2. The Steady State and the Diffusion Equation

The Neutron Field

• Basic field quantity in reactor physics is the neutron angular flux density distribution:

 $\Phi(\vec{r}, E, \vec{\Omega}, t) = v(E)n(\vec{r}, E, \vec{\Omega}, t)$

- -- distribution in space (\vec{r}) , energy (E), and direction $(\vec{\Omega})$ of the neutron flux in the reactor at time *t*.
- Need to solve the transport equation for an accurate estimate of local reaction rates, particularly near fuel rods and strong neutron absorbers. At steady state, we have:

$$\Sigma(\vec{r}, E)\Phi(\vec{r}, E, \vec{\Omega}) + \vec{\Omega} \cdot \vec{\nabla}\Phi(\vec{r}, E, \vec{\Omega}) = \int_{0}^{\infty} dE' \int_{0}^{4\pi} d^{2}\Omega' \Sigma(\vec{r}, E' \to E, \vec{\Omega}' \to \Omega)\Phi(\vec{r}, E', \vec{\Omega}')$$

- Domain is large and heterogeneous, with extremely complex energy dependence of cross sections
- Transport equation cannot be applied to the entire domain, yet it is required for accurate estimate of local reaction rates. Therefore,

\Rightarrow task must be segmented

 \Rightarrow unit cells with reflective boundary conditions

$\Rightarrow \textit{transport theory within unit cells} \\ \Rightarrow \textit{diffusion theory for global flux distribution in reactor}$

Transport Equation

• At steady state, within the phase-space elementary volume, neutron losses (L.H.S.) are equal to neutron production (R.H.S.)

LOSSES

 $\begin{array}{ll} \sum \bullet \Phi & \\ \vec{\Omega} \bullet \vec{\nabla} \Phi & \\ \end{array} & \text{neutrons lost by collision} \\ \text{streaming term, net losses through leakage} \end{array}$

PRODUCTION

- 1) elastic scattering
- 2) inelastic scattering
- 3) (n, 2n),...
- 4) <u>fission</u>

• Fission is ISOTROPIC

-direction of emission $\vec{\Omega}$ is independent of $\vec{\Omega}'$ and E'-probability is uniform $\Rightarrow \frac{1}{4\pi}$ -number of neutrons is function of incident energy v = v(E')-emission energy (*E*) is independent of $E' \Rightarrow \chi(E)$

$$\therefore \sum_{\text{fission}} \left(\vec{r}; E' \to E, \vec{\Omega}' \to \Omega \right) = \frac{1}{4\pi} \chi(E) v \sum_{f} (\vec{r}, E')$$

(Note: We have neglected the delayed neutron source)

Separation of cell and reactor calculations



The DRAGON Neutron Transport Code



- entirely developed at Ecole Polytechnique
- many options | cartesian, hexagonal geometry clusters, cylinders
- can also solve 3D Transport problems in "supercell" geometries, required for calculating properties of reactivity mechanisms

The Scalar Flux

- The angular flux density is of no interest per se.
- The ultimate objective is to determine the fission rate (power). Since fission is isotropic, we have:

$$\frac{\text{fission rate}}{\text{cm}^3} = \int_0^\infty \Sigma_f(\vec{r}, E, t) \phi(\vec{r}, E, t) dE$$

• The neutron scalar flux is the actual quantity of interest for the neutron field in the reactor. It is formally related to the angular density by:

$$\phi(\vec{r}, E, t) = \int_{4\pi} n(\vec{r}, E, \vec{\Omega}, t) \cdot v(E) d^2 \Omega$$

- The scalar flux distribution will be *obtained directly* by solving the *diffusion equation* over the entire reactor.
- Reaction rates are conserved by using appropriately *homogenized macroscopic cross sections* for each unit cell in the reactor.
- The homogenized cross sections are obtained from the transport calculations in the unit cells (using transport codes such as WIMS, APPOLLO or DRAGON).

Note:

• Advanced Monte Carlo methods can be used to solve accurately the neutron field over an entire domain in transport theory (no approximations). However, this stochastic approach is presently limited to small systems, and is not practical to deal with the problem of nuclide depletion (fuel management).

Neutron Balance and the Diffusion Equation

- By integrating the transport equation over all angles, we obtain an equation for the scalar flux density which can be solved over the entire domain. This will yield the required neutron balance equation for the reactor.
 - In time-dependent form, we must account for:
 - The *delayed neutron source* S_d, which varies locally according to the concentration of the delayed neutron precursors;
 - The presence of any *external source* of neutrons, S, which might be placed in the reactor (e.g. at startup). This source, if it is present, will produce a fixed number of neutrons per unit time, independent of the current state of the reactor.
 - The local *production of prompt fission neutrons*, proportional to the instantaneous fission rate.
- One obtains the continuity equation:



Prompt Neutrons Delayed Neutrons

- This equation is exact (no approximations), but contains an additional *independent* variable, the neutron current *J*, which is not simply related to the scalar flux.
- We can close the system by making the *diffusion approximation* (Fick's Law):

$$\vec{J}(\vec{r}, E, t) = -D(\vec{r}, E, t)(\vec{\nabla}\phi(\vec{r}, E, t)$$

to obtain the time-dependent diffusion equation.

The Diffusion Equation

• For clarity, the diffusion equation can be put in operator notation. In practice, it would be discretized and the operators would appear as matrices:

$$\frac{1}{v}\frac{\partial\phi}{\partial t} = (\mathbf{F}_p - \mathbf{M})\phi + S_d + S$$

• The delayed neutron source results from the radioactive decay of the precursors. Assuming that there are *K* precursors, with decay constants λ_k , we can write:

$$S_d(\vec{r}, E, t) = \sum_{k=1}^{K} \chi_{dk}(E) \lambda_k C_k(\vec{r}, t)$$

where χ_{dk} is the delayed neutron emission spectrum (different from the prompt neutron emission spectrum χ_p) and where the precursor concentrations are given by the precursor depletion equations:

$$\frac{\partial C_k(\vec{r},t)}{\partial t} = -\lambda_k C_k(\vec{r},t) + \int_0^\infty dE' v_{dk} \Sigma_f(\vec{r},E',t)$$

• We note that the delayed neutron source is not completely independent of the scalar flux (it is a function of the flux history). The precursor equations are therefore coupled to the diffusion equation, and must be solved simultaneously.

• Interpretation:

The diffusion equation simply states that the rate of change of the neutron scalar flux at position \vec{r} for neutrons of energy *E* is the result of differences between:

- The production of fission neutrons (prompt operator $\mathbf{F}_p \phi$ and the delayed source S_d), plus any external source of neutrons S, if present, and
- The removal of neutrons (operator $\mathbf{M}\phi$) via absorption and scattering plus net leakage of neutrons to other points in the reactor;
- It is the presence of the leakage term $(-\vec{\nabla} \cdot D\vec{\nabla}\phi)$ in operator **M** that introduces the spatial coupling between points in the reactor and provides for a *continuous distribution of the flux.*

TIME DEPENDENT DIFFUSION EQUATION

- Operator notation (continuous) $\mathbf{F}_{p}\phi = \chi_{p}(E) \int_{\vartheta}^{\infty} dE' v_{p}(E') \Sigma_{f}(\vec{r}, E', t) \phi(\vec{r}, E', t) \quad \text{prompt fission source}$ $\mathbf{M}\phi = -\vec{\nabla} \cdot D(r, E)\vec{\nabla}\phi + \Sigma_{a}\phi(r, E, t)$ $-\int_{0}^{\infty} dE' \Sigma_{s}(r, E' \to E, t) \phi(r, E', t)$ scattering "source"
- In practice we use themultigroup formulation (matrix notation, discrete energy groups)

group flux:
$$\phi_g(r,t) = \int_{Eg}^{Eg-1} dE' \phi(r,E',t)$$

For

$$\left[\frac{1}{\mathbf{v}}\right]\frac{\partial}{\partial t}\underline{\phi} = \left[\mathbf{F}_{p}\right]\underline{\phi} - \left[\mathbf{M}\right]\underline{\phi} + \underline{S}_{d} + \underline{S}$$

$$\left[\frac{1}{\mathbf{v}}\right] = \begin{bmatrix}\frac{1}{\mathbf{v}_{1}} & 0 \\ & \ddots \\ 0 & \frac{1}{\mathbf{v}_{G}}\end{bmatrix}$$

with
$$\begin{bmatrix} \mathbf{F}_p \end{bmatrix} \boldsymbol{\phi} = \begin{bmatrix} \boldsymbol{\chi}_p \end{bmatrix} \begin{bmatrix} \mathbf{F}_p \end{bmatrix}^T \boldsymbol{\phi}$$

 $\begin{bmatrix} \boldsymbol{\chi}_p \end{bmatrix} = \begin{bmatrix} \boldsymbol{\chi}_{p1(r)} \\ \vdots \\ \boldsymbol{\chi}_{pG(r)} \end{bmatrix}, \begin{bmatrix} \mathbf{F}_p \end{bmatrix}^T = \begin{bmatrix} \boldsymbol{v}_{p1} \boldsymbol{\Sigma}_{f1}, \cdots, \boldsymbol{v}_{pG} \boldsymbol{\Sigma}_{fG} \end{bmatrix}$

 $[\mathbf{M}] \underline{\phi} = [\mathbf{L}] \underline{\phi} + [\mathbf{A}] \underline{\phi}$ age scattering and absorption and leakage $\begin{bmatrix} \mathbf{A} \end{bmatrix} = \begin{pmatrix} \Sigma_{11} & \mathbf{0} & \mathbf{0} \\ -\Sigma_{21} & \Sigma_{22} & \\ \vdots & \ddots & \\ -\Sigma & -\Sigma & -\Sigma & \Sigma_{11} \end{pmatrix}$ $\begin{bmatrix} \mathbf{L} \end{bmatrix} = \begin{bmatrix} -\vec{\nabla} \cdot D_1 \vec{\nabla} & & \\ & \ddots & \\ & & -\vec{\nabla} \cdot D_G \vec{\nabla} \end{bmatrix}$ 2nd order partial derivatives

DIFFUSION EQUATION

Example: 2 energy groups

$$\begin{split}
\varphi &= \begin{bmatrix} \phi_{1}(r,t) \\ \phi_{2}(r,t) \end{bmatrix} \text{ "fast" flux "thermal" flux} \\
\begin{bmatrix} \frac{1}{v_{1}} & 0 \\ 0 & \frac{1}{v_{2}} \end{bmatrix} \xrightarrow{\partial} \left[\phi_{1} \\ \phi_{2} \end{bmatrix} = \overbrace{\left[\begin{array}{c} \chi_{p1} v \Sigma_{f1} & \chi_{p1} v \Sigma_{f2} \\ \chi_{p2} v \Sigma_{f1} & \chi_{p2} v \Sigma_{f2} \end{bmatrix} \left[\phi_{1} \\ \phi_{2} \end{bmatrix} \\
& + \overbrace{\left[\begin{array}{c} -\vec{\nabla} \cdot D_{1} \vec{\nabla} + \Sigma_{11} & 0 \\ -\Sigma_{21} & -\vec{\nabla} \cdot D_{2} \vec{\nabla} + \Sigma_{22} \end{bmatrix} \left[\phi_{2} \end{bmatrix} \\
& + \overbrace{\left[\begin{array}{c} -\vec{\nabla} \cdot D_{1} \vec{\nabla} + \Sigma_{11} & 0 \\ -\Sigma_{21} & -\vec{\nabla} \cdot D_{2} \vec{\nabla} + \Sigma_{22} \end{bmatrix} \left[\phi_{2} \end{bmatrix} \\
& + \overbrace{\left[\begin{array}{c} S_{D} \\ + \sum_{k=1}^{K} \left[\begin{array}{c} \chi_{dk1} \\ \chi_{dk2} \end{array} \right] \lambda_{k} C_{k} + \begin{bmatrix} S_{1} \\ S_{2} \end{bmatrix} \right] \\
\end{split}$$

usually:

• $\left[\chi_{p}\right] = \begin{bmatrix} 1\\ 0 \end{bmatrix}$ $\chi_{dk} = \begin{bmatrix} 1\\ 0 \end{bmatrix}$

i.e. all fission neutrons appear in fast group

- no up-scattering $(\Sigma_{12} = 0)$
- These equations must be discretized in \vec{r} :
 - finite difference approximation for spatial derivatives in leakage terms $\left(-\vec{\nabla}\cdot D\vec{\nabla}\right)$

- typically 15 000 unknowns for each energy group

- yields a set of algebraic equations which must be integrated over time

BOUNDARY CONDITIONS

a) internal surfaces between material regions

- angular flux density must be continuous:
 - $\Phi_{(1)}\left(r_{s}, E, \vec{\Omega}, t\right) = \Phi_{(2)}\left(r_{s}, E, \vec{\Omega}, t\right)$
- Net Current must be continuous: $\vec{J}_{(1)}(r_s E, t) = \vec{J}_{(2)}(r_s E, t)$

For diffusion theory, this implies

- continuity of flux $\phi_{(1)} = \phi_{(2)}$

- continuity of current $-D_{(1)}\vec{\nabla}\phi_{(1)} = -D_{(2)}\vec{\nabla}\phi_{(2)}$

b) outer boundaries (free surfaces)

 \hat{e}_s : normal unit vector (1) $if \begin{vmatrix} \hat{e}_s \cdot \vec{\Omega} > 0 \text{ neutron is leaving the system} \\ \hat{e}_s \cdot \vec{\Omega} < 0 \text{ neutron is entering the domain} \end{vmatrix}$

Free surface boundary condition (no re-entry)

$$\Phi(r_s E, \Omega, t) = 0$$

for r_s on surface, and $\hat{e}_s \cdot \vec{\Omega} < 0$

• Diffusion theory; the true B.C. is approximated by imposing J - (r, E, t) = 0, which can be written generally as:

$$D(r_{s})\hat{e}_{s} \cdot \vec{\nabla} \phi(r_{s}, E, t) + \frac{1}{2} \left(\frac{1-\alpha}{1+\alpha} \right) \phi(r_{s}, E, t) = 0$$

albedo
$$\begin{cases} \alpha = 0 & \text{free surface} \\ \alpha = 1 & \text{reflection} \end{cases}$$

establishes a relation between flux and gradient of the flux at the boundary

The Steady State and Criticality

$$\frac{1}{v}\frac{\partial\phi}{\partial t} = (\mathbf{F}_p - \mathbf{M})\phi + S_d + S$$

- Let us postulate that a steady state exists in the reactor.
- Under this condition:
 - -- the delay between fission and the emission of the delayed neutrons is not significant;
 - -- the delayed neutron source is in equilibrium with the flux distribution;
 - -- the fission production operator becomes:

$$\mathbf{F}\phi = \chi(E)\int_{0}^{\infty} dE' \nu \Sigma_{f}(\vec{r}, E)\phi(\vec{r}, E) \equiv \mathbf{F}_{p}\phi + \mathbf{F}_{d}\phi$$

where v is the total number of neutrons emitted in fission, including delayed neutrons, and $\chi(E)$ is the total neutron emission spectrum.

• Let us also postulate that there is no external source present in the reactor (S=0). In that case, the *steady state neutron balance equation* reduces to:

$$\widetilde{\mathbf{F}} \overrightarrow{\boldsymbol{\phi}} = \widetilde{\mathbf{M}} \overrightarrow{\boldsymbol{\phi}}$$

Interpretation:

For a steady state to exist in the absence of an external neutron source, the number of neutrons (of energy E) at each point in the domain must be exactly equal to the number of neutrons (of energy E) eliminated at that point, including leakage to other regions or to the exterior of the reactor.

In this situation only will the reactor be declared *critical*.

Criticality and the External Source

$\overrightarrow{\mathbf{F}} \overrightarrow{\boldsymbol{\phi}}$	$= \mathbf{M}\phi^{losses}$
$\widetilde{\mathbf{F}\phi}$	$=\widetilde{\mathbf{M}q}$

We observe:

- The flux level is arbitrary in a critical reactor (homogeneous equation).
- If production were to exceed losses, the flux level would increase. The reactor then would be said to be *supercritical*;
- If production were to be less than losses, the flux level would decrease. The reactor then would be said to be in a *subcritical* state.
- Let us now suppose that there is an external source present in the steady-state reactor (S≠0). The balance equation then becomes:

$\overrightarrow{\mathbf{F}} \phi$ +	external source	- Mo
$\mathbf{\Gamma} \boldsymbol{\psi}_s = \mathbf{T}$	5	-1 VI ψ

We observe:

- For a steady state to exist in a reactor in the presence of an external source, the reactor must necessarily be subcritical;
- The steady-state flux level is not arbitrary in a subcritical reactor (inhomogeneous equation). It is in fact proportional to the intensity of the source *S*.

Conclusion:

- There can be only one of two conditions leading to a steady-state neutron flux (and power) in a fission chain reactor:
 - \Rightarrow The reactor is critical with no source, or
 - \Rightarrow The reactor is subcritical with an external source.

Static Reactivity – The λ Eigenvalue

- Consider solutions to the steady-state diffusion equation for the following hypothetical situations:
 - 1) A reactor is known to be in a critical state
 - 2) A reactor is known to be in a near-critical configuration

For case 2), we get only the trivial solution $\phi = 0$. For case 1) we also get a trivial solution because our knowledge of the material properties (homogenized cross sections) is never perfect. In order to obtain a non-trivial solution we introduce an *eigenvalue* λ which will multiply the fission source term:

$\mathbf{M}\phi = \lambda \mathbf{F}\phi$

This is the appropriate form of the static diffusion equation.

- The constant λ (the eigenvalue) is unique for the whole reactor.
- It is uniformly adjusted until the critical balance between both sides of the equation is assured at every point. The corresponding distribution φ is called the eigenfunction.
- Mathematically, many solutions are possible. However, there is only one value of λ which corresponds to non-singular and positive values of φ at every point inside the domain (the fundamental solution):

 \Rightarrow unique physically realizable solution

• The closer λ is to 1.0, the closer the system is to being critical. If λ = 1.0, the reactor is critical, and the fundamental solution is physically realized:

 \Rightarrow the actual (steady state) flux distribution

• The difference between 1.0 and λ is called the *static reactivity*:

$$\rho_s = 1.0 - \lambda$$

Static Reactivity

$$\rho_s = 1.0 - \lambda$$

- The static reactivity is a measure of the uniform correction needed to make the reactor critical (for ex. an arbitrary correction to the average number of neutrons per fission).
- The static reactivity is a characteristic of the entire reactor, and not of any region in particular. The solution to the static diffusion equation is extremely valuable in reactor design because it provides:
 - an estimate of how close the system is to critical (the value of ρ_s)

- an estimate of the flux distribution (hence power) if the reactor were actually

critical.

• An estimate of the static reactivity can be obtained with Rayleigh's quotient:

$$\lambda = rac{\left\langle \phi_0^*, \mathbf{M} \phi
ight
angle}{\left\langle \phi_0^*, \mathbf{F} \phi
ight
angle}$$

where the < > bracket notation denotes integration over all space and energy and where ϕ_0^* is a weighting function (called the *adjoint flux*). For static reactivity, we therefore can write:

$$\lambda = rac{\left\langle \phi_0^*, (\mathbf{F} - \mathbf{M}) \phi
ight
angle}{\left\langle \phi_0^*, \mathbf{F} \phi
ight
angle}$$

Note that ρ_s and λ have no physical units (being ratios of reaction rates).

A related concept is the effective multiplication factor, called $k_{eff}.$ We have k_{eff} = 1/ $\!\lambda$, so that:

$$\rho_{s} = 1.0 - \frac{1.0}{k_{\rm eff}} = \frac{k_{\rm eff} - 1}{k_{\rm eff}}$$

PERTURBATION THEORY AND THE ADJOINT FLUX

Reference:

$$\mathbf{M}_0 \boldsymbol{\phi}_0 = \boldsymbol{\lambda}_0 \mathbf{F}_0 \boldsymbol{\phi}_0$$

- ϕ_0 is a known solution - $1 - \lambda_0$ is the reference static reactivity

Perturbation:

Ex: - control rod layout

- refuellings

- structural material

We wish to evaluate $-\Delta\lambda$ (change in static reactivity) due to perturbations ΔM and ΔF without solving the perturbed systems equations $\left(\mathbf{M}\phi = \lambda \mathbf{F}\phi\right)$

Perturbation formula (first order)



• Second order $O(\Delta \phi)^2$ accuracy is achieved when ADJOINT flux ϕ_0^* is chosen as a weighting function.

Adjoint flux

 $\mathbf{M}_{0}^{*}\boldsymbol{\phi}_{0}^{*}=\boldsymbol{\lambda}_{0}\mathbf{F}_{0}^{*}\boldsymbol{\phi}_{0}^{*}$ (importance function) \Rightarrow

 $(\lambda_0^* = \lambda_0)$

 $\Delta \lambda = \lambda - \lambda_{0}$

The Effective Multiplication Factor



- We see that the effective multiplication factor is simply the effective number of ۲ neutrons produced for each neutron eliminated in the system (by absorption and leakage).
- In elementary reactor theory, this factor is often expressed as the product of factors ۲ relating to the reproduction cycled of neutrons from one generation to the next (the six factor formula):

$$keff = k_{\infty} \cdot \Lambda_f \Lambda_t$$
$$= \varepsilon \eta f p \cdot (\Lambda_f \Lambda_t)$$

Ex.: CANDU ε fast fission factor 1.027 η resonance escape probability 0.907 thermal utilization factor f 0.906 Thermal reproduction factor $(v\Sigma_f / \Sigma_a \text{ in fuel})$ 1.224 Λ_f non-leakage probability for fast neutrons 0.994 0.974 non-leakage probability for thermal neutrons Λ_{t}

Thus we have:

$0 < k_{\rm eff} < \infty$
$-\infty < \rho_s < 1.0$

with:

State	Flux	k _{eff}	$ ho_s$
subcritical	\downarrow	<1.0	<0
critical	\rightarrow	=1.0	=0
supercritical	\uparrow	>1.0	>0

where:

• ADJOINT WEIGHTING (simple example)



With uniform properties in one energy group, the reference solution is obtained:

$$\begin{bmatrix} -D_0 \frac{d^2}{dx^2} + \Sigma_{a0} \end{bmatrix} \phi_0(x) = \lambda_0 v \Sigma_{f0} \phi_0(x)$$

with $\phi_0(x) = 0$ at $x = \pm a$
$$\frac{d^2 \phi}{dx^2} + B^2 \phi = 0, \quad \therefore \ \phi_0(x) = \phi_0 \cos Bx$$

$$B^{2} = \left(\frac{\pi}{2a}\right)^{2}$$
 from boundary conditions; B^{2} is geometric buckling (curvature)

Inserting

Inserting $\frac{d^2\phi}{dx^2} = -B^2\phi$ into the reference solution above gives:



- **Perturbation:** localized at center, with small effect on flux. We will assume $\phi = \phi_0$ in the range from $-x_p \le x \le x_p$ (i.e. cos Bx~1.0)
- Adjoint equation: with one energy group,

$$\begin{array}{c} \mathbf{M}_{0}^{*} = \mathbf{M} \\ \mathbf{F}_{0}^{*} = \mathbf{F} \end{array} \right\} \text{ so that } \phi_{0}^{*} = \phi; \quad \text{adjoint flux is equal to real flux}$$

Consider two cases, for localized perturbation $\Delta \Sigma_a$:

No Adjoint Weighting

$$\Delta \rho = \frac{-\int\limits_{-x_p}^{x_p} dx \Delta \Sigma_a \phi_0(x)}{\int\limits_{-a}^{a} dx \nu \Sigma_{f0} \phi_0(x)}$$
$$= \frac{\pi}{2} \left(\frac{\Delta \Sigma_a}{\nu \Sigma_{f0}}\right) \frac{x_p}{a}$$

Correct Formula

$$\Delta \rho = \frac{-\int\limits_{-x_p}^{x_p} dx \Delta \Sigma_a [\phi_0(x)]^2}{\int\limits_{-a}^{a} dx v \Sigma_{f0} [\phi_0(x)]^2}$$
$$= 2 \left(\frac{\Delta \Sigma_a}{v \Sigma_{f0}}\right) \frac{x_p}{a}$$

27% higher, which accounts for the fact that neutron importance is greater in center than at the periphery.

Conclusion:

- -- Importance weighting is essential
- -- Generally, $\phi_{g}^{*}(r) \neq \phi_{g}(r)$ (with more than one energy group)