Introduction to the modeling of light diffusion by radiative transfer

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I Introduction :

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The transport theory of light diffusion (also called radiative transfer formalism) is a powerful method to model light diffusion through a medium containing particles. It accounts for absorption and multiple scattering (possibly anisotropic scattering), but neglects any kind of wave effects (diffraction, and interferences effects). The specific intensity (or spectral luminance) can be calculated in this approach, allowing to investigate detailed angular dependent effects.
The radiative transfer approach has been extensively investigated since the 50's, following the pioneering work of Chandrasekhar (Nobel Prize in 1983 for his theoretical studies of the physical processes of importance to the structure and evolution of the stars).
It has many applications in the field of skin optics, marine biology, paper optics, virtual reality (BRDF modeling) and the propagation of radiant energy in the atmosphere of planets, stars and galaxies.

A simpler approach, the diffusion approximation will be also discussed in this lecture. Extensively used in the field of optical tomography, the diffusion model approximates the transfer formalism in the limit of high scattering (and poorly absorbing) medium. Theses lectures have been essentially inspired by :

- Akira Ishimaru "Wave Propagation and Scattering in Random Media" January 1999, Wiley-IEEE Press
- S. Chandrasekhar "Radiative Transfer". Dover Publications Inc. (1960).

II Definition of important physical quantities in transport theory

2.1 Plane-Parallel geometry

In these lectures, only the case of the plane parallel geometry (also called "slab") (see Fig. 1) is considered. The incident flux is for simplicity assumed to be specular, normal to the surface, and thus we can assume an **azimuthal symmetry** (no φ dependency in spherical coordinates). It will not be the case for oblique incidence.

Physical quantities only depend in this case on z and θ (Note that the incident flux is uniform on the incident surface, i.e. no (x,y) dependency).

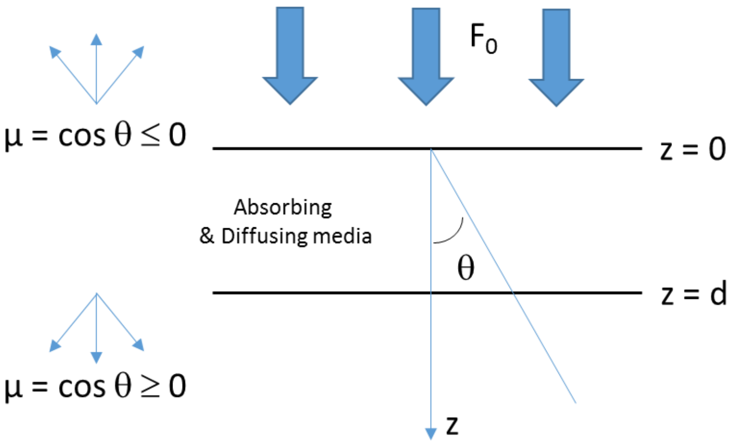


Fig. 1 : the plane parallel geometry. The axis z and angle θ are defined.

The semi-infinite medium $d \to \infty$ is a particular case of this problem. In this latter case, in absence of absorption, it is sometimes considered that the light is coming from the deep inside ($d \to \infty$).

2.2 Specific intensity, flux, energy density

The physical quantities used in radiative transfer are the same as in radiometry. The most important quantity is the **specific intensity I**, also sometimes called **luminance, radiance** or **brightness** (luminance en Français). The specific intensity is defined as follows. The power flowing within a solid angle dΩ around a direction $\vec{\Omega}$ through a surface dS located around a point $\vec{r}$ in a frequency interval (ν, ν + dν) is (see Fig. 1) :

$$d\Phi = I(\vec{r},\vec{\Omega},\nu)\ cos\alpha\ dS\ d\Omega\ d\nu$$

The specific intensity units are $Wm^{-2}sr^{-1}Hz^{-1}$. $\cos\alpha = \vec{n}\cdot\vec{\Omega}$.

Usually, the frequency (or wavelength) dependency of I is not explicitly specified, as in most case, this is no exchange of energy between each frequency (i.e each wavelength). Thus the ETR can be solved independently for each wavelength.

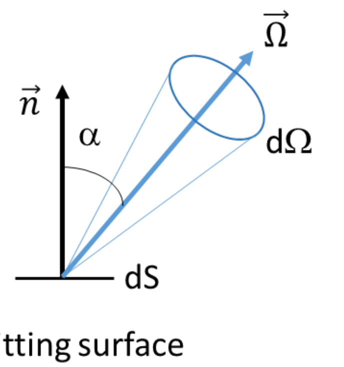


Fig. 2 : Definition of the specific intensity

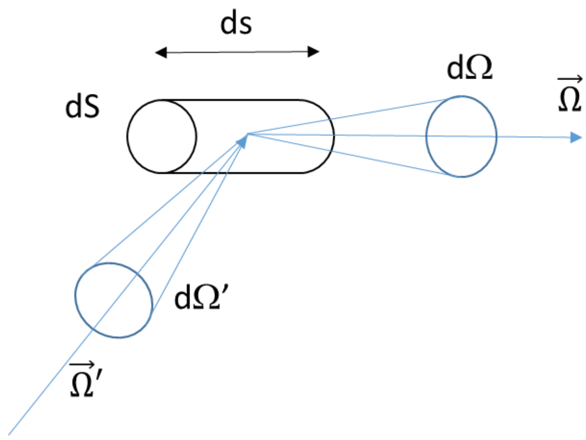


Fig. 3 : Energy balance in a elementary volume

The flux (W/m^2) is given by :

$$\vec{F}(M) = \int_{4\pi} I(M,\vec{\Omega})\,\vec{\Omega}\ d\Omega$$

Coming back to the parallel plane problem, the positive flowing flux per unit area (W/m^2) is thus given by :

$$F^{+}(z) = \int_{0}^{2\pi} I(z,\theta)\ cos\theta\ d\Omega = 2\pi\int_{0}^{\pi/2} I(z,\theta)\ cos\theta\ sin\theta\ d\theta$$

F, name here as a flux, is an **irradiance** for incoming flux on a surface, and **emittance** of outcoming flux in radiometric terminology. Introducing μ = cosθ (note that θ = 0 is obtained for μ = 1)

$$F^{+}(z) = 2\pi\int_{0}^{1} I(z,\mu)\ \mu\ d\mu$$

Similarly:

$$F^{-}(z) = -2\pi\int_{-1}^{0} I(z,\mu)\ \mu\ d\mu$$

The total flux F is :

$$F(z) = 2\pi \int_{-1}^{1} I(z,\mu)\,\mu\, d\mu = F^{+}(z) - F^{-}(z)$$

The energy density u (J / m^3) is given by :

$$u(z) = \frac{1}{c}\int_{0}^{4\pi} I(z,\theta)\, d\Omega = \frac{1}{c}\int_{-1}^{1} I(z,\mu)\, d\mu$$

This equation can be derived with the following arguments. The elementary variation of energy density du in a solid angle $d\Omega$ during a short time duration dt is given by :

$$du = \frac{I\, dS\, d\Omega\, \mathrm{dt}}{dS\, c\, \mathrm{dt}}$$

III Equation of transfer in radiative transport theory

3.1 Derivation of the radiative transfer equation

In this section, the balance equation governing the evolution of the specific intensity is derived (see Fig. 3). Let us consider a cylindrical elementary volume with a cross section dS and a length ds. This cylinder is designed around one light direction $\vec{\Omega}$ of solid angle dΩ. The variation of power in this solid angle is by definition:

$$\left(I(s+ds,\vec{\Omega}) - I(s,\vec{\Omega})\right) dS d\Omega = \frac{dI}{ds} dS d\Omega \mathrm{ds}$$

This variation has several origins : 1 / light absorption, 2 / light scattered out of the solid angle dΩ, 3/ light scattered in the solid angle dΩ coming from other directions dΩ', 4/ potentially light emission (not included here).

Introducing the **absorption (resp. scattering) coefficient** μ_a (resp. μ_s) (unit m^{-1}), the fraction of incident power absorbed or scattered out (mechanism 1/ and 2/) of the elementary volume of length ds is given by :

$$-(\mu_a + \mu_s)\, I(s,\vec{\Omega}) dS d\Omega ds$$

These coefficients are related to the **particle cross section**: $\mu_a = \rho\, \sigma_a$ and $\mu_s = \rho\, \sigma_s$, where ρ is the particles concentration (unit m^{-3}), and σ_a is the absorption cross section (unit m^2), σ_s is the scattering cross section if particles are all the same and scattering events independent. Such cross sections can be calculated using electromagnetic theory, such as the Mie theory for spherical particles for instance. In most cases however, μ_a and μ_s are extracted from experiments (for each wavelength).

To calculate the third contribution to flux variation (light scattered into the considered volume), the so called "**phase function**" $p(\vec{\Omega},\vec{\Omega}')$ needs to be introduced. This function describes the dependence of scattered radiance on scattering angle. It is the fraction of flux arriving with a $\vec{\Omega}'$ direction, and scattered in the $\vec{\Omega}$ direction. There are several ways of normalizing this function. In these lectures, we use the following equation:

$$\frac{1}{4\pi}\int_{4\pi} p\left(\vec{\Omega},\vec{\Omega'}\right) d\vec{\Omega}' = \omega_0 = \frac{\mu_s}{\mu_a + \mu_s}$$

ω_0 is the albedo. $\omega_0 = 1$ means that there is no absorption (conservative transport). This normalization condition has the advantage of simplifying the writing of the radiative transfer equation (see later).

In the case of a homogenous medium, the phase function is in fact only a function of $\cos\Theta = \vec{\Omega}\cdot\vec{\Omega}'$. In consequence, $p(\vec{\Omega},\vec{\Omega}') = p(\vec{\Omega}'\cdot\vec{\Omega})$. For the parallel plane problem, we have :

$$cos\Theta = \cos\theta' \cos\theta + \sin\theta' \sin\theta \, cos(\varphi - \varphi'), = \mu'\mu \, + \sqrt{1-\mu'^2}\sqrt{1-\mu^2} cos(\varphi - \varphi')$$

Indeed, in spherical coordinate,

$$\vec{\Omega} = \begin{pmatrix} \sin\theta \, cos\varphi \\ \sin\theta \, sin\varphi \\ \cos\theta \end{pmatrix} \text{ and } \vec{\Omega}\,' = \begin{pmatrix} \sin\theta' \, cos\varphi' \\ \sin\theta' \, sin\varphi' \\ \cos\theta' \end{pmatrix}$$

$$\vec{\Omega}\cdot\vec{\Omega}' = \sin\theta \, cos\varphi \, \sin\theta' cos\varphi' + \sin\theta \, sin\varphi \, \sin\theta' sin\varphi' + \cos\theta\cos\theta'$$

$$\vec{\Omega}\cdot\vec{\Omega}' = \cos\theta\cos\theta' + \sin\theta\sin\theta'(cos\varphi \, cos\varphi' + \, sin\varphi \, sin\varphi')$$

$$\vec{\Omega}\cdot\vec{\Omega}' = \cos\theta\cos\theta' + \sin\theta\sin\theta' cos(\varphi - \varphi')$$

The most used phase functions are:

- Uniform phase function (isotropic scattering)
- Rayleigh phase function (for particles smaller than the wavelength) : $p(cos\Theta) \propto 1 + cos\Theta$
- The Mie phase function (for spherical metallic or dielectric particles of any size), solution of Maxwell equations,
- Henyey-Greenstein phase function, which is an empirical phase function, with a parameter g which allows to tune the degree of anisotropy. $p(cos\Theta) \propto \frac{1-g^2}{(1+g^2-2g\, cos\Theta)^{3/2}}$

The normalization condition becomes in spherical coordinates :

$$\frac{1}{4\pi}\int_{4\pi} p\left(\vec{\Omega},\vec{\Omega'}\right) d\vec{\Omega}' = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} d\Theta \, sin\Theta \, p(\Theta) = \omega_0$$

Using the phase function concept, the contribution of light scattered in the solid angle dΩ coming from other directions dΩ' to the power variation is:

$$\frac{\mu_a \, + \, \mu_s}{4\pi} dSd\Omega ds \int_{4\pi} p(\vec{\Omega},\vec{\Omega}') \, I\left(s,\vec{\Omega'}\right) d\vec{\Omega}\,'$$

We thus have :

$$\frac{d\, I}{ds} = -(\mu_a + \mu_s)\, I\left(s,\vec{\Omega}\right) + \frac{\mu_a \, + \, \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}') \, I\left(s,\vec{\Omega'}\right) d\vec{\Omega'}$$

The s variable depends on the considered light direction $\vec{\Omega}$. We can detail this derivative in cartesian coordinate:

$$dI = \frac{\partial\, I}{\partial x}dx + \frac{\partial\, I}{\partial y}dy + \frac{\partial\, I}{\partial z}dz = \vec{\nabla} I \cdot d\vec{r}$$

$$ds = \vec{\Omega}\cdot d\vec{r} = \Omega_x dx + \Omega_y dy + \Omega_z dz$$

Thus :

$$\frac{d\, I}{ds} = \vec{\nabla}\cdot\left(I\,\vec{\Omega}\right) = \vec{\Omega}\cdot\overrightarrow{\text{grad}}\, \text{I} = div(I\,\vec{\Omega})$$

This equation can be simplified in the case of the plane parallel problem. Indeed, first of all, for specular incidence at normal incidence or for diffuse lighting, we have an azimuthal symmetry (the specific intensity or luminance does not depend on φ). Moreover, let us notice that s = z/μ (Fig.1 and 3)

Finally :

$$\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\, I\left(s,\vec{\Omega'}\right) d\vec{\Omega'} = \frac{1}{4\pi}\int_0^{2\pi} d\varphi' \int_0^{\pi} d\theta' \, sin\theta' p(\theta,\varphi,\theta',\varphi')\, I(z,\theta',\varphi')$$

$$\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\, I\left(s,\vec{\Omega'}\right) d\vec{\Omega'} = \frac{1}{4\pi}\int_0^{2\pi} d\varphi' \int_{-1}^{1} d\mu' \, p(\mu,\varphi,\mu',\varphi')\, I(z,\mu',\varphi')$$

To eliminate the φ dependence, we integrate the previous equation with respect to φ on the full 2π range. The equation thus reduces to :

$$\mu \frac{d\, I}{dz} = (\mu_a + \mu_s)\left[-I + \frac{1}{2}\int_{-1}^{1} p_0(\mu,\mu')\, I(z,\mu')\, d\mu' \right]$$

with:

$$p_0(\mu,\mu') = \frac{1}{2\pi}\int_0^{2\pi} d\varphi' \int_0^{2\pi} d\varphi\, p(\mu,\varphi,\mu',\varphi')$$

The normalization condition being:

$$\frac{1}{2}\int_0^{\pi} p_0(\Theta)\, sin\Theta\, d\Theta = \omega_0$$

(This new phase function can be simplified using an expansion in term of Legendre polynomials). In the next, for simplification, we will note p the p_0 phase function.

Introducing the optical distance $\boxed{\tau = (\mu_a + \mu_s)\, z}$,

$$\boxed{\mu \frac{d\, I}{d\tau} = -I + \frac{1}{2}\int_{-1}^{1} p(\mu,\mu')\, I(\tau,\mu')\, d\mu'}$$

Solutions of this equation will be discussed in the next section.

3.2 Flux conservation

Let us examine the conservation of the flux F(z) by integrating the previous equation along all solid angle. As

$$F(z) = 2\pi \int_{-1}^{1} I(z,\mu)\, \mu\, d\mu$$

$$\frac{d\, F}{dz} = (\mu_a + \mu_s)\left[-2\pi \int_{-1}^{1} I(z,\mu)\, d\mu + \pi \int_{-1}^{1}\int_{-1}^{1} p(\mu,\mu')\, I(z,\mu')\, d\mu'\, d\mu \right]$$

Using the fact that :

$$\frac{1}{2}\int_{-1}^{1} p(\mu,\mu')\, d\mu' = \omega_0$$

We thus have :

$$\frac{d\,F}{dz} = 2\pi\,(\mu_a + \mu_s)(\omega_0 - 1)\int_{-1}^{1} I(z,\mu)\, d\mu$$

Therefore, dF / dz is equal to zero (conservative system) if the albedo is equal to 1 (no absorption).

3.3 Reduced incident intensity I_r and diffuse intensity I_d

The specific intensity can be split between reduced incident intensity I_r and diffuse intensity I_d.
The reduced incident intensity relates to light from the initial incident beam that retains its original collimated wave form and has not been absorbed or scattered. It therefore obeys the following "easy to solve" differential equation:

$$\frac{d\,I_r}{ds} = -(\mu_a + \mu_s)\, I_r$$

In the plane parallel problem, the collimated incident flux can be written as :

$$I_r(z = 0, \vec{\Omega}) = F_0\, \delta_\Omega(\vec{\Omega})$$

Where $\delta_\Omega(\vec{\Omega})$ denotes a Dirac peak in the positive z direction (θ = 0), defined in standard physicist notation, with the well known properties :

$$\int_\Omega \delta_\Omega(\vec{\Omega}) d\Omega = 1$$

$$\int_\Omega \delta_\Omega(\vec{\Omega}) g(\vec{\Omega}) d\Omega = g(\theta = 0, \varphi)$$

Where g is an arbitrary function of $\vec{\Omega}$ continuous at $\theta = 0$.

The Dirac function on the $\vec{\Omega}$ direction satisfies:

$$\int_\Omega \delta_\Omega(\vec{\Omega}) d\Omega = 1 \qquad \int_\Omega 2\pi\, sin\theta\, \delta_\Omega(\vec{\Omega}) d\theta = \int_\Omega 2\pi\, \delta_\Omega(\vec{\Omega}) d\mu = 1$$

Other Dirac functions can be introduced:

$$\int_0^\pi \delta_\theta(\theta) d\theta = 1 \qquad \int_{-1}^{1} \delta_\mu(\mu - 1) d\mu = 1$$

We thus have :

$$I_r(z = 0, \vec{\Omega}) = F_0\, \delta_\Omega(\vec{\Omega}) = \frac{F_0}{2\pi}\frac{\delta_\theta(\theta)}{sin\theta} = \frac{F_0}{2\pi}\delta_\mu(\mu - 1)$$

The solution of the reduced specific intensity equation: $\mu\frac{d\,I_r}{d\tau} = -\,I_r$ is:

$$\boxed{I_r(\tau,\theta) = \frac{F_0}{2\pi}\, e^{-\tau/\mu}\frac{\delta_\theta(\theta)}{sin\theta} = \frac{F_0}{2\pi}\, e^{-\tau/\mu}\delta_\mu(\mu - 1)}$$

The diffuse specific intensity is solution of :

$$\frac{d\,I_d}{ds} = -(\mu_a + \mu_s)\,I_d + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\,I_d(s,\vec{\Omega}')d\vec{\Omega}' + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\,I_r\left(s,\vec{\Omega}'\right)d\vec{\Omega}'$$

Leading to

$$\mu\frac{d\,I_d}{d\tau} = -I_d + \frac{1}{2}\int_{-1}^{1} p(\mu,\mu')\,I_d(\tau,\mu')\,d\mu' + \frac{1}{2}\int_{-1}^{1} p(\mu,\mu')\frac{F_0}{2\pi}\,e^{-\tau/\mu'}\delta(\mu'-1)\,d\mu'$$

$$\boxed{\mu\frac{d\,I_d}{d\tau} = -I_d + \frac{1}{2}\int_{-1}^{1} p(\mu,\mu')\,I_d(\tau,\mu')\,d\mu' + \frac{1}{4\pi}F_0\,e^{-\tau}p(\mu,1)}$$

In many cases, there is no incident diffuse flux on both side of the layer, which make easier the application of boundary conditions. As an example, in the plan parallel problem:

$$I_d(z=0,\mu>0) = 0 \quad I_d(z=d,\mu<0) = 0$$

IV Solution of the transfer radiative equation in the first order approximation

The radiative transfer equation can thus be written as:

$$\mu\frac{d\,I_d}{d\tau} = -I_d + S(\tau,\mu)$$

where S is a "source term" given by:

$$S(\tau,\mu) = \frac{1}{2}\int_{-1}^{1} p(\mu,\mu')\,I_d(\tau,\mu')\,d\mu' + \frac{1}{4\pi}F_0\,e^{-\tau}p(\mu,1)$$

The former equation can be further compacted by the following variable change:

$$I_d(\tau,\mu) = J(\tau,\mu)e^{-\tau/\mu}$$

$$\mu\frac{d\,I_d}{d\tau} = \mu\frac{d\,J}{d\tau}e^{-\tau/\mu} - Je^{-\frac{\tau}{\mu}} = \mu\frac{d\,J}{d\tau}e^{-\tau/\mu} - I_d$$

We thus have:

$$\mu\frac{d\,J}{d\tau} = S(\tau,\mu)e^{\tau/\mu} = \frac{1}{2}\int_{-1}^{1} p(\mu,\mu')J(\tau,\mu')e^{-\tau/\mu'}e^{\tau/\mu}\,d\mu' + \frac{1}{4\pi}F_0\,e^{-\tau}e^{\tau/\mu}p(\mu,1)$$

The "formal" solution of this equation is:

$$\boxed{J(\tau,\mu) = \int_0^{\tau}\frac{S(u,\mu)}{\mu}e^{u/\mu}du + C}$$

$$I_d(\tau,\mu) = e^{-\tau/\mu}\int_0^{\tau}\frac{S(u,\mu)}{\mu}e^{u/\mu}\,du + Ce^{-\tau/\mu}$$

By applying the proper boundary conditions $I_d(\tau=0,\mu>0)=0 \quad I_d(\tau=\tau_d,\mu<0)=0$

$$I_d(\tau,\mu>0) = e^{-\tau/\mu}\int_0^{\tau}\frac{S(u,\mu)}{\mu}e^{u/\mu}\,du$$

$$I_d(\tau,\mu<0) = -e^{-\tau/\mu}\int_{\tau}^{\tau_d}\frac{S(u,\mu)}{\mu}e^{u/\mu}\,du$$

As S depends on I_d, these solutions are useless in the general case. However, in the first order approximation:

$$S(\tau, \mu) \approx \frac{1}{4\pi} F_0 \, e^{-\tau} p(\mu, 1)$$

$$I_d(\tau, \mu > 0) = e^{-\tau/\mu} \frac{1}{4\pi} F_0 \, \frac{p(\mu, 1)}{\mu} \int_0^{\tau} e^{-u} e^{u/\mu} \, du$$

$$\boxed{I_d(\tau, \mu > 0) \approx \frac{1}{4\pi} F_0 \, \frac{p(\mu, 1)}{1 - \mu} \left(e^{-\tau} - e^{-\frac{\tau}{\mu}} \right)}$$

$$I_d(\tau, \mu < 0) = -e^{-\tau/\mu} \frac{1}{4\pi} F_0 \, \frac{p(\mu, 1)}{\mu} \int_{\tau}^{\tau_d} e^{-u} e^{u/\mu} \, du$$

$$I_d(\tau, \mu < 0) \approx \frac{1}{4\pi} F_0 \, \frac{p(\mu, 1)}{1 - \mu} e^{-\tau/\mu} \left(e^{\tau_d \left(\frac{1}{\mu} - 1\right)} - e^{\tau \left(\frac{1}{\mu} - 1\right)} \right)$$

$$\boxed{I_d(\tau, \mu < 0) \approx -\frac{1}{4\pi} F_0 \, \frac{p(\mu, 1)}{1 - \mu} \left(e^{\frac{\tau_d}{\mu} - \frac{\tau}{\mu} - \tau_d} - e^{-\tau} \right)}$$

We can deduce from these equations the diffuse reflectance and transmittance (for normal incidence) Rd_0 and Td_0.

Indeed, the incident normal irradiance is F_0, which can be double checked as:

$$F_r = 2\pi \int_0^1 I_r(0, \mu) \, \mu \, d\mu = 2\pi \int_0^1 \frac{F_0}{2\pi} \delta_\mu(\mu - 1) \, \mu \, d\mu = F_0$$

Consequently:

$$T_{d0} = \frac{1}{F_0} 2\pi \int_0^1 I_d(\tau_d, \mu > 0) \, \mu \, d\mu = \frac{1}{2} \int_0^1 \frac{\mu}{1 - \mu} p(\mu, 1) \left(e^{-\tau_d} - e^{-\frac{\tau_d}{\mu}} \right) d\mu$$

$$R_{d0} = \frac{1}{F_0} 2\pi \int_{-1}^0 I_d(0, \mu < 0) \, \mu \, d\mu = -\frac{1}{2} \int_{-1}^0 \frac{\mu}{1 - \mu} p(\mu, 1) \left(e^{\frac{\tau_d}{\mu} - \tau_d} - 1 \right) d\mu$$

These solutions are valid when the diffuse contribution is much lower than the specular one, in particular in case of absorbing medium ($\omega_0 < 0.9$) or poorly diffusing ($\tau < 0.4$).

V Solution of the radiative transfer equation by the discrete ordinates method

5.1 Discretization of the radiative transfer equation by the discrete ordinates method

We intend to solve the equation:

$$\mu \frac{d \, I_d}{d\tau} = -I_d + \frac{1}{2} \int_{-1}^{1} p(\mu, \mu') \, I_d(\tau, \mu') \, d\mu' + \frac{1}{4\pi} F_0 \, e^{-\tau} p(\mu, 1)$$

with the boundary conditions:

$$I_d(\tau = 0, \mu > 0) = 0 \quad I_d(\tau = \tau_d, \mu < 0) = 0$$

Note that in the particular case of isotropic scattering, $p(\mu, \mu') = \omega_0$.

The principle of the "discrete ordinates methods" consists in expanding $I_d(\tau, \mu)$ on a discrete set of 2N μ_n values. The discretization of μ was carefully chosen in order to get the best accuracy with a minimum N values when evaluating the scattering integral. To this aim, the Gauss's quadrature formula is used. This method allows approximating an integral by a sum with a very good approximation:

$$\int_{-1}^{1} f(x)dx \approx \sum_{j=-N}^{N} a_j f(x_j)$$

This result is obtained by a Lagrange interpolation formula:

$$f(x) \approx \sum_{j=-N}^{N} f(x_j) \frac{P_{2N}(x)}{(x-x_j){P_{2N}}'(x_j)}$$

where P_{2N} is the Legendre polynomial of degree 2N, x_j its roots, which satisfy:

$$\frac{P_{2N}(x_j)}{(x-x_j){P_{2N}}'(x_j)} = 1$$

a_j are the Christoffel number associated with P_{2N}, given by:

$$a_j = \int_{-1}^{1} \frac{P_{2N}(x)}{(x-x_j){P_{2N}}'(x_j)} dx$$

Which, in the case of Legrendre polynomial, reduces to: $a_j = \frac{2}{(1-{x_j}^2){P_{2N}}'(x_j)^2}$

Introducing the Gauss's quadrature formula into the ETR equation:

$$\mu \frac{d\, I_d}{d\tau} = -I_d + \frac{1}{2} \sum_{j=-N}^{N} a_j\, p(\mu, \mu_j)\, I_d(\tau, \mu_j) + \frac{1}{4\pi} F_0\, e^{-\tau} p(\mu, 1)$$

where μ_j are the roots of the Legrendre polynomial of degree 2N, and a_j the corresponding Christoffel number. We thus obtain a set of 2N discrete equations:

$$\frac{d\, I_d(\tau, \mu_i)}{d\tau} + \frac{I_d(\tau, \mu_i)}{\mu_i} - \sum_{j=-N}^{N} a_j\, p(\mu_i, \mu_j) \frac{I_d(\tau, \mu_j)}{2\mu_i} = \frac{1}{4\pi} F_0\, e^{-\tau} \frac{p(\mu_i, 1)}{\mu_i}$$

which can be written as a compact matrix formula:

$$\frac{d}{d\tau} I(\tau) + S\, I(\tau) = Be^{-\tau}$$

Where I, B are 2N sized vectors and S a 2N × 2N matrix. Matrix elements are:

$$S_{ii} = \frac{1}{\mu_i} - \frac{1}{2\mu_i} a_i\, p(\mu_i, \mu_i)$$

$$S_{ij} = -\frac{1}{2\mu_i} a_j\, p(\mu_i, \mu_j)$$

$$B_i = \frac{1}{4\pi} F_0\, \frac{p(\mu_i, 1)}{\mu_i}$$

The system of coupled ordinary differential equation is linear, and can be solved by the classical procedure. First, a particular solution is obtained:

$$I_p(\tau) = Ae^{-\tau}$$

$$A = (S - 1)^{-1} B$$

Then, the complementary solution is:

$$\frac{d}{d\tau} I_c(\tau) + S\, I_c(\tau) = 0$$

Assuming that the complementary solution is given by $I_c = X e^{-\lambda\tau}$, the λ and X value must satisfy:

$$S\, X = \lambda\, X$$

which means that X and λ can be found by solving a matrix eigenvalue problem. The final complementary solution is a linear combination of all the eigenvectors of the S matrix:

$$I_c = \sum_{n=-N}^{N} C_n\, X^{<n>} e^{-\lambda_n \tau}$$

Let us stress out that $X^{<n>}$ is a vector, while C_n and λ_n are scalar. The resulting diffuse luminance I is thus:

$$I = I_c + I_p = \sum_{n=-N}^{N} C_n\, X^{<n>} e^{-\lambda_n \tau} + A e^{-\tau}$$

The C_n coefficient are found by using the boundary conditions, as explained in the following.

5.2 Boundary conditions

5.2.1 Boundary conditions for the slab geometry (index matching)

For $i \in [1, N]$

$$I_d(\tau = 0, \mu_i > 0) = 0$$

$$\sum_{n=-N}^{N} C_n\, X_{i,n} + A_i = 0$$

For $i \in [-N, -1]$

$$I_d(\tau = \tau_d, \mu_i < 0) = 0$$

$$\sum_{n=-N}^{N} C_n\, X_{i,n} e^{-\lambda_n \tau_d} + A_i e^{-\tau_d} = 0$$

These two conditions can be put in one single matrix inversion (where the C vector is the unknown variable).

$$\begin{pmatrix} X_{N,N} & \cdots & X_{N,1} & X_{N,-1} & \cdots & X_{N,-N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ X_{1,N} & \cdots & X_{1,1} & X_{1,-1} & \cdots & X_{1,-N} \\ X_{-1,N} e^{-\lambda_N \tau_d} & \cdots & X_{-1,1} e^{-\lambda_1 \tau_d} & X_{-1,-1} e^{-\lambda_{-1} \tau_d} & \cdots & X_{-1,-N} e^{-\lambda_{-N} \tau_d} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ X_{-N,N} e^{-\lambda_N \tau_d} & \cdots & X_{-N,1} e^{-\lambda_1 \tau_d} & X_{-N,-1} e^{-\lambda_{-1} \tau_d} & \cdots & X_{-N,-N} e^{-\lambda_{-N} \tau_d} \end{pmatrix} \begin{pmatrix} C_N \\ \cdots \\ C_1 \\ C_{-1} \\ \cdots \\ C_{-N} \end{pmatrix} = - \begin{pmatrix} A_N \\ \cdots \\ A_1 \\ A_{-1} e^{-\tau_d} \\ \cdots \\ A_{-N} e^{-\tau_d} \end{pmatrix}$$

5.2.2 Boundary conditions for the semi-infinite plane geometry (index matching):

In this case, we need to suppress half of the λ_n eigenvalues: the ones that are negative. We thus need to find only N C_n scalar, and not 2N, as previously. The top interface boundary condition becomes :

For $i \in [1, N]$

$$I_d(\tau = 0, \mu_i > 0) = 0$$

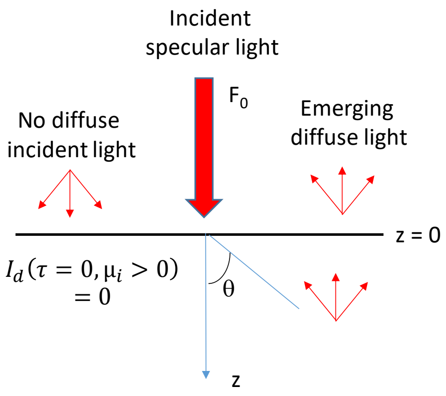
$$\sum_{\substack{n=1 \\ \lambda_n > 0}}^{N} C_n X_{i,n} + A_i = 0$$

For these particular n values, we have :

$$\begin{pmatrix} X_{N,N} & \cdots & X_{N,1} \\ \vdots & \ddots & \vdots \\ X_{1,N} & \cdots & X_{1,1} \end{pmatrix} \begin{pmatrix} C_N \\ \cdots \\ C_1 \end{pmatrix} = -\begin{pmatrix} A_N \\ \cdots \\ A_1 \end{pmatrix}$$

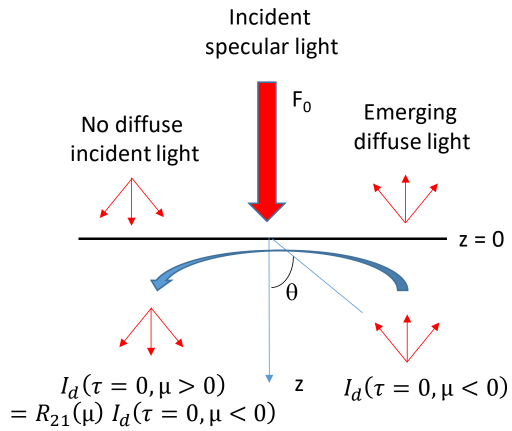
5.2.3 Boundary conditions for the slab geometry (no index matching, Fresnel reflections)

Usually, the diffusing slab medium (let us call it “2”) does not have the same optical index than the entrance medium at the front (let us call it “1”) and the exit medium on the back (let us call it “3”).



$$R_{cd} = \frac{\int_{\mu \leq 0} \mu \, I_d(\tau = 0, \mu) \, d\mu}{F_0}$$

Diagram illustrating boundary condition with index matching at the front interface. R_{cd} is the collimated to diffuse reflectance.



$$R_{cd} = \frac{\int_{\mu \leq 0} T_{21}(\mu) \, \mu \, I_d(\tau = 0, \mu) \, d\mu}{F_0}$$

Diagram illustrating boundary condition without index matching at the front interface. R_{cd} is the collimated to diffuse reflectance.

Boundary conditions than become:

$$I_d(\tau = 0, \mu > 0) = R_{21}(\mu) \, I_d(\tau = 0, \mu < 0)$$

$$I_d(\tau = \tau_d, \mu < 0) = R_{23}(\mu) \, I_d(\tau = \tau_d, \mu > 0)$$

Note that, according to Fresnel formulas, $R_{21}(\mu) \neq R_{12}(\mu)$ and $\mu = \cos(\theta) = \cos(-\theta)$.

It has to be noted that, if the optical index of the slab is higher than the surrounding media, a particular attention has to be paid to internal total reflection.

Moreover, the specular light is also subject to reflection at the back interface.

Let’s us first detail the application of the boundary condition in the RTE where reflection of the specular light at the back interface are neglected.

Consequently, for $i \in [1, N]$, we have N equations given by:

$$\sum_{n=-N}^{N} C_n X_{i,n} + A_i = R_{21}(\mu_i)\left(\sum_{n=-N}^{N} C_n X_{-i,n} + A_{-i}\right)$$

Here

$$\sum_{n=-N}^{N} C_n \left(X_{i,n} - R_{21}(\mu_i)X_{-i,n}\right) = R_{21}(\mu_i)A_{-i} - A_i$$

Consequently, for $i \in [-N, -1]$, we have again N equations given by :

$$\sum_{n=-N}^{N} C_n X_{i,n}e^{-\lambda_n\tau_d} + A_i e^{-\tau_d} = R_{23}(\mu_i)\left(\sum_{n=-N}^{N} C_n X_{-i,n}e^{-\lambda_n\tau_d} + A_{-i}e^{-\tau_d}\right)$$

$$\sum_{n=-N}^{N} C_n \left(X_{i,n} - R_{23}(\mu_i)X_{-i,n}\right)e^{-\lambda_n\tau_d} = R_{23}(\mu_i)A_{-i}e^{-\tau_d} - A_i e^{-\tau_d}$$

The C_n coefficient are found by inversing the corresponding matrix.

If the reflection at the back interface are included, the source term of the RTE changes and becomes:

$$\frac{1}{4\pi}p(\mu, 1)\, T_{1,2}(\mu = 1)\, F_0\, \frac{e^{-\tau} + R_n \exp(-(2\tau_d - \tau))}{1 - {R_n}^2 \exp(-2\tau_d)}$$

Where Rn is the Fresnel reflection at μ = 1 (0.04 % for n = 1.5).

We thus have :

$$\frac{d}{d\tau}I(\tau) + S\, I(\tau) = Be^{-\tau} + B'e^{\tau}$$

$$B_i = \frac{1}{4\pi}T_{1,2}(\mu = 1)\, F_0\, \frac{p(\mu_i, 1)}{\mu_i}\frac{1}{1 - {R_n}^2 \exp(-2\tau_d)}$$

$$B'_i = \frac{1}{4\pi}T_{1,2}(\mu = 1)\, F_0\, \frac{p(\mu_i, 1)}{\mu_i}\frac{R_n \exp(-2\tau_d)}{1 - {R_n}^2 \exp(-2\tau_d)}$$

We thus need to find two particular solutions:

$$I_p(\tau) = Ae^{-\tau} + A'e^{-\tau}$$

By linearity :

$$A = (S - 1)^{-1}B$$

$$A' = (S + 1)^{-1}B'$$

Finally, the application of the boundary conditions is also impacted. Indeed, for $i \in [1, N]$, we have N equations given by:

$$\sum_{n=-N}^{N} C_n X_{i,n} + A_i + A'_i = R_{21}(\mu_i)\left(\sum_{n=-N}^{N} C_n X_{-i,n} + A_{-i} + A'_{-i}\right)$$

Here

$$\sum_{n=-N}^{N} C_n \left(X_{i,n} - R_{21}(\mu_i) X_{-i,n}\right) = R_{21}(\mu_i) A_{-i} - A_i + R_{21}(\mu_i) A'_{-i} - A'_i$$

For the second interface, for $i \in [-N, -1]$, we have again N equations given by :

$$\sum_{n=-N}^{N} C_n X_{i,n} e^{-\lambda_n \tau_d} + A_i e^{-\tau_d} + A'_i e^{\tau_d} = R_{23}(\mu_i) \left(\sum_{n=-N}^{N} C_n X_{-i,n} e^{-\lambda_n \tau_d} + A_{-i} e^{-\tau_d} + A'_{-i} e^{\tau_d} \right)$$

$$\sum_{n=-N}^{N} C_n \left(X_{i,n} - R_{23}(\mu_i) X_{-i,n}\right) e^{-\lambda_n \tau_d} = R_{23}(\mu_i) A_{-i} e^{-\tau_d} - A_i e^{-\tau_d} + R_{23}(\mu_i) A'_{-i} e^{\tau_d} - A'_i e^{\tau_d}$$

Again, the C_n coefficient are found by inversing the corresponding matrix.

5.2.4 Boundary conditions for the semi-infinite plane geometry (no index matching, Fresnel reflections)

$$I_d(\tau = 0, \mu > 0) = R_{21}(\mu)\, I_d(\tau = 0, \mu < 0)$$

$$\sum_{\substack{n=-N \\ \lambda_n > 0}}^{N} C_n \left(X_{i,n} - R_{21}(\mu_i) X_{-i,n}\right) = R_{21}(\mu_i) A_{-i} - A_i$$

VI The diffusion approximation of the transfer equation

The diffusion approximation is an approximated solution of the radiative transfer equation, valid in highly scattering media (turbid media). This simple approximation has been extensively used to model light scattering in extremely diffusing medium such as the skin (and living tissue) or paper for instance. Contrary to the RTE, it provides easy 2D and 3D solutions, and also time dependent solution. The major difficulty in using the diffusion approximation relies in the application of boundary conditions, which is discussed in here after. Moreover, note that the diffusion approximation may not be valid in the first step of the light propagation (at the early step of light scattering).

6.1 Derivation of the diffusion equations

If the medium is extremely diffusing, the diffuse specific intensity I_d is approximately uniform (Lambertian), i.e. for every point M :

$$I_d(M,\vec{\Omega}) \approx I_d(M,-\vec{\Omega}) \approx C^{st}(M)$$

The constant C is simply the **average diffuse specific intensity** given by:

$$\boxed{U(M) = \int_{4\pi} I_d(M,\vec{\Omega}) \frac{d\Omega}{4\pi}}$$

However, the specific intensity cannot be strictly considered isotropic, otherwise there would not be any light transport. Indeed, the flux or **irradiance F** (W/m^2) is:

$$\boxed{\vec{F}(M) = \int_{4\pi} I_d(M,\vec{\Omega})\, \vec{\Omega}\, d\Omega}$$

And in the case of a strictly isotropic diffusion:

$$\vec{F}(M) = \int_{4\pi} I_d(M,\vec{\Omega})\, \vec{\Omega}\, d\Omega = U(M) \int_{4\pi} \vec{\Omega}\, d\Omega = 0$$

(As $\int_{4\pi} \vec{\Omega}\, d\Omega = 0$ (see appendix 1)).

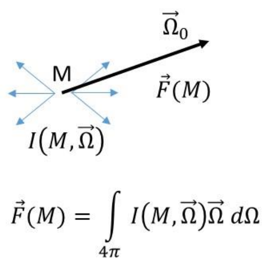


Fig. 4 : Flux and specific intensity in the diffusion approximation

Consequently, the diffuse specific intensity is written as a purely isotropic term + non isotropic term, assumed proportional to the total flux :

$$I_d(M,\vec{\Omega}) \approx U(M) + C^{st}\vec{F}(M)\cdot\vec{\Omega}$$

The constant C^{st} is fixed by:

$$\vec{F}(M) = \int_{4\pi} I_d(M,\vec{\Omega})\, \vec{\Omega}\, d\Omega = C^{st} \int_{4\pi} (\vec{F}(M)\cdot\vec{\Omega})\, \vec{\Omega}\, d\Omega = C^{st}\frac{4\pi}{3}\vec{F}$$

(As for any vector F, $\int_{4\pi}(\vec{F}(M)\cdot\vec{\Omega})\ \vec{\Omega}\ d\Omega = \frac{4\pi}{3}\vec{F}$, see appendix 2)

$$I_d(M,\vec{\Omega}) \approx U(M) + \frac{3}{4\pi}\vec{F}(M)\cdot\vec{\Omega}$$

The RTE for diffuse specific intensity is:

$$\frac{d\,I_d}{ds} = -(\mu_a + \mu_d)\ I_d(s,\vec{\Omega}) + \frac{\mu_a\ +\ \mu_d}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\ I_d\left(s,\vec{\Omega'}\right)d\Omega' + \frac{\mu_a\ +\ \mu_d}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\ I_r\left(s,\vec{\Omega'}\right)d\Omega'$$

In order to get an equation where the main unknown variable is the flux F (and not the intensity), we integrate the RTE over all possible direction, noticing that:

$$\frac{d\,I_d}{ds} = \vec{\Omega}\cdot\vec{\nabla}I_d = div(\vec{\Omega}\cdot I_d)$$

$$div(\vec{F}) = -(\mu_a + \mu_s)\ 4\pi\ U(\vec{r}) + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi}\left(\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')d\vec{\Omega}\right) I_d\left(s,\vec{\Omega'}\right)d\vec{\Omega}' + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi}\left(\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')d\vec{\Omega}\right) I_r\left(s,\vec{\Omega'}\right)d\vec{\Omega}'$$

$$\frac{1}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')d\vec{\Omega} = \omega_0 = \frac{\mu_s}{\mu_a\ +\ \mu_s}$$

$$div(\vec{F}) = -(\mu_a + \mu_s)\ 4\pi\ U(\vec{r}) + \mu_s\int_{4\pi} I_d\left(s,\vec{\Omega'}\right)d\vec{\Omega}' + \mu_s\int_{4\pi} I_r\left(s,\vec{\Omega'}\right)d\vec{\Omega}'$$

$$\boxed{div(\vec{F}) = -\mu_a\ 4\pi\ U(\vec{r}) + \mu_s\ 4\pi\ U_r(\vec{r})}$$

Where :

$$\boxed{U_r(\vec{r}) = \int_{4\pi} I_r(\vec{r},\vec{\Omega})\frac{d\Omega}{4\pi}}$$

A second equation can be obtained replacing the expression of I_d into the RTE :

$$\vec{\Omega}\cdot\vec{\nabla}I_d = -(\mu_a + \mu_s)\ I_d(s,\vec{\Omega}) + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\ I_d\left(s,\vec{\Omega'}\right)d\Omega' + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\ I_r\left(s,\vec{\Omega'}\right)d\Omega'$$

$$\vec{\Omega}\cdot\vec{\nabla}\left(U(M) + \frac{3}{4\pi}\vec{F}(M)\cdot\vec{\Omega}\right) = -(\mu_a + \mu_s)\ \left[U(M) + \frac{3}{4\pi}\vec{F}(M)\cdot\vec{\Omega}\right] + \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\left[U(M) + \frac{3}{4\pi}\vec{F}(M)\cdot\vec{\Omega}'\right]d\Omega' + S_r(s,\vec{\Omega})$$

Where :

$$S_r(s,\vec{\Omega}) = \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega},\vec{\Omega}')\ I_r\left(s,\vec{\Omega'}\right)d\Omega'$$

$$\vec{\Omega}\cdot\vec{\nabla}\left(U(M)+\frac{3}{4\pi}\vec{F}(M)\cdot\vec{\Omega}\right)$$
$$=-(\mu_a+\mu_s)\left[U+\frac{3}{4\pi}\vec{F}\cdot\vec{\Omega}\right]+\mu_s U+\frac{\mu_a+\mu_s}{4\pi}\frac{3}{4\pi}\vec{F}(M)\cdot\int_{4\pi}p(\vec{\Omega},\vec{\Omega}')\,\vec{\Omega}'d\Omega'+S_r(s,\vec{\Omega})$$

Introducing $\vec{p}_1$:

$$\vec{p}_1=\frac{1}{4\pi}\int_{4\pi}p(\vec{\Omega},\vec{\Omega}')\,\vec{\Omega}'d\Omega'$$

Note that in the case of isotropic scattering,

$$\vec{p}_1=\frac{1}{4\pi}\omega_0\int_{4\pi}\vec{\Omega}'d\Omega'=0$$

Moreover in the case where $p(\vec{\Omega},\vec{\Omega}')=p(\Theta)$, $\vec{p}_1$ is oriented along $\vec{\Omega}$ and its norm p_1 does not depend on $\vec{\Omega}$.

In this common case,

$$\vec{p}_1=p_1\vec{\Omega}$$

$$\vec{\Omega}\cdot\vec{\nabla}U+\frac{3}{4\pi}\vec{\Omega}\cdot\vec{\nabla}\left(\vec{F}(M)\cdot\vec{\Omega}\right)=-\mu_a\,U+(\mu_a+\mu_s)\frac{3}{4\pi}[-1+p_1]\,\vec{F}\cdot\vec{\Omega}+S_r(s,\vec{\Omega})$$

We now multiply by $\vec{\Omega}$ and integrate over all 4π, noticing that:

$$\int_{\Omega}(\vec{F}\cdot\vec{\Omega})\;\vec{\Omega}\,d\Omega=\frac{4\pi}{3}\vec{F}\quad\text{(see appendix 2)}$$

$$\int_{4\pi}\vec{\Omega}\left(\vec{\Omega}\cdot\vec{\nabla}U\right)\,d\Omega=\frac{4\pi}{3}\vec{\nabla}U\quad\text{(see appendix 2)}$$

$$\int_{4\pi}\vec{\Omega}\left[\vec{\Omega}\cdot\vec{\nabla}\left(\vec{F}\cdot\vec{\Omega}\right)\right]d\Omega=0\quad\text{(see appendix 3)}$$

$$\frac{4\pi}{3}\vec{\nabla}U=(\mu_a+\mu_s)\vec{F}\cdot[-1+p_1]+\int_{4\pi}S_r(s,\vec{\Omega})\,\vec{\Omega}\;d\Omega$$

$$\boxed{\vec{\nabla}U=-\frac{3}{4\pi}(\mu_a+\mu_s)\vec{F}\cdot[1-p_1]+\frac{3}{4\pi}\int_{4\pi}S_r(s,\vec{\Omega})\,\vec{\Omega}\;d\Omega}$$

The quantity $(\mu_a+\mu_s)\cdot[1-p_1]$ is called the transport extinction coefficient, it means that in the case of anisotropic transport, the extinction coefficient is reduced by a factor $[1-p_1]$.

The former equation can be simplified replacing F as a function of U, as :

$$div(\vec{F})=-\mu_a\,4\pi\,U(\vec{r})+\mu_s\,4\pi\,U_r(\vec{r})$$

$$\Delta U=-\frac{3}{4\pi}(\mu_a+\mu_s)(1-p_1)(-\mu_a\,4\pi\,U+\mu_s\,4\pi\,U_r)+\frac{3}{4\pi}\vec{\nabla}\int_{4\pi}S_r(s,\vec{\Omega})\,\vec{\Omega}\;d\Omega$$

$$\Delta U=3\,\mu_a(\mu_a+\mu_s)(1-p_1)U-3\,\mu_s(\mu_a+\mu_s)(1-p_1)U_r+\frac{3}{4\pi}\vec{\nabla}\int_{4\pi}S_r(s,\vec{\Omega})\,\vec{\Omega}\;d\Omega$$

$$\Delta U-{\kappa_d}^2U=-3\,\mu_s(\mu_a+\mu_s)(1-p_1)U_r+\frac{3}{4\pi}\vec{\nabla}\int_{4\pi}S_r(s,\vec{\Omega})\,\vec{\Omega}\;d\Omega$$

$$\kappa_d=\sqrt{3\,\mu_a(\mu_a+\mu_s)(1-p_1)}$$

The diffusion model consists in solving the former equation, with the proper boundary conditions.
Once U is known, F can be deduced form :

$$\vec{F} = \frac{4\pi}{3(\mu_a + \mu_s)(1 - p_1)}\left(-\vec{\nabla}U + \frac{3}{4\pi}\int_{4\pi} S_r(s, \vec{\Omega})\,\vec{\Omega}\ \mathrm{d}\Omega\right)$$

$$\vec{F} = -\frac{4\pi}{3(\mu_a + \mu_s)(1 - p_1)}\vec{\nabla}U + \frac{1}{(\mu_a + \mu_s)(1 - p_1)}\int_{4\pi} S_r(s, \vec{\Omega})\,\vec{\Omega}\ \mathrm{d}\Omega$$

$$S_r(s, \vec{\Omega}) = \frac{\mu_a\ +\ \mu_s}{4\pi}\int_{4\pi} p(\vec{\Omega}, \vec{\Omega}')\, I_r\left(s, \vec{\Omega'}\right) d\Omega'$$

This equation, similar to Fick's law of particle diffusion, is usually written as:

$$\boxed{\vec{F} = -\frac{4\pi}{3(\mu_a + \mu_s)(1 - p_1)}\vec{\nabla}U + \vec{Q}_1}$$

The second term, Q_1 is:

$$\vec{Q}_1 = \frac{1}{4\pi(1 - p_1)}\int_{4\pi}\left(\int_{4\pi} p(\vec{\Omega}, \vec{\Omega}')\, I_r\left(s, \vec{\Omega'}\right) d\Omega'\right)\vec{\Omega}\ \mathrm{d}\Omega$$

$$\vec{Q}_1 = \frac{1}{4\pi(1 - p_1)}\int_{4\pi}\left(\int_{4\pi} p(\vec{\Omega}, \vec{\Omega}')\,\vec{\Omega}\ \mathrm{d}\Omega\right) I_r\left(s, \vec{\Omega'}\right) d\Omega'$$

If scattering are isotropic, then :

$$\int_{4\pi} p(\vec{\Omega}, \vec{\Omega}')\,\vec{\Omega}\ \mathrm{d}\Omega = p(\vec{\Omega}, \vec{\Omega}')\int_{4\pi}\vec{\Omega}\ \mathrm{d}\Omega = 0$$

Thus Q_1 represents the impact of anisotropy on the reduce intensity. Moreover:

$$\vec{Q}_1 = \frac{\vec{p}_1}{(1 - p_1)}U_r$$

Similarly,

$$\boxed{\Delta U - {\kappa_d}^2 U = -3\ \mu_s(\mu_a + \mu_s)(1 - p_1)U_r + \frac{3}{4\pi}(\mu_a + \mu_s)(1 - p_1)\vec{\nabla}\vec{Q}_1}$$

For isotropic scattering, the flux is simply:

$$\boxed{\vec{F} = -\frac{4\pi}{3(\mu_a + \mu_s)}\vec{\nabla}U}$$

Similarly :

$$\boxed{\Delta U - {\kappa_d}^2 U = -3\ \mu_s(\mu_a + \mu_s)U_r}$$

With

$$\kappa_d = \sqrt{3\ \mu_a(\mu_a + \mu_s)}$$

Appendix 1: Proof that $\int_{\Omega}\ \vec{\Omega}\, d\Omega = 0$

Noticing that :

$$\vec{\Omega} = \begin{pmatrix}\sin\theta\ cos\varphi\\ \sin\theta\ sin\varphi\\ \cos\theta\end{pmatrix}$$

We thus found that :

$$\int_{\Omega} \vec{\Omega}\, d\Omega = \begin{pmatrix} \int_0^{\pi} (\sin\theta)^2 d\theta \times \int_0^{2\pi} \cos\varphi\, d\varphi \\ \int_0^{\pi} (\sin\theta)^2 d\theta \times \int_0^{2\pi} \sin\varphi\, d\varphi \\ 2\pi \int_0^{\pi} \cos\theta \sin\theta\, d\theta \end{pmatrix} = 0$$

Appendix 2: Proof that, for any vector F, $\int_{\Omega} (\vec{F} \cdot \vec{\Omega})\ \vec{\Omega}\, d\Omega = \frac{4\pi}{3}\vec{F}$

$$\int_{\Omega} \left(\vec{F}(M) \cdot \vec{\Omega}\right) \vec{\Omega}\, d\Omega = \begin{pmatrix} F_x \times \int_0^{\pi} (\sin\theta)^3 d\theta \times \int_0^{2\pi} (\cos\varphi)^2\, d\varphi \\ F_y \times \int_0^{\pi} (\sin\theta)^3 d\theta \times \int_0^{2\pi} (\sin\varphi)^2\, d\varphi \\ F_z \times 2\pi \int_0^{\pi} \cos\theta^2 \sin\theta\, d\theta \end{pmatrix} = \begin{pmatrix} F_x \times \frac{4}{3} \times \pi \\ F_y \times \frac{4}{3} \times \pi \\ F_z \times 2\pi \frac{2}{3} \end{pmatrix} = \frac{4\pi}{3}\vec{F}$$

Appendix 3: Proof that for any vector F : $\int_{4\pi} \vec{\Omega}\ \left[\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right)\right] d\Omega = 0$

Indeed,

$$\vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right) = \begin{pmatrix} \partial F_x \Omega_x / \partial x \\ \partial F_y \Omega_y / \partial y \\ \partial F_z \Omega_z / \partial z \end{pmatrix}$$

$$\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right) = (\sin\theta \cos\varphi)^2 \frac{\partial F_x}{\partial x} + (\sin\theta \sin\varphi)^2 \frac{\partial F_y}{\partial y} + \cos\theta^2 \frac{\partial F_z}{\partial z}$$

$$\int_{4\pi} \vec{\Omega}\ \left[\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right)\right] d\Omega = \begin{pmatrix} \int_{4\pi} \sin\theta \cos\varphi\ \left[\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right)\right] \sin\theta d\theta d\varphi \\ \int_{4\pi} \sin\theta \sin\varphi\ \left[\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right)\right] \sin\theta d\theta d\varphi \\ \int_{4\pi} \cos\theta\ \left[\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right)\right] \sin\theta d\theta d\varphi \end{pmatrix}$$

$$\int_{4\pi} \sin\theta \cos\varphi\ \left[\vec{\Omega} \cdot \vec{\nabla}\left(\vec{F} \cdot \vec{\Omega}\right)\right] \sin\theta d\theta d\varphi$$

$$= \frac{\partial F_x}{\partial x} \int_{4\pi} \sin\theta^2 \cos\varphi\, (\sin\theta \cos\varphi)^2 d\theta d\varphi + \frac{\partial F_y}{\partial y} \int_{4\pi} \sin\theta^2 \cos\varphi\, (\sin\theta \sin\varphi)^2 d\theta d\varphi$$

$$+ \frac{\partial F_z}{\partial z} \int_{4\pi} \sin\theta^2 \cos\varphi \cos\theta^2 d\theta d\varphi$$

$$\int_{4\pi} \sin\theta^2 \cos\varphi\, (\sin\theta \cos\varphi)^2 d\theta d\varphi = \int_0^{2\pi} (\cos\varphi)^3 d\varphi \times \int_0^{\pi} (\sin\theta)^3 d\theta = \frac{4}{3} \times 0$$

$$\int_{4\pi} \sin\theta^2 \cos\varphi\, (\sin\theta \sin\varphi)^2 d\theta d\varphi = \int_0^{2\pi} \cos\varphi\, (\sin\varphi)^2 d\varphi \times \int_0^{\pi} (\sin\theta)^4 d\theta = 0 \times \frac{3\pi}{8}$$

$$\int_{4\pi} \sin\theta^2 \, cos\varphi \, \cos\theta^2 d\theta d\varphi = \int_0^{2\pi} cos\varphi \, d\varphi \times \int_0^{\pi} (sin\theta)^2 (cos\theta)^2 d\theta = 0 \times \frac{\pi}{8}$$

6.2 Boundary conditions for diffusion equations

6.2.1 Boundary conditions with index matching : general case

In the plane parallel problem, we have seen the following boundary conditions :

$$I_d(\tau = 0, \mu > 0) = 0 \quad I_d(\tau = \tau_d, \mu < 0) = 0$$

In the diffusion approximation, the main variable is no longer the specific intensity, but the average diffuse specific intensity, which make more difficult to apply the same boundary condition.

Indeed, the average diffuse specific intensity, is :

$$U(\vec{r}) = \int_{4\pi} I_d(\vec{r}, \vec{\Omega}) \frac{d\Omega}{4\pi}$$

Leading to in the case of the parallel plane problem:

$$U(\tau) = \frac{1}{2} \int_1^1 I_d(\tau, \mu) d\mu$$

It is not possible to apply the exact boundary condition to U, with contains both $I_d(\mu > 0)$ and $I_d(\mu < 0)$ at each point. An approximate solution consists in assuming that the total inward diffuse flux (instead of the specific intensity) is equal to zero.

If $\vec{n}$ is a normal vector to the surface directed inward, then :

$$\int_{2\pi} I_d(\vec{r}_s, \vec{\Omega}) \left(\vec{\Omega} \cdot \vec{n}\right) d\Omega = 0$$

Note that the integration is performed only for the half of the solid angle $\theta \epsilon \left[0, \frac{\pi}{2}\right]$.

For the parallel plane problem, we would have :

$$F^+(0) = 0 = 2\pi \int_0^1 I(0, \mu) \, \mu \, d\mu$$

$$F^-(\tau_d) = 0 = -2\pi \int_{-1}^0 I(\tau_d, \mu) \, \mu \, d\mu$$

Let us derive the boundary condition as a function of U and F only. As:

$$I_d(\vec{r}, \vec{\Omega}) \approx U(\vec{r}) + \frac{3}{4\pi} \vec{F}(\vec{r}) \cdot \vec{\Omega}$$

$$\int_{2\pi} I_d(\vec{r}_s, \vec{\Omega}) \left(\vec{\Omega} \cdot \vec{n}\right) d\Omega = \int_{2\pi} \left(U(\vec{r}_s) \left(\vec{\Omega} \cdot \vec{n}\right) + \frac{3}{4\pi} \vec{F}(\vec{r}_s) \cdot \vec{\Omega} \left(\vec{\Omega} \cdot \vec{n}\right) \right) d\Omega = 0$$

The first term is:

$$\int_{2\pi} U(\vec{r}_s) \left(\vec{\Omega} \cdot \vec{n}\right) d\Omega = U(\vec{r}_s) \int_0^{\pi/2} \cos\theta \, 2\pi \sin\theta \, d\theta = U(\vec{r}_s)\pi$$

For the second term, we first introduce normal and tangential flux to the surface:

$$\vec{F}(\vec{r}_s) = F_n(\vec{r}_s)\vec{n} + F_t(\vec{r}_s)\vec{t}$$

$$\int_{2\pi} \left(\frac{3}{4\pi} F_n(\vec{r}_s)(\vec{n}\cdot\vec{\Omega})\,(\vec{\Omega}\cdot\vec{n}) \right) d\Omega = \frac{3}{4\pi} F_n(\vec{r}_s) \int_0^{\pi/2} (\cos\theta)^2\, 2\pi \sin\theta\, d\theta = \frac{F_n(\vec{r}_s)}{2}$$

$$\int_{2\pi} \left(\frac{3}{4\pi} F_t(\vec{r}_s)(\vec{t}\cdot\vec{\Omega})\,(\vec{\Omega}\cdot\vec{n}) \right) d\Omega = \frac{3}{4\pi} F_t(\vec{r}_s) \int_0^{2\pi}\int_0^{\pi/2} \cos\varphi\, \sin\theta \cos\theta \sin\theta\, d\theta d\varphi = 0$$

Finally:

$$\boxed{\int_{2\pi} I_d(\vec{r}_s,\vec{\Omega})\,(\vec{\Omega}\cdot\vec{n})\, d\Omega = U(\vec{r}_s)\pi + \frac{F_n(\vec{r}_s)}{2} = 0}$$

Note that, in the parallel plane problem,

$$F^+(z) = 2\pi \int_0^1 I(z,\mu)\,\mu\, d\mu \approx U(z)\pi + \frac{F(z)}{2}$$

$$F^-(z) = -2\pi \int_0^1 I(z,\mu)\,\mu\, d\mu \approx U(z)\pi - \frac{F(z)}{2}$$

We know express F_n as a function of U using :

$$\vec{F} = -\frac{4\pi}{3(\mu_a+\mu_s)(1-p_1)}\vec{\nabla}U + \vec{Q}_1$$

$$U(\vec{r}_s) + \frac{F_n(\vec{r}_s)}{2\pi} = U(\vec{r}_s) - \frac{2}{3(\mu_a+\mu_s)(1-p_1)}\vec{\nabla}U\cdot\vec{n} + \frac{\vec{Q}_1\cdot\vec{n}}{2\pi}$$

We thus have :

$$\boxed{U(\vec{r}_s) - \frac{2}{3(\mu_a+\mu_s)(1-p_1)}\vec{\nabla}U\cdot\vec{n} + \frac{\vec{Q}_1\cdot\vec{n}}{2\pi} = 0}$$

In the isotropic case:

$$\boxed{U(\vec{r}_s) - \frac{2}{3(\mu_a+\mu_s)}\vec{\nabla}U\cdot\vec{n} = 0}$$

6.2.2 Boundary conditions with index matching : plane parallel case

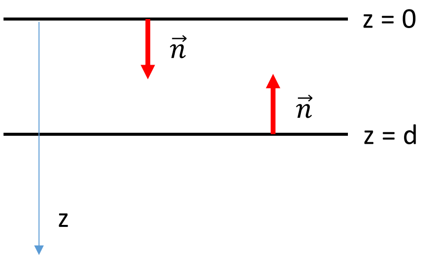


Fig. 5 : Definition of the normal vector n for the slab geometry for the incoming flux at z=0 and z=d

By applying the last formula (isotropic scattering), in the parallel plane problem, taking into account the sign of the $(\vec{u}_z\cdot\vec{n})$ scalar product, we have at z = 0:

$$U(0) - \frac{2}{3(\mu_a+\mu_s)}\frac{dU}{dz}(0) = 0$$

And at z = d :

$$U(d) + \frac{2}{3(\mu_a + \mu_s)} \frac{dU}{dz}(d) = 0$$

Note that the outcoming flux at z = 0 is thus :

$$F^-(0) \approx U(0)\pi + \frac{2\pi}{3(\mu_a + \mu_s)} \frac{dU}{dz}(0)$$

As :

$$U(0) = \frac{2}{3(\mu_a + \mu_s)} \frac{dU}{dz}(0)$$

$$F^-(0) \approx U(0)\pi + \frac{2\pi}{3(\mu_a + \mu_s)} \frac{dU}{dz}(0) = \frac{4\pi}{3(\mu_a + \mu_s)} \frac{dU}{dz}(0) = -F_z(0)$$

Thus, when U(z) is know, the outcouming flux can simply be calculated using the Fourier'law :

$$F_z(0) = -\frac{4\pi}{3(\mu_a + \mu_s)} \frac{dU}{dz}(0)$$

6.2.3 Boundary conditions without index matching (Fresnel conditions):

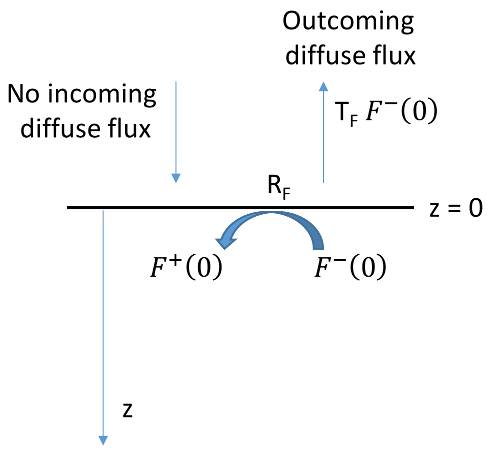


Fig. 6 : Boundary conditions with Fresnel reflection at the top interface

When Fresnel reflection occurs at the top interface, $F^+(0)$ can not be considered null because of internal reflexion. We thus have :

$$F^+(0) = R_F\, F^-(0)$$

$$U(0)\,\pi + \frac{F(0)}{2} = R_F \left(U(0)\,\pi - \frac{F(0)}{2} \right)$$

$$U(0)\,\pi(1 - R_F) + \frac{F(0)}{2}(1 + R_F) = 0$$

$$U(0)\,\pi + \frac{1 + R_F}{1 - R_F} \frac{F(0)}{2} = 0$$

$$U(0) - \frac{2}{3(\mu_a + \mu_s)} \frac{1 + R_F}{1 - R_F} \frac{dU}{dz}(0) = 0$$

R_F is the effective Fresnel reflection coefficient (Rogers, 1997) (0.574 for n = 1.5).

6.4.4 Approximated boundary conditions by a Dirichlet boundary condition

A commonly used simplification to apply the former boundary condition consists in extrapolating U(z) in z < 0 by a linear expression. Then :

$$U(0) - \frac{2}{3(\mu_a + \mu_s)} \frac{U(0) - U(-\Delta z)}{\Delta z} = 0$$

$$U(0)\left[\Delta z - \frac{2}{3(\mu_a + \mu_s)}\right] + \frac{2}{3(\mu_a + \mu_s)} U(-\Delta z) = 0$$

Let'us take :

$$\Delta z = \frac{2}{3(\mu_a + \mu_s)}$$

Then, the former boundary condition is equivalent to :

$$U(-\Delta z) = 0$$

which is easier to implement (especially in 2D or 3D real space problems).

The same equation holds in case of Fresnel reflections, with :

$$\Delta z = \frac{2}{3(\mu_a + \mu_s)} \frac{1 + R_F}{1 - R_F}$$