

PHYS-E0562 Nuclear Engineering, advanced course Lecture 2 – Deterministic transport theory

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Topics of this lecture

Introduction to the coupled problem:

- Non-linearity caused by coupling to thermal hydraulics and fuel depletion
- Scale of the coupled problem
- Reactor physics calculation chain

Transport theory:

- Neutron density, flux and current
- Formulation of the neutron transport equation

Physical properties of the transport problem:

- Fundamental and transient mode solutions
- Eigenvalue problem and criticality calculations
- Point kinetics approximation



What is expected to be known before the lecture

Reactor physics:

- Basic concepts: neutron flux, cross section, reaction rates
- Prompt and delayed neutrons

Misc:

- Basic stuff about differential equations
- Basic idea on how to solve neutron transport problems



The operation of a nuclear reactor is based on the self-sustaining chain reaction, carried on by fission neutrons. Consequently, a major part of reactor analysis involves the transport and interaction physics of neutrons.

Solution to the neutron transport problem provides sufficient information on neutron-induced reaction rate distributions within the reactor core, which can be used for calculating output, power distribution, depletion and production rates of nuclides, etc.

There are major challenges in the solution of the transport problem:

- High level of heterogeneity, as neutrons are not uniformly distributed in the fuel
- Reaction probabilities (microscopic cross sections) are strongly dependent on neutron energy
- Time-scales of prompt and delayed neutrons differ by several orders of magnitude ([µs] or [ms] vs. [s])

Reactor analysis relies heavily on computational modeling, and any transport method used for solving reactor physics problems needs to be able to cope with these challenges.





Figure 1 : Neutron density distribution in reactor geometry. Left: BWR fuel assembly. Right: Small test reactor core (ATR reactor, Idaho National Laboratory). When frozen in time, most of the neutrons in thermal systems are found in large moderator regions. Density is considerably lower in fuel and absorbers.²

²The neutron density distribution is not to be confused with flux distribution, which also depends on neutron speed, therefore emphasizing higher energies (see Fig. 2).



Even though microscopic cross sections are complicated functions of neutron energy, the transport problem is linear by nature with the following assumptions:

- Neutrons do not interact with each other³
- Reaction probabilities are independent of reaction rates

The linearity assumption applies to criticality experiments and very low power research reactors. For commercial power reactors, the reality is unfortunately different, because reaction probabilities depend on:

- 1) Material temperatures and densities
- 2) Material compositions

This creates a non-linear problem, in which the neutronics solution is coupled to:

- 1) Heat transfer and coolant flow (via reactivity feedbacks)
- 2) Isotopic changes in fuel during the reactor operating cycle (via fuel depletion)

Solving the transport problem alone is not sufficient for the modeling of an operating nuclear reactor – the calculation scheme needs to be able to handle also reactivity feedbacks and fuel depletion

³Neutron density in a power reactor is in the order of 10¹⁰ 1/cm³, which can be compared to the density of hydrogen atoms in water or uranium atoms in fuel (\sim 10²² 1/cm³).



The coupling between neutronics and thermal hydraulics is particularly strong in light water reactors, because the reactor operates on thermal neutrons (\sim 80% of fissions), and the slowing-down process is sensitive to operating conditions:

- Neutrons are born with a mean energy of 2 MeV, and they require ~20 elastic collisions with hydrogen nuclei to reach the thermal region (< 1 eV)</p>
- If the neutron returns to fuel too early, it is more likely to be absorbed in the capture resonances of ²³⁸U than cause fission in ²³⁵U
- Since coolant serves the purpose of moderator as well, any change in the reactor operating state is immediately reflected in the slowing-down process

Reactivity feedbacks represent fast, almost immediate coupling between neutronics and reactor operating conditions. In the long time-scale, similar non-linearity is induced by changes in fuel composition by neutron irradiation:

- ²³⁵U is depleted and replaced by ²³⁹Pu as the primary fissile isotope
- Non-fissile plutonium, minor actinides (Np, Am, Cm) and fission products are accumulated in the fuel, increasing absorption
- Burnable absorber used for passive reactivity control is depleted

Nuclear fuel in light water reactors is loaded in the reactor core for the duration of the entire operating cycle, which is typically 12 or 18 months. A single fuel assembly remains in the core for several cycles, and is exposed to intense neutron irradiation for 3 to 4 years.



In practice, the real challenge in reactor modeling is to obtain the solution to the coupled problem by assuming that the problem can be linearized over some time interval and performing iterations between the different solvers.

Obtaining high-fidelity solutions to neutronics, heat transfer, coolant flow and fuel depletion becomes a tremendous task:

- Typical LWR core contains 50,000 100,000 fuel rods, number of fuel pellets is counted in millions
- Fuel temperature varies by hundreds of degrees, depending on local power⁴
- Significant variation in coolant density, especially in BWR's
- Accurate simulation of fuel burnup would require tracking the concentrations of hundreds of isotopes in millions of depletion zones

Calculations involving a single state-point without burnup are barely within the capabilities of modern super-computers.

Reactor design and safety analyses require covering various operating states, time-dependent simulations, modeling of core depletion over multiple cycles, modeling of reactivity control, etc., which renders the direct approach unfeasible in practice.

⁴Even the difference between surface and center-line temperature in a fuel pellet can exceed 400 K during normal operation.



Instead, the traditional approach to coupled problems is to divide the neutronics solution in parts:



- The scale of the modeled system is gradually increased, while simultaneously moving towards more simplified description of physics
- ▶ Spatial resolution: nuclide-level \rightarrow pin-level \rightarrow assembly-level \rightarrow core-level
- ► Energy resolution: continuous-energy → micro-group structure → macro-group structure → few-group structure
- Transition from one stage to the next is carried out in such way that local reaction rate balance is preserved
- The details of the calculation chain depend on the modeled system and the methods used

The final stage involves a simplified description of the full-scale system, which can be coupled to the solution of heat transfer and coolant flow.



From an engineering point of view, the typical LWR calculation chain can be divided into three computational tasks:

- (i) Production of nuclide-wise microscopic interaction data for neutron transport codes from evaluated nuclear data
- (ii) Solution of the local heterogeneous transport problem at fuel assembly level using higher-order transport methods
- (iii) Solution of the global homogeneous transport problem using reduced-order methods, such as diffusion theory

The second step is called spatial homogenization, and it provides the sufficient building blocks for the full-scale simulation:

- Traditionally carried out using deterministic 2D lattice transport codes
- Input: isotopic micro-group reaction cross sections, detailed description of the geometry at fuel assembly level
- Output: handful of macroscopic few-group constants representing the transport physics



Dividing the calculation chain into separate steps enables running coupled full-core simulations at an acceptable computational cost without compromising the accuracy.

The cost of reducing the physical complexity by spatial homogenization is that all information on reactivity feedback effects and dependence of reaction rates on fuel burnup is completely lost.

This information is recovered by repeating the procedure over and over again in such way that all reactor operating conditions are covered:

- Assembly types
- Variation in thermal-hydraulic state variables: fuel temperature, coolant temperature and density
- Reactivity control: soluble boron, insertion of control rods
- Fuel depletion

The result is a parametrized library of reactor-specific group constants, from which the data corresponding to local operating conditions can be obtained by interpolation.



The neutronics solution in LWR core calculations is typically based on two-group nodal diffusion methods, and coupled simulations can be used, for example, for:

- Steady state fuel cycle simulations, modeling normal reactor operation over one or several cycles
- Dynamic simulations, modeling the behavior of the reactor core in transients

Fuel cycle simulations are needed for core design, to make sure that the reactor remains critical and within the safety margins. Dynamic simulations are needed for safety analyses, and to study the behavior in abnormal operating conditions.⁵

The multi-stage calculation chain based on spatial homogenization and nodal diffusion methods has the potential to produce very accurate results in full-scale 3D simulations at an acceptable computational cost ...

⁵Nuclear power plant simulations require modeling the reactor core as part of the coolant loop(s), including pumps, valves, heat exchangers, etc. This type of simulations are carried out using system codes, in which the reactor is modeled using similar methods as in core simulations, or using simplified methods, such as 1D neutronics or point-kinetics approximation.



- ... but the approach also has its limitations:
 - Homogenized group constants are case-specific, i.e. they must be generated separately for each problem
 - Different reactor types (LWR, SFR, HTGR) may require different methods both in assembly and core-level calculations
 - Traditional deterministic lattice transport codes usually rely on a 2D solution, which is not sufficient for describing 3D effects encountered in some advanced reactor types
 - Dividing the full-scale transport problem into isolated sub-problems creates artificial interfaces, which affect the quatility of the solution

In general, there is a multitude of deterministic transport codes and methods developed for different purposes, and no universal calculation scheme that could handle all applications with the same level of reliability. The two-group nodal diffusion methods covered in this course apply mainly to conventional LWR analyses.

The results are always subject to uncertainties and errors in both methodology and input data, and the calculation scheme can be validated by comparison to experimental data and high-fidelity methods.



The remaining lectures in this course cover the various stages of the multi-stage calculation scheme and method used for obtaining the solution to the coupled problem:

- This and the following lecture cover the deterministic and stochastic (Monte Carlo) approach to transport theory
- Diffusion theory, which forms the basis of nodal diffusion methods, is derived from transport theory in Lecture 4
- Lecture 5 deals with fuel depletion and the solution of the burnup problem
- Lecture 6 covers the basics of heat transfer and coolant flow
- Lectures 7 and 8 cover spatial homogenization and nodal diffusion methods, i.e. the solution of the full-scale transport problem
- Lectures 9 and 10 cover the methods used thermal hydraulics and fuel behaviour modeling
- Lecture 11 covers reactor dynamics (time-dependent solution of the coupled problem)
- Lecture 12 covers design and simulation of reactor operating cycle



Basic concepts of transport theory

The main objective of neutron transport calculation is to solve the nuclear reaction rate distribution within the reactor core. All deterministic solution methods rely on transport theory, which is based on relatively simple conservation laws and a few mathematical definitions.

Transport theory of neutrons shares some similarities with other transport problems, for example, in fluid dynamics and plasma physics, with a few significant differences:

- 1) The interaction probabilities are very strongly dependent on neutron energy
- The forces acting in collisions have very limited range, and the neutron path is broken into a "random walk" from one collision to the next
- 3) Neutron-neutron interactions can be ignored

As discussed later on, neutron transport can be considered a linear problem under certain approximations.



Basic concepts of transport theory: cross sections

The probabilities of neutron-induced reactions are characterized by cross sections. As discussed in Lecture 1, the total macroscopic cross section, Σ , gives the total interaction probability per traveled path length:

$$dP = \Sigma(\boldsymbol{r}, E)ds \tag{1}$$

Scattering reactions are associated with a change in neutron energy and direction of motion, and they are described by double-differential cross sections, which combine the probability of the scattering event to distributions of energy transfer and scattering angle. The probability of a neutron scattering from direction $\hat{\Omega}$ to $\hat{\Omega}'$ and energy E to E' per traveled path length is given by:

$$dP = \Sigma_{\rm s}(\mathbf{r}, \hat{\mathbf{\Omega}} \to \hat{\mathbf{\Omega}}', E \to E') ds d\Omega' dE'$$
⁽²⁾

The change in direction is often written using the scattering cosine $\mu = \cos \theta = \hat{\Omega} \cdot \hat{\Omega}'$, i.e. the cosine of the angle θ between the direction vectors before and after the collision (the second angle, φ , describing the rotation of the scattered direction vector around the incident direction is called the azimuthal angle).



The double-differential scattering cross section is then written as $\Sigma_s(\mathbf{r}, \mu, E \to E')$. This is a valid approximation in an isotropic medium, in which case the scattering rate does not depend on the absolute direction of the incident neutron.



Basic concepts of transport theory: cross sections

Macroscopic cross section is related to microscopic cross section, σ , by:

$$\Sigma(\mathbf{r}, E) = N(\mathbf{r})\sigma(E) \tag{3}$$

where N is the nuclide density. Microscopic cross section can therefore be interpreted as the interaction probability per traveled path length and nuclide density. An alternative interpretation is that this parameter represents the effective cross-sectional area of the nucleus.

Microscopic cross sections are nuclide-specific constants, which depend on the reaction type and neutron energy. The total cross section can be written as the sum over partial reaction modes:

$$\sigma(E) = \sigma_{\text{capt}}(E) + \sigma_{\text{fiss}}(E) + \sigma_{\text{ela}}(E) + \dots$$
(4)

The same applies to macroscopic cross sections:

$$\Sigma(\mathbf{r}, E) = \Sigma_{\text{capt}}(\mathbf{r}, E) + \Sigma_{\text{fiss}}(\mathbf{r}, E) + \Sigma_{\text{ela}}(\mathbf{r}, E) + \dots$$

= $N(\mathbf{r}) [\sigma_{\text{capt}}(E) + \sigma_{\text{fiss}}(E) + \sigma_{\text{ela}}(E) + \dots]$ (5)

And if the medium consists of multiple nuclides:

$$\Sigma(\mathbf{r}, E) = \sum_{i} \Sigma_{i}(\mathbf{r}, E) = \sum_{i} N_{i}(\mathbf{r})\sigma_{i}(E)$$
(6)

where the summation is carried over all the constituent nuclides.



Basic concepts of transport theory: neutron population

All deterministic transport methods treat neutrons as a collective population of independent particles, with the help of three concepts:

- Neutron density
- Neutron flux
- Neutron current (or current density)

Neutron density and flux are best understood as two closely related density-like functions in the six-dimensional phase-space, depending on the position and momentum variables, although the momentum variable is usually replaced by energy and direction of motion.

(7)

The direction of motion $\hat{\Omega}$ depends on two angular variables, and it can be written using the three Cartesian direction vectors as:

where $\eta \in [0, \pi]$ is the polar and $\vartheta \in [0, 2\pi]$ is the azimuthal

$$\Omega_x = \sin \eta \cos \vartheta$$
$$\Omega_y = \sin \eta \sin \vartheta$$
$$\Omega_z = \cos \eta$$





angle.

Angular neutron density, $n(\mathbf{r}, \hat{\mathbf{\Omega}}, E)$, gives the number of neutrons inside an infinitesimal volume element dV at position \mathbf{r} :

$$n(\mathbf{r}, \hat{\mathbf{\Omega}}, E) dV d\hat{\mathbf{\Omega}} dE$$
 (8)

The infinitesimal element in the angular space is the differential solid angle $d\hat{\Omega}$ about the direction of motion $\hat{\Omega}$. The energy is distributed within interval dE about E.



The density of neutrons moving in all directions, also called the scalar density, is given by:

$$n(\mathbf{r}, E) = \int_{4\pi} n(\mathbf{r}, \hat{\mathbf{\Omega}}, E) d\hat{\mathbf{\Omega}}$$
(9)

and the density of neutrons moving in all directions at all energies:

$$n(\mathbf{r}) = \int_{4\pi} \int_{E} n(\mathbf{r}, \hat{\mathbf{\Omega}}, E) d\hat{\mathbf{\Omega}} dE$$
(10)



Neutron flux, or more precisely, angular neutron flux, has no straightforward physical interpretation, but it is defined as the angular neutron density multiplied by speed:

$$\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = vn(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)$$
(11)

The difference between the two concepts can be understood by considering a randomly distributed population of neutrons passing through a volume at different energies:

- If a snapshot, frozen in time, is taken of the population, it shows the distribution of neutrons in different positions, energies and directions of motion – the angular neutron density in the six-dimensional phase space.
- If another snapshot is taken a short time interval dt later, each neutron has moved forward by distance ds = vdt. The faster the neutrons are moving, the longer the combined distance covered by the entire population. This distance will be later related to the integral of the neutron flux and the number of neutron-induced reactions within the volume.







Figure 2 : Neutron density and flux distribution in a BWR fuel assembly integrated over energy and direction. Left: Density distribution peaks in the internal and external moderator channels where thermal neutrons are collected. Right: Flux distribution is clearly more uniform, because the neutron speed multiplier ($\psi = vn$) emphasizes the contribution of high-energy neutrons with longer mean-free-paths and more uniform distribution over the geometry.



The neutron flux is not a physical, measurable quantity,⁶ and its practical significance actually results from a simple connection to reaction rates. The rate of reaction x in the infinitesimal phase-space element can be written as the product of angular flux and the corresponding macroscopic cross section:

$$dR_x = \Sigma_x(\mathbf{r}, E)\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E)dVd\hat{\mathbf{\Omega}}dE$$
(12)

When integrated over variables, the result is a physical reaction rate:

$$R_x = \int_V \int_{\hat{\Omega}} \int_E \Sigma_x(\boldsymbol{r}, E) \psi(\boldsymbol{r}, \hat{\Omega}, E) dV d\hat{\Omega} dE$$
(13)

that gives the number of reactions x per second, induced by neutrons within the domain of integration. For example, the total capture rate in volume V is given by:

$$\int_{V} \int_{4\pi} \int_{0}^{\infty} \Sigma_{\gamma}(\boldsymbol{r}, E) \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) dV d\hat{\boldsymbol{\Omega}} dE$$
(14)

and the total number of fission neutrons produced by thermal neutron-induced fission:

$$\int_{V} \int_{4\pi} \int_{0}^{E_{1}} \nu \Sigma_{\rm f}(\boldsymbol{r}, E) \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) dV d\hat{\boldsymbol{\Omega}} dE$$
(15)

where E_1 is the boundary between thermal and fast energy group.

⁶This interpretation is subject to argument, but what cannot be argued is that flux can only be measured via physical reaction rates.



For scattering reactions the product of angular flux and the double-differential scattering cross section describes the differential reaction rate density, i.e. the rate at which neutrons are scattering from direction $\hat{\Omega}$ to $\hat{\Omega}'$ and energy *E* to *E'*:⁷

$$dR_{\rm s} = \Sigma_{\rm s}(\mathbf{r}, \hat{\mathbf{\Omega}} \to \hat{\mathbf{\Omega}}', E \to E')\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E)dVd\hat{\mathbf{\Omega}}dEd\hat{\mathbf{\Omega}}'dE'$$
(16)

Or if the change in direction is written using the scattering cosine:

$$dR_{\rm s} = \Sigma_{\rm s}(\mathbf{r}, \mu, E \to E')\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E)dVd\hat{\mathbf{\Omega}}dEd\mu dE'$$
(17)

Similar to total reaction rate, the differential reaction rate can be integrated over variables, scattering angles and emission energies. The total scattering rate is given by:

$$R_{\rm s} = \int_{V} \int_{4\pi} \int_{0}^{\infty} \int_{-1}^{1} \int_{0}^{\infty} \Sigma_{\rm s}(\mathbf{r}, \mu, E \to E') \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E) dV d\hat{\mathbf{\Omega}} dE d\mu dE'$$
(18)

Or similarly for the down-scattering rate, i.e. scattering from fast to thermal group:

$$R_{\rm s12} = \int_{V} \int_{4\pi} \int_{E_1}^{\infty} \int_{-1}^{1} \int_{0}^{E_1} \Sigma_{\rm s}(\mathbf{r}, \mu, E \to E') \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E) dV d\hat{\mathbf{\Omega}} dE d\mu dE'$$
(19)

where E_1 is the group boundary.

⁷To be precise, $d {f \hat\Omega}$ about ${f \hat\Omega}$, etc.



The neutron direction of motion plays no role in capture and fission events,⁸ which means that the reaction rate can be integrated over direction of motion:

$$dR_{x} = \int_{4\pi} \Sigma_{x}(\mathbf{r}, E)\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E)dVd\hat{\mathbf{\Omega}}dE = \Sigma_{x}(\mathbf{r}, E) \left[\int_{4\pi} \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E)d\hat{\mathbf{\Omega}}\right]dVdE$$

= $\Sigma_{x}(\mathbf{r}, E)\phi(\mathbf{r}, E)dVdE$ (20)

where the scalar neutron flux is defined similar to the scalar neutron density (9):

$$\phi(\mathbf{r}, E) = \int_{4\pi} \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E) d\hat{\mathbf{\Omega}} = vn(\mathbf{r}, E)$$
(21)

The scalar flux can be interpreted as the distance covered by neutrons with energy dE about E inside an infinitesimal volume element dV at r in time interval dt:

$$ds = \phi(\mathbf{r}, E) dV dE dt \tag{22}$$

When integrated over volume, energy and time, the result is the total combined distance covered by the neutrons, as suggested by the previous example illustrating the differences between neutron density and flux.

⁸The incident neutron is lost in capture and fission neutrons are typically assumed to be emitted isotropically, which is a very good approximation in the energy range of fission reactors.



The connection to reaction rates is seen by recalling that the macroscopic cross section Σ is defined as the neutron interaction probability per traveled path length.

This connection reflects the fact that the rate of neutron-induced reactions is increased if:

- 1) Neutron density is increased, increasing the number of neutrons that may collide with the nuclides in the medium
- Neutron velocity is increased, increasing the path length traveled within the given time interval and the number of chances of colliding with the nuclides

The same connection applies in the opposite case, when the neutron flux (density, velocity or both) is decreased.

The reaction rate also naturally depends on the macroscopic cross section:

$$\Sigma(\mathbf{r}, E) = N(\mathbf{r})\sigma(E)$$
(23)

which in turn depends on:

- 1) The nuclide density $N, {\rm which} \ {\rm affects} \ {\rm the} \ {\rm number} \ {\rm of} \ {\rm nuclides} \ {\rm encountered} \ {\rm by} \ {\rm the} \ {\rm neutron} \ {\rm within} \ {\rm its} \ {\rm path}$
- 2) The microscopic cross section σ , representing the interaction probability between the neutron and a single target nucleus





Figure 3 : Neutron flux is connected to reaction rates by multiplication with macroscopic cross sections and integration over variables. Reaction rates therefore also depend on flux spectrum. This emphasizes the contribution of low-energy neutrons, as cross sections increase towards lower energies. Left: Total collision rate distribution in the previous BWR fuel assembly. Right: Total fission rate ("hot" shades) and thermal flux ("cold" shades). Dark and bright colors indicate low and high values, respectively. Since more than 80% of fissions are induced by thermal neutrons, the fission rate distribution follows the distribution of thermal flux.



Angular and scalar neutron flux are both density-like functions describing the neutron population, and their differences become apparent in how they are primarily used:

- Angular flux, $\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E)$, is used for determining the rate at which neutrons are moving from one phase-space position to another by streaming or scattering
- Scalar flux, \u03c6(r, E), is used for determining the rate of reactions where the incident neutron is lost and secondary neutrons, if emitted, have no preferential direction.

It is important to note that, even though (angular) neutron density and flux depend on the direction of motion, they are both scalar functions. The direction is a variable, similar to position and energy, and it provides two of the six phase-space coordinates.⁹

⁹Since human senses are limited to three geometric dimensions, it is not possible to visualize angular or scalar flux accurately, but if you must, think about density (scalar field) instead of flow (vector field).



The vector equivalent of angular flux is the angular current density:10

$$\begin{aligned} \boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) &= \boldsymbol{v}n(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \\ &= \hat{\boldsymbol{\Omega}}\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \end{aligned}$$
(24)

where $\mathbf{v} = \hat{\mathbf{\Omega}}v$ is the neutron velocity. The angular current density describes the rate at which neutrons with energy dE about E and direction $d\hat{\mathbf{\Omega}}$ about $\hat{\mathbf{\Omega}}$ pass through an infinitesimal surface element $d\mathbf{S}$ located at \mathbf{r} :

$$dL = \boldsymbol{j}(\boldsymbol{r}, \boldsymbol{\hat{\Omega}}, E) \cdot d\mathbf{S}$$
⁽²⁵⁾

When the angular current density is integrated over the full solid angle, the result is another vector quantity called neutron current density:

$$\mathbf{J}(\boldsymbol{r}, E) = \int_{4\pi} \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) d\hat{\boldsymbol{\Omega}}$$
(26)

which gives the net rate of neutrons with energy dE about E passing through an infinitesimal surface element $d\mathbf{S}$ located at \mathbf{r} :

$$dL = \mathbf{J}(\mathbf{r}, E) \cdot d\mathbf{S} \tag{27}$$

¹⁰The terminology used in the literature for different flux and current quantities is not unambiguous. It should also be noted that the concept of flux in neutron transport theory is not equivalent with the mathematical definition of flux, used correctly, for example, in electromagnetic field theory.





Figure 4 : Illustration of angular and neutron current densities as vector fields in a BWR fuel assembly. Left: Angular current density of thermal neutrons traveling in a 30° direction with respect to the positive x-axis. Right: Neutron current density, representing the net flow of thermal neutrons. Distribution of thermal neutron density is plotted in the background.



One of the crucial differences between the flux and the current quantities is seen by comparing Eqs. (21) and (26). If the neutron density is completely isotropic (all directions equally likely), then:

$$\begin{aligned} \mathbf{J}(\boldsymbol{r}, E) &= \int_{4\pi} \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) d\hat{\boldsymbol{\Omega}} = 0 \\ \phi(\boldsymbol{r}, E) &= \int_{4\pi} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) d\hat{\boldsymbol{\Omega}} > 0 \end{aligned}$$
(28)

Whereas the neutron flux can be associated with the total distance covered by neutrons in a volume and the rate of neutron-induced reactions, the current density can be associated with the flow of neutrons over boundary surfaces.

Neutron current, i.e. the rate at which neutrons are crossing surface S is given by surface integral:

$$J = \int_{\hat{\mathbf{\Omega}}} \int_{S} \int_{E} \mathbf{j}(\mathbf{r}, \hat{\mathbf{\Omega}}, E) \cdot d\mathbf{S} d\hat{\mathbf{\Omega}} dE = \int_{\hat{\mathbf{\Omega}}} \int_{S} \int_{E} \left[\mathbf{j}(\mathbf{r}, \hat{\mathbf{\Omega}}, E) \cdot \hat{\mathbf{u}} \right] d\hat{\mathbf{\Omega}} dS dE$$
(29)

where $\hat{\mathbf{u}}$ is the surface normal.



Similar to integral reaction rates, neutron current can also be divided into components with respect to space, energy and direction. If surface S defines the boundary of a volume, the rate at which neutrons are streaming in is given by the inward current

$$J^{-} = \int_{-1}^{0} \int_{S} \int_{E} \left[\mathbf{j}(\mathbf{r}, \hat{\mathbf{\Omega}}, E) \cdot \hat{\mathbf{u}} \right] d\mu dS dE$$
(30)

and the rate at which neutrons are streaming out by the outward current:

$$J^{+} = \int_{0}^{1} \int_{S} \int_{E} \left[\mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) \cdot \hat{\mathbf{u}} \right] d\mu dS dE$$
(31)

where $\mu = \hat{\Omega} \cdot \hat{\mathbf{u}}$ is the cosine between the neutron direction of motion and the surface normal.¹¹ The values of inward and outward currents are negative and positive, respectively.

Integral of the neutron current density yields the net current:

$$J_{\rm net} = \int_{S} \int_{E} \left[\mathbf{J}(\boldsymbol{r}, E) \cdot \hat{\mathbf{u}} \right] dS dE$$
(32)

The value is positive for outward and negative for inward flow. The net current is related to the partial currents (30) and (31) by:

$$J_{\rm net} = J^- + J^+$$
 (33)

¹¹Assuming that $\hat{\mathbf{u}}$ points in the outward direction.



Basic concepts of transport theory: summary

Angular neutron flux, ψ , can be thought of as a mathematical density-like function in the sixdimensional phase space that connects the behavior of the neutron population to physical reaction rates:

$$R_{x} = \int_{V} \int_{\hat{\mathbf{\Omega}}} \int_{E} \Sigma_{x}(\mathbf{r}, \hat{\mathbf{\Omega}}, E) \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E) dV d\hat{\mathbf{\Omega}} dE$$
(34)

The directional dependence is important in scattering reactions, described by double-differential cross sections, which combine the probability of the scattering event to the distributions of energy transfer and scattering angle.

In reactions where the incident neutron is lost or secondary neutrons are emitted isotropically, angular flux can be replaced by the scalar flux, which is obtained by integration over full solid angle:

$$\phi(\mathbf{r}, E) = \int_{4\pi} \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E) d\hat{\mathbf{\Omega}}$$
(35)

The integral reaction rate is then reduced to:

$$R_x = \int_V \int_E \Sigma_x(\mathbf{r}, E) \phi(\mathbf{r}, E) dV dE$$
(36)

The integration of flux over the phase space variables and time yields the total combined distance traveled by the neutrons. This is intuitively associated with reaction rate by recalling that the macroscopic cross section is defined as the interaction probability per path length traveled by the neutron.



Basic concepts of transport theory: summary

The vector equivalent of angular flux is the angular current density:

$$\boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = \hat{\boldsymbol{\Omega}} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)$$
 (37)

which integrated over full solid angle yields the neutron current density:

$$\mathbf{J}(\boldsymbol{r}, E) = \int_{4\pi} \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) d\hat{\boldsymbol{\Omega}}$$
(38)

It should be noted that, even though angular flux and angular current density are related by (37), similar connection does not apply for scalar flux and neutron current density:

$$\mathbf{J}(\boldsymbol{r}, E) \neq \hat{\mathbf{\Omega}}\phi(\boldsymbol{r}, E)$$
(39)

The current densities are associated with the rates at which neutrons cross the boundaries of a specified volume. When (37) is integrated over a surface, direction, energy and time, the result is the net number of neutrons that have passed through the surface.

Reaction rate integrals appear in the source and removal terms of the neutron transport equation. The streaming term can be written using the neutron current density, and in diffusion theory it is associated to flux gradient by an approximation known as Fick's law.



Neutron transport equation

General neutron transport theory forms the basis of all deterministic transport calculation methods, including diffusion theory, which is used in full-scale reactor simulator calculations. The theory is based on the following fundamental assumptions:

- 1) Neutrons can be treated as independent particles, traveling in straight lines between collisions
- 2) Neutron-neutron interactions can be ignored
- 3) Reaction cross sections are independent of flux and constant in time

With these assumptions the neutron transport equation describes a linear problem.¹² Additional approximations include:

- All materials are isotropic, i.e. differential scattering cross sections depend only on scattering angles and not on neutron direction of motion
- 5) Fission neutrons are emitted isotropically
- 6) Fission spectrum is independent of incident neutron energy

Approximations 5 and 6 are valid at energies relevant for fission reactor applications.

¹²As pointed out earlier, assumption 3) does not hold in coupled problems describing an operating nuclear reactor subject to reactivity feedbacks and fuel burnup, in which case the transport problem actually becomes non-linear. The solution to the coupled problem is obtained by iteration between the different solvers, assuming that the transport problem can be linearized over sufficiently short time intervals.



Neutron transport equation

The transport equation is formulated simply by considering the particle density balance inside an infinitesimal element of the six-dimensional phase space.¹³

- Position: dV about r
- Direction: $d \hat{\Omega}$ about $\hat{\Omega}$
- Energy: dE about E

The equation can be written as:

$$\underbrace{\frac{1}{v}\frac{\partial}{\partial t}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)}_{(A)} + \underbrace{\hat{\boldsymbol{\Omega}}\cdot\nabla\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)}_{(B)} + \underbrace{\Sigma(\boldsymbol{r},E)\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)}_{(C)} = q(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E,t)$$
(40)

where q is the general source term and:

- (A) is the time-rate of change in neutron density inside the phase-space element¹⁴
- (B) is the streaming term, i.e. the net rate at which neutrons moving in direction $\hat{\Omega}$ with energy *E* are entering and leaving the volume element (see next slide)
- (C) is the removal term, i.e. the rate at which neutrons are removed from the phase-space element by absorption or scattering to new energy and direction

¹⁴Results from the relation between flux and neutron density: $\psi = vn \Longrightarrow \frac{1}{v} \frac{\partial \psi}{\partial t} = \frac{\partial n}{\partial t}$



¹³See figure on slide 19.

Neutron transport equation

The form of terms (A) and (C) is easily understood, but the streaming term is less straightforward. It was stated earlier that the rate at which neutrons with energy E and direction $\hat{\Omega}$ pass through an infinitesimal surface element $d\mathbf{S}$ located at \mathbf{r} is given by the angular current density:

$$dL = \boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) \cdot d\mathbf{S}$$
(41)

If S is the complete boundary of the infinitesimal volume element dV, then the net rate at which neutrons are flowing in or out is given by surface integral:

$$\oint_{S} \boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) \cdot d\mathbf{S}$$
(42)

Since angular current density is a vector field, divergence theorem yields:

$$\oint_{S} \boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) \cdot d\mathbf{S} = \int_{V} \nabla \cdot \boldsymbol{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) dV$$
(43)

Angular current density can be written using angular flux $j=\hat{\Omega}\psi$, which results in:

$$\int_{V} \nabla \cdot \hat{\Omega} \psi(\boldsymbol{r}, \hat{\Omega}, E, t) dV = \int_{V} \hat{\Omega} \cdot \nabla \psi(\boldsymbol{r}, \hat{\Omega}, E, t) dV$$
(44)

showing the final form of the streaming term integrated over volume.


The source term can be written as the sum of external, scattering and fission source:

$$q(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) = Q(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) + S(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) + F(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t)$$
(45)

The external source term, Q, is independent of flux and it gives the rate at which neutrons are emitted into the phase-space element by external sources.

The scattering source can be written using the double-differential scattering cross section, by integration over all incident energies and directions:¹⁵

$$S(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) = \int_{4\pi} \int_0^\infty \Sigma_s(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}' \to \hat{\boldsymbol{\Omega}}, E' \to E) \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}', E', t) d\hat{\boldsymbol{\Omega}}' dE'$$
(46)

Since fission neutrons are emitted isotropically, the fission source term can be written using the scalar flux:

$$F(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) = \frac{\chi(E)}{4\pi} \int_0^\infty \nu \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE'$$
(47)

where $\nu \Sigma_{\rm f}$ is the fission neutron production cross section and $\chi(E)$ is the fission spectrum, i.e. the probability that the energy of the emitted neutron falls on interval dE about E. Factor $1/4\pi$ results from the source isotropy.

¹⁵It is assumed here that the double-differential scattering cross section is written as the sum over all nuclides and scattering modes. Neutron-multiplying (n,2n), (n,3n), etc. reactions are accounted for in the distribution of secondary energies and scattering angles (normalization to 2 or 3 instead of 1).



The transport equation describes accurately the balance in angular neutron density with the help of angular flux. Similar equation can be derived for the scalar density and flux, by integrating (40) over the full solid angle.

The integration of the time-derivative term and the removal term is straightforward:

$$\int_{4\pi} \frac{1}{v} \frac{\partial}{\partial t} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) d\hat{\boldsymbol{\Omega}} = \frac{1}{v} \frac{\partial}{\partial t} \int_{4\pi} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) d\hat{\boldsymbol{\Omega}} = \frac{1}{v} \frac{\partial}{\partial t} \phi(\boldsymbol{r}, E, t)$$
(48)

and

$$\int_{4\pi} \Sigma(\boldsymbol{r}, E) \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) d\hat{\boldsymbol{\Omega}} = \Sigma(\boldsymbol{r}, E) \int_{4\pi} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) d\hat{\boldsymbol{\Omega}} = \Sigma(\boldsymbol{r}, E) \phi(\boldsymbol{r}, E, t)$$
(49)

The fission source term (47) was already written using the scalar flux and integration over full solid angle cancels the $1/4\pi$ factor:

$$\int_{4\pi} \frac{\chi\left(E\right)}{4\pi} \int_{0}^{\infty} \nu \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' d\hat{\mathbf{\Omega}} = \chi\left(E\right) \int_{0}^{\infty} \nu \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE'$$
(50)

The external source is independent of the flux and its angular dependence depends on the source type. The integration of the two remaining terms is less straightforward.



The integration of the scattering source (46) is written as:

$$\int_{4\pi} \left[\int_{4\pi} \int_0^\infty \Sigma_{\rm s}(\mathbf{r}, \hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}}, E' \to E) \psi(\mathbf{r}, \hat{\mathbf{\Omega}}', E', t) d\hat{\mathbf{\Omega}}' dE' \right] d\hat{\mathbf{\Omega}}$$
(51)

Since the integration is carried over the full solid angle, and because the double-differential scattering cross section depends only on the angle between directions $\hat{\Omega}'$ and $\hat{\Omega}$, the integral over the double-differential scattering cross section can be written using the scattering cosine:

$$\int_{4\pi} \int_0^\infty \left[\int_{-1}^1 \Sigma_{\rm s}(\mathbf{r},\mu,E'\to E) d\mu \right] \psi(\mathbf{r},\hat{\mathbf{\Omega}}',E',t) d\hat{\mathbf{\Omega}}' dE'$$
(52)

The term in brackets describes the total scattering probability from energy E' to E, and can be written as:

$$\int_{4\pi} \int_{0}^{\infty} \Sigma_{s}(\mathbf{r}, E' \to E) \psi(\mathbf{r}, \hat{\mathbf{\Omega}}', E', t) d\hat{\mathbf{\Omega}}' dE'$$

$$= \int_{0}^{\infty} \Sigma_{s}(\mathbf{r}, E' \to E) \left[\int_{4\pi} \psi(\mathbf{r}, \hat{\mathbf{\Omega}}', E', t) d\hat{\mathbf{\Omega}}' \right] dE'$$
(53)

The term in brackets is the scalar flux, and the final form can be written as:

$$\int_{0}^{\infty} \Sigma_{\rm s}(\mathbf{r}, E' \to E) \phi(\mathbf{r}, E', t) dE'$$
(54)



The final term in (40) left to be integrated is the streaming term, which can also be written using the angular current density (24):

$$\hat{\boldsymbol{\Omega}} \cdot \nabla \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = \nabla \cdot \hat{\boldsymbol{\Omega}} \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) = \nabla \cdot \mathbf{j}(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E)$$
(55)

Integration over the full solid angle yields

$$\int_{4\pi} \nabla \cdot \mathbf{j}(\mathbf{r}, \mathbf{\hat{\Omega}}, E) d\mathbf{\hat{\Omega}} = \nabla \cdot \int_{4\pi} \mathbf{j}(\mathbf{r}, \mathbf{\hat{\Omega}}, E) d\mathbf{\hat{\Omega}} = \nabla \cdot \mathbf{J}(\mathbf{r}, E)$$
(56)

where $\mathbf{J}(\mathbf{r}, E)$ is the neutron current density (26).

When the results of Eqs. (48)–(56) are collected and external source term is omitted for convenience, the result can be written as:

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\mathbf{r}, E, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, E) + \Sigma(\mathbf{r}, E) \phi(\mathbf{r}, E, t)$$

$$= \int_{0}^{\infty} \left[\Sigma_{s}(\mathbf{r}, E' \to E) \phi(\mathbf{r}, E', t) + \chi(E) \nu \Sigma_{f}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) \right] dE'$$
(57)

This form of transport equation is also known as the neutron continuity equation, and it forms the starting point for the derivation of diffusion theory, discussed in Lecture 4. It should be noted that no approximations were made in the derivation of (57) from the original transport equation (40).



Even though the transport equation is linear, it is extremely difficult to solve because:

- 1) The geometries are complex and heterogeneous
- 2) Cross sections are complicated functions of neutron energy
- 3) The angular dependence of streaming and scattering source term are difficult to handle

In practice, the integrals over space, direction and energy cannot be resolved while holding on to the continuous dependence on phase-space variables.

For practical reasons, most deterministic transport methods therefore rely on at least three approximations:

- 1) The geometry is discretized into a number of homogeneous material regions
- The continuous energy dependence of cross sections is condensed into a number of discrete energy groups
- 3) The angular dependence of double-differential scattering cross sections is represented by functional expansions, the directional dependence of flux is represented by functional expansions or discrete directions

The first two approximations are common to all deterministic transport methods, the treatment of angular dependence is what differentiates the methods from each other $(S_n, P_n, \text{method of characteristics}, \text{diffusion theory, etc.})$.



The solution by applying diffusion approximation is left for Lecture 4, and the remainder of this lecture is devoted to looking at the different physical aspects of the transport problem from the viewpoint of deterministic transport theory.¹⁶

From here on, the transport equation is written for the sake of simplicity without the phase space variables:

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla\psi + \Sigma\psi = Q + F + S$$
(58)

It is assumed that the accurate solution is available, even though this is clearly not the case in reality.

Integration of (58) over variables preserves the neutron balance, and turns streaming term into total leakage rate:

$$\int_{V} \int_{\hat{\mathbf{\Omega}}} \int_{E} \hat{\mathbf{\Omega}} \cdot \nabla \psi \, dV d\hat{\mathbf{\Omega}} dE = \oint_{S} \int_{E} \mathbf{J} \cdot d\mathbf{S} dE \tag{59}$$

Integration of the removal term yields the total reaction rate, and the absorption rate is given by:

$$\int_{V} \int_{\hat{\Omega}} \int_{E} \left[\Sigma \psi - S \right] dV d\hat{\Omega} dE$$
(60)

Integration of fission and external source terms yields the corresponding total source rates.

¹⁶In Lecture 3 the perspective is switched to that of the individual neutron with the introduction of Monte Carlo neutron transport simulation.



Equilibrium state and criticality

When no difference is made between prompt and delayed neutrons, the criticality state of the reactor can be related to whether the chain reaction is below, at or above the self-sustaining condition:¹⁷

- When the system is in sub-critical state, the chain reaction is not self-sustained, and the fission chains die out after a number of generations
- When the system is in critical state, the chain reaction is self-sustained, and each terminated fission chain is replaced, on the average, by exactly one new chain
- When the system is in super-critical state, the chain reaction is self-sustained, and each terminated fission chain is replaced, on the average, by more than one new chain

In the absence of external sources, it is easy to see that the time-dependence of neutron population takes the form of:

$$n(t) \sim n_0 e^{\omega t} \tag{61}$$

where ω depends on the source and loss terms. Steady-state condition ($\omega = 0$) always implies criticality, i.e. that the chain reaction is in a self-sustained state, and fission source rate equals the sum of absorption and leakage rates.

The absolute population size is not fixed, which results from the fact that the system is characterized by a homogeneous linear differential equation.

¹⁷In contrast to the description given in Lecture 1, the fission chains here are assumed to consist of both prompt and delayed neutrons.



Equilibrium state and criticality

In the presence of constant external source, time-dependence of neutron population takes the form of:

$$n(t) \sim n_0 e^{\omega t} - \frac{Q}{\omega} \left[1 - e^{\omega t} \right]$$
(62)

where $\omega \neq 0$. If the system is sub-critical ($\omega < 0$), the asymptotic solution is constant in time:

$$\lim_{t \to \infty} n(t) = -\frac{Q}{\omega}$$
(63)

reflecting the fact that source neutrons are multiplied in fission chains that are finite in length. In fact, a steady state solution in the presence of external source can only exist if the system is sub-critical.

In the special case of criticality, the transport equation with external source is reduced to:

$$\frac{1}{v}\frac{\partial\psi}{\partial t} = Q \tag{64}$$

as the streaming, removal, and fission and scattering source terms are summed to zero. The time-dependence of neutron population is then of form:

$$n(t) \sim Qt \tag{65}$$

which is also understood by recalling that in critical state each neutron replicates itself (on the average) without additional multiplication. In other words, the external source initiates new nonbranching infinitely long fission chains at a constant rate.



Equilibrium state and criticality



Figure 5 : Neutron population as function of time in sub-critical, critical and super-critical states. Left: Equilibrium in the absence of external sources implies criticality. When the system is sub- or super-critical, the population is exponentially decreasing or increasing, respectively. Right: Equilibrium in the presence of external sources may only exist if the system is sub-critical (and the source is constant). The growth rate is linear at criticality and exponential when the system is super-critical.



Fundamental and transient flux modes

Since the transport problem is characterized by a linear equation, its solution can be written as a linear combination of different flux modes:

$$\psi = \psi_0 + \psi_1 + \psi_2 + \dots \tag{66}$$

where ψ_0 is called the fundamental mode and the remaining modes the transient modes. The different flux modes ψ_n are associated with the eigenfunctions of the transport equation and time constants ω_n , such that:

$$\omega_0 > \omega_1 > \omega_2 > \dots \tag{67}$$

Since the time dependence of flux is characterized by an exponential amplitude function, and:

$$e^{\omega_0 t} > e^{\omega_1 t} > e^{\omega_2 t} > \dots$$
 (68)

it is easy to see that the fundamental mode is the asymptotic solution to the transport equation, which persists after the transient modes, excited by changes in the physical conditions, fade away.

Time constants ω_n can be associated to eigenvalues k_n , in such way that:

$$k_0 > k_1 > k_2 > \dots$$
 (69)

Eigenvalue k_0 corresponding to the fundamental flux mode is interpreted as the multiplication factor.



Fundamental and transient flux modes



Figure 6 : Left: First four axial flux modes in a PWR full core calculation (amplitudes not to scale). The solutions are asymmetric, because of axial profiling of burnable absorber. Total flux and fundamental flux mode ψ_0 are always positive, but transient modes may have negative components. Right: First 50 eigenvalues. As the plot shows, $k_0 > k_1 > k_2 > \ldots$ Each eigenvalue is associated with a time constant, and the transient modes fade away as $t \to \infty$.



Fundamental and transient flux modes



Figure 7 : First 15 radial flux modes in the PWR core calculation. The fundamental flux mode (top left) corresponds to the flux shape in steady-state condition. Calculated by Monte Carlo simulation using the fission matrix method. See also Lecture2_anim1.gif for an animation on the convergence of flux into fundamental mode in a fast criticality experiement (Pu-Flattop).



Criticality eigenvalue problem

Several applications in reactor physics involve the solution of the steady-state transport equation, even though there is no balance between the physical source and loss rates. An example of such task is criticality calculation, which essentially means determining how far the system is from the self-sustaining state.¹⁸

In such case, the transport equation is usually written in the criticality- or k-eigenvalue form:

$$\hat{\mathbf{\Omega}} \cdot \nabla \psi + \Sigma \psi = \frac{1}{k} F + S \tag{70}$$

i.e. time-dependence and external source are dropped, and balance between source and loss rates is attained by scaling the fission term with constant 1/k.

In theory the solution consists of an infinite number of eigenfunctions $\psi_0, \psi_1, \psi_2, \ldots$ with associated eigenvalues k_0, k_1, k_2, \ldots , but in practice it is the fundamental flux mode ψ_0 which is taken as the solution to (70).

The fact that the higher flux modes can be dropped is based on the idea that the solution represents a steady-state system. As discussed earlier, this is the asymptotic solution that persists as $t \to \infty$ and the higher modes fade away.

¹⁸As will be discussed in Lecture 7, this type of problems are also encountered in spatial homogenization, in which the neutronics solution is obtained in some sub-domain of the full-scale geometry, and the accurate description of boundary leakage currents is not available.



Criticality eigenvalue problem

Eigenvalue k_0 corresponding to the fundamental flux mode is also called the effective multiplication factor, $k_{\rm eff}$, which is used to define the criticality condition as:

$$k_{\rm eff} \begin{cases} < 1 \implies \text{system is sub-critical} \\ = 1 \implies \text{system is critical} \\ > 1 \implies \text{system is super-critical} \end{cases}$$
(71)

If the integral source and loss rates 19 are known, $k_{\rm eff}$ can be associated to neutron balance:

$$k_{\rm eff} = \frac{F}{T - S + L} \tag{72}$$

where

- F is the integral fission source rate
- T is the integral total reaction rate
- S is the integral scattering source rate
- L is the integral leakage rate

The integral scattering source rate includes neutron production from multiplying (n,2n), (n,3n), etc. reactions.

¹⁹integrals over space, direction and energy



Criticality eigenvalue problem

It is important to note that using the criticality eigenvalue form of the transport equation as a representation of the physical transport problem is an approximation. Consequently, the solution to (70) is not the the solution to the physical problem, but rather to a modified problem in which:

- ▶ The fission source term is scaled up when $k_{\rm eff} < 1$
- ▶ The fission source term is scaled down when $k_{\rm eff} > 1$

The result is that the contribution of fission source on flux distribution and spectrum is correspondingly over- $(k_{\rm eff} > 1)$ or under-estimated $(k_{\rm eff} < 1)$.

The root cause of this issue is not in the way the transport problem is solved,²⁰ but rather in its formulation: a time-dependent system is forced into a steady-state condition by adjusting one of the source terms. There is no solution to this problem, which can have a significant impact in the results when the system is far from criticality.

In infinite-lattice calculations performed for the purpose of group constant generation the distortion in flux spectrum is often adjusted using leakage corrections, which account for the contribution of inward or outward net current, which in a realistic steady-state system would balance the source and loss rates.

²⁰The same bias appears in the Monte Carlo method when the transport simulation is run in criticality source mode, as discussed in Lecture 3.



Other eigenvalue forms of the steady-state transport equation

The k-eigenvalue form is just one approach to approximating the system with a steady-state transport equation. Similar scaling to attain balance between source and loss rates could be accomplished using the collision eigenvalue, c, which adjusts the total source term:

$$\hat{\mathbf{\Omega}} \cdot \nabla \psi + \Sigma \psi = \frac{1}{c} (F + S) \tag{73}$$

The solution to this equation is again an approximation to the physical problem, with its biases when $c \neq 1$.

PWR full-core reactor simulator calculations are often run to obtain critical boron concentration, which can be formally thought of as an eigenvalue problem, in which the contribution to boron absorption is separated from the removal term and adjusted to attain balance between source and loss rate:

$$\hat{\mathbf{\Omega}} \cdot \nabla \psi + (\Sigma' + N_{\mathrm{B}} \sigma_{\mathrm{B}}) \psi = F + S \tag{74}$$

where Σ' is the total cross section excluding absorption to coolant boron, and $N_{\rm B}$ and $\sigma_{\rm B}$ are the atomic density and microscopic absorption cross section of $^{10}{\rm B}$, respectively.

Another example of a similar approach is introduced in Lecture 7 along with leakage corrections, in which the balance between terms is attained by critical buckling search.



Other eigenvalue forms of the steady-state transport equation

Another interesting approach to obtain a steady-state form of the transport equation is to assume that the time-dependence of flux can be fully separated from the rest of the variables. Time-dependence takes an exponential form and the separation of variables can be written as:

$$\psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E, t) = \psi(\boldsymbol{r}, \hat{\boldsymbol{\Omega}}, E) e^{\alpha t} .$$
(75)

The substitution of this into the time-dependent transport equation (40), yields for the time-derivative term:

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E)e^{\alpha t} = \frac{\alpha}{v}\psi(\boldsymbol{r},\hat{\boldsymbol{\Omega}},E)e^{\alpha t}$$
(76)

When the exponential multiplier is canceled in all terms, the transport equation can be written as:

$$\frac{\alpha}{v}\psi + \hat{\mathbf{\Omega}} \cdot \nabla\psi + \Sigma\psi = F + S \tag{77}$$

where α is the eigenvalue that can be adjusted to attain balance between the source and loss rates.²¹ The criticality condition can be written correspondingly as:

$$\alpha \begin{cases} < 0 \quad \Rightarrow \text{ system is sub-critical} \\ = 0 \quad \Rightarrow \text{ system is critical} \\ > 0 \quad \Rightarrow \text{ system is super-critical} \end{cases}$$
(78)

 $^{^{21}}$ To be precise, α is the eigenvalue corresponding to the fundamental flux mode.



Other eigenvalue forms of the steady-state transport equation

The additional multiplier α/v has the same units as macroscopic cross section, and it can be interpreted as an absorption ($\alpha > 0$) or production ($\alpha < 0$) reaction with cross section inversely proportional to neutron velocity. The reaction can also be interpreted as time-absorption or -production, as seen by writing the probability per traveled path length:

$$dP = -\frac{\alpha}{v}ds = \alpha dt \tag{79}$$

It should be noted that the α -eigenvalue form makes no adjustments to any of the physical source or loss terms, and it can be shown that the solution to (77) corresponds to the asymptotic (fundamental mode) solution of the time-dependent transport equation.

The shape and spectrum of the flux is adjusted by the time-absorption / production term, which can be understood by considering slow neutrons, for which the adjustment is most significant:

- When the system is super-critical, the slowest neutrons cannot keep up with the exponentially increasing neutron population, and their contribution is scaled down by time-absorption
- When the system is sub-critical, it is the slow neutrons that are dominating the exponentially decreasing population, and their contribution is scaled up by time-production

The differences between the k- and $\alpha\text{-}eigenvalue$ solutions to the transport equation are best illustrated by an example.



Comparison of k- and $\alpha\text{-}eigenvalue mode}$

Example:Comparison of k- and $\alpha\text{-}eigenvalue mode$

Consider the k- and $\alpha\text{-}\text{eigenvalue}$ solutions to transport equation in an infinite 20 cm thick uranium plate with 30% ^{235}U enrichment:

- 1) The *k*-eigenvalue solution gives $k_{\rm eff}$ = 1.23, suggesting that the system is (prompt) super-critical, and the balance between the source and loss rates is attained by adjusting the fission term by factor 1/1.23 = 0.81.
- 2) The α -eigenvalue solution gives $\alpha = 1.04 \cdot 10^7$ 1/s, which also means that the system is super-critical. The balance between source and loss rates is obtained by adding a time-absorption term with effective macroscopic cross section $1.04 \cdot 10^7/v$ 1/cm.

In the first case, the fission source is *artificially* adjusted to obtain a solution to the *modified* transport equation.

In the second case, the solution to the asymptotic fundamental flux mode is obtained by separating time-dependence from the rest of the variables, without modifications in the original problem.



Comparison of k- and $\alpha\text{-}eigenvalue mode}$

Example:Comparison of k- and $\alpha\text{-}eigenvalue mode$

The differences are emphasized when the uranium plate is surrounded by an infinite water reflector. The thermalization of neutrons has a major effect in the *k*-eigenvalue solution, in which $k_{\rm eff}$ is increased to 1.46. The α -eigenvalue for the reflected geometry is 1.23·10⁷ 1/s.

The most dramatic differences between the two methods are seen in the corresponding flux solutions. The k-eigenvalue solution completely ignores the time-dependence of flux, which emphasizes the contribution of thermal neutrons returning to the fissile material with high probability to cause new fissions.

In reality, the exponentially growing chain reaction is maintained by fast neutrons alone, and the flux grows several orders of magnitude during the time it takes for a thermal neutron to return from the reflector.

The α -eigenvalue flux represents the asymptotic solution to the time-dependent problem, and reflects the correct shape of the exponentially growing flux. The contribution of thermal neutrons is scaled down by time-absorption, which is inversely proportional to neutron speed.

The time-dependent behavior of the systems is illustrated in animations Lecture2_anim2.gif and Lecture2_anim3.gif. It is seen that in the given time-scale, neutrons scattered to low energy appear to be stopped in the reflector, unable to contribute in the continuation of the chain reaction.



Comparison of k- and $\alpha\text{-}eigenvalue mode}$



Figure 8 : k- and α -eigenvalue solutions to transport equation in an infinite slab geometry (20 cm thick uranium plate with 30% ²³⁵U enrichment). Left: unreflected system, Right: infinite water reflector. The unreflected system is prompt super-critical, with $k_{\rm eff}$ = 1.23 given by the k-eigenvalue calculation. The reflector increases the value to $k_{\rm eff}$ = 1.46. Both eigenvalue modes result in very similar flux shape for the unreflected system, but the thermalization of neutrons in the reflected geometry is clearly emphasized in the k-eigenvalue calculation. In reality, fast neutrons are sufficient for maintaining an exponentially-growing chain reaction, and the fact that thermal neutrons follow far behind is not properly represented. Calculated by k- and α -eigenvalue Monte Carlo simulation.



Comparison of k- and α -eigenvalue mode

The previous example is an extreme case, presented to demonstrate the fact that the solution of the k-eigenvalue form of the transport equation can lead to completely false conclusions on the physical behavior of the system.

The k-eigenvalue method is still the most commonly used approach to solving reactor physics problems, and when close to criticality, the flux solution can be a good approximation on what the solution would look like if the system was critical.

It is important to note that the modeled system itself is often an approximation of physical reality, for example, an infinite lattice of identical fuel assemblies. In such case, the asymptotic shape and spectrum of the time-dependent flux (solution to α -eigenvalue problem) may not be any closer to physical reality than the solution to the adjusted transport equation (solution to *k*-eigenvalue problem).

There are also differences in the numerical algorithms used for solving different eigenvalue problems. α -eigenvalue problems can be subject to numerical instabilities when the system is well below criticality, and *k*-eigenvalue problems are easier to solve using iterative techniques.



Point-kinetics approximation: prompt neutrons

The simplest way to account for time dependence in deterministic transport theory is the so-called point kinetics approximation, in which the flux is approximated by the fundamental mode solution, assuming separation of variables:

$$\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E, t) \approx \psi_0(\mathbf{r}, \hat{\mathbf{\Omega}}, E) \mathcal{T}_0(t)$$
 (80)

where ψ_0 is time-independent form function and \mathcal{T}_0 is the time-dependent amplitude function. When the sub-indexes are dropped for convenience, the flux amplitude takes the form:

$$\mathcal{T}(t) = \mathcal{T}(0)e^{\omega t} \tag{81}$$

In the absence of delayed neutrons, the coefficient in the exponential can be written as:

$$\omega = \frac{\rho}{\Lambda} \tag{82}$$

where reactivity ρ represents the branching of the fission chains and the amount of multiplication in the system, and generation time Λ can be interpreted as the average time taken for a single prompt neutron to reproduce itself by fission.

Coefficient ω is the inverse period, related to the reactor period T:

$$T = \frac{1}{\omega}$$
(83)

which is time taken for the neutron population to grow by factor 2.7 (positive reactivity) or decrease by factor 0.37 (negative reactivity).



Point-kinetics approximation: prompt neutrons

Reactivity can be written using the eigenvalue corresponding to the fundamental mode solution, i.e. the effective multiplication factor, $k_{\rm eff}$:

$$\rho = \frac{k_0 - 1}{k_0} = \frac{k_{\rm eff} - 1}{k_{\rm eff}}$$
(84)

In other words, reactivity gives the fractional deviation of the system from criticality.²²

In some text books, generation time is related to another time constant, known as the prompt removal lifetime

$$\tau_{\rm r} = \Lambda k_{\rm eff} \tag{85}$$

which represents the effective mean time between the generation and the removal of a neutron from the system by new fission. $^{\rm 23}$

The emission of delayed neutrons complicates the solution of the transport equation, by coupling fission rate to the decay of delayed neutron precursors. Time dependence of flux still follows an exponential form, but the simple relation between ω and ρ in Eq. (82) is lost.

 $^{^{23}}$ Since this time interval has the physical interpretation as the average lifetime of the emitted fission neutron, $\tau_{\rm r}$ is often called the prompt neutron lifetime.



 $^{^{22}}$ One of the common units for reactivity is pcm (per cent mille), 1 pcm = 10⁻⁵ and 1000 pcm = 1%.

As discussed in Lecture 1, delayed neutron emission results from the radioactive decay of certain fission products, known as delayed neutron precursors. For example:

$${}^{87}_{35}\text{Br} \xrightarrow{\beta^{-}}_{55.7\text{s}} {}^{87}_{36}\text{Kr}^{*} \longrightarrow {}^{86}_{36}\text{Kr} + {}^{1}_{0}\text{n}$$
(86)

The decay of the excited state of 87 Kr is practically instantaneous, and the delay between fission and neutron emission depends on the half-life of the precursor isotope 87 Br.

There are hundreds of fission products that act as delayed neutron precursors,²⁴ but most of them are either short lived or have very low fission yields. The half-lives of significant precursor isotopes range from hundreds of milliseconds to almost a minute (for ⁸⁷Br above).

In practice, all precursor chains are not handled separately, but the reactions are instead divided into a number of representative precursor groups with different lifetimes and neutron yields. The most conventional representation uses six groups, with half-lives ranging from about 0.02 to 55 seconds.²⁵

The physical total delayed neutron fraction β depends on the yields of prompt and delayed neutrons, which depend on isotope and neutron energy.

²⁵The six-group representation is used in the ENDF/B and JENDL evaluated nuclear data files. The European JEFF-3.1 file and later evaluations are based on eight precursor groups.



²⁴Fission yield data typically consists of about 1000 fission product isotopes and isomeric states.

Table 1 : Ten most abundant delayed neutron precursor isotopes in thermal fission of ²³⁵U and ²³⁹Pu and fast fission of ²³⁸U. The yields are cumulative, and they refer to average nuclide production per fission.

Nuclide	Half-life (s)	²³⁵ U yield	²³⁹ Pu yield	²³⁸ U yield
⁸⁷ Br	55.70	0.021	0.007	0.016
¹³⁷	24.51	0.036	0.023	0.056
⁸⁸ Br	16.50	0.018	0.005	0.019
¹³⁸	6.46	0.015	0.007	0.040
⁹³ Rb	5.80	0.035	0.017	0.046
⁸⁹ Br	4.37	0.014	0.003	0.021
⁹⁷ Y	3.75	0.021	0.012	0.032
⁹⁴ Rb	2.70	0.015	0.007	0.034
^{98m} Y	2.00	0.020	0.019	0.026
¹⁴³ Cs	1.79	0.016	0.006	0.035
¹⁴¹ Xe	1.73	0.016	0.005	0.034
⁹⁹ Y	1.48	0.019	0.013	0.047
^{97m} Y	1.17	0.028	0.025	0.023
⁹⁷ Sr	0.43	0.017	0.007	0.033
⁹⁵ Rb	0.38	0.007	0.003	0.022



Table 2 : Half-lives (in seconds), decay constants and relative yields of delayed neutron precursor groups in 235 U, 238 U and 239 Pu fission. The physical total delayed neutron fraction depends on neutron energy.

	²³⁵ U			²³⁸ U			²³⁹ Pu		
j	$T_{1/2}$	λ_j	$\overline{ u}_j/\overline{ u}_{ m d}$	$T_{1/2}$	λ_j	$\overline{ u}_j/\overline{ u}_{ m d}$	$T_{1/2}$	λ_j	$\overline{ u}_j/\overline{ u}_{ m d}$
1	54.51	0.013	0.038	52.38	0.013	0.013	53.75	0.013	0.038
2	21.84	0.032	0.213	21.58	0.032	0.137	22.29	0.032	0.280
3	6.00	0.116	0.188	5.00	0.139	0.162	5.19	0.134	0.216
4	2.23	0.311	0.407	1.93	0.359	0.388	2.09	0.332	0.328
5	0.50	1.398	0.128	0.49	1.406	0.225	0.55	1.263	0.103
6	0.18	3.872	0.026	0.17	4.030	0.075	0.22	3.209	0.035





Figure 9 : Physical total delayed neutron yield (left) and fraction (right) of selected actinides as function of neutron energy. The fraction also depends on the prompt neutron yield, which varies from nuclide to nuclide and increases practically linearly as function of neutron energy.



The emission of delayed neutrons changes the fission source (47) into:

$$F(\mathbf{r}, \hat{\mathbf{\Omega}}, E, t) = (1 - \beta) \frac{\chi(E)}{4\pi} \int_{0}^{\infty} \nu \Sigma_{\mathrm{f}}(\mathbf{r}, E') \phi(\mathbf{r}, E', t) dE' + \sum_{j}^{J_{\mathrm{d}}} \left[\frac{\chi_{j}(E)}{4\pi} \lambda_{j} C_{j}(\mathbf{r}, t) \right]$$
(87)

where β is the total delayed neutron fraction²⁶ and the second term gives the emission rate in J_d precursor groups. The delayed neutron source depends on precursor concentration C_j , which is coupled to decay equations:

$$\frac{\partial}{\partial t}C_{j}(\boldsymbol{r},t) = \int_{0}^{\infty} \beta_{j}\nu\Sigma_{\rm f}(\boldsymbol{r},E')\phi(\boldsymbol{r},E',t)dE' - \lambda_{j}C_{j}(\boldsymbol{r},t)$$
(88)

where λ_j is the decay constant and β_j is the delayed neutron fraction in precursor group j. It is also assumed that the precursor nuclides are not transmuted by neutron interactions.

As pointed out in Lecture 1, the concentrations of delayed neutron precursors follow changes in fission power with a considerable delay. Consequently, the momentary precursor concentrations in Eq. (87) depend on the immediate operating history.

²⁶For now, β is written without dependence on E.



When the reactor has operated at constant power for a sufficiently long time, the precursor concentrations are in equilibrium, and

$$\frac{\partial}{\partial t}C_j(\boldsymbol{r},t) = 0 \tag{89}$$

The saturation concentrations are then given by:

$$C_j(\boldsymbol{r}) = \frac{1}{\lambda_j} \int_0^\infty \beta_j \nu \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E') dE'$$
(90)

which yields for the fission source term:

$$F(\mathbf{r}, \hat{\mathbf{\Omega}}, E) = (1 - \beta) \frac{\chi(E)}{4\pi} \int_0^\infty \nu \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E') dE' + \sum_j^{\rm Jd} \left[\beta_j \frac{\chi_j(E)}{4\pi} \int_0^\infty \nu \Sigma_{\rm f}(\mathbf{r}, E') \phi(\mathbf{r}, E') dE' \right]$$
(91)

Fraction (1 - β) of fission neutrons is then emitted as prompt with spectrum χ and fraction β as delayed with spectra χ_j , suggesting that in steady-state operation the impact of delayed neutrons is seen only in the energy distribution of emitted fission neutrons.²⁷

²⁷It is pointed out later that this is not exactly the case, as the time constants depend on the importance of neutrons for the continuation of the fission chain.



In the point-kinetics approximation it is assumed that the spatial distribution of delayed neutron precursor concentrations is separable from the time-dependence, which results from the similar separability for flux and, consequently, fission rate.

The relation between inverse period and reactivity depends on delayed neutron constants β_j and λ_j . The relation is not easily resolved in simple closed form, but it can be written as:

$$\rho = \omega \Lambda + \sum_{j=1}^{J_{\rm d}} \left[\frac{\omega \beta_j}{\omega + \lambda_j} \right]$$
(92)

This is known as the inhour equation. When the number of precursor groups J_d is six, the timedependent amplitude function can be written using its seven roots $(\omega_0, \omega_1, \dots, \omega_6)^{28}$ as:

$$\mathcal{T}(t) = \mathcal{T}(0) \sum_{j=0}^{6} A_j e^{\omega_j t}$$
(93)

where constants A_i are:

$$A_{j} = \frac{\Lambda + \sum_{i=1}^{6} \left[\frac{\beta_{i}}{\omega_{j} + \lambda_{i}}\right]}{\Lambda + \frac{1}{1 - \rho} \sum_{i=1}^{6} \left[\frac{\beta_{i}\lambda_{i}}{(\omega_{j} + \lambda_{i})^{2}}\right]}$$
(94)

 $^{\rm 28}{\rm Not}$ to be confused with the ω_n 's of the different eigenmodes.



Components corresponding to smaller ω_j decay faster, and the time dependence becomes dominated by the solution determined by the largest root ω_0^{29}

$$\mathcal{T}(t) \simeq \mathcal{T}(0) A_0 e^{\omega_0 t} \tag{95}$$

The corresponding period $T_0 = 1/\omega_0$ is known as the asymptotic or stable reactor period, and it can be measured experimentally by monitoring the rate of change in fission power.

The relation between (92) and (82) is seen by setting $\beta = 0$. This corresponds to the prompt super-critical state,³⁰ in which $\rho \gg \beta$.

The relation between ρ , ω and the time constants is illustrated in Fig. 10. The transfer to prompt super-critical state is shown as a steep drop in the asymptotic period. It is also seen that:

$$\lim_{\rho \to -\infty} \omega(\rho) = -\lambda_1 \tag{96}$$

which means that the decrease rate of neutron population is limited by the slowest decaying precursor group.

³⁰Another common practice is to measure reactivity in units of delayed neutron fraction, or dollars. When reactivity is above 1\$, the system is in prompt super-critical state.



²⁹When ρ > 0, only ω_0 is positive, leading to exponential growth. When ρ < 0, ω_0 is the least negative root, corresponding to slowest exponential decay.



Figure 10: Relation between ρ , ω and the time constants. Left: Illustration of the 7 roots $\omega_0, \omega_1, \ldots, \omega_6$. of Eq. (92) with fictitious delayed neutron constants. The roots are found at the crossing points between the curves and a horizontal line corresponding to ρ . Right: Asymptotic reactor period corresponding to the largest root as function of reactivity. The top curve shows the negative of reactor period (decaying amplitude function) as function of negative of reactivity.



Point-kinetics approximation: summary

The point kinetics approximation relies on separation of variables, and essentially assumes that the time-dependence of the system can be approximated by a single form function and the associated amplitude function, and that all higher-order (transient) flux modes can be discarded.

The method is best applied to transients caused by uniform changes in the operating conditions, or in small or otherwise closely coupled systems, for example:

- Criticality experiments
- Small research reactors
- Fast reactors

The approximation breaks down especially in localized transients in neutronically large systems, such as PWR control rod ejections, which require more elaborate methods and time-space resolved solution.

LWR transient analyses are typically performed using reactor dynamics codes with time-dependent one- or three-dimensional neutronics. This topic is covered in Lecture 11.

It should also be noted that the inhour equation (92) describes the dynamic behavior of the reactor after a step change in reactivity. In reality, both positive and negative reactivity insertions take time, and the results are not accurate when ρ is changing.



Calculation of time constants

The delayed neutron fractions in the coupled fission source (87) and precursor concentration (88) equations was written without energy dependence. This is not because β is independent of neutron energy, but rather because the use of physical delayed fractions leads to inaccurate results for the dynamic reactor response.

The reason is that some source neutrons are more likely to introduce long fission chains than others, because they are born further away from boundaries or strong absorbers, in a region of higher reactivity, or simply at a different energy. The point-kinetics approximation fails to capture these effects, even though the separation variables is otherwise well justified.

In order to account for the fact that fission chains that are terminated early contribute less to the asymptotic neutron population than those forming longer chains, the reactor time constants must be calculated by importance-weighting. In deterministic transport theory this implies using the adjoint neutron flux ψ^{\dagger} :

$$\beta_{\mathrm{eff},j} = \frac{\int_{V} \int_{\hat{\Omega}} \int_{E} \int_{\hat{\Omega}'} \int_{E'} \psi^{\dagger}(\boldsymbol{r}, \hat{\Omega}', E') \mathbf{B}_{j}(\mathbf{r}, E, E') \psi(\boldsymbol{r}, \hat{\Omega}, E) dV d\hat{\Omega} dE d\hat{\Omega}' dE'}{\int_{V} \int_{\hat{\Omega}} \int_{E} \int_{\hat{\Omega}'} \int_{E'} \psi^{\dagger}(\boldsymbol{r}, \hat{\Omega}', E') \mathbf{F}(\mathbf{r}, E, E') \psi(\boldsymbol{r}, \hat{\Omega}, E) dV dE d\hat{\Omega} dE d\hat{\Omega}' dE'}$$
(97)

where F is the fission operator:

$$\mathbf{F}(\mathbf{r}, E, E') = \chi(E')\nu\Sigma_{\rm f}(\mathbf{r}, E), \qquad (98)$$

and \mathbf{B}_{i} is the delayed neutron emission source operator:

$$\mathbf{B}_{j}(\mathbf{r}, E, E') = \chi_{\mathrm{d},j}(E')\nu_{\mathrm{d},j}\Sigma_{\mathrm{f}}(\mathbf{r}, E)$$
(99)



Calculation of time constants

The adjoint flux is a measure of neutron importance, and it is the solution to the adjoint transport equation, obtained by inverting the scattering and fission operators.³¹ Similar adjoint flux weighting can be written from the calculation of prompt generation time:

$$\Lambda_{\rm eff} = \frac{\int_{V} \int_{\hat{\Omega}} \int_{E} \int_{\hat{\Omega}'} \int_{E'} \psi^{\dagger}(\boldsymbol{r}, \hat{\Omega}', E') \frac{1}{v} \psi(\boldsymbol{r}, \hat{\Omega}, E) dV d\hat{\Omega} dE d\hat{\Omega}' dE'}{\int_{V} \int_{\hat{\Omega}} \int_{E} \int_{\hat{\Omega}'} \int_{E'} \psi^{\dagger}(\boldsymbol{r}, \hat{\Omega}', E') \mathbf{F}(\mathbf{r}, E, E') \psi(\boldsymbol{r}, \hat{\Omega}, E) dV d\hat{\Omega} dE d\hat{\Omega}' dE'} \quad (100)$$

The importance-weighted β and Λ calculated from (97) and (100) are called the effective delayed neutron fraction and effective generation time, respectively.

Neutron importance and adjoint flux play a major role in sensitivity and uncertainty analysis, and it also has use in shielding applications and variance reduction techniques used in Monte Carlo simulation. These topics, however, are beyond the scope of this course.

³¹ In Monte Carlo simulation, the adjoint transport problem can be intuitively understood as tracking the neutron histories backwards, for example, starting from a fission event and following the path to its origin. Keeping track of the neutron's descendants and calculating their contribution to the asymptotic population forms the basis of the iterated fission probability (IFP) method, used by Monte Carlo codes to calculate importance-weighted time constants.


Summary of main topics

The modeling of an operating nuclear reactor is a complicated task, involving the couple solution of neutronics, heat transfer from fuel to coolant, heat removal from the core by coolant flow and fuel depletion.

Reactivity feedbacks and fuel burnup turn linear transport problem into a non-linear coupled problem. The solution is obtained by iterating between different solvers. The calculations are based on a multi-stage scheme, in which the scale of the problem is gradually increased while simultaneously moving towards simplified physics.

All deterministic transport methods are based on the solution to the transport equation, which is formulated based neutron balance in the six-dimensional phase space. The transport problem cannot be solved without approximations.

Transport calculations can be roughly divided into time-dependent and eigenvalue calculations. The most commonly used method is the k-eigenvalue criticality calculation, in which the balance between neutron source and loss terms is obtained by artificially scaling the number of emitted fission neutrons.

The simplest approach to time-dependent problems is the point-kinetics approximation, in which the flux is approximated by the fundamental mode solution and separated into space-, direction and energy-dependent form function and time-dependent amplitude function. The approximation is commonly used in small or otherwise closely-coupled systems, but the simulation of LWR transients requires more elaborated time-space resolved solution.



Topics of next lecture

The next lecture (9.3.2018) introduces the Monte Carlo method, which provides an alternative insight into the transport problem from the viewpoint of an individual neutron

Specific topics include:

- Basics of Monte Carlo calculation, probability and statistics
- CSG geometry model used in Monte Carlo codes
- Particle tracking routines
- Interaction physics
- Simulating the neutron population
- Collection of results

