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Definition of Two Band Parameters for Use in Photon Transport Calculations*

by

Dermott E. Cullen

This write-up is designed to:

1. Derive the multi-group photon diffusion equations starting from the Boltzmann equation. This is mostly for my own edification so that I can plainly see all of the limitations and assumptions imposed by the diffusion equation. However, it also serves to define all of the required diffusion parameters in terms of cross sections, so that I can clearly establish the relationship to the multi-band parameters that we use in neutron transport calculations.

2. Define all required two band parameters in terms of Planckian and Rosseland mean values.

For reference to the multi-band method, see Nucl. Sci. Eng. 55, 387-400 (1974). When the multi-band method is applied to photon transport, only two bands per group are used. In order to avoid spatially dependent band weights, each band weight is defined to be equal to one-half. Band cross sections are selected to simultaneously conserve both the Planckian and Rosseland means. The following methods can be used in either transport (e.g., Monte Carlo) or diffusion calculations.

Band total cross sections and diffusion coefficients are given by Eq. (28) and band cross sections for individual cross sections (i.e., absorption, scattering, etc.) are given by Eq. (32). In addition, see Eq. (35) for the constant cross section case; i.e., Planckian $\equiv$ Rosseland mean.

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Derivation of Diffusion Equation

Consider the Boltzmann equation

$$\frac{1}{v} \frac{\partial N}{\partial t}(\vec{r}, \vec{\Omega}, E, t) + \vec{\Omega} \cdot \vec{\nabla} N(\vec{r}, \vec{\Omega}, E, t) + \Sigma_t(\vec{r}, E, t) N(\vec{r}, \vec{\Omega}, E, t) = R(\vec{r}, \vec{\Omega}, E, t) \quad (1)$$

$$R(\vec{r}, \vec{\Omega}, E, t) = \frac{1}{4\pi} \int_{\vec{\Omega}'} \int_{E'} f(\vec{r}, t; \vec{\Omega}', E' + \vec{\Omega}, E) N(\vec{r}, \vec{\Omega}', E', t) d\vec{\Omega}' dE' + S(\vec{r}, \vec{\Omega}, E, t) \quad (2)$$

For photons the total source (extraneous plus scattered plus re-emitted) is simplified to

$$R(\vec{r}, \vec{\Omega}, E, t) = \frac{1}{2} \left\{ \Sigma_{a0} B + \Sigma_{\sin 0} N_0(\vec{r}, E, t) + S_0(\vec{r}, E, t) \right\} \quad (3)$$

which is isotropic (i.e., independent of $\vec{\Omega}$). The P_n equations are obtained by multiplying the Boltzmann equation by the Legendre Polynomial $P_n(\vec{\Omega})$ and integrating over $\vec{\Omega}$ to find,

$$(2n+1) \frac{1}{v} \frac{\partial N_n}{\partial t} + \left[(n+1) \nabla N_{n+1} + n \nabla N_{n-1} \right] + (2n+1) \Sigma_{tn} N_n = (2n+1) R_n \quad (4)$$

where

$$R_n = \Sigma_{a0} B + \Sigma_{\sin 0} N_0 + S_0 \quad n = 0$$

$$= 0 \quad \text{otherwise}$$

and Σ_{tn} is the N_n weighted total cross section.

The two equations of interest for the diffusion equation are

$$n = 0 \quad \frac{1}{v} \frac{\partial N_0}{\partial t} + \nabla N_1 + \Sigma_{t0} N_0 = R_0 \quad (6)$$

$$n = 1 \quad \frac{3}{v} \frac{\partial N_1}{\partial t} + (2\nabla N_2 + \nabla N_0) + 3\Sigma_{t1} N_1 = 0 \quad (7)$$

In order to obtain Fick's law, $\frac{3}{v} \frac{\partial N_1}{\partial t} + 2\nabla N_2$ must be eliminated (8) from the $n = 1$ equation, either by assuming the sum of these two terms is zero or somehow related to N_0 and ∇N_1 . The result of assuming these two terms are zero is

$$n = 1 \quad N_1 = - \frac{1}{3\Sigma_{t1}} \nabla N_0 \quad (\text{Fick's law}) \quad (9)$$

Any other assumption merely replaces $\frac{1}{3\Sigma_{t1}}$ by some other term to again obtain Fick's law with a modified diffusion coefficient. Substituting for N_1 in the $n = 0$ equation yields,

$$\frac{1}{v} \frac{\partial N_0}{\partial t} - \nabla \left[\frac{1}{3\Sigma_{t1}} \nabla N_0 \right] + \Sigma_{t0} N_0 = \Sigma_{a0} N_0 + \Sigma_{\text{sin0}} N_0 + S_0 \quad (10)$$

The total cross section may be written as,

$$\Sigma_{t0} = \Sigma_{a0} + \Sigma_{\text{sin0}} + \Sigma_{\text{sout0}} \quad (11)$$

where

Σ_{ao} - absorption

Σ_{sino} - ingroup scattering (for group g , $\Sigma_{sino} = \Sigma_{sg} \rightarrow g$)

Σ_{souto} - scattering out of group (for group g , $\Sigma_{souto} = \sum_{g' \neq g} \Sigma_{sg' \rightarrow g'}$)

S_o - include extraneous sources plus scattering from all other groups

s_o = extraneous source

Therefore,

$$S_o = s_o + \sum_{g' \neq g} \Sigma_{sg' \rightarrow g} N_{og'}$$

Therefore we find,

$$\frac{1}{V} \frac{\partial N_o}{\partial t} - \nabla \left[\frac{1}{3\Sigma_{t1}} \nabla N_o \right] = \Sigma_{ao} (B - N_o) - \Sigma_{souto} N_o + S_o \quad (12)$$

Two band equations [see: Nuc. Sci. and Eng. 55, 387-400 (1974)]

Assuming a weight p_k of $\frac{1}{2}$ for each band the equations are,

$$\frac{1}{V} \frac{\partial N_{ok}}{\partial t} - \nabla \left[\frac{1}{3\Sigma_{tk}} \nabla N_{ok} \right] = \Sigma_{aok} (B - N_{ok}) - \Sigma_{soutk} N_{ok} + \frac{1}{2} S_o \quad (15)$$

$K = 1, 2$

The required parameters needed to define these equations are,

$$\Sigma_{t01}, \Sigma_{t02}, \Sigma_{a01}, \Sigma_{a02}, \Sigma_{sout1}, \Sigma_{sout2}$$

For any cross section the group averaged value is,

$$\langle \Sigma(\omega) \rangle = \frac{\int_{E_1}^{E_2} \Sigma(E) \omega(E) dE}{\int_{E_1}^{E_2} \omega(E) dE} \quad (17)$$

Where the cross section is a function of the weighting function $\omega(E)$.

For,

$$\left. \begin{array}{l} \text{Planckian } \omega(E) = B_V(T) \\ \text{Rosseland } \omega(E) = \frac{1}{\Sigma_T} \frac{dB_V(T)}{dT} \end{array} \right\} = f(\Sigma_T)g(E) \text{ in each case}$$

In order to convert the definition of the group averaged cross section from an integral over energy to an integral over total cross section re-write the definition of the group average in the equivalent form,

$$\langle \Sigma(\omega) \rangle = \frac{\int_{\Sigma_T^*} \int_{E_1}^{E_2} \delta(\Sigma_T^* - \Sigma_T(E)) \Sigma(E) \omega(E) dE d\Sigma_T^*}{\int_{\Sigma_T^*} \int_{E_1}^{E_2} \delta(\Sigma_T^* - \Sigma_T(E)) \omega(E) dE d\Sigma_T^*} \quad (18)$$

If the integration over Σ_T^* is performed first we return to the normal definition. However if we perform the integral over E first, since the weighting function $\omega(E)$ can be written as a product of two terms, $f(\Sigma_T)g(E)$ we find,

$$\langle \Sigma(\omega) \rangle = \frac{\int_{\Sigma_t^*} \Sigma(\Sigma_t^*) f(\Sigma_t^*) d\Sigma_t^* \int_{\Gamma_1}^{\Gamma_2} \delta(\Sigma_t^* - \Sigma_t(E)) g(E) dE}{\int_{\Sigma_t^*} f(\Sigma_t^*) d\Sigma_t^* \int_{\Gamma_1}^{\Gamma_2} \delta(\Sigma_t^* - \Sigma_t(E)) g(E) dE} \quad (19)$$

Defining the total cross section probability density

$$p(\Sigma_t^*) = \int_{\Gamma_1}^{\Gamma_2} \delta(\Sigma_t^* - \Sigma_t(E)) g(E) dE / \int_{\Gamma_1}^{\Gamma_2} g(E) dE \quad (20)$$

We obtain a definition of the multi-group cross section in terms of an integral over cross section,

$$\langle \Sigma(\omega) \rangle = \int_{\Sigma_t^*} \Sigma(\Sigma_t^*) f(\Sigma_t^*) p(\Sigma_t^*) d\Sigma_t^* / \int_{\Sigma_t^*} f(\Sigma_t^*) p(\Sigma_t^*) d\Sigma_t^* \quad (21)$$

Where $f(\Sigma_t^*)$ is the cross section dependent portion of the weighting function $\omega(E)$

Planckian $f(\Sigma_t^*) = 1$

Rosseland $f(\Sigma_t^*) = \frac{1}{\Sigma_t^*}$

In the multi-band method the total cross section probability density, $p(\Sigma_t^*)$ is assumed to be given by a series of Dirac delta functions,

$$p(\Sigma_t^*) = \sum_k p_k \delta(\Sigma_t^* - \Sigma_{tk}) \quad (22)$$

In particular for two band photon transport when two bands each of weight $\frac{1}{2}$ are used,

$$p(\Sigma_t^*) = \frac{1}{2} [\delta(\Sigma_t^* - \Sigma_{t1}) + \delta(\Sigma_t^* - \Sigma_{t2})] \quad (23)$$

With this assumption the group averaged cross section is given by,

$$\langle \Sigma(\omega) \rangle = \frac{\frac{1}{2} [\Sigma(\Sigma_{t1})f(\Sigma_{t1}) + \Sigma(\Sigma_{t2})f(\Sigma_{t2})]}{\frac{1}{2} [f(\Sigma_{t1}) + f(\Sigma_{t2})]} \quad (24)$$

The two band cross sections $\Sigma(\Sigma_{t1})$ and $\Sigma(\Sigma_{t2})$ are selected by insuring that both the Planckian and Rosseland mean cross sections are exactly conserved,

$$\text{Planckian } \langle \Sigma \rangle_{Pl} = \frac{1}{2} [\Sigma(\Sigma_{t1}) + \Sigma(\Sigma_{t2})] \quad ; \quad f(\Sigma_t) = 1 \quad (25)$$

$$\text{Rosseland } \langle \Sigma \rangle_R = \frac{\frac{1}{2} \left[\frac{\Sigma(\Sigma_{t1})}{\Sigma_{t1}} + \frac{\Sigma(\Sigma_{t2})}{\Sigma_{t2}} \right]}{\frac{1}{2} \left[\frac{1}{\Sigma_{t1}} + \frac{1}{\Sigma_{t2}} \right]} \quad ; \quad f(\Sigma_t) = \frac{1}{\Sigma_t}$$

Total cross section

$$1) \quad \langle \Sigma_t \rangle_{Pl} = \frac{1}{2} [\Sigma_{t1} + \Sigma_{t2}] \quad (26)$$

$$2) \quad \langle \Sigma_t \rangle_R = 1 / \left[\frac{1}{2} \left(\frac{1}{\Sigma_{t1}} + \frac{1}{\Sigma_{t2}} \right) \right]$$

$$\text{or } \frac{1}{2} (\Sigma_{t1} + \Sigma_{t2}) \langle \Sigma_t \rangle_R = \Sigma_{t1} \Sigma_{t2}$$

changing variables let

$$\Sigma_{t1} = A - B \quad ; \quad \Sigma_{t2} = A + B \quad + \quad \Sigma_{t1} + \Sigma_{t2} = 2A \quad ; \quad \Sigma_{t1} \Sigma_{t2} = A^2 - B^2$$

$$1) \quad \left[\langle \Sigma_t \rangle_{p1} = A \right] \quad (27)$$

$$2) \quad A \langle \Sigma_t \rangle_R = A^2 - B^2$$

$$B^2 = A^2 - A \langle \Sigma_t \rangle_R = \langle \Sigma_t \rangle_{p1}^2 \left[1 - \frac{\Sigma_{tR}}{\Sigma_{tp1}} \right]$$

$$\Sigma_{t1} = \langle \Sigma_t \rangle_{p1} \left[1 - \sqrt{1 - \frac{\langle \Sigma_t \rangle_R}{\langle \Sigma_t \rangle_{p1}}} \right]$$

$$\Sigma_{t2} = \langle \Sigma_t \rangle_{p1} \left[1 + \sqrt{1 - \frac{\langle \Sigma_t \rangle_R}{\langle \Sigma_t \rangle_{p1}}} \right]$$

In terms of diffusion coefficients

$$\begin{aligned} D_1 &= \langle D \rangle_{p1} / \left[1 - \sqrt{1 - \frac{\langle D \rangle_{p1}}{\langle D \rangle_R}} \right] \\ D_2 &= \langle D \rangle_{p1} / \left[1 + \sqrt{1 - \frac{\langle D \rangle_{p1}}{\langle D \rangle_R}} \right] \end{aligned} \quad (28)$$

Partial cross sections (i.e. absorption, scattering)

$$1) \quad \langle \Sigma_i \rangle_{p1} = \frac{1}{2} (\Sigma_{i1} + \Sigma_{i2}) \quad ; \quad i = \text{absorption or scattering} \quad (29)$$

$$2) \quad \langle \Sigma_i \rangle_R = \frac{\frac{1}{2} \left[\frac{\Sigma_{t1}}{\Sigma_{t1}} + \frac{\Sigma_{t2}}{\Sigma_{t2}} \right]}{\frac{1}{2} \left[\frac{1}{\Sigma_{t1}} + \frac{1}{\Sigma_{t2}} \right]} = \frac{1}{2} \langle \Sigma_t \rangle_R \left[\frac{\Sigma_{i1}}{\Sigma_{t1}} + \frac{\Sigma_{i2}}{\Sigma_{t2}} \right]$$

$$\Sigma_{t1} \Sigma_{t2} \langle \Sigma_i \rangle_R = \frac{1}{2} \langle \Sigma_t \rangle_R [\Sigma_{A1} \Sigma_{T2} + \Sigma_{A2} \Sigma_{T1}]$$

changing variables let,

$$\varepsilon_{i1} = C - D \quad ; \quad \varepsilon_{i2} = C + D \Rightarrow \varepsilon_{i1} + \varepsilon_{i2} = 2C$$

$$1) \quad \langle \varepsilon_i \rangle_{p1} = C \quad (30)$$

$$2) \quad (A^2 - B^2) \langle \varepsilon_i \rangle_R = \frac{1}{2} \langle \varepsilon_t \rangle_R \left[(C - D)(A + B) + (C + D)(A - B) \right]$$

$$\langle \varepsilon_t \rangle_{p1} \langle \varepsilon_t \rangle_R \langle \varepsilon_i \rangle_R = \frac{1}{2} \langle \varepsilon_t \rangle_R \left[C(A + B + A - B) - D(A + B - A + B) \right]$$

$$\langle \varepsilon_t \rangle_{p1} \langle \varepsilon_i \rangle_R = \frac{1}{2} \left[2CA - 2DB \right]$$

$$\langle \varepsilon_t \rangle_{p1} \langle \varepsilon_i \rangle_R = C \langle \varepsilon_t \rangle_{p1} - D \langle \varepsilon_t \rangle_{p1} \sqrt{1 - \frac{\langle \varepsilon_t \rangle_F}{\langle \varepsilon_t \rangle_{p1}}}$$

$$\langle \varepsilon_i \rangle_R = \langle \varepsilon_i \rangle_{p1} - D \sqrt{1 - \frac{\langle \varepsilon_t \rangle_R}{\langle \varepsilon_t \rangle_{p1}}}$$

$$D = \langle \varepsilon_i \rangle_{p1} \frac{\left[1 - \frac{\langle \varepsilon_i \rangle_F}{\langle \varepsilon_i \rangle_{p1}} \right]}{\sqrt{1 - \frac{\langle \varepsilon_t \rangle_R}{\langle \varepsilon_t \rangle_{p1}}}} \quad (31)$$

therefore,

$$\varepsilon_{i1} = \langle \varepsilon_i \rangle_{p1} \left[1 - \frac{\left[1 - \frac{\langle \varepsilon_i \rangle_R}{\langle \varepsilon_i \rangle_{p1}} \right]}{\sqrt{1 - \frac{\langle \varepsilon_t \rangle_R}{\langle \varepsilon_t \rangle_{p1}}}} \right] \quad (32)$$

i = absorbtion, scattering, etc.

$$\varepsilon_{i1} = \langle \varepsilon_i \rangle_{p1} \left[1 + \frac{\left[1 - \frac{\langle \varepsilon_i \rangle_F}{\langle \varepsilon_i \rangle_{p1}} \right]}{\sqrt{1 - \frac{\langle \varepsilon_t \rangle_R}{\langle \varepsilon_t \rangle_{p1}}}} \right]$$

These definitions are consistent in the sense that if any cross section is equal to the total (e.g. no scattering $\Sigma_a = \Sigma_t$) the band total cross section is equal to the partial cross section since,

$$D = \langle \Sigma_t \rangle_{pl} \frac{\left[1 - \frac{\langle \Sigma_t \rangle_R}{\langle \Sigma_t \rangle_{pl}} \right]}{\sqrt{1 - \frac{\langle \Sigma_t \rangle_R}{\langle \Sigma_t \rangle_{pl}}}} = \langle \Sigma_t \rangle_{pl} \sqrt{1 - \frac{\langle \Sigma_t \rangle_R}{\langle \Sigma_t \rangle_{pl}}} = B \quad (33)$$

$C \pm D = A \pm B$ for the two bands.

special case

#1 when $\langle \Sigma_t \rangle_{pl} \approx \langle \Sigma_t \rangle_R$, which normally implies $\langle \Sigma_i \rangle_{pl} \approx \langle \Sigma_i \rangle_R$ the expression,

$$\frac{\left[1 - \frac{\langle \Sigma_i \rangle_R}{\langle \Sigma_i \rangle_{pl}} \right]}{\sqrt{1 - \frac{\langle \Sigma_t \rangle_R}{\langle \Sigma_t \rangle_{pl}}}} \quad (34)$$

approaches an indeterminate form, since the two equations used to define C and D are approaching the point of becoming no longer linearly independent; i.e. they can be satisfied for $C = \langle \Sigma_i \rangle_{pl}$ and any arbitrary D. By expanding terms it can be shown that in this case we can simply define,

$$\left. \begin{aligned} \Sigma_{i1} &= \langle \Sigma_i \rangle_R \\ \Sigma_{i2} &= \langle \Sigma_i \rangle_{pl} \end{aligned} \right\} \quad i = \text{total, absorption, scattering} \quad (35)$$

this condition should be applied whenever $\left| \langle \epsilon_T \rangle_P \geq 0.9999 \langle \epsilon_T \rangle_{P1} \right|$

$$\text{i.e. } \sqrt{1 - \frac{\langle \epsilon_T \rangle_R}{\langle \epsilon_T \rangle_{P1}}} < 0.01 \quad (36)$$

#2 This is not really a special case but it is worth mentioning. For any cross section if $\langle \epsilon_i \rangle_{P1} = \langle \epsilon_i \rangle_P$ (e.g. Compton scattering in which only one unique cross section is defined) the cross section for this reaction will be the same in all bands, i.e.,

$$\epsilon_{ik} = \langle \epsilon_i \rangle, k = 1, 2 \quad (37)$$

Equivalent multi-group quantities

Equivalent multi-group quantities can be obtained by summing over the bands within each group. For two bands the equivalent multi-group $\tilde{N}_0$ is simply $\tilde{N}_0 = N_{01} + N_{02}$ where N_{01} and N_{02} are the two band quantities. The equivalent multi-group cross sections for any process i ($i = \text{total, absorption, scattering}$) should be defined to conserve observable reaction rates (i.e. as a ratio of reactions to $\tilde{N}_0$). For two bands the equivalent multi-group cross section for process i is simply,

$$\tilde{\epsilon}_i = (\epsilon_{i1}N_{01} + \epsilon_{i2}N_{02}) / (N_{01} + N_{02}) \quad (38)$$

where N_{01} , N_{02} , ϵ_{i1} and ϵ_{i2} are the two band quantities.

An advantage of this two band algorithm is that starting from spatially independent band cross sections Σ_{i1} and Σ_{i2} , the equivalent multi-group cross section $\tilde{\Sigma}_i$ (in Eq. 38) can be continuously spatially dependent and properly reflect the correct average value over the entire range from optically thin to optically thick spatial regions.