

[Hydrogenous Moderators]  
(Chapter 1.9.3 of Elements)

### Slowing-down in hydrogenous material

In hydrogenous materials of interest, e.g., H<sub>2</sub>O, hydrogen dominates the scattering, so we take  $\alpha = 0$ . In an infinite medium ( $\nabla^2 = 0$ ), for steady-state conditions ( $\frac{\partial}{\partial t} = 0$ ), the diffusion equation is

$$\Sigma_{total}(E)\varphi(E) = \int_E^\infty \Sigma_{scatt}(E')\varphi(E')\frac{dE'}{E'} + S(E). \quad (1)$$

The equation simplifies upon introducing the *collision density*,  $\psi(E) = \Sigma_{total}(E)\varphi(E)$ ,

$$\psi(E) = \int_E^\infty \frac{\Sigma_{scatt}(E')}{\Sigma_{total}(E')}\psi(E')\frac{dE'}{E'} + S(E). \quad (2)$$

This is an inhomogeneous *Volterra integral equation of the second kind*, about which we will say nothing more except that it converts upon differentiation into an inhomogeneous first-order ordinary differential equation

$$\frac{d\psi(E)}{dE} + \frac{\Sigma_{scatt}(E)}{E\Sigma_{total}(E)}\psi(E) = S'(E), \quad (3)$$

where

$$S'(E) = \frac{dS(E)}{dE}. \quad (4)$$

This procedure does not work for the general case  $\alpha \neq 0$  because both integration limits then depend on the variable. The differential equation for the hydrogen case,  $\alpha = 0$ , is easily solved by introducing an *integrating factor*,  $r(E)$ , explained in most books on advanced calculus,

$$r(E) = \exp\left(\int_\varepsilon^E \frac{\Sigma_{scatt}(E')}{\Sigma_{total}(E')}\frac{dE'}{E'}\right); \quad \frac{dr(E)}{dE} = r'(E) = \frac{\Sigma_{scatt}(E)}{E\Sigma_{total}(E)}r(E). \quad (5)$$

The lower limit  $\varepsilon$  is arbitrary and the integrand is well behaved for any choice of range that does not include  $E = 0$ . Moreover, whatever  $\varepsilon$  is, it leads to an irrelevant constant factor in  $r(E)$ .

Then, multiplying both sides by  $r(E)$ , the differential equation becomes

$$\frac{d}{dE}(r(E)\psi(E)) = r(E)S'(E), \quad (6)$$

and the solution is

$$r(E)\psi(E) = \int_{\varepsilon}^E r(E')S'(E')dE' + c, \quad (7)$$

where  $c$  is a constant of integration to be determined later. Integrating the right-hand side by parts, we find

$$r(E)\psi(E) = (r(E')S(E')) \Big|_E^{\infty} - \int_{\varepsilon}^E S(E')r'(E')dE' + c. \quad (8)$$

Because  $S(E)$  and therefore  $\psi(E)$  and  $\varphi(E)$  vanish for energies greater than some energy  $E_{\max}$ ,

$$\lim_{E \rightarrow \infty} r(E)\psi(E) = 0, \quad (9)$$

$$c = r(\varepsilon)S(\varepsilon) + \int_{\varepsilon}^{\infty} S(E')r'(E')dE', \quad (10)$$

and

$$r(E)\psi(E) = r(E')S(E') + \int_E^{\infty} S(E')r'(E')dE'. \quad (11)$$

So, for  $E \leq E_{\max}$ , we have the general result for slowing-down in hydrogenous media

$$\varphi(E) = \frac{\psi(E)}{\Sigma_{total}(E)} = \frac{S(E)}{\Sigma_{total}(E)} + \frac{1}{\Sigma_{total}(E)} \int_E^{\infty} S(E') \frac{\Sigma_{scatt}(E')}{\Sigma_{total}(E')} \exp\left(\int_E^{E'} \frac{\Sigma_{scatt}(E'')}{\Sigma_{total}(E'')} \frac{dE''}{E''}\right) \frac{dE'}{E'}. \quad (12)$$

In the following we proceed using familiar mathematical operations, without bringing in the concept of slowing-down density, which appears in some treatments of this subject, hoping to make more clear the mathematical aspects of the theory.

Taking the source function to be a *delta function*,  $S(E) = S_o\delta(E - E_Q)$ , we have the result for a specific source energy

$$\varphi(E) = \frac{S_o\delta(E - E_Q)}{\Sigma_{total}(E_Q)} + \frac{S_o}{E_Q} \frac{\Sigma_{scatt}(E_Q)}{\Sigma_{total}(E)\Sigma_{total}(E_Q)} \exp\left(\int_E^{E_Q} \frac{\Sigma_{scatt}(E'')}{\Sigma_{total}(E'')} \frac{dE''}{E''}\right) U(E < E_Q), \quad (13)$$

where the unit function  $U(E < E_Q) = 1$  for  $E < E_Q$  and  $U(E < E_Q) = 0$  otherwise, is frequently called the *Heaviside step function*. The exponential factor,

$$\exp\left(\int_E^{E_Q} \frac{\Sigma_{scatt}(E'')}{\Sigma_{total}(E'')} dE''\right) = \exp\left(\int_E^{E_Q} 1 - \frac{\Sigma_{abs}(E'')}{\Sigma_{total}(E'')} dE''\right) = \left(\frac{E_Q}{E}\right) P_{R.E.}(E) \quad (14)$$

involves the *resonance escape probability*,

$$P_{R.E.}(E) = \exp\left[-\int_E^{E_Q} \frac{\Sigma_{abs}(E'')}{\Sigma_{total}(E'')} dE''\right], \quad (15)$$

which, for  $1/v$  absorption and constant scattering is

$$P_{R.E.}(E) = \left(\frac{1 + \Sigma_{abs}(E_Q)/\Sigma_{scatt}}{1 + \Sigma_{abs}(E_Q)/\Sigma_{scatt} \sqrt{E_Q/E}}\right)^2. \quad (16)$$

Thus the flux per unit energy for a delta-function source is

$$\phi(E) = \frac{S_o \delta(E - E_Q)}{\Sigma_{total}(E_Q)} + \frac{S_o \Sigma_{scatt}(E_Q) P_{R.E.}(E)}{\Sigma_{total}(E) \Sigma_{total}(E_Q)} \left(\frac{1}{E}\right) U(E < E_Q). \quad (17)$$

The differential inelastic scattering cross section (assumed constant in space and for a monoisotopic material) is

$$\frac{\partial \Sigma_{scat}}{\partial E}(E_o \rightarrow E) = \frac{\Sigma_o}{(1 - \alpha)E_o} \begin{cases} 1 & \text{for } \alpha E_o < E < E_o \text{ and} \\ 0 & \text{for } E < \alpha E_o \text{ or } E > E_o \end{cases}. \quad (18)$$

The minimum relative final energy of the neutron,  $\alpha$ , is

$$\alpha = \frac{(A - 1)^2}{(A + 1)^2}. \quad (19)$$

The total scattering cross section is then

$$\Sigma_{scat}(E_o) = \int_0^\infty \frac{\partial \Sigma_{scat}}{\partial E}(E_o \rightarrow E) dE = \frac{\Sigma_o}{(1 - \alpha)E_o} \int_{\alpha E_o}^{E_o} dE = \Sigma_o. \quad (20)$$

That is, the constant  $\Sigma_o$  in the expression for the inelastic scattering cross section is the total scattering cross section,  $\Sigma_{scat}(E_o)$ . For scattering from hydrogen,  $\alpha = 0$ : the neutron can lose all of its kinetic energy in a single, head-on collision, and the minimum energy after scattering is zero.

Because it is conventional in discussing the present subject, we now go over to the energy  $E$  rather than the speed  $v$  to represent the energy-related variable, using the same function names in spite of the risk of confusing functions having different arguments but distinguishing between them in terms of the argument names. (Tables and computers, which expect numerical values for the arguments of functions, can't do this—different functions must have different names.)

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$$\Sigma_{total}(E)\varphi(E) = \int_E^\infty \Sigma_{scatt}(E')\varphi(E')\frac{dE'}{E'} + S(E). \quad (21)$$

The equation simplifies upon introducing the *collision density*,  $\psi(E) = \Sigma_{total}(E)\varphi(E)$ ,

$$\psi(E) = \int_E^\infty \frac{\Sigma_{scatt}(E')}{\Sigma_{total}(E')}\psi(E')\frac{dE'}{E'} + S(E). \quad (22)$$

This is an inhomogeneous *Volterra integral equation of the second kind*, about which we will say nothing more except that it converts upon differentiation into an inhomogeneous first-order ordinary differential equation

$$\frac{d\psi(E)}{dE} + \frac{\Sigma_{scatt}(E)}{E\Sigma_{total}(E)}\psi(E) = S'(E), \quad (23)$$

where

$$S'(E) = \frac{dS(E)}{dE}. \quad (24)$$

This procedure does not work for the general case  $\alpha \neq 0$  because both integration limits then depend on the variable. The differential equation for the hydrogen case,  $\alpha = 0$ , is easily solved by introducing an *integrating factor*,  $r(E)$ , explained in most books on advanced calculus,

$$r(E) = \exp\left(\int_\varepsilon^E \frac{\Sigma_{scatt}(E')}{\Sigma_{total}(E')}\frac{dE'}{E'}\right); \quad \frac{dr(E)}{dE} = r'(E) = \frac{\Sigma_{scatt}(E)}{E\Sigma_{total}(E)}r(E). \quad (25)$$

The lower limit  $\varepsilon$  is arbitrary and the integrand is well behaved for any choice of range that does not include  $E = 0$ . Moreover, whatever  $\varepsilon$  is, it leads to an irrelevant constant factor in  $r(E)$ .

Then, multiplying both sides by  $r(E)$ , the differential equation becomes

$$\frac{d}{dE}(r(E)\psi(E)) = r(E)S'(E) \quad , \quad (26)$$

and the solution is

$$r(E)\psi(E) = \int_{\varepsilon}^E r(E')S'(E')dE' + c, \quad (27)$$

where  $c$  is a constant of integration to be determined later. Integrating the right-hand side by parts, we find

$$r(E)\psi(E) = (r(E')S(E')) \Big|_E^{\infty} - \int_{\varepsilon}^E S(E')r'(E')dE' + c \quad . \quad (28)$$

Because  $S(E)$  and therefore  $\psi(E)$  and  $\varphi(E)$  vanish for energies greater than some energy  $E_{\max}$ ,

$$\lim_{E \rightarrow \infty} r(E)\psi(E) = 0, \quad (29)$$

$$c = r(\varepsilon)S(\varepsilon) + \int_{\varepsilon}^{\infty} S(E')r'(E')dE' \quad , \quad (30)$$

and

$$r(E)\psi(E) = r(E')S(E') + \int_E^{\infty} S(E')r'(E')dE' \quad . \quad (31)$$

So, for  $E \leq E_{\max}$ , we have the general result for slowing-down in hydrogenous media

$$\varphi(E) = \frac{\psi(E)}{\Sigma_{total}(E)} = \frac{S(E)}{\Sigma_{total}(E)} + \frac{1}{\Sigma_{total}(E)} \int_E^{\infty} S(E') \frac{\Sigma_{scatt}(E')}{\Sigma_{total}(E')} \exp \left( \int_E^{E'} \frac{\Sigma_{scatt}(E'')}{\Sigma_{total}(E'')} \frac{dE''}{E''} \right) \frac{dE'}{E'} \quad . \quad (32)$$

In the following we proceed using familiar mathematical operations, without bringing in the concept of slowing-down density, which appears in some treatments of this subject, hoping to make more clear the mathematical aspects of the theory.

Taking the source function to be a *delta function*,  $S(E) = S_o\delta(E - E_Q)$ , we have the result for a specific source energy

$$\varphi(E) = \frac{S_o\delta(E - E_Q)}{\Sigma_{total}(E_Q)} + \frac{S_o}{E_Q} \frac{\Sigma_{scatt}(E_Q)}{\Sigma_{total}(E)\Sigma_{total}(E_Q)} \exp \left( \int_E^{E_Q} \frac{\Sigma_{scatt}(E'')}{\Sigma_{total}(E'')} \frac{dE''}{E''} \right) U(E < E_Q) \quad , \quad (33)$$

where the unit function  $U(E < E_0) = 1$  for  $E < E_0$  and  $U(E < E_0) = 0$  otherwise, is frequently called the *Heaviside step function*. The exponential factor, called the *resonance escape probability*, represents the fraction of neutrons surviving absorption while slowing down to energy  $E$ . Typically the factor is significant in materials with strong absorption resonances and more relevant in nuclear reactor technology than in neutron moderators.