

Neutron leakage

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- Types on neutron leakage
- The B_n leakage calculation
- The homogeneous fundamental mode
- The leakage coefficient
- Leakage rates with the CP method

A leakage model is required in a lattice calculation performed with a **fundamental mode** approximation, i.e., when the elementary cell or assembly calculation is performed in 2D and/or is surrounded by reflection or translation boundary conditions.

- Any axial and/or radial leakage rate not taken into account by an explicit boundary condition must be represented by the leakage model.
- The leakage rate depends of the following factors:
 - scattering anisotropy
 - streaming effects caused by strong heterogeneities and/or low optical density regions in the lattice
- Moreover the leakage model is used to obtain consistent values of the diffusion coefficients that can be used in a full core reactor calculation performed with the diffusion equation.
- Taking into account the streaming effects leads to a truly heterogeneous definition of the diffusion coefficient.

Streaming effects:

The streaming effect can be isotropic or anisotropic, depending if the leakage rate is identical or different for the three spatial dimensions.

- Homogeneous (aka., no-streaming) approximation. **Sufficient for situations where the lattice geometry is completely homogenized.**
- Isotropic streaming is mainly caused by heterogeneities of the lattice, such as poison pins or finite regions of small optical density. **Sufficient for CANDU and PWR reactors.**
- Anisotropic streaming is due to the fact that the lattice may not have the same properties along the axial dimension and over the radial plane of the lattice. **Required for small FRB and gas-cooled reactors.**

Scattering anisotropy:

- The scattering anisotropy can be neglected in some fast reactor cases.
- In a pressurized water reactor (PWR), the effect of scattering anisotropy on the leakage is of prime importance, due to the presence of hydrogen in the moderator. Its effect on the leakage model is therefore **always** taken into account by using a consistent B_1 approximation. **Here, a transport-corrected B_0 approximation is not acceptable.** In most cases, an homogeneous consistent B_1 calculation is sufficient.

In a lattice calculation

- we need to determine neutron fluxes, leakage and reaction rates of a unit cell **without** the knowledge of the exact operating conditions and materials surrounding it.
- However, we can always assume that the real neutron flux of the unit cell or assembly is under steady-state conditions (i.e., we know that $K_{\text{eff}} = 1$).

Without more information, the best that we can do in the lattice calculation is

- to assume that all the surrounding cells or assemblies are **identical** to the one being considered and
- to adjust the neutron leakage in each group g in such a way that $K_{\text{eff}} = 1$.

The B_n leakage calculation

1. The flux calculation inside the unit cell or assembly will be performed under **closed** conditions. An infinite domain or a finite domain closed with reflective (i.e., with an albedo set to one) or periodic boundary conditions will be used.
2. A leakage model will be introduced to enforce $K_{\text{eff}} = 1$ in the unit cell. The **fundamental mode** approximation consists to represent the neutron flux as the product of a macroscopic distribution in space $\psi(\mathbf{r})$ with a homogeneous or periodic **fundamental flux** $\varphi(\mathbf{r}, E, \boldsymbol{\Omega})$:

$$(1) \quad \phi(\mathbf{r}, E, \boldsymbol{\Omega}) = \psi(\mathbf{r}) \varphi(\mathbf{r}, E, \boldsymbol{\Omega}) \quad .$$

3. The macroscopic distribution is assumed to be a property of the complete reactor and to be the solution of a **Laplace equation**:

$$(2) \quad \nabla^2 \psi(\mathbf{r}) + B^2 \psi(\mathbf{r}) = 0$$

where the **buckling** B^2 is a real number that is used to adjust the curvature of $\psi(\mathbf{r})$ in such a way to obtain $K_{\text{eff}} = 1$. The buckling is positive or negative if the lattice is originally over-critical or sub-critical. The curvature thus obtained must be similar to what is observed for the real neutron flux in the complete reactor.

The B_n leakage calculation

- There exist homogeneous and heterogeneous variants of the fundamental mode theory, depending on whether the fundamental flux $\varphi(\mathbf{r}, E, \boldsymbol{\Omega})$ is assumed to be homogeneous or periodic according to the lattice pitch.
- The heterogeneous fundamental mode approximation is used to take into account the streaming effects in the lattice.

Without any knowledge of the complete reactor geometry, we will use the following generic solution of Eq. (2):

$$(3) \quad \psi(\mathbf{r}) = \psi_0 e^{i\mathbf{B} \cdot \mathbf{r}}$$

where the vector \mathbf{B} is chosen in such a way that $B^2 = \mathbf{B} \cdot \mathbf{B}$. The neutron flux will therefore be factorized as

$$(4) \quad \phi(\mathbf{r}, E, \boldsymbol{\Omega}) = \varphi(\mathbf{r}, E, \boldsymbol{\Omega}) e^{i\mathbf{B} \cdot \mathbf{r}}$$

where $\varphi(\mathbf{r}, E, \boldsymbol{\Omega})$ is a complex quantity.

The determination of the corresponding leakage rates in each energy group will be obtained through the **homogeneous** or **heterogeneous B_1 equations**. These equations are obtained after substituting the factorization of Eq. (4) into the neutron transport equation applied to a finite lattice of cells or assemblies.

This model assumes that the leakage rates can be computed in a unit cell (or assembly) completely homogenized in space. Note that the collision rates are nevertheless computed in the heterogeneous representation of the lattice.

The idea is therefore to compute the curvature of the macroscopic flux distribution in the homogenized unit cell (or assembly). A flux–volume homogenization is generally performed. In this case, the factorization of Eq. (4) is rewritten as

$$(5) \quad \phi(\mathbf{r}, E, \boldsymbol{\Omega}) = \varphi(E, \boldsymbol{\Omega}) e^{i\mathbf{B} \cdot \mathbf{r}}$$

where we note the non–dependence of $\varphi(E, \boldsymbol{\Omega})$ with the spatial coordinates. This value is complex.

The next step consists to obtain the neutron transport equation for the case of a finite and homogeneous geometry:

$$(6) \quad \begin{aligned} \boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, E, \boldsymbol{\Omega}) &+ \Sigma(E) \phi(\mathbf{r}, E, \boldsymbol{\Omega}) \\ &= \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(E \leftarrow E', \boldsymbol{\Omega} \leftarrow \boldsymbol{\Omega}') \phi(\mathbf{r}, E', \boldsymbol{\Omega}') \\ &+ \frac{\chi(E)}{4\pi K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \phi(\mathbf{r}, E') \end{aligned}$$

The corresponding **homogeneous B_1 equations** are obtained by substituting the factorization (5) into Eq. (6). We obtain

$$(7) \quad [\Sigma(E) + i\mathbf{B} \cdot \boldsymbol{\Omega}] \varphi(E, \boldsymbol{\Omega}) = \int_{4\pi} d^2\Omega' \int_0^\infty dE' \Sigma_s(E \leftarrow E', \boldsymbol{\Omega} \leftarrow \boldsymbol{\Omega}') \varphi(E', \boldsymbol{\Omega}') + \frac{\chi(E)}{4\pi K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E')$$

where the integrated fundamental flux is given in terms of the angular fundamental flux using

$$(8) \quad \varphi(E) = \int_{4\pi} d^2\Omega \varphi(E, \boldsymbol{\Omega}) \quad .$$

We expand the differential scattering term using zero and first order Legendre polynomials (linearly anisotropic collision in the LAB). We obtain

$$(9) \quad \Sigma_s(E \leftarrow E', \boldsymbol{\Omega} \leftarrow \boldsymbol{\Omega}') = \frac{1}{2\pi} \Sigma_s(E \leftarrow E', \mu) = \sum_{\ell=0}^1 \frac{2\ell+1}{4\pi} \Sigma_{s,\ell}(E \leftarrow E') P_\ell(\mu)$$

where $\mu = \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}'$, $P_0(\mu) = 1$ and $P_1(\mu) = \mu$.

Substituting Eq. (9) into Eq. (7), we get

$$\begin{aligned}
 [\Sigma(E) + i\mathbf{B} \cdot \boldsymbol{\Omega}] \varphi(E, \boldsymbol{\Omega}) &= \int_0^\infty dE' \left\{ \frac{1}{4\pi} \Sigma_{s0}(E \leftarrow E') \varphi(E') \right. \\
 &+ \left. \frac{3}{4\pi} \Sigma_{s1}(E \leftarrow E') \mathcal{J}(E') \cdot \boldsymbol{\Omega} \right\} \\
 (10) \quad &+ \frac{\chi(E)}{4\pi K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E')
 \end{aligned}$$

where the **fundamental current** is given in terms of the angular fundamental flux using

$$(11) \quad \mathcal{J}(E) = \int_{4\pi} d^2\Omega \boldsymbol{\Omega} \varphi(E, \boldsymbol{\Omega}) \quad .$$

Equation (10) is weighted and integrated over Ω as required by the B_1 model:

1. A simple integration, without weighting, leads to the first B_1 equation (a conservation relation). Some terms have been removed due to parity properties:

$$(12) \quad \begin{aligned} \Sigma(E) \varphi(E) + iB \mathcal{J}(E) &= \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E') \varphi(E') \\ &+ \frac{\chi(E)}{K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E') \end{aligned}$$

where the dependency against the direction of vector B was removed by defining

$$(13) \quad \mathcal{J}(E) = \frac{1}{B} [\mathbf{B} \cdot \mathbf{J}(E)] \quad .$$

2. The weight factor

$$\omega(\Omega) = \frac{1}{\Sigma(E) + i\mathbf{B} \cdot \Omega}$$

is next used to multiply each member of Eq. (10) before its integration

The second B_1 equation is therefore written

$$\begin{aligned} \varphi(E) = & \int_0^\infty dE' \left\{ \frac{1}{4\pi} \Sigma_{s0}(E \leftarrow E') \varphi(E') \int_{4\pi} d^2\Omega \frac{\Sigma(E) - i\mathbf{B} \cdot \boldsymbol{\Omega}}{\Sigma(E)^2 + (\mathbf{B} \cdot \boldsymbol{\Omega})^2} \right. \\ & + \left. \frac{3}{4\pi} \Sigma_{s1}(E \leftarrow E') \mathcal{J}(E') \cdot \int_{4\pi} d^2\Omega \frac{\boldsymbol{\Omega} \Sigma(E) - i(\boldsymbol{\Omega} \otimes \boldsymbol{\Omega}) \cdot \mathbf{B}}{\Sigma(E)^2 + (\mathbf{B} \cdot \boldsymbol{\Omega})^2} \right\} \\ & + \frac{\chi(E)}{4\pi K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E') \int_{4\pi} d^2\Omega \frac{\Sigma(E) - i\mathbf{B} \cdot \boldsymbol{\Omega}}{\Sigma(E)^2 + (\mathbf{B} \cdot \boldsymbol{\Omega})^2} \end{aligned}$$

where $\boldsymbol{\Omega} \otimes \boldsymbol{\Omega}$ is the **dyadic product** of the solid angle by itself. After some simplification relating to parity properties, we obtain

$$\begin{aligned} \varphi(E) = \alpha [B, \Sigma(E)] & \left\{ \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E') \varphi(E') + \frac{\chi(E)}{K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E') \right\} \\ & - 3i\beta [B, \Sigma(E)] B \int_0^\infty dE' \Sigma_{s1}(E \leftarrow E') \mathcal{J}(E') \end{aligned}$$

(14)

where we used the following identities:

$$\boldsymbol{\Omega} \otimes \boldsymbol{\Omega} = \begin{bmatrix} \Omega_x^2 & \Omega_x \Omega_y & \Omega_x \Omega_z \\ \Omega_x \Omega_y & \Omega_y^2 & \Omega_y \Omega_z \\ \Omega_x \Omega_z & \Omega_y \Omega_z & \Omega_z^2 \end{bmatrix}$$

$$\frac{1}{4\pi} \int_{4\pi} d^2\Omega \frac{\Sigma^2}{\Sigma^2 + (\mathbf{B} \cdot \boldsymbol{\Omega})^2} = \alpha(B, \Sigma) \Sigma \quad \text{and} \quad \frac{1}{4\pi} \int_{4\pi} d^2\Omega \frac{(\boldsymbol{\Omega} \otimes \boldsymbol{\Omega}) \cdot \mathbf{B}}{\Sigma^2 + (\mathbf{B} \cdot \boldsymbol{\Omega})^2} = \beta(B, \Sigma) \mathbf{B} .$$

The functions $\alpha(B, \Sigma)$ and $\beta(B, \Sigma)$ are defined as

$$(15) \quad \alpha(B, \Sigma) = \begin{cases} \frac{1}{B} \tan^{-1} \frac{B}{\Sigma} & \text{if } B^2 > 0; \\ \frac{1}{\Sigma} - \frac{B^2}{3\Sigma^3} + \frac{B^4}{5\Sigma^5} - \frac{B^6}{7\Sigma^7} + \dots & \text{if } B^2 \simeq 0; \\ \frac{1}{2\Im(B)} \ln \frac{\Sigma + \Im(B)}{\Sigma - \Im(B)} & \text{if } B^2 < 0. \end{cases}$$

where $\Im(B)$ is the imaginary component of B and

$$(16) \quad \beta(B, \Sigma) = \frac{1}{B^2} [1 - \alpha(B, \Sigma) \Sigma] .$$

$$(12) \quad \Sigma(E) \varphi(E) + iB \mathcal{J}(E) = \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E') \varphi(E') + \frac{\chi(E)}{K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E')$$

The second B_1 equation is finally obtained by substituting Eq. (12) into Eq. (14):

$$(17) \quad \frac{i\mathcal{J}(E)}{B} = \frac{1}{\Sigma(E) \gamma[B, \Sigma(E)]} \left\{ \frac{1}{3} \varphi(E) + \int_0^\infty dE' \Sigma_{s1}(E \leftarrow E') \frac{i\mathcal{J}(E')}{B} \right\}$$

where

$$(18) \quad \gamma(B, \Sigma) = \frac{1}{3\Sigma} \frac{\alpha(B, \Sigma)}{\beta(B, \Sigma)} \simeq 1 + \frac{4}{15} \left(\frac{B}{\Sigma} \right)^2 - \frac{12}{175} \left(\frac{B}{\Sigma} \right)^4 + \frac{92}{2625} \left(\frac{B}{\Sigma} \right)^6 + \dots$$

- Equations (12) and (17) form the coupled set of the two B_1 equations.
- We did assume linearly anisotropic scattering in the LAB, but no Ω -expansion of the angular fundamental flux was required.
- In homogeneous cases, the quantity $i\mathcal{J}(E)/B$ is always real and remains finite when the buckling approaches zero.

- This system can be solved using a multigroup discretization, taking care to use a sufficiently large number of energy groups to ensure that $\langle \gamma(B, \Sigma) \rangle_g \simeq \gamma(B, \Sigma_g)$.
- These equations are also used to find the **critical buckling**, i.e., the value of B^2 that will lead to an **effective multiplication factor** K_{eff} equal to one.
- The **inconsistent** B_1 (or inconsistent P_1) form of the homogeneous leakage model is obtained by assuming the **micro-reversibility principle**

$$(19) \quad \Sigma_{s1}(E \leftarrow E') \frac{i\mathcal{J}(E')}{B} = \Sigma_{s1}(E' \leftarrow E) \frac{i\mathcal{J}(E)}{B}$$

in Eq. (17).

- The inconsistent approximation should generally be avoided if epithermal neutrons are present because it leads to the **outscatter approximation** which is not valid at high energy.

The **leakage coefficient** is defined as

$$(20) \quad d(B, E) = \frac{1}{B} \frac{i\mathcal{J}(E)}{\varphi(E)}$$

and used as a change of variable relation to transform Eqs. (12) and (17). A new set of B_1 equations are then obtained:

$$(21) \quad \begin{aligned} [\Sigma(E) + d(B, E) B^2] \varphi(E) &= \int_0^\infty dE' \Sigma_{s0}(E \leftarrow E') \varphi(E') \\ &+ \frac{\chi(E)}{K_{\text{eff}}} \int_0^\infty dE' \nu(E') \Sigma_f(E') \varphi(E') \end{aligned}$$

and

$$(22) \quad d(B, E) = \frac{1}{3\gamma[B, \Sigma(E)] \Sigma(E)} \left\{ 1 + 3 \int_0^\infty dE' \Sigma_{s1}(E \leftarrow E') d(B, E') \frac{\varphi(E')}{\varphi(E)} \right\} .$$

The leakage coefficient




Equation (21) can be easily condensed over any energy group structure if we introduce

$$(23) \quad \varphi_g = \int_{E_g}^{E_{g-1}} dE \varphi(E) \quad ,$$

$$(24) \quad d_g = \frac{1}{\varphi_g} \int_{E_g}^{E_{g-1}} dE d(B, E) \varphi(E) \quad \text{and} \quad \Sigma_g = \frac{1}{\varphi_g} \int_{E_g}^{E_{g-1}} dE \Sigma(E) \varphi(E) \quad .$$

The group-dependent leakage rate L_g appears naturally as

$$(25) \quad L_g = d_g B^2 \bar{\varphi}_g \quad .$$

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 The principle behind an homogeneous leakage model is to modify the heterogeneous flux equation with an additional term defined in such a way to force the homogeneous leakage rate of Eq. (25).
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 With this correction, the volume average of the heterogeneous flux $\bar{\phi}_g$ is equal to the fundamental flux φ_g of the homogeneous B_1 model.
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 This approach can be applied to all deterministic solution techniques of the neutron transport equation.

The collision probability technique is based on a multigroup discretization and allow the calculation of the neutron flux into the heterogeneous regions of the cell or of the assembly.

The flux is given by the relation

$$(26) \quad \phi_{i,g} = \sum_j Q_{j,g} \tilde{p}_{ij,g}$$

where

$\phi_{i,g}$ = neutron flux in region g and region i

$Q_{j,g}$ = isotropic scattering (in LAB) and fission neutron source

$\Sigma_{i,g}$ = macroscopic total cross section

$\tilde{p}_{ij,g}$ = reduced collision probability. $\tilde{p}_{ij,g} \Sigma_{j,g}$ is the probability for a neutron born uniformly and isotropically in region i to undergo its first collision in region j .

In order to reach a faster convergence, the within-group scattering term is removed from the source term:

$$(27) \quad \phi_{i,g} - \sum_j p_{ij,g} \Sigma_{s0,j,g \leftarrow g} \phi_{j,g} = \sum_j Q_{j,g}^* \tilde{p}_{ij,g}$$

where the source term $Q_{i,g}^*$ does not include the contributions from the within-group scattering rates in group g .

The modified source term is written as

$$(28) \quad Q_{i,g}^* = \sum_{h \neq g} \Sigma_{s0,i,g \leftarrow h} \phi_{i,h} + \frac{1}{K_{\text{eff}}} Q_{i,g}^{\text{fiss}}$$

where

$\Sigma_{s0,i,g \leftarrow h}$ = macroscopic transfer cross section for the scattering reaction

$Q_{i,g}^{\text{fiss}}$ = source of secondary neutrons from fission.

Equation (27) can be written in matrix form as

$$(29) \quad \Phi_g = \mathbb{W}_g \mathbf{Q}_g^*$$

where $\Phi_g = \{\phi_{i,g} ; \forall i\}$ and $\mathbf{Q}_g^* = \{Q_{i,g}^* ; \forall i\}$.

\mathbb{W}_g is a scattering reduced collision probability matrix, defined as

$$(30) \quad \mathbb{W}_g = [\mathbb{I} - \mathbb{P}_g \mathbb{S}_{s0,g \leftarrow g}]^{-1} \mathbb{P}_g$$

where \mathbb{I} is the identity matrix, $\mathbb{P}_g = \{p_{ij,g} ; \forall i \text{ et } j\}$ and $\mathbb{S}_{s0,g \leftarrow g} = \text{diag}\{\Sigma_{s0,i,g \leftarrow g} ; \forall i\}$.

Group-dependent leakage coefficients $d_g(B)$ and leakage rates $d_g(B) B^2$ can be obtained as described previously. Leakage rates can be included in Eq. (28) in many different ways:

1. By subtracting $d_g(B) B^2$ from the within-group scattering cross sections. Eq. (29) is then replaced by $\Phi_g = \mathbb{W}_g [\mathbf{Q}_g^* - d_g(B) B^2 \Phi_g]$ where transport-corrected total cross sections are used to compute the \mathbb{W}_g matrix. The iterative strategy of the power method is simplified as

$$(31) \quad \Phi_g^{(k+1)} = \mathbb{W}_g \left[\mathbf{Q}_g^{*(k)} - d_g^{(k)}(B) (B^{(k)})^2 \Phi_g^{(k)} \right]$$

where k is the outer iteration index.

2. By multiplying each element of the \mathbb{P}_g matrix by a non-leakage probability $P_{\text{NL},g}$. This non-leakage probability is computed in term of $\bar{\Sigma}_{0,g}$, the average transport-corrected macroscopic total cross section in group g . Eq. (29) is then replaced by

$$(32) \quad \Phi_g^{(k+1)} = \mathbb{W}_g \left[P_{\text{NL},g}^{(k)} \mathbf{Q}_g^{*(k)} - (1 - P_{\text{NL},g}^{(k)}) \mathbb{S}_{s0,g \leftarrow g} \Phi_g^{(k)} \right]$$

where $\mathbb{S}_{s0,g \leftarrow g} = \text{diag}\{\Sigma_{s0,i,g \leftarrow g} ; \forall i\}$ and the total cross sections used to compute the \mathbb{W}_g matrix are also transport-corrected.