

VI. ONE-GROUP DIFFUSION THEORY

References: Duderstadt & Hamilton Chapter 4

M. L. Adams, Reactor Theory Course Notes, Chapter 4

E. W. Larsen, Reactor Theory Course Notes, Chapter 4

L. Grossman, Nuclear Reactor Theory Course Notes

VI.1. Derivation of Diffusion Equation by P₁ Assumption

In order to derive somewhat simpler equation than the neutron transport equation, we will assume that the angular flux at a given position is almost the same in all directions, i.e., the angular flux depends weakly on $\underline{\Omega}$. Thus, *if* the angular flux depends weakly on $\underline{\Omega}$, then the diffusion equation is a good approximation to the transport equation.

The Balance Equation

We begin this derivation by recalling the one-group transport equation, assuming that the external source is isotropic:

(VI.1)

$$\begin{aligned} \frac{1}{v} \frac{\partial}{\partial t} \psi(\underline{r}, \underline{\Omega}, t) + \underline{\Omega} \cdot \nabla \psi(\underline{r}, \underline{\Omega}, t) + \Sigma_t(\underline{r}, t) \psi(\underline{r}, \underline{\Omega}, t) \\ = v \Sigma_f(\underline{r}, t) \phi(\underline{r}, t) \frac{1}{4\pi} + \int_{4\pi} d\Omega' \psi(\underline{r}, \underline{\Omega}', t) \Sigma_s(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega}, t) + \frac{1}{4\pi} S(\underline{r}, t) . \end{aligned}$$

We integrate this equation over all angle $\underline{\Omega}$, obtaining:

$$\begin{aligned} \frac{1}{v} \frac{\partial}{\partial t} \int_{4\pi} d\Omega \psi(\underline{r}, \underline{\Omega}, t) + \nabla \cdot \int_{4\pi} d\Omega \underline{\Omega} \psi(\underline{r}, \underline{\Omega}, t) + \Sigma_t(\underline{r}, t) \int_{4\pi} d\Omega \psi(\underline{r}, \underline{\Omega}, t) \\ = v \Sigma_f(\underline{r}, t) \phi(\underline{r}, t) + \left(\int_{4\pi} d\Omega' \psi(\underline{r}, \underline{\Omega}', t) \right) \left(\int_{4\pi} d\Omega \Sigma_s(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega}, t) \right) + S(\underline{r}, t) . \end{aligned}$$

We have used here the identity $\underline{\Omega} \cdot (\nabla f) = \nabla \cdot (\underline{\Omega} f)$, which is true because $\underline{\Omega}$ is not a function of position. [Note that $\nabla \cdot (\underline{\Omega} f) \equiv f (\nabla \cdot \underline{\Omega}) + \underline{\Omega} \cdot (\nabla f)$, and $\nabla \cdot \underline{\Omega} = 0$.]

Using the definitions of the scalar flux ϕ , the net current density \underline{J} , and the scattering cross section Σ_s , we can rewrite the last equation as:

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\underline{r}, t) + \nabla \cdot \underline{J}(\underline{r}, t) + \Sigma_t(\underline{r}, t) \phi(\underline{r}, t) = v \Sigma_f(\underline{r}, t) \phi(\underline{r}, t) + \Sigma_s(\underline{r}, t) \phi(\underline{r}, t) + S(\underline{r}, t) .$$

If we recognize that $\Sigma_a = \Sigma_t - \Sigma_s$ (and suppress the arguments \underline{r} and t), we have:

$$(VI.2)$$

$$\frac{1}{v} \frac{\partial}{\partial t} \phi + \nabla \cdot \underline{J} + \Sigma_a \phi = v \Sigma_f \phi + S .$$

This is commonly called the *neutron balance equation*. It is also called the “*0th-moment equation*” (because it is the 0th angular moment of the transport equation), and occasionally the “*neutron continuity equation*”. Equation (VI.2) states that the total number of neutrons must be preserved, what we can see if we integrate it over some spatial volume D :

$$\frac{1}{v} \frac{\partial}{\partial t} \int_D d^3r \phi + \int_D d^3r \nabla \cdot \underline{J} + \int_D d^3r \Sigma_a \phi = \int_D d^3r v \Sigma_f \phi + \int_D d^3r S .$$

We use the divergence theorem on the leakage term to obtain:

$$(VI.3)$$

$$\frac{1}{v} \frac{\partial}{\partial t} \int_D d^3r \phi + \int_{\partial D} d^3r \underline{n} \cdot \underline{J} + \int_D d^3r \Sigma_a \phi = \int_D d^3r v \Sigma_f \phi + \int_D d^3r S ,$$

which, basically, says:

$$\left[\begin{array}{c} \text{rate of} \\ \text{change of} \\ \text{neutrons in D} \end{array} \right] + \left[\begin{array}{c} \text{net} \\ \text{leakage rate} \\ \text{out of D} \end{array} \right] + \left[\begin{array}{c} \text{absorption} \\ \text{rate in D} \end{array} \right] = \left[\begin{array}{c} \text{production} \\ \text{rate from} \\ \text{fission in D} \end{array} \right] + \left[\begin{array}{c} \text{prod. rate} \\ \text{from external} \\ \text{source in D} \end{array} \right].$$

At this point we have made *no approximations* to the one-group transport equation — we have simply integrated it over angle. However, we have four unknown functions of position in our balance equation: $\phi(\underline{r})$, $J_x(\underline{r})$, $J_y(\underline{r})$, and $J_z(\underline{r})$. Thus, we need three more equations.

First-Moment Equation(s)

To obtain some more equations, we multiply the transport equation, Eq. (VI.1), by $\underline{\Omega}$ and then integrate over angle:

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} \int_{4\pi} d\Omega \underline{\Omega} \psi(\underline{r}, \underline{\Omega}, t) + \underline{\nabla} \cdot \int_{4\pi} d\Omega \underline{\Omega} \underline{\Omega} \psi(\underline{r}, \underline{\Omega}, t) + \Sigma_t(\underline{r}, t) \int_{4\pi} d\Omega \underline{\Omega} \psi(\underline{r}, \underline{\Omega}, t) \\ & = \left[v \Sigma_f(\underline{r}, t) \phi(\underline{r}, t) + S(\underline{r}, t) \right] \int_{4\pi} d\Omega \underline{\Omega} \frac{1}{4\pi} + \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}', t) \int_{4\pi} d\Omega \underline{\Omega} \Sigma_s(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega}, t) \right). \end{aligned}$$

(We have taken the “first angular moment” of the transport equation. Each term is a vector, so this is really three equations.) We can recognize some of the integrals, giving:

(VI.4)

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} \underline{J}(\underline{r}, t) + \underline{\nabla} \cdot \int_{4\pi} d\Omega \underline{\Omega} \underline{\Omega} \psi(\underline{r}, \underline{\Omega}, t) + \Sigma_t(\underline{r}, t) \underline{J}(\underline{r}, t) \\ & = \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}', t) \int_{4\pi} d\Omega \underline{\Omega} \Sigma_s(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega}, t) \right). \end{aligned}$$

We have not yet evaluated the scattering term. Let us consider one component, say the x-component, of this term:

$$\begin{aligned}
& \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}') \int_{4\pi} d\Omega \Omega_x \Sigma_s(\underline{r}, \underline{\Omega}' \cdot \underline{\Omega}) \right) \\
&= \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}') \sum_{k=0}^K \Sigma_{sk}(\underline{r}) \int_{4\pi} d\Omega \Omega_x P_k(\mu_0) \right) \\
&= \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}') \sum_{k=0}^K \Sigma_{sk}(\underline{r}) \int_{4\pi} d\Omega \Omega_x \sum_{m=-k}^k Y_{km}^*(\underline{\Omega}') Y_{km}(\underline{\Omega}) \right).
\end{aligned}$$

It is not difficult to show that

$$\begin{aligned}
\Omega_x = & \quad (VI.5) \\
& C_x \left(Y_{1,1}^*(\underline{\Omega}) + Y_{1,-1}^*(\underline{\Omega}) \right).
\end{aligned}$$

Thus,

$$\begin{aligned}
& \quad (VI.6) \\
& \int_{4\pi} d\Omega \Omega_x Y_{km}(\underline{\Omega}) = C_x \delta_{k1} (\delta_{m1} + \delta_{m,-1}),
\end{aligned}$$

and we have:

$$\begin{aligned}
& \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}', t) \int_{4\pi} d\Omega \underline{\Omega}_x \Sigma_s(\underline{r}, \underline{\Omega}' \cdot \underline{\Omega}, t) \right) \quad (\text{VI.7}) \\
&= \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}', t) \sum_{k=0}^K \Sigma_{sk}(\underline{r}, t) \sum_{m=-k}^k C_x Y_{km}^*(\underline{\Omega}') \delta_{k1} (\delta_{m1} + \delta_{m,-1}) \right) \\
&= \int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}', t) \Sigma_{s1}(\underline{r}, t) C_x \left(Y_{1,1}^*(\underline{\Omega}') + Y_{1,-1}^*(\underline{\Omega}') \right) \right) \\
&= \Sigma_{s1}(\underline{r}, t) \int_{4\pi} d\Omega' \underline{\Omega}'_x \psi(\underline{r}, \underline{\Omega}', t) \\
&= \Sigma_{s1}(\underline{r}, t) J_x(\underline{r}, t) .
\end{aligned}$$

The other components are similar. Thus, the scattering term is simply:

$$\int_{4\pi} d\Omega' \left(\psi(\underline{r}, \underline{\Omega}', t) \int_{4\pi} d\Omega \underline{\Omega} \Sigma_s(\underline{r}, \underline{\Omega}' \cdot \underline{\Omega}, t) \right) = \Sigma_{s1}(\underline{r}, t) \underline{J}(\underline{r}, t) . \quad (\text{VI.8})$$

We now define the *transport cross section*:

$$\Sigma_{tr}(\underline{r}) = \Sigma_t(\underline{r}) - \Sigma_{s1}(\underline{r}) . \quad (\text{VI.9})$$

If we collect what we have so far, we find that our first-moment equation is:

$$\frac{1}{v} \frac{\partial}{\partial t} \underline{J}(\underline{r}, t) + \underline{\nabla} \cdot \int_{4\pi} d\Omega \underline{\Omega} \underline{\Omega} \psi(\underline{r}, \underline{\Omega}, t) + \Sigma_{tr}(\underline{r}, t) \underline{J}(\underline{r}, t) = 0 . \quad (\text{VI.10})$$

We still have made *no approximations!* In order to obtain a closed system of equations (i.e., to keep the leakage term from introducing new unknowns other than ϕ and \underline{J}), we shall now make an approximation: **we assume that ψ varies at most linearly in angle:**

Assume: (VI.11)

$$\psi(\underline{r}, \underline{\Omega}, t) \approx a(\underline{r}, t) + b(\underline{r}, t) \Omega_x + c(\underline{r}, t) \Omega_y + d(\underline{r}, t) \Omega_z .$$

This is equivalent to an expansion in the spherical harmonics Y_{00} , $Y_{1,-1}$, Y_{10} , and Y_{11} ; thus, this is sometimes called a P_1 approximation. Another way to say it is that we are assuming ψ is *linearly anisotropic*. We can now express a, b, c, and d in terms of scalar flux ϕ and net current \underline{J} . Note:

$$(VI.12)$$

$$\phi = \int_{4\pi} d\Omega \psi = \int_{4\pi} d\Omega (a + b\Omega_x + c\Omega_y + d\Omega_z) = 4\pi a ;$$

$$\underline{J} = \int_{4\pi} d\Omega \underline{\Omega} \psi = \int_{4\pi} d\Omega \underline{\Omega} (a + b\Omega_x + c\Omega_y + d\Omega_z) = \frac{4\pi}{3} (b\underline{e}_x + c\underline{e}_y + d\underline{e}_z) .$$

We solve for a, b, c, and d, then insert the solutions into our assumption (VI.11) to obtain:

$$(VI.13)$$

$$\psi(\underline{r}, \underline{\Omega}, t) \approx \frac{1}{4\pi} (\phi(\underline{r}, t) + 3 \underline{\Omega} \cdot \underline{J}(\underline{r}, t)) .$$

We insert our *assumed* linearly anisotropic angular flux into the leakage term to obtain:

$$(VI.14)$$

$$\begin{aligned} \underline{\nabla} \cdot \int_{4\pi} d\Omega \underline{\Omega} \underline{\Omega} \left(\frac{1}{4\pi} [\phi(\underline{r}, t) + 3 \underline{\Omega} \cdot \underline{J}(\underline{r}, t)] \right) &= \underline{\nabla} \cdot \int_{4\pi} d\Omega \underline{\Omega} \underline{\Omega} \left(\frac{1}{4\pi} \phi(\underline{r}, t) \right) \\ &= \underline{\nabla} \cdot \left(\frac{4\pi}{3} \underline{I} \right) \left(\frac{1}{4\pi} \phi(\underline{r}, t) \right) \\ &= \frac{1}{3} \underline{\nabla} \phi(\underline{r}, t) . \end{aligned}$$

Here we have used the notation \underline{I} to represent the *identity tensor*. If this is confusing, the

\underline{I}

following might be easier to digest (we use the x-component as an example):

(VI.15)

$$\begin{aligned}
& \underline{\nabla} \cdot \int_{4\pi} d\Omega \underline{\Omega}_x \underline{\Omega} \left(\frac{1}{4\pi} [\phi(\underline{r}, t) + 3 \underline{\Omega} \cdot \underline{\mathbf{J}}(\underline{r}, t)] \right) \\
&= \frac{1}{4\pi} \int_{4\pi} d\Omega \underline{\Omega}_x \underline{\Omega} \cdot [\underline{\nabla} \phi + 3 \underline{\nabla} (\underline{\Omega}_x J_x + \underline{\Omega}_y J_y + \underline{\Omega}_z J_z)] \\
&= \frac{1}{4\pi} \int_{4\pi} d\Omega \underline{\Omega}_x \left[\underline{\Omega}_x \frac{\partial \phi}{\partial x} + \underline{\Omega}_y \frac{\partial \phi}{\partial y} + \underline{\Omega}_z \frac{\partial \phi}{\partial z} + 3 \underline{\Omega} \cdot \underline{\nabla} (\underline{\Omega}_x J_x + \underline{\Omega}_y J_y + \underline{\Omega}_z J_z) \right] \\
&= \dots = \frac{1}{3} \frac{\partial \phi(\underline{r}, t)}{\partial x} .
\end{aligned}$$

Thus, under the assumption of a *linearly-anisotropic angular flux*, our system of equations is:

(VI.16)

$$\begin{aligned}
& \frac{1}{v} \frac{\partial}{\partial t} \phi(\underline{r}, t) + \underline{\nabla} \cdot \underline{\mathbf{J}}(\underline{r}, t) + \Sigma_a(\underline{r}, t) \phi(\underline{r}, t) = v \Sigma_f(\underline{r}, t) \phi(\underline{r}, t) + S(\underline{r}, t) , \\
& \frac{1}{v} \frac{\partial}{\partial t} \underline{\mathbf{J}}(\underline{r}, t) + \frac{1}{3} \underline{\nabla} \phi(\underline{r}, t) + \Sigma_{tr}(\underline{r}, t) \underline{\mathbf{J}}(\underline{r}, t) = 0 .
\end{aligned}$$

These are called the ***P₁ equations***, for they were obtained by assuming a P₁ angular flux. To obtain the diffusion equation from the P₁ system, we require one additional assumption:

Assume:(VI.17)

$$\frac{\partial}{\partial t} \underline{\mathbf{J}}(\underline{r}, t) = \text{negligible compared to } \frac{1}{3} \underline{\nabla} \phi(\underline{r}, t) .$$

Under this assumption, the first-moment equation yields the following expression for the net current density:

$$\mathbf{J}(\mathbf{r},t) = - \frac{1}{3\Sigma_{tr}(\mathbf{r},t)} \nabla\phi(\mathbf{r},t). \quad (\text{VI.18})$$

This is *Fick's Law*, which describes diffusion processes: the net current is proportional to the negative of the gradient of the concentration. The constant of proportionality is called the *diffusion coefficient*; in our case it is:

$$D(\mathbf{r},t)=\text{diffusion coefficient} = \frac{1}{3\Sigma_{tr}(\mathbf{r},t)}. \quad (\text{VI.19})$$

Finally, we can now eliminate the current from the balance equation to obtain a single diffusion equation for the scalar flux:

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\mathbf{r},t) - \nabla \cdot (D(\mathbf{r},t) \nabla \phi(\mathbf{r},t)) + \Sigma_a(\mathbf{r},t) \phi(\mathbf{r},t) = v\Sigma_f(\mathbf{r},t) \phi(\mathbf{r},t) + S(\mathbf{r},t). \quad (\text{VI.20})$$

Equation VI.20 is known as the *one-speed neutron diffusion equation*. To obtain this equation, we made two assumptions:

- 1) that ψ was a linear function of angle, and
- 2) that the time derivative of the current \ll the spatial derivative of scalar flux.

Note that our first assumption (and, thus, the diffusion equation) is not valid in the following cases:

- 1) near boundaries or where material properties change dramatically over the distance of several mean free paths,
- 2) near localized sources, and
- 3) in strongly absorbing media.

VI.1.1 Initial Conditions for the One-Group Diffusion Equation

The diffusion equation (Eq. VI.20) is a linear second order partial differential equations of the parabolic type, that requires initial and boundary conditions. The initial condition for the diffusion equation is the same as the initial condition for the transport equation:

(VI.21)

$$\phi(\underline{r}, t)|_{t=0} = \int_{4\pi} d\Omega \psi(\underline{r}, \underline{\Omega}, t)|_{t=0} = \int_{4\pi} d\Omega I(\underline{r}, \underline{\Omega}) .$$

VI.1.2 Boundary Conditions for the One-Group Diffusion Equation

As was mentioned above, the diffusion equation is not valid near the boundaries. We ignore this and do our best to come up with the boundary conditions which will produce the proper flux distribution in the interior of the reactor, several mean free paths away from the reactor boundary. Let's first consider the interface conditions:

VI.1.3 Interface Conditions

The correct transport theory condition at the interface of two regions is

, for all $\underline{\Omega}$.

$$\psi_1(\underline{r}_s, \underline{\Omega}, t) = \psi_2(\underline{r}_s, \underline{\Omega}, t)$$

In the diffusion theory we cannot satisfy this boundary condition. The best we can do is to require that the first two angular flux moments (scalar flux and net current) are continuous across the interface.

In general, three different kinds of transport boundary conditions are used:

- 1) specified incident: $\psi(\underline{r}, \underline{\Omega}, t) = b(\underline{r}, \underline{\Omega}, t)$ for $\underline{n} \cdot \underline{\Omega} < 0$ and $\underline{r} \in \partial D_{\text{inc}}$.
- 2) reflecting: $\psi(\underline{r}, \underline{\Omega}, t) = \psi(\underline{r}, \underline{\Omega}', t)$ for $\underline{n} \cdot \underline{\Omega} < 0$ and $\underline{r} \in \partial D_{\text{ref}}$.
- 3) periodic: $\psi(\underline{r}, \underline{\Omega}, t) = \psi(\underline{r} - \underline{d}, \underline{\Omega}, t)$ for $\underline{n} \cdot \underline{\Omega} < 0$ and $\underline{r} \in \partial D_{\text{periodic}}$.

In this section, we shall derive analogous boundary conditions for the one-group diffusion equation.

Reflecting

We first recall the diffusion approximation for the angular flux (linearly anisotropic, or P_1):

(VI.22)

$$\psi(\underline{r}, \underline{\Omega}, t) = \frac{1}{4\pi} \left(\phi(\underline{r}, t) - 3D(\underline{r}, t) \underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}, t) \right) .$$

We insert this approximation into the transport reflecting boundary condition, defining \underline{r}_s to be on the reflecting part of the boundary of D , and we obtain:

$$\frac{1}{4\pi} \left(\phi(\underline{r}_s, t) - 3D(\underline{r}_s, t) \underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}_s, t) \right) = \frac{1}{4\pi} \left(\phi(\underline{r}_s, t) - 3D(\underline{r}_s, t) \underline{\Omega}' \cdot \underline{\nabla} \phi(\underline{r}_s, t) \right) ,$$

or

(VI.23)

$$\underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}_s, t) = \underline{\Omega}' \cdot \underline{\nabla} \phi(\underline{r}_s, t) ,$$

where $\underline{\Omega}'$ is the angle that reflects onto $\underline{\Omega}$ at position \underline{r}_s . Consider the relationship between $\underline{\Omega}'$ and $\underline{\Omega}$, plotted below (both vectors are in the plane of the paper):

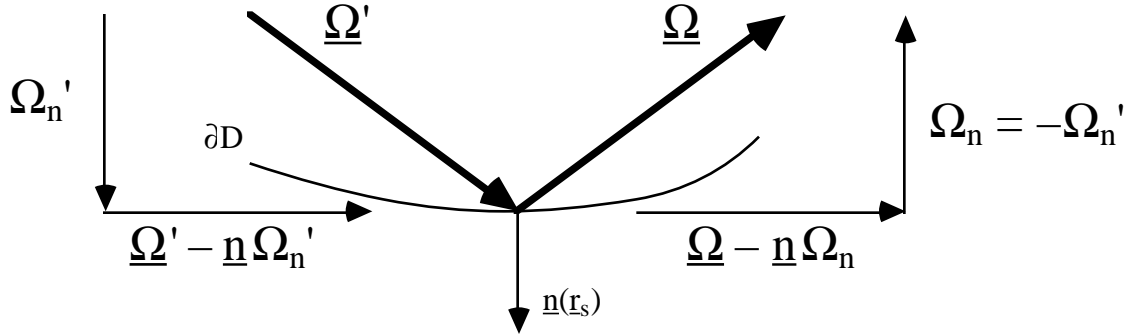


Figure VI.1

Let us rewrite Eq. (VI.23), using the trivial identity $\underline{\Omega} = \underline{n} \Omega_n + (\underline{\Omega} - \underline{n} \Omega_n)$:

$$\Omega_n \underline{n} \cdot \underline{\nabla} \phi + (\underline{\Omega} - \Omega_n \underline{n}) \cdot \underline{\nabla} \phi = \Omega_n' \underline{n} \cdot \underline{\nabla} \phi + (\underline{\Omega}' - \Omega_n' \underline{n}) \cdot \underline{\nabla} \phi ,$$

or

$$-\Omega_n' \underline{n}(\underline{r}_s) \cdot \underline{\nabla} \phi(\underline{r}_s, t) = \Omega_n \underline{n}(\underline{r}_s) \cdot \underline{\nabla} \phi(\underline{r}_s, t) ,$$

which can be true for all $\underline{\Omega}$ only if:

(VI.24)

$$\underline{n}(\underline{r}_s) \cdot \underline{\nabla} \phi(\underline{r}_s, t) = 0 , \quad \underline{r}_s \in \partial D_{\text{ref}} .$$

This is the diffusion boundary condition on reflecting boundaries. It is sometimes called a *zero-current* boundary condition, because it says there is no net flow of particles across the reflecting boundary.

Periodic

Let us once again insert the diffusion approximation for the angular flux into the transport boundary condition. For \underline{r}_s defined to be on the periodic part of the boundary, we have:

$$\frac{1}{4\pi} \left(\phi(\underline{r}, t) - 3D(\underline{r}, t) \underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}, t) \right)_{\underline{r}=\underline{r}_s} = \frac{1}{4\pi} \left(\phi(\underline{r}, t) - 3D(\underline{r}, t) \underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}, t) \right)_{\underline{r}=\underline{r}_s - \underline{d}} ,$$

which can be true for all $\underline{\Omega}$ if:

$$\phi(\underline{r}, t) = \phi(\underline{r} - \underline{d}, t) , \underline{r} \in \partial D_{\text{periodic}} , \quad (\text{VI.25a})$$

and

$$D(\underline{r}, t) \underline{\nabla} \phi(\underline{r}, t) = D(\underline{r} - \underline{d}, t) \underline{\nabla} \phi(\underline{r} - \underline{d}, t) , \underline{r} \in \partial D_{\text{periodic}} , \quad (\text{VI.25b})$$

Graphical definition of \underline{d} is given in Fig. (VI.2).

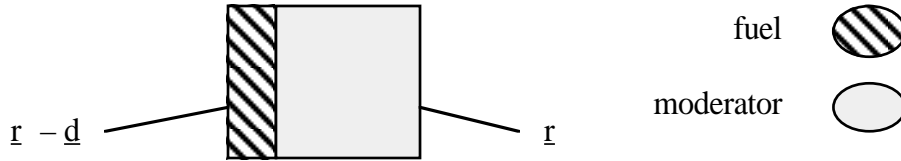


Figure VI.2

Thus, on a periodic boundary, the *scalar flux* and *current* are specified. In fact, this is the general *interface condition* that goes with the diffusion equation: the scalar flux and current are each continuous across the interface. We shall use this later.

Specified Incident (Includes Vacuum)

Insert the diffusion approximation for the angular flux into the transport boundary condition:

$$\frac{1}{4\pi} \left(\phi(\underline{r}_s, t) - 3D(\underline{r}_s, t) \underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}_s, t) \right) \stackrel{?}{=} b(\underline{r}_s, \underline{\Omega}, t) , \quad n(\underline{r}_s) \cdot \underline{\Omega} < 0 \quad \& \quad \underline{r}_s \in \partial D_{\text{inc}} .$$

On the right-hand side is an arbitrary function of $\underline{\Omega}$. On the left-hand side is a linear function of $\underline{\Omega}$. Thus, in general, this cannot be an equality. This is more evidence that the dif-

fusion equation is not accurate near boundaries — the diffusion approximation to the angular flux cannot (in general) satisfy the transport boundary condition.

Since we cannot satisfy it exactly, we try to do something that makes sense. If we multiply both sides of our “equation” by the cosine $|\underline{n} \cdot \underline{\Omega}|$, then integrate over all incoming angles, then at least we will make our diffusion equation have the correct particle inleakage rate:

$$\frac{1}{4\pi} \int_{\underline{n} \cdot \underline{\Omega} < 0} d\Omega |\underline{n} \cdot \underline{\Omega}| (\phi(\underline{r}_s, t) - 3D(\underline{r}_s, t) \underline{\Omega} \cdot \underline{\nabla} \phi(\underline{r}_s, t)) = \int_{\underline{n} \cdot \underline{\Omega} < 0} d\Omega |\underline{n} \cdot \underline{\Omega}| b(\underline{r}_s, \underline{\Omega}, t),$$

or

(VI.26)

$$\frac{1}{4} \phi(\underline{r}_s, t) + \frac{1}{2} D(\underline{r}_s, t) \underline{n} \cdot \underline{\nabla} \phi(\underline{r}_s, t) = J_{\text{inc}}(\underline{r}_s, t) \quad , \quad \underline{r}_s \in \partial D_{\text{inc}} \quad .$$

This is one possibility for a diffusion boundary condition on a specified-incident-flux boundary. In the case of a vacuum, J_{inc} is zero, and we have:

(VI.27)

$$\frac{1}{4} \tilde{\phi}(\tilde{\underline{r}}_s, t) = 0 \quad , \quad \underline{r}_s \in \partial D_{\text{inc}} \quad ,$$

where

(VI.28)

$$\bar{\phi}(\underline{r}_s, t) = \phi(\underline{r}_s, t) + d_{\text{ext}} \underline{n} \cdot \underline{\nabla} \phi(\underline{r}_s, t)$$

with the extrapolated distance

$$d_{\text{ext}} = 2D = \frac{2}{3\Sigma_{\text{tr}}} = \frac{2}{3} \lambda_{\text{tr}}$$

This is called an “extrapolated” boundary condition — the scalar flux, if *linearly extrapolated*, would reach zero at a distance d_{ext} past the boundary.

Remember three things:

- 1) The extrapolation is linear.
- 2) The scalar flux doesn't really go to zero.
- 3) Eqs. (VI.26) and (VI.27) are equivalent.

Figure VI.3 shows the actual and extrapolated flux shape.

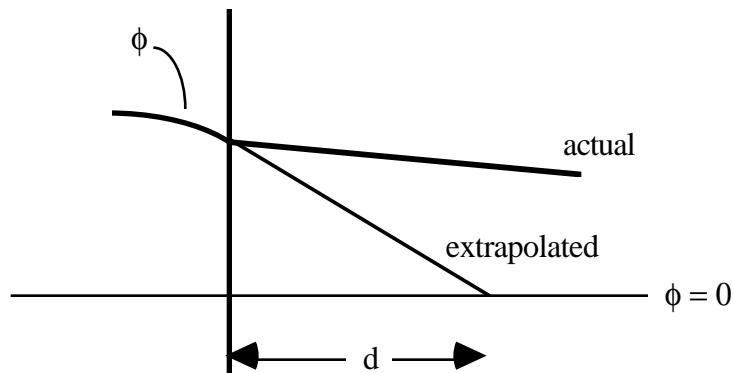


Figure VI.3

The extrapolated boundary condition simply *specifies the relative sizes of the ϕ and $\underline{n} \cdot \nabla \phi$* at the boundary.

The extrapolated boundary condition is used extensively in diffusion theory. It is often used with a transport-corrected version of the extrapolation distance:

(VI.29)

$$d_{\text{ext}} = (0.7104\dots)\lambda_{\text{tr}} .$$

The usual way to obtain the number 0.7104 is to analytically solve the transport equation for a semi-infinite uniform slab, and then ask what extrapolation distance would give the best solution.