The neutron flux – part 1

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Content (week 6)

- Definition of neutron flux and current
  - Spherical harmonics expansion of the neutron flux
  - The Fick law
- Derivation of the transport equation
  - The characteristics form
  - The integral form
- Boundary and continuity conditions

The particle flux

We use an approach of statistical mechanics in which each particle is moving in a six-dimensional phase space made of three position and three velocity coordinate axes. The position of a single particle is identified by a set of seven quantities:

- three position coordinates $\boldsymbol{r} = x\,\boldsymbol{i} + y\,\boldsymbol{j} + z\,\boldsymbol{k}$;
- three velocity coordinates. We use the velocity module $V_{\rm n} \equiv |\boldsymbol{V}_{\rm n}|$ with $\boldsymbol{V}_{\rm n} = d\boldsymbol{r}/dt$ and the two components of the direction $\boldsymbol{\Omega} \equiv \boldsymbol{V}_{\rm n}/V_{\rm n}$;
- the time t, used in transient situations, when the steady-state hypothesis is not valid.

A population of particles is represented by the population density $n(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)$ such that:

> $n(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)\, d^3r\, dV_{\rm n}\, d^2\Omega$ is the number of particles, at time t, in the volume element d^3r surrounding point $\boldsymbol{r}$, in the velocity element $dV_{\rm n}$ surrounding $V_{\rm n}$, and in the solid angle element $d^2\Omega$ surrounding $\boldsymbol{\Omega}$.

We note that $n(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)$ is a distribution with respect to variables $\boldsymbol{r}$, $V_{\rm n}$ and $\boldsymbol{\Omega}$. It is a function with respect to t.

The dependent variable used in reactor physics is the particle flux. The angular flux is a distribution, related to the population density, and defined as

$$\phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) \equiv V_{\rm n}\, n(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) \quad . \tag{1}$$

The particle flux

The angular flux defined in Eq(1) gives the maximum information about the population of particles. In many applications a more global representation is preferred. The integrated flux is obtained by performing a distribution reduction on variable $\boldsymbol{\Omega}$:

(2) $$\phi(\boldsymbol{r}, V_\mathrm{n}, t) = \int_{4\pi} d^2\Omega \, \phi(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t)$$

where we have used the same symbol to represent the two distributions.

The integrated flux is the total distance travelled in one second by all the particles in the one cm^3 volume

as it is obtained by multiplying the number of particles in that cm^3 by the speed of each one. This is equivalent to the total length of all the particle tracks laid down in one cm^3 in one second.

The integrated flux may be written with the particle energy E or lethargy u as independent variable, in replacement of V_n. Change of variables leads to

(3) $$E = \frac{1}{2} m \, V_\mathrm{n}^2 \quad \text{and} \quad u = \ln \frac{E_0}{E} \quad ,$$

The particle flux

where m is the mass of a particle and E_0 is the maximum energy of a particle, so that

(4) $$\phi(\boldsymbol{r}, E, t) = \frac{1}{m\,V_{\rm n}}\,\phi(\boldsymbol{r}, V_{\rm n}, t)\ , \quad 0 < E \le E_0$$

and

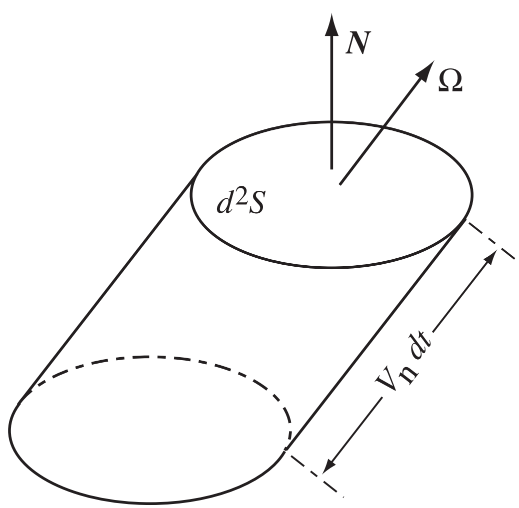
(5) $$\phi(\boldsymbol{r}, u, t) = E\,\phi(\boldsymbol{r}, E, t)\ , \quad 0 \le u < \infty \ .$$

The particle current

We have represented in figure an element of surface d^2S with a unit normal vector $\boldsymbol{N}$ located on point $\boldsymbol{r}$. The number d^3n of particles, of velocity $V_{\rm n}$ and direction $\boldsymbol{\Omega}$, crossing d^2S during an element of time dt is equal to the number of particles located in the represented slanted cylinder in figure.

This number is

$$d^3n = n(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)\left[d^2S\,(V_{\rm n}\,dt)\,\boldsymbol{\Omega}\cdot\boldsymbol{N}\right] \quad .$$



The angular current $\boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)$ is a vector defined in such a way that

$$\frac{d^3n}{d^2S\,dt} = \boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)\cdot\boldsymbol{N}$$

so that

$$\boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) = \boldsymbol{\Omega}\,\phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) \quad . \tag{6}$$

The particle current

We can define the integrated current as

(7) $$\boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, t) = \int_{4\pi} d^2\Omega \, \boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) = \int_{4\pi} d^2\Omega \, \boldsymbol{\Omega} \, \phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) \ .$$

The angular current is positive if the particle crosses d^2S in the direction of $\boldsymbol{N}$, and negative otherwise. We can also define the outgoing current J^+ and incoming current J^- by integrating the angular current over outgoing and incoming directions, respectively. We write

(8) $$J^+(\boldsymbol{r}, V_{\rm n}, t) = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{N}>0} d^2\Omega \ (\boldsymbol{\Omega}\cdot\boldsymbol{N}) \, \phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)$$

and

(9) $$J^-(\boldsymbol{r}, V_{\rm n}, t) = -\int_{\boldsymbol{\Omega}\cdot\boldsymbol{N}<0} d^2\Omega \ (\boldsymbol{\Omega}\cdot\boldsymbol{N}) \, \phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)$$

so that

(10) $$\boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, t) \cdot \boldsymbol{N} = J^+(\boldsymbol{r}, V_{\rm n}, t) - J^-(\boldsymbol{r}, V_{\rm n}, t) \ .$$

Spherical harmonics expansion

A frequently used approximation consists to develop the angular flux in spherical harmonics. We are using the standard closure condition, assuming that the $(L+1)$–th Legendre coefficients of the angular flux are zero, at all spatial points.

$$\phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi} \sum_{m=-\ell}^{\ell} \phi_\ell^m(\boldsymbol{r}, V_{\rm n}, t)\, R_\ell^m(\boldsymbol{\Omega}) \tag{11}$$

where $R_\ell^m(\boldsymbol{\Omega})$ are the real spherical harmonics. The summation over index ℓ in Eq. (11) corresponds to the more general case of a three-dimensional (3D) geometry.

- In one-dimensional (1D) slab and spherical geometries, only the $m=0$ value is required, due to symmetry reasons.
- In 1D cylindrical geometry, only $0 \le m \le \ell$ values with $m+\ell$ even are required.
- In 2D geometries defined in the $x-y$ plane, only even $m+\ell$ values are required.

Spherical harmonics expansion

There are important relations between the spherical harmonic moments of the angular flux and the integrated flux and current values. We can show that

$$\phi(\boldsymbol{r}, V_\mathrm{n}, t) = \phi_0^0(\boldsymbol{r}, V_\mathrm{n}, t) \tag{12}$$

and that

$$\boldsymbol{J}(\boldsymbol{r}, V_\mathrm{n}, t) = \phi_1^0(\boldsymbol{r}, V_\mathrm{n}, t)\, \boldsymbol{i} + \phi_1^1(\boldsymbol{r}, V_\mathrm{n}, t)\, \boldsymbol{j} + \phi_1^{-1}(\boldsymbol{r}, V_\mathrm{n}, t)\, \boldsymbol{k} \ \ . \tag{13}$$

Equation (11) can be truncated after the $\ell = 1$ component, leading to the linearly anisotropic flux approximation. We write:

$$\begin{aligned} \phi(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t) &= \frac{1}{4\pi} \left[\phi_0^0(\boldsymbol{r}, V_\mathrm{n}, t) + 3 \sum_{m=-1}^{1} \phi_1^m(\boldsymbol{r}, V_\mathrm{n}, t)\, R_1^m(\boldsymbol{\Omega}) \right] \\ &= \frac{1}{4\pi} \left[\phi(\boldsymbol{r}, V_\mathrm{n}, t) + 3\, \boldsymbol{\Omega} \cdot \boldsymbol{J}(\boldsymbol{r}, V_\mathrm{n}, t) \right] \ \ . \end{aligned} \tag{14}$$

Spherical harmonics expansion

Analytical expressions for $J^+(\boldsymbol{r}, V_\mathrm{n}, t)$ and $J^-(\boldsymbol{r}, V_\mathrm{n}, t)$ can be found in the special case of the linearly anisotropic flux approximation. We substitute Eq. (14) into Eq. (8) and set $\boldsymbol{N} = \boldsymbol{i}$ with $\boldsymbol{\Omega} = \mu\, \boldsymbol{i} + \sqrt{1-\mu^2}\, \cos\omega\, \boldsymbol{j} + \sqrt{1-\mu^2}\, \sin\omega\, \boldsymbol{k}$, so that

$$\begin{aligned}
J^+(\boldsymbol{r}, V_\mathrm{n}, t) &= \frac{1}{4\pi} \int_{\boldsymbol{\Omega}\cdot\boldsymbol{N}>0} d^2\Omega\ (\boldsymbol{\Omega}\cdot\boldsymbol{N}) \left[\phi(\boldsymbol{r}, V_\mathrm{n}, t) + 3\, \boldsymbol{\Omega}\cdot\boldsymbol{J}(\boldsymbol{r}, V_\mathrm{n}, t)\right] \\
&= \frac{1}{4\pi} \int_0^1 d\mu\, \mu \int_0^{2\pi} d\omega \Big[\phi(\boldsymbol{r}, V_\mathrm{n}, t) + 3\mu\, J_x(\boldsymbol{r}, V_\mathrm{n}, t) \\
&\quad + 3\sqrt{1-\mu^2}\, \cos\omega\, J_y(\boldsymbol{r}, V_\mathrm{n}, t) \\
&\quad + 3\sqrt{1-\mu^2}\, \sin\omega\, J_z(\boldsymbol{r}, V_\mathrm{n}, t) \Big] \\
&= \frac{1}{4}\, \phi(\boldsymbol{r}, V_\mathrm{n}, t) + \frac{1}{2}\, \boldsymbol{J}(\boldsymbol{r}, V_\mathrm{n}, t)\cdot\boldsymbol{N} \ .
\end{aligned}$$

Similarly, we can show that

(15)
$$J^-(\boldsymbol{r}, V_\mathrm{n}, t) = \frac{1}{4}\, \phi(\boldsymbol{r}, V_\mathrm{n}, t) - \frac{1}{2}\, \boldsymbol{J}(\boldsymbol{r}, V_\mathrm{n}, t)\cdot\boldsymbol{N}$$

The Fick law

The Fick law is an approximation relating the integrated flux with the integrated current:

$$\boldsymbol{J}(\boldsymbol{r}, V_{\rm n}, t) = -D(\boldsymbol{r}, V_{\rm n})\boldsymbol{\nabla}\phi(\boldsymbol{r}, V_{\rm n}, t)$$

where $D(\boldsymbol{r}, V_{\rm n})$ is the diffusion coefficient. It is used in the context of the diffusion approximation. It is computed by the lattice code.

In some applications with anisotropic streaming, the diffusion coefficient $D(\boldsymbol{r}, V_{\rm n})$ can be replaced by a 3×3 diagonal tensor $\mathbb{D}(\boldsymbol{r}, V_{\rm n})$ containing directional diffusion coefficients. These applications are not usual.

The Fick law is not a fundamental relation.

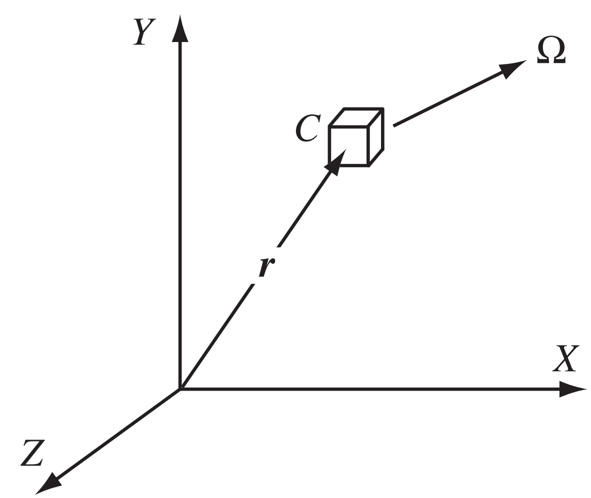
Derivation of the transport equation 1

The absence of particle-particle interactions produces a linear form of the Boltzmann equation. The transport equation is obtained as the phase-space balance relation for the neutral particles located in a control volume.

We first define a control volume C, surrounded by surface ∂C, as illustrated in figure. We consider the particles located in C travelling in direction $\boldsymbol{\Omega}$ (within a $d^2\Omega$ interval), with a velocity equal to $V_{\rm n}$ (within a $dV_{\rm n}$ interval). [a] The number of such particles, initially equal to

$$\int_C d^3r\, n(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)\, dV_{\rm n}\, d^2\Omega$$

is going to change during a small period of time Δt.



[a] The reader should not confuse d^3r, the elemental volume with $d\boldsymbol{r} = \boldsymbol{r}' - \boldsymbol{r}$.

Derivation of the transport equation 2

We define the following quantities:

- the rate of change of particles in V during Δt is

(16) $$d^3\mathcal{A} = \int_C d^3r \, [n(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t + \Delta t) - n(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t)] \, dV_\mathrm{n} \, d^2\Omega \ ;$$

- the net number of particles streaming out of V during Δt is obtained by integrating the particle current over ∂C as

(17) $$d^3\mathcal{B} = \int_{\partial C} d^2r \, (\boldsymbol{\Omega} \cdot \boldsymbol{N}) \, \phi(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t) \, dV_\mathrm{n} \, d^2\Omega \, \Delta t$$

where $\boldsymbol{N}$ is the unit vector, normal to ∂C, and pointing outside ∂C at point $\boldsymbol{r}$. We now use the divergence theorem to transform Eq. (17) into

(18) $$d^3\mathcal{B} = \int_C d^3r \, \boldsymbol{\nabla} \cdot \boldsymbol{\Omega} \, \phi(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t) \, dV_\mathrm{n} \, d^2\Omega \, \Delta t$$

Derivation of the transport equation 3

- the number of collisions in d^3r during Δt is

(19) $$d^3\mathcal{C} = \int_C d^3r\, \Sigma(\boldsymbol{r}, V_\mathrm{n})\ [V_\mathrm{n}\, n(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t)]\, dV_\mathrm{n}\, d^2\Omega\, \Delta t$$

  where we assume that the macroscopic total cross section Σ is independent of $\boldsymbol{\Omega}$ and t. The independence of cross sections with t is generally not valid and is introduced here to simplify the notation.

- the number of new particles created in d^3r during Δt is

(20) $$d^3\mathcal{D} = \int_C d^3r\, Q(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t)\, dV_\mathrm{n}\, d^2\Omega\, \Delta t$$

  where $Q(\boldsymbol{r}, V_\mathrm{n}, \boldsymbol{\Omega}, t)$ is the source density.

The particle balance is written

(21) $$d^3\mathcal{A} = -d^3\mathcal{B} - d^3\mathcal{C} + d^3\mathcal{D}$$

Derivation of the transport equation 4

so that the integral over the control volume can be discarded from the four terms, leading to

$$\frac{n(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t+\Delta t)-n(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t)}{\Delta t} = -\boldsymbol{\nabla}\cdot\boldsymbol{\Omega}\,\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) - \Sigma(\boldsymbol{r},V_{\rm n})\,[V_{\rm n}\,n(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t)] + Q(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) \ .$$

Taking the limit as $\Delta t \to 0$ and introducing the angular flux as dependent variable, we obtain the differential form of the transport equation:

$$\frac{1}{V_{\rm n}}\frac{\partial}{\partial t}\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) + \boldsymbol{\nabla}\cdot\boldsymbol{\Omega}\,\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) + \Sigma(\boldsymbol{r},V_{\rm n})\,\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) = Q(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) \ .$$

Using the identity $\boldsymbol{\nabla}\cdot\boldsymbol{w}\,f(\boldsymbol{r}) = \boldsymbol{w}\cdot\boldsymbol{\nabla} f(\boldsymbol{r})$, this equation can be rewritten as

$$\frac{1}{V_{\rm n}}\frac{\partial}{\partial t}\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) + \Sigma(\boldsymbol{r},V_{\rm n})\,\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) = Q(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega},t) \ .$$

In steady-state conditions, this equation reduces to

(22) $$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega}) + \Sigma(\boldsymbol{r},V_{\rm n})\,\phi(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega}) = Q(\boldsymbol{r},V_{\rm n},\boldsymbol{\Omega}) \ .$$

Derivation of the transport equation 5

We finally note that the source density can be written in a spherical harmonic expansion:

$$Q(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi} \sum_{m=-\ell}^{\ell} Q_\ell^m(\boldsymbol{r}, V_{\rm n}, t)\, R_\ell^m(\boldsymbol{\Omega}) \tag{23}$$

where the value of L is smaller or equal to the value used to expand the angular flux.

The characteristics form 1

- The characteristics form of the transport equation corresponds to an integration of the streaming operator $\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi$ over the characteristics, a straight line of direction $\boldsymbol{\Omega}$.
- At each time of its motion, the particle is assumed to be at distance s from a reference position $\boldsymbol{r}$ on its characteristics, so that its actual position is $\boldsymbol{r} + s\,\boldsymbol{\Omega}$.

The streaming operator can be transformed using the chain rule. We first write

(24) $$\frac{d}{ds} = \frac{\partial}{\partial x}\frac{dx}{ds} + \frac{\partial}{\partial y}\frac{dy}{ds} + \frac{\partial}{\partial z}\frac{dz}{ds} \quad \text{with} \quad ds\,\boldsymbol{\Omega} = d\boldsymbol{r} = dx\,\boldsymbol{i} + dy\,\boldsymbol{j} + dz\,\boldsymbol{k} \ .$$

Taking the dot product with $\boldsymbol{i}$, we obtain $ds\,\boldsymbol{\Omega} \cdot \boldsymbol{i} = dx$. Similarly, $ds\,\boldsymbol{\Omega} \cdot \boldsymbol{j} = dy$ and $ds\,\boldsymbol{\Omega} \cdot \boldsymbol{k} = dz$. After substitution in Eq. (24), we obtain

(25) $$\frac{d}{ds} = (\boldsymbol{\Omega} \cdot \boldsymbol{i})\,\frac{\partial}{\partial x} + (\boldsymbol{\Omega} \cdot \boldsymbol{j})\,\frac{\partial}{\partial y} + (\boldsymbol{\Omega} \cdot \boldsymbol{k})\,\frac{\partial}{\partial z} = \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \ .$$

Substituting Eq. (25) into the (steady-state) differential form, we obtain the backward characteristics form:

(26) $$\frac{d}{ds}\phi(\boldsymbol{r} + s\,\boldsymbol{\Omega}, V_{\rm n}, \boldsymbol{\Omega}) \ + \ \Sigma(\boldsymbol{r} + s\,\boldsymbol{\Omega}, V_{\rm n})\,\phi(\boldsymbol{r} + s\,\boldsymbol{\Omega}, V_{\rm n}, \boldsymbol{\Omega}) = Q(\boldsymbol{r} + s\,\boldsymbol{\Omega}, V_{\rm n}, \boldsymbol{\Omega}) \ .$$

The integral form

We first introduce an integrating factor $\mathrm{e}^{-\tau(s,\,V_\mathrm{n})}$ where the optical path is defined as a function of the macroscopic total cross section $\Sigma(\boldsymbol{r}, V_\mathrm{n})$ using

(27) $$\tau(s, V_\mathrm{n}) = \int_0^s ds' \, \Sigma(\boldsymbol{r} - s' \, \boldsymbol{\Omega}, V_\mathrm{n}) \quad .$$

We next compute the following relation:

(28) $$\begin{aligned} \frac{d}{ds}\left[\mathrm{e}^{-\tau(s,V_\mathrm{n})}\,\phi(\boldsymbol{r} - s\boldsymbol{\Omega}, V_\mathrm{n}, \boldsymbol{\Omega})\right] \;&=\; \mathrm{e}^{-\tau(s,V_\mathrm{n})}\Big[-\Sigma(\boldsymbol{r} - s\boldsymbol{\Omega}, V_\mathrm{n})\,\phi(\boldsymbol{r} - s\boldsymbol{\Omega}, V_\mathrm{n}, \boldsymbol{\Omega}) \\ &\quad + \frac{d}{ds}\phi(\boldsymbol{r} - s\boldsymbol{\Omega}, V_\mathrm{n}, \boldsymbol{\Omega})\Big] \end{aligned}$$

where we used the identity $\frac{d}{ds}\int_0^s ds' \, g(s') = g(s)$.

Substitution of the forward characteristics form into Eq. (28) leads to

(29) $$-\frac{d}{ds}\left[\mathrm{e}^{-\tau(s,V_\mathrm{n})}\,\phi(\boldsymbol{r} - s\boldsymbol{\Omega}, V_\mathrm{n}, \boldsymbol{\Omega})\right] \;=\; \mathrm{e}^{-\tau(s,V_\mathrm{n})}\,Q(\boldsymbol{r} - s\boldsymbol{\Omega}, V_\mathrm{n}, \boldsymbol{\Omega}) \quad .$$

The integral form

Equation (29) can be integrated between 0 and ∞, so that

(30) $$-\int_0^\infty ds\, \frac{d}{ds}\left[\mathrm{e}^{-\tau(s,V_\mathrm{n})}\,\phi(\boldsymbol{r}-s\boldsymbol{\Omega},V_\mathrm{n},\boldsymbol{\Omega})\right] = \int_0^\infty ds\,\mathrm{e}^{-\tau(s,V_\mathrm{n})}\,Q(\boldsymbol{r}-s\boldsymbol{\Omega},V_\mathrm{n},\boldsymbol{\Omega})$$

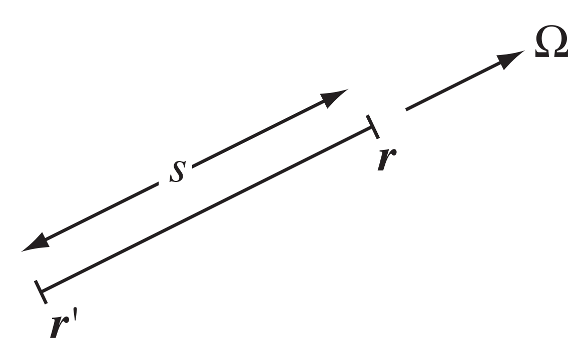
or

(31) $$\phi(\boldsymbol{r},V_\mathrm{n},\boldsymbol{\Omega}) = \int_0^\infty ds\ \mathrm{e}^{-\tau(s,V_\mathrm{n})}\ Q(\boldsymbol{r}-s\,\boldsymbol{\Omega},V_\mathrm{n},\boldsymbol{\Omega}) \ .$$

This form of the transport equation is generally limited to isotropic sources in the LAB:

(32) $$Q(\boldsymbol{r},V_\mathrm{n},\boldsymbol{\Omega}) = \frac{1}{4\pi}\,Q(\boldsymbol{r},V_\mathrm{n}) \ .$$

Equation (31) is the integral form of the transport equation for the infinite-domain case. A particle from source $Q(\boldsymbol{r}',V_\mathrm{n},\boldsymbol{\Omega})$ will travel with an exponential attenuation factor in direction $\boldsymbol{\Omega}$ and contribute to the flux at point $\boldsymbol{r}$.



Boundary and continuity conditions 1

The domain V where the particles move may be surrounded by a boundary ∂V where boundary conditions are imposed. We also introduce $\boldsymbol{N}(\boldsymbol{r}_{\rm s})$, the outward normal at $\boldsymbol{r}_{\rm s} \in \partial V$. Solution of the transport equation in V requires the knowledge of the angular flux $\phi(\boldsymbol{r}_{\rm s}, V_{\rm n}, \boldsymbol{\Omega}, t)$ for $\boldsymbol{\Omega} \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s}) < 0$.

- The albedo boundary condition is used to relate the incoming flux with the known outgoing flux. This condition is written

  (33) $$\phi(\boldsymbol{r}_{\rm s}, V_{\rm n}, \boldsymbol{\Omega}) = \beta\, \phi(\boldsymbol{r}_{\rm s}, V_{\rm n}, \boldsymbol{\Omega}') \;\; \text{with} \;\; \boldsymbol{\Omega} \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s}) < 0$$

  where $\boldsymbol{\Omega}'$ is the direction of the outgoing particle. The albedo β is equal to zero and one for a vacuum and reflective boundary condition, respectively. Intermediate values can also be used. Specular reflection corresponds to the case where

  (34) $$\boldsymbol{\Omega} \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s}) = -\boldsymbol{\Omega}' \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s}) \;\; \text{and} \;\; (\boldsymbol{\Omega} \times \boldsymbol{\Omega}') \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s}) = 0 \;\; .$$

Boundary and continuity conditions 2

- The white boundary condition is a reflective condition where all particles leaving V return back in V with an isotropic angular distribution:

(35) $$\phi(\boldsymbol{r}_{\rm s}, V_{\rm n}, \boldsymbol{\Omega}) = \frac{1}{\pi} \int_{\boldsymbol{\Omega}' \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s})>0} d^2\Omega' \, \left[\boldsymbol{\Omega}' \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s})\right] \phi(\boldsymbol{r}_{\rm s}, V_{\rm n}, \boldsymbol{\Omega}')$$

with $\boldsymbol{\Omega} \cdot \boldsymbol{N}(\boldsymbol{r}_{\rm s}) < 0$.

- The periodic boundary condition corresponds to the case where the flux on one boundary is equal to the flux on another parallel boundary in a periodic lattice grid:

(36) $$\phi(\boldsymbol{r}_{\rm s}, V_{\rm n}, \boldsymbol{\Omega}, t) = \phi(\boldsymbol{r}_{\rm s} + \Delta\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t) \quad \text{where } \Delta\boldsymbol{r} \text{ is the lattice pitch.}$$

- The zero-flux boundary condition corresponds to the absence of particles on ∂V. This condition is non-physical as particles are continuously leaving the domain V, producing a non-zero number density on ∂V. The vacuum boundary condition must always be preferred to represent an external boundary.

Inside V, the angular flux $\phi(\boldsymbol{r}, V_{\rm n}, \boldsymbol{\Omega}, t)$ must be continuous across all internal interfaces in the direction $\boldsymbol{\Omega}$ of the moving particle. The continuity condition is not required along directions which are not parallel to the path of travel.