t\varphi(x,E,\mu,t)$$
$$= \int_{-1}^{1} d\mu' \int_0^{\infty} dE'\Sigma_s(E'\to E,\mu'\to\mu)\varphi(x,E',\mu',t) + S(x,E,\mu,t)$$