Boltzmann Transport Equation (Considering Delayed Neutrons)

Shim, Hyung Jin

Nuclear Engineering Department,
Seoul National University

References

1. George I. Bell and Samuel Glasstone, "Nuclear Reactor Theory," Van Nostrand Reinhold, NY, 1970.
2. James J. Duderstadt and Louis J. Hamilton, "Nuclear Reactor Analysis," John Wiley & Sons, Inc., 1976.
3. Raymond E. Alcouffe and R. Douglas O'Dell, "Transport Calculations for Nuclear Reactors, CRC Handbook of Nuclear Reactors Calculations Volume I," CRC Press Inc., FL, 1986.
4. Eugene P. Wigner, "Mathematical Problems of Nuclear Reactor Theory," Proceedings of Symposium in Applied Mathematics, American Mathematical Society, Providence, Vol. 11, pp. 89-104 (1961).
5. Z. Akcasu, G. S. Lellouche, L. M. Shotkin, *Mathematical Methods in Nuclear Reactor Dynamics*, Academic Press, NY (1971).
6. E. E. Lewis, W. F. Miller, *Computational Methods of Neutron Transport*, American Nuclear Society, Inc., IL, 1993.

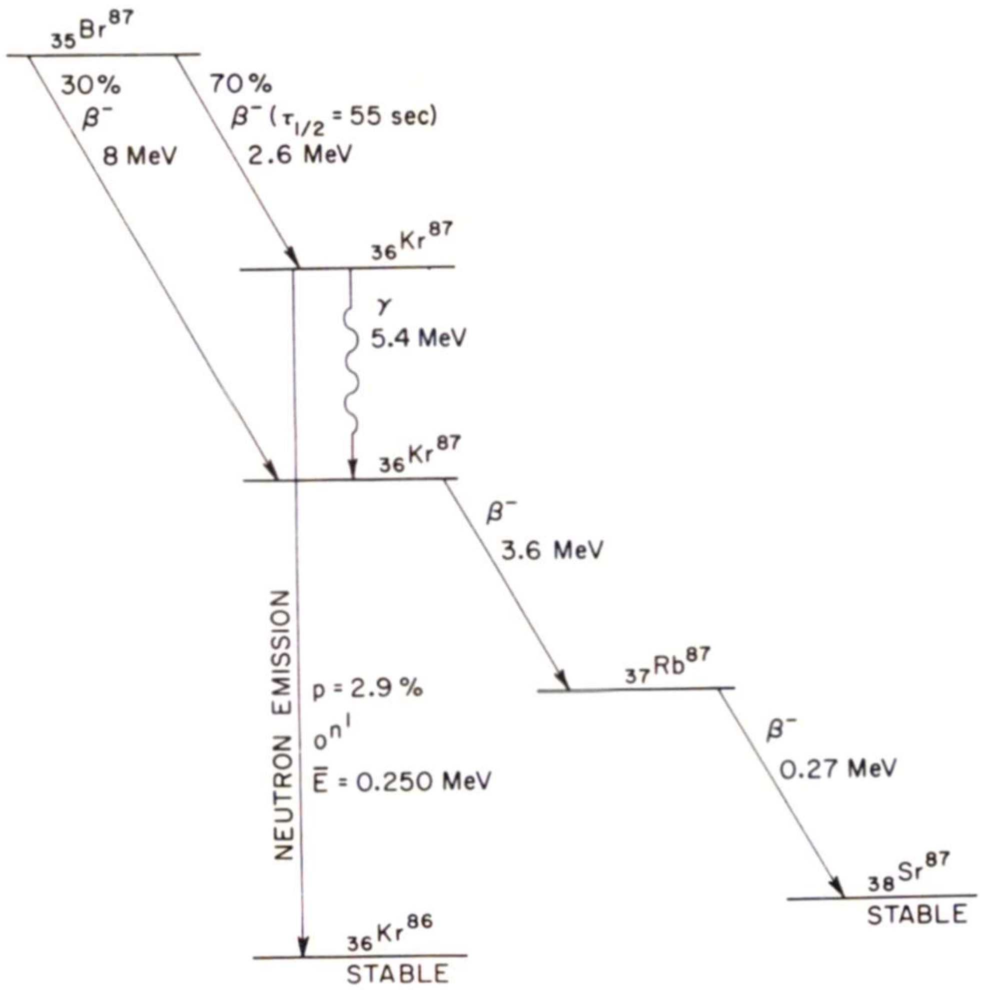
Delayed Neutron

- For the precise time-dependent neutron transport equation, we must incorporate into the following NTE the fact that some of the neutrons produced as the result of fission events may be delayed by decays of unstable fission fragments.

$$\begin{aligned}
&\frac{1}{v}\frac{\partial \Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t}+\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t)+\Sigma_t(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t)\\
&\quad=\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\,\Sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\
&\quad+\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\,\chi(\mathbf{r},E'\to E)\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E',\mathbf{\Omega}'\to\mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\
&\quad+Q(\mathbf{r},E,\mathbf{\Omega},t) \qquad\qquad \cdots\cdots (1)
\end{aligned}$$

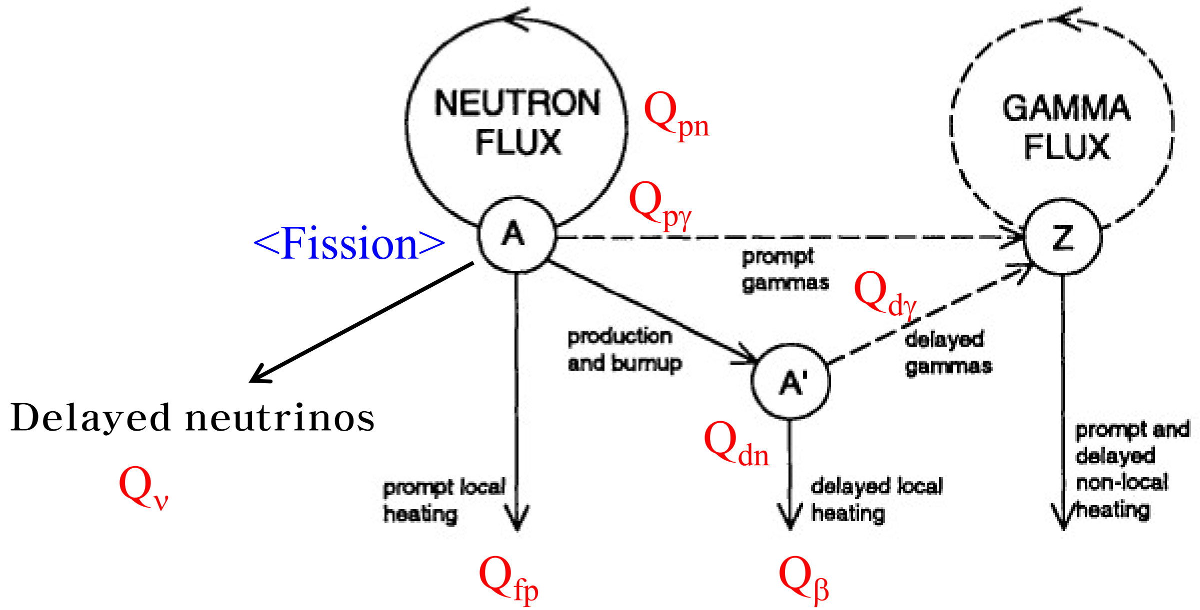
- Delayed Neutron
  - Not all the ν neutrons emitted in an average fission event appear at once.
  - A small fraction (0.65 percent for U^{235}) are emitted from certain of the fission fragments after a β decay makes these fragments unstable with respect to their neutron content.
  - The β decay that precedes the emission of these *delayed neutrons* is a relatively slow process, the half-lives of the unstable fission fragments involved being between ~0.2 sec and ~54 sec.
  - Once the β decay occurs, a neutron appears essentially instantaneously.
  - Such fission fragments are called *delayed-neutron precursors*.

Decay Scheme of a Typical Delayed Neutron Precursor



[5] Z. Akcasu, G. S. Lellouche, L. M. Shotkin, "Mathematical Methods in Nuclear Reactor Dynamics," Academic Press, NY (1971).

Particles Produces from Fission



〈from NJOY Manual〉

$$\boxed{Q_{FIS}=Q_{fp}+Q_{pn}+Q_{dn}+Q_{p\gamma}+Q_{d\gamma}+Q_\beta+Q_\nu}$$

Q_{fp}=Kinetic energy of the fragments

Q_{pn}=Kinetic energy of the prompt neutron

Q_{dn}=Kinetic energy of the delayed neutron

$Q_{p\gamma}$=Kinetic energy of the prompt gammas

$Q_{d\gamma}$=Kinetic energy of the delayed gammas

Q_β =Total energy released by the delayed betas

Q_ν =Energy carried away by the neutrinos

Components of energy release in fission

Quantity	Value(eV)	Uncertainty
Kinetic energy of the fragments	1.6912E+08	4.9000E+05
Kinetic energy of the prompt neutrons	4.7900E+06	7.0000E+04
Kinetic energy of the delayed neutrons	7.4000E+03	1.1100E+03
Kinetic energy of the prompt gammas	6.9700E+06	5.0000E+05
Kinetic energy of the delayed gammas	6.3300E+06	5.0000E+04
Total energy released by delayed betas	6.5000E+06	5.0000E+04
Energy carried away by the neutrinos	8.7500E+06	7.0000E+04
Total energy release per fission (sum)	2.0247E+08	1.3000E+05
Total energy less neutrino energy	1.9372E+08	1.5000E+05

Interpreted ENDF file for U-235e (ENDF/B-VI)

〈Ref: LA-UR-08-05891, www.physor2008.ch〉

(Delayed Neutron) Precursor Concentration

- In order to quantitatively describe the effect of the NTE of Eq. (1), we need to introduce another function, the **fictitious** concentration of the *i*-th one of the delayed neutron precursors at location **r** in a reactor, $C_i(\mathbf{r},t)$ [precursor nuclei/cc].
  - $\underline{C_i(\mathbf{r},t)d\mathbf{r}}$ is the expected number of **fictitious** precursor of *i*-th kind in d**r** at **r** at time t **which always decay by emitting a delayed neutron**.

  ✓ Question about the meaning of the fictitious concentration
    - When the actual nuclide density function of ^{87}Br is expressed as $^{87}\mathrm{Br}(\mathbf{r},t)$, what's the number which satisfies the following relationship between the precursor concentration of ^{87}Br, $C_{^{87}\mathrm{Br}}(\mathbf{r},t)$, and $^{87}\mathrm{Br}(\mathbf{r},t)$?

$$C_{^{87}\mathrm{Br}}(\mathbf{r},t) = \boxed{}\,^{87}\mathrm{Br}(\mathbf{r},t)$$

- There are about twenty of these precursors, but most of them have such a small yield that it is possible to fit the data by assuming six groups.

Delayed Neutron Data

- The decay constant of the *i*-th delayed neutron precursor group and the fraction of fission neutrons due to its decay are denoted by λ_i and β_i, respectively.

< Delayed neutron data for thermal fission of ^{235}U >

Group	Decay Const. [sec^{-1}]	Yield [neutrons per fission]	Relative fraction β_i/β	Fraction β_i
1	0.0124	0.00052	0.033	0.000215
2	0.0305	0.00346	0.219	0.001424
3	0.111	0.00310	0.196	0.001274
4	0.301	0.00624	0.395	0.002568
5	1.14	0.00182	0.115	0.000748
6	3.01	0.00066	0.042	0.000273
Total	-	0.0158	1.000	0.00650

$$\beta = \sum_{i=1}^{I} \beta_i \qquad (2)$$

< David L. Hetrick, "Dynamics of Nuclear Reactors," American Nuclear Society, Inc., IL, USA (1993) >

- In the table, note that the unit of the yield of the precursor is [neutrons per fission], not [nuclei per fission] because the precursor is assumed to always decay by emitting a delayed neutron.

Questions on Delayed Neutron Production

- Question #1
  - ✓ Calculate the half-life [sec^{-1}] from the given decay constant of each precursor group.
  - ✓ What's the relationship between the yield and β_i?
  - ✓ Calculate the mean time [sec], $\overline{t_i}$, for each precursor group to produce a delayed neutron.
  - ✓ Calculate the mean time to generate all the fission neutrons from the instant of fission assuming that the prompt neutrons are produced instantaneously.

$$\overline{t} = (1-\beta)\cdot(0[\text{sec}]) + \sum_{i=1}^{6}\beta_i \cdot \overline{t_i} \cong 0.085[\text{sec}]$$

Why do we have to consider this small amount of delayed neutrons?

Reactor Period

- Let l be the *neutron lifetime*, that is, the average time from the emission of a neutron in fission to the absorption of the neutron somewhere in the reactor.
- In view of the definition of the multiplication factor, the absorption of one neutron in a reactor leads, on the average, to the emission of k neutrons for the next generation, that is, l sec later from its birth:

$$n(t+l) = kn(t) \qquad \text{①}$$

- And since

$$n(t+l) \cong n(t) + l\frac{dn(t)}{dt} \qquad \text{②}$$

it follows that $n(t)$ is determined by the equation

$$\frac{dn(t)}{dt} \cong \frac{k-1}{l}n(t) \Rightarrow n(t) = n(0)\exp\left(t/T\right) \qquad \text{③}$$

- T called the period of the reactor or "e-folding time" in which the delayed neutrons have been omitted gives

$$\boxed{T = \frac{l}{k-1}} \qquad \text{④}$$

Infinite Reactor with No Delayed Neutrons

- Let l_p be the *prompt neutron lifetime*, that is, the average time from the emission of a prompt neutron in fission to the absorption of the neutron somewhere in the reactor.
- In view of the definition of the multiplication factor, the absorption of one neutron in an infinite reactor leads, on the average, to the emission of k_∞ neutrons for the next generation, that is, l_p sec later from its birth:

$$n(t+l_p) = k_\infty n(t)$$

- And since

$$n(t+l_p) \cong n(t) + l_p \frac{dn(t)}{dt}$$

  it follows that $n(t)$ is determined by the equation

$$\frac{dn(t)}{dt} \cong \frac{k_\infty - 1}{l_p} n(t) \Rightarrow n(t) = n(0)\exp\left(t/T\right)$$

- Then the reactor period becomes

$$T = \frac{l_p}{k_\infty - 1}$$

Reactor Period w/o Considering Delayed Neutrons

- As an illustration of these results, consider an infinite thermal reactor consisting of a homogeneous mixture of H_2O and ^{235}U in which k_∞ is increased by only 0.1%, that is, from $(k_\infty)_0$=1.00000 to k_∞=1.00100.
- In this case, the prompt neutron lifetime is about 10^{-4} sec.

  (J. R. Lamarsh, "Introduction to Nuclear Reactor Theory," New York Univ., 1966.)
- Then from Eq. ④, the reactor period becomes

$$T = \frac{10^{-4}}{1.001 - 1} = 0.1\sec$$

- This is very short period: in one second the reactor would pass through 10 periods and the fission rate (and power) would increase by a factor of $e^{10} = 2.2 \times 10^4$.
- Had the reactor originally been operating at 1MW, the power would increase to 22GW in only one second. A reactor with such a short period would be very difficult to control, to say the least.
- **The period of a finite reactor** is even shorter than computed above because the prompt neutron lifetime in the finite reactor is less than in the infinite reactor.

Mean Lifetime

- If l_p is the prompt neutron lifetime, and l_i is the mean lifetime of a delayed neutron in the *i*-th group measured from the instant of fission to the time when the neutron is ultimately absorbed, the mean-life of all fission neutrons, prompt and delayed, is

$$l = (1-\beta)l_p + \sum_{i=1}^{6} \beta_i l_i \quad \text{......} \quad ⑤$$

- It may be noted that the delayed neutrons slow down and are captured in a time which is short compared with the mean lifetime of their precursors.

$$l \cong (1-\beta)l_p + \sum_{i=1}^{6} \beta_i \overline{t_i} \quad \text{......} \quad ⑥$$

- Finally, since β<<1 for all fissile nuclei, Eq. ⑥ can be written as

$$l \cong l_p + \sum_{i=1}^{6} \beta_i \overline{t_i} \quad \text{......} \quad ⑦$$

Mean Lifetime (Contd.)

< Delayed neutron data for thermal fission of ^{235}U >

Group	Half-Life (sec)	Decay Const. (sec^{-1})	Yield (neutrons per fission)	Relative fraction β_i/β	Fraction β_i
1	55.72	0.0124	0.00052	0.033	0.000215
2	22.72	0.0305	0.00346	0.219	0.001424
3	6.22	0.111	0.00310	0.196	0.001274
4	2.30	0.301	0.00624	0.395	0.002568
5	0.610	1.14	0.00182	0.115	0.000748
6	0.230	3.01	0.00066	0.042	0.000273
Total	-	-	0.0158	1.000	0.00650

< David L. Hetrick, "Dynamics of Nuclear Reactors," American Nuclear Society, Inc., IL, USA (1993) >

- Using the values of the upper table, the term $\sum_{i=1}^{6} \beta_i \overline{t_i}$ is found to be 0.085sec~0.1sec.
- Then a 0.1% change in k_∞ now leads to a period of T = 0.1/0.001 = 100sec.

Precursor Density Equation

- When β_i^j is the fraction of the neutrons from a fission of isotope j (^{235}U, ^{239}Pu, etc.) that eventually appear from the decay of the precursor i, we have:

Creation rate of precursors of i-th kind per unit volume at location **r** at time t

$$= \sum_j \beta_i^j \int_{4\pi} d\mathbf{\Omega} \int_E dE \;\; \nu^j(\cancel{\mathbf{r}}, E)\Sigma_f^j(\mathbf{r}, E, \mathbf{\Omega}, t)\Phi(\mathbf{r}, E, \mathbf{\Omega}, t) \qquad (3)$$

where

$\nu^j(E)$ = average number of neutrons produced from a fission of isotope j due to a neutron with energy E

$\Sigma_f^j(\mathbf{r}, E, \mathbf{\Omega}, t)$ = the macroscopic cross section of isotope j for fission induced by neutrons with energy E and direction $\mathbf{\Omega}$

- Because the precursors are removed only by their decays, the removal rate of the i-th group precursors at r becomes

Remvoal rate of precursors of i-th kind per unit volume at location **r** at time t

$$= \lambda_i C_i(\mathbf{r}, t) \qquad (4)$$

Delayed Precursor Density Equation (Contd.)

- Then the number balance of the *i*-th group precursor per unit volume at location **r** at time t, i.e. the balance of $C_i(\mathbf{r},t)$, can be written as

$$\boxed{\frac{\partial C_i(\mathbf{r},t)}{\partial t} = \sum_j \beta_i^j \int_{4\pi} d\mathbf{\Omega} \int_E dE \ \nu^j(E)\Sigma_f^j(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t) - \lambda_i C_i(\mathbf{r},t)} \quad \cdots\cdots\cdots \quad (5)$$

- Note that the migration of the precursors before the emission of a delayed neutron is neglected in Eq. (5) because they lose their kinetic energy very rapidly in solid-fuel reactors. They are stopped in a short distance from the point of their formation by fission (e.g., the range of light fission fragments in aluminum is approximately 1.4×10^{-3}cm)*.

  * A. M. Weinberg and E. P. Wigner, "The Physical Theory of Neutron Chain Reactors," Univ. of Chicago Press, Chicago, IL (1958).

- Consequently, the delayed neutrons is assumed to be produced at the same point where the fission event takes place as the prompt neutrons.

Considering Delayed Neutrons in NTE

- Now, let us divide the fission production rate term in Eq. (1) of

$$\int_{4\pi} d\mathbf{\Omega}' \int_{E'} dE' \chi(\mathbf{r}, E' \to E) \nu(\mathbf{r}, E') \Sigma_f(\mathbf{r}, E', \mathbf{\Omega}' \to \mathbf{\Omega}, t) \Phi(\mathbf{r}, E', \mathbf{\Omega}', t)$$

into the fission production rate terms of prompt and delayed neutrons.

- With χ_p^j defined as the corresponding neutron spectrum of prompt neutrons emitted by fission of isotope j, we have:

<u>Rate at which prompt neutrons appear in unit volume at **r** at *t*</u>

$$= \sum_j \chi_p^j (E' \to E)(1 - \beta^j) \int_{4\pi} d\mathbf{\Omega}' \int_{E'} dE' \; \nu^j (E') \Sigma_f(\mathbf{r}, E', \mathbf{\Omega}' \to \mathbf{\Omega}, t) \Phi(\mathbf{r}, E', \mathbf{\Omega}', t) \quad \text{(6)}$$

where β^j is the total yield of the precursors from a fission of isotope j:

$$\beta^j = \sum_{i=1}^{I} \beta_i^j \quad \text{(7)}$$

Considering Delayed Neutrons in NTE (Contd.)

- Because a precursor inevitably produces a delayed neutron from its β decay, the delayed neutron production rate becomes

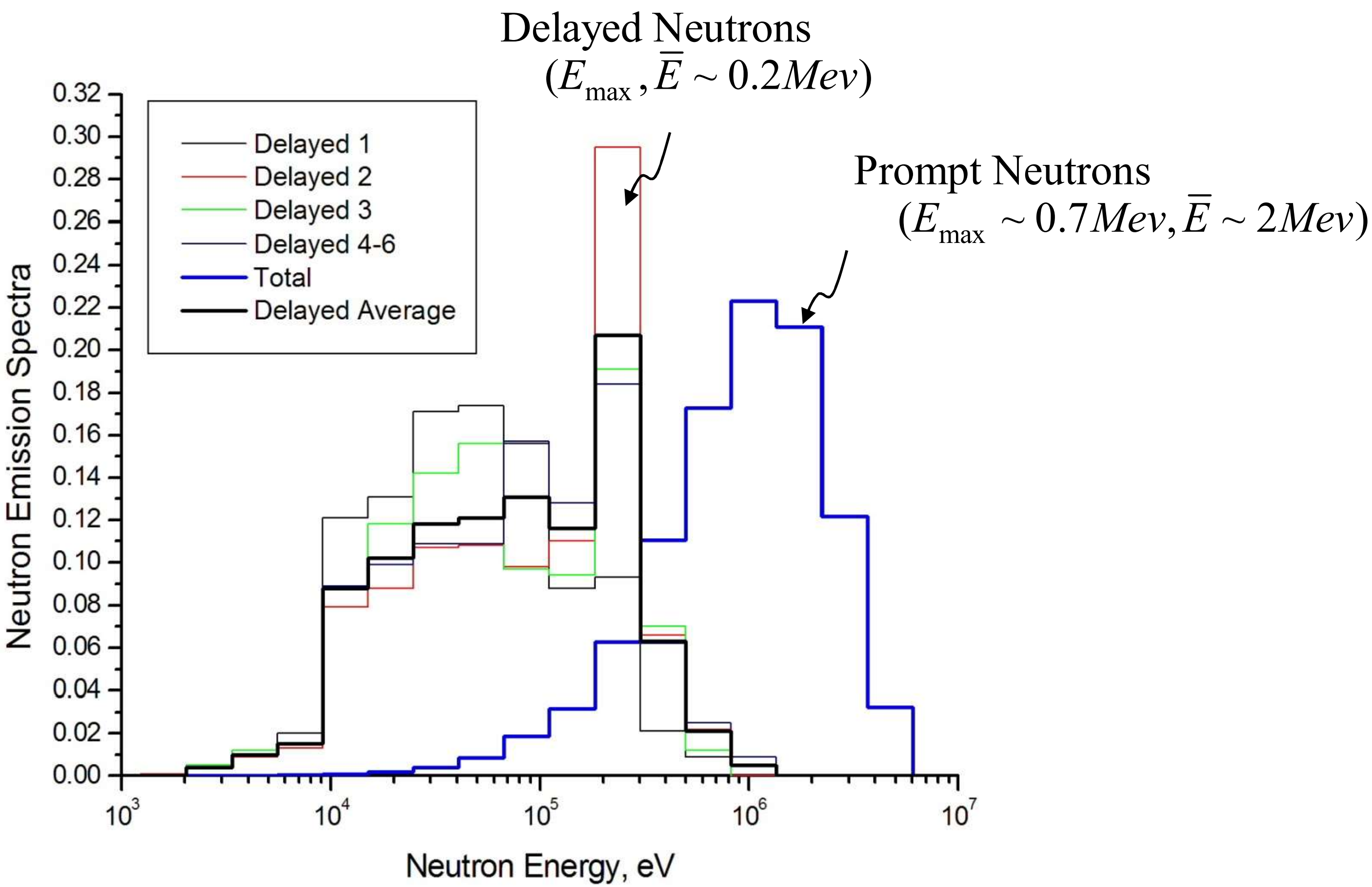
Rate at which delayed neutrons are emitted per unit volume per unit steradian at **r** at *t*

$$= \sum_{i=1}^{I} \frac{\chi_i(E)}{4\pi} \lambda_i C_i(\mathbf{r},t) \quad \cdots\cdots \quad (8)$$

where

$\chi_i(E)$ = the probability of delayed neutrons appearing at energy E as a result of a decay of the i-th group precursor

Prompt and Delayed Neutron Spectra



Time-Dependent Neutron Transport Equation

- Then, by replacing the neutron production rate term in Eq. (1) by Eq. (6) plus Eq. (8), the time-dependent NTE is obtained as

$$
\begin{aligned}
\frac{1}{v}\frac{\partial \Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} = & -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t) - \Sigma_t(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t) \\
& + \int_{4\pi} d\mathbf{\Omega}' \int_{E'} dE' \, \Sigma_s(\mathbf{r},E' \to E,\mathbf{\Omega}' \to \mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t) \\
& + \sum_j \int_{4\pi} d\mathbf{\Omega}' \int_{E'} dE' \chi_p^j(E' \to E)\left(1-\beta^j\right)\nu^j(E')\Sigma_f^j(\mathbf{r},E',\mathbf{\Omega}' \to \mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t) \\
& + \sum_{i=1}^{I} \frac{\chi_i(E)}{4\pi}\lambda_i C_i(\mathbf{r},t) \\
& + Q(\mathbf{r},E,\mathbf{\Omega},t) \qquad \cdots\cdots \quad (9a)
\end{aligned}
$$

Time-Dependent Neutron Transport Equation

- Assuming that the direction of prompt neutrons produced from a fission reaction follows the isotropic distribution and that their energy is independent of the incident neutron energy, Eq. (9a) can be expressed as

$$
\begin{aligned}
\frac{1}{v}\frac{\partial\Phi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} &= -\mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega},t)-\Sigma_t(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t)\\
&+\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\,\Sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\
&+\sum_j\frac{\chi_p^j(E)}{4\pi}\left(1-\beta^j\right)\int_{4\pi}d\mathbf{\Omega}'\int_{E'}dE'\nu^j(E')\Sigma_f^j(\mathbf{r},E',\mathbf{\Omega}',t)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\\
&+\sum_{i=1}^{I}\frac{\chi_i(E)}{4\pi}\lambda_i C_i(\mathbf{r},t)\\
&+Q(\mathbf{r},E,\mathbf{\Omega},t) \qquad \cdots\cdots (9b)
\end{aligned}
$$

- Note that Eq. (5) should be accompanied with Eq. (9) to calculate the precursor density distribution function.

$$
\frac{\partial C_i(\mathbf{r},t)}{\partial t}=\sum_j\beta_i^j\int_{4\pi}d\mathbf{\Omega}\int_E dE\;\nu^j(E)\Sigma_f^j(\mathbf{r},E,\mathbf{\Omega},t)\Phi(\mathbf{r},E,\mathbf{\Omega},t)-\lambda_i C_i(\mathbf{r},t) \qquad \cdots\cdots (5)
$$

Boundary Conditions [6]

- Suppose that the spatial domain within which the neutron transport equation is to be solved has volume V surrounded by a surface Γ.

- Suppose that the spatial domain within which the neutron transport equation is to be solved has volume V surrounded by a surface Γ.

- To solve the equation, the flux at t=0, $\Phi(\mathbf{r},E,\mathbf{\Omega},0)$ must be specified. In addition, the flux distribution entering V across Γ must be known.

$$\Phi(\mathbf{r},E,\mathbf{\Omega},t)=\tilde{\Phi}(\mathbf{r},E,\mathbf{\Omega},t),\quad \mathbf{\Omega}\cdot\mathbf{n}<0,\quad \mathbf{r}\in\Gamma$$

- The frequent case in which $\tilde{\Phi}$ is identically zero is referred to as the vacuum boundary condition.

$$\Phi(\mathbf{r},E,\mathbf{\Omega},t)=0,\quad \mathbf{\Omega}\cdot\mathbf{n}<0,\quad \mathbf{r}\in\Gamma$$

Implicit Boundary Condition – Albedo BC

- Implicit boundary conditions are relationship **between the incoming and outgoing fluxes**.

1. Albedo boundary conditions
   - The incoming flux on a boundary is set equal to a known isotropic albedo, $\alpha(E)$, times the outgoing flux on the same boundary in the direction corresponding to spectral reflection,

$$\Phi(\mathbf{r}, E, \boldsymbol{\Omega}, t) = \alpha(E)\Phi(\mathbf{r}, E, \boldsymbol{\Omega}', t), \quad \boldsymbol{\Omega}\cdot\mathbf{n} < 0, \quad \mathbf{r} \in \Gamma$$

   Here Ω is the reflection angle corresponding to an incident angle **Ω'**

$$\mathbf{n}\cdot\boldsymbol{\Omega} = -\mathbf{n}\cdot\boldsymbol{\Omega}' \quad \text{and} \quad (\boldsymbol{\Omega}\times\boldsymbol{\Omega}')\cdot\mathbf{n} = 0$$

   - The special case of α=1.0 is referred to as a reflective boundary condition.

White & Periodic BC's

2. White boundary condition
   - All particles passing out of V over a surface increment return with an isotropic distribution

3. Periodic boundary condition
   - The flux distribution on one boundary is equal to the flux distribution on another boundary in a periodic lattice structure

$$\Phi(\mathbf{r}, E, \mathbf{\Omega}, t) = \Phi(\mathbf{r} + \mathbf{r}_l, E, \mathbf{\Omega}', t)$$

Time-Dependent Diffusion Equation

- Question #2
  - ✓ By integrating Eqs. (9) and (5) over $\mathbf{\Omega}$, show that the time-dependent neutron diffusion equation is

$$
\begin{aligned}
\frac{1}{v(E)}\frac{\partial \phi(\mathbf{r},E,t)}{\partial t} = {} & \nabla \cdot D(\mathbf{r},E,t)\nabla \phi(\mathbf{r},E,t) - \Sigma_t(\mathbf{r},E,t)\phi(\mathbf{r},E,t) \\
& + \int_{E'} \Sigma_s(\mathbf{r},E' \to E,t)\phi(\mathbf{r},E',t)dE' \\
& + \sum_j \chi_p^j(E)(1-\beta^j)\int_{E'} \nu^j(E')\Sigma_f^j(\mathbf{r},E',t)\phi(\mathbf{r},E',t)dE' \\
& + \sum_{i=1}^{I} \chi_i(E)\lambda_i C_i(\mathbf{r},t) \\
& + Q(\mathbf{r},E,t) \qquad \cdots\cdots (10)
\end{aligned}
$$

$$
\frac{\partial C_i(\mathbf{r},t)}{\partial t} = \sum_j \beta_i^j \int_E dE\ \nu^j(E)\Sigma_f^j(\mathbf{r},E,t)\phi(\mathbf{r},E,t) - \lambda_i C_i(\mathbf{r},t) \qquad \cdots\cdots (11)
$$