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# Numerical Simulation of Polarized Light and Temperature with a Refractive Interface

Olivier Pironneau<sup>1</sup>

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## Abstract

In this article we propose a numerical algorithm to compute the intensity and polarization of a multichromatic electromagnetic radiation crossing a medium with non constant refractive index and modeled by the Vector Radiative Refractive Transfer Equations (VRRTE). Special attention is given to the case where the refractive index has a discontinuity for which the Fresnel conditions are necessary. We assume that the only spatial variable of interest is the altitude (stratified medium). An algorithm based on iterations of the sources is shown to be monotone and convergent. Numerical examples are given with highly varying absorption coefficient  $\kappa$  and Rayleigh scattering as in the Earth atmosphere. To study the effect of CO<sub>2</sub> in the atmosphere  $\kappa$  is changed in the frequency ranges where CO<sub>2</sub> is absorbing.

*Keywords:* Radiative transfer, Polarization, Fresnel's law, Integral equation, Numerical analysis, Climate modeling. MSC classification 3510, 35Q35, 35Q85, 80A21, 80M10

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## 1. Introduction

Understanding and computing a multichromatic electromagnetic radiation crossing a medium with non constant refractive index and non constant absorption and scattering is a challenge for which the works of S. Chandrasekhar [3] and G. Pomraning [12] are fundamental. Applications are numerous in astrophysics, nuclear engineering, atmospheric sciences [4] and more recently image synthesis [1].

The medium is too large and the wavelengths too small to use Maxwell's equations, so the Radiative Transfer Equation (RTE) is used. It is an integro partial differential system in 6 dimensions, 3 for space, 2 for ray directions, 1 for frequencies; so it is a serious numerical challenge. With his coauthors the present author proposed to analyze the coupling of RTE with the temperature equation to understand the effect of the numerous physical parameters on the temperature in the Earth atmosphere. An algorithm based on iterations on the source was shown to be monotone and convergent for stratified media in [7] and in 3D for a general topography in [6]. The method was generalized to polarized light by using the vector RTE (VRTE) for stratified media [10]. Then it was further generalized to VRRTE (the second R is for refractive) for media with non-constant but smooth refractive index [9].

In this article the method is generalized to VRRTE with discontinuous refractive index for which the Fresnel conditions are necessary to match the Stokes vector on both sides of the discontinuity. We have used a formulation of Fresnel's conditions given by A. Garcia [5] which is well adapted to the VRRTE.

While Fresnel's conditions are natural jump conservations for the Maxwell equations, they are not natural to the VRRTE. Hence we had to include them in the integral semi-analytic solution of the VRRTE rather than in the partial differential equations (see sections 5 and 6).

By coupling the VRRTE with the temperature equation the problem becomes nonlinear. Iterations on the sources is a very simple idea in which the equations are solved with given right hand side (the sources) and then the sources are updated with the new solution. The temperature equation is solved with Newton iterations as explained in [7]. We prove here that the sequences are monotonous and that the solution can be approached from above and below, at least when the jump in the refractive index is not too large.

The method is tested numerically on two set of cases, one in which the light comes from the Sun and the other where the (infrared) light comes from Earth. These waves cross a medium which has a layer of large refractive index (like the sea) and the atmosphere above it which has a refractive index close to unity.

We intend to generalize the method to non stratified atmosphere as in [6].

## 2. Fundamental Equations

Light in a medium  $\Omega$  is an electromagnetic radiation satisfying Maxwell's equations. The electric field  $\mathbf{E} = \mathbf{E}_0 \exp(i(\mathbf{k} \cdot \mathbf{x} - \nu t))$  of a monochromatic plane wave of frequency  $\nu$  propagating in direction  $\mathbf{k}$ , is a solution to Maxwell equations which is suitable to describe the propagation of a ray for which  $\nu$  is very large.

Such radiations are characterized either by  $\mathbf{k}$  and  $\mathbf{E}_0$  or equivalently [3] by their Stokes vectors  $\mathbf{I} = [I, Q, U, V]^T$ , made of the irradiance  $I$  and 3 functions  $Q, U, V$  to define its state of polarization.

The radiation comes from the boundary but also from a the Planck law, a volume source  $\mathbf{F} = [\kappa_a B_\nu(T), 0, 0, 0]^T$  for an unpolarized-emitting black-body (for example due to the black-body radiation of air or water). It is defined in terms of the rescaled Planck function  $B_\nu(T) = \nu^3 (e^{\frac{\nu}{T}} - 1)^{-1}$ , and the rescaled temperature  $T$ . The range of frequencies of interest is  $\nu \in (0.01, 20) \times 10^{14}$ , hence a scaling is applied (see [7]):  $\nu$  is divided by  $10^{14}$  and  $T_K$  in Kelvin is divided by 4798:  $T = 10^{-14} \frac{k}{h} T_K = \frac{T_K}{4798}$ , where  $k$  and  $h$  are the Boltzmann and Planck constants. The parameter  $\kappa_a$  is related to absorption and scattering (see (3.3) below), which, by the way, are quantum effects, not described by Maxwell's equations.

Absorption and scattering are modeled by a system of integro-differential partial differential equations, known as VRRTE – short for Vector Radiative Refractive Transfer Equations – [12] p152. With  $\tilde{\mathbf{I}} := \mathbf{I}/n^2$ ,

$$\frac{n}{c} \partial_t \tilde{\mathbf{I}} + \boldsymbol{\omega} \nabla_{\mathbf{x}} \tilde{\mathbf{I}} + \frac{\nabla_{\mathbf{x}} n}{n} \cdot \nabla_{\boldsymbol{\omega}} \tilde{\mathbf{I}} + \kappa_{\nu} \tilde{\mathbf{I}} = \int_{\mathbb{S}_2} \mathbb{Z}(\mathbf{x}, \boldsymbol{\omega}' : \boldsymbol{\omega}) \tilde{\mathbf{I}} d\boldsymbol{\omega}' + \tilde{\mathbf{F}}, \quad (2.1)$$

for all  $\mathbf{x} \in \Omega$ ,  $\boldsymbol{\omega} \in \mathbb{S}_2$ , where  $c$  is the speed of light,  $n$  the refractive index of the medium,  $\mathbb{S}_2$  the unit sphere,  $\kappa$  the absorption and  $\mathbb{Z}$  the phase scattering matrix for rays  $\boldsymbol{\omega}'$  scattered in direction  $\boldsymbol{\omega}$  for each frequency  $\nu$ . It is assumed that  $n$  depends continuously on position  $\mathbf{x} \in \Omega$  except on surfaces of discontinuities on which additional jump conditions will be applied (Fresnel's laws);  $\kappa$  depends on  $\mathbf{x}$  and strongly on  $\nu$ , except at interfaces of strong discontinuities where the transmission, reflection and refraction are subject to Fresnel's law.

Because  $c$  is very large, the term  $\frac{1}{c} \partial_t \mathbf{I}$  is neglected. The thermal conductivity is also small so that ‘‘Thermal Equilibrium’’ is assumed:

$$\nabla_{\mathbf{x}} \cdot \int_{\mathbb{R}_+} \int_{\mathbb{S}_2} \tilde{I} \boldsymbol{\omega} d\boldsymbol{\omega} d\nu = 0. \quad (2.2)$$

**Notation 1.** *On all variables, the tilde indicates a division by  $n^2$ . Arguments of functions are sometimes written as indices like  $\kappa_{\nu}$  and  $n_z$ .*

Following [8], given a cartesian frame  $\mathbf{i}, \mathbf{j}, \mathbf{k}$ , the third term on the left in (2.1) is computed in polar coordinates, with

$$\boldsymbol{\omega} := \mathbf{i} \sin \theta \cos \varphi + \mathbf{j} \sin \theta \sin \varphi + \mathbf{k} \cos \theta, \quad \mathbf{s}_1 := -\mathbf{i} \sin \varphi + \mathbf{j} \cos \varphi,$$

$$\nabla_{\mathbf{x}} \log n \cdot \nabla_{\boldsymbol{\omega}} \tilde{\mathbf{I}} = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left\{ \tilde{\mathbf{I}} (\cos \theta \boldsymbol{\omega} - \mathbf{k}) \cdot \nabla_{\mathbf{x}} \log n \right\} + \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} \left\{ \tilde{\mathbf{I}} \mathbf{s}_1 \cdot \nabla_{\mathbf{x}} \log n \right\}.$$

When  $n$  does not depend on  $x, y$  but only on  $z$ , it simplifies to

$$\nabla_{\mathbf{x}} \log n \cdot \nabla_{\boldsymbol{\omega}} \tilde{\mathbf{I}} = (\partial_z \log n) \cdot \partial_{\mu} \left\{ (1 - \mu^2) \tilde{\mathbf{I}} \right\} \quad \text{where } \mu = \cos \theta.$$

### 3. The Stratified Case

For an atmosphere of thickness  $Z$  over a flat ground, the domain is  $\Omega = \mathbb{R}^2 \times (0, Z)$ , and all variables are independent of  $x, y$ . In [3], p40-53, expressions

for the phase matrix  $\mathbb{Z}$  are given for Rayleigh and isotropic scattering for  $I$  and  $Q$ ,

$$\mathbb{Z}_R = \frac{3}{2} \begin{bmatrix} 2(1-\mu^2)(1-\mu'^2) + \mu^2\mu'^2 & \mu^2 \\ \mu'^2 & 1 \end{bmatrix}, \quad \mathbb{Z}_I = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

For a given  $\beta \in [0, 1]$ , we shall consider a combination of  $\beta\mathbb{Z}_R$  (Rayleigh scattering) plus  $(1-\beta)\mathbb{Z}_I$  (isotropic scatterings) [3],[12],[13].

The two other components of the Stokes vectors have autonomous equations,

$$\mu\partial_z\tilde{U} + \partial_z \log n \cdot \partial_\mu \{(1-\mu^2)\tilde{U}\} + \kappa\tilde{U} = 0, \quad (3.1)$$

$$\mu\partial_z\tilde{V} + \partial_z \log n \cdot \partial_\mu \{(1-\mu^2)\tilde{V}\} + \kappa\tilde{V} = \frac{\mu}{2} \int_{-1}^1 \mu'\tilde{V}(z, \mu')d\mu'. \quad (3.2)$$

**Notation 2.** Denote the scattering coefficient  $a_s \in [0, 1)$ , which, as  $\kappa$ , is a function of altitude  $z$  and frequency  $\nu$ . Define

$$\kappa_s = \kappa a_s, \quad \kappa_a = \kappa - \kappa_s = \kappa(1 - a_s). \quad (3.3)$$

From (3.1),(3.2) we see that, if the light source at the boundary is unpolarized then  $U = V = 0$  and the light can be described either by  $I$  and  $Q$  or two orthogonal components  $I_l, I_r$ , such that  $I = I_l + I_r$  and  $Q = I_l - I_r$  (see [3]):

$$\left\{ \begin{array}{l} \mu\partial_z\tilde{I}_l + \partial_z \log n \cdot \partial_\mu \{(1-\mu^2)\tilde{I}_l\} + \kappa\tilde{I}_l \\ \quad = \frac{3\beta\kappa_s}{8} \int_{-1}^1 ([2(1-\mu'^2)(1-\mu^2) + \mu'^2\mu^2]\tilde{I}_l + \mu^2\tilde{I}_r)d\mu' \\ \quad + \frac{(1-\beta)\kappa_s}{4} \int_{-1}^1 [\tilde{I}_l + \tilde{I}_r]d\mu' + \frac{\kappa_a}{2} \tilde{B}_\nu(T(z)), \\ \mu\partial_z\tilde{I}_r + \partial_z \log n \cdot \partial_\mu \{(1-\mu^2)\tilde{I}_r\} + \kappa\tilde{I}_r = \frac{3\beta\kappa_s}{8} \int_{-1}^1 (\mu'^2\tilde{I}_l + \tilde{I}_r)d\mu' \\ \quad + \frac{(1-\beta)\kappa_s}{4} \int_{-1}^1 [\tilde{I}_l + \tilde{I}_r]d\mu' + \frac{\kappa_a}{2} \tilde{B}_\nu(T(z)), \end{array} \right. \quad (3.4)$$

Using an appropriate linear combination of (3.4), the system for  $\tilde{I}$  and  $\tilde{Q}$  is derived,

$$\left\{ \begin{array}{l} \mu\partial_z\tilde{I} + \partial_z \log n \cdot \partial_\mu \{(1-\mu^2)\tilde{I}\} + \kappa\tilde{I} \\ \quad = \kappa_a \tilde{B}_\nu + \frac{\kappa_s}{2} \int_{-1}^1 \tilde{I}d\mu' + \frac{\beta\kappa_s}{4} P_2(\mu) \int_{-1}^1 [P_2\tilde{I} - (1-P_2)\tilde{Q}]d\mu', \\ \mu\partial_z\tilde{Q} + \partial_z \log n \cdot \partial_\mu \{(1-\mu^2)\tilde{Q}\} + \kappa\tilde{Q} \\ \quad = -\frac{\beta\kappa_s}{4} (1-P_2(\mu)) \int_{-1}^1 [P_2\tilde{I} - (1-P_2)\tilde{Q}]d\mu', \end{array} \right. \quad (3.5)$$

where  $P_2(\mu) = \frac{1}{2}(3\mu^2 - 1)$ . The temperature  $T(z)$  is linked to  $I$  by (2.2) which, in the case of (3.5) is as follows.

**Proposition 1.** *Thermal equilibrium for (3.4) or (3.5) is*

$$\int_{\mathbb{R}_+} \kappa_a [\tilde{B}_\nu(T) - \frac{1}{2} \int_{-1}^1 \tilde{I} d\mu] d\nu = 0.$$

*Proof* Averaging in  $\mu$  the first equation of (3.5) leads to

$$\begin{aligned} \nabla_{\mathbf{x}} \cdot \int_{\mathbb{S}_2} \boldsymbol{\omega} \tilde{I} = \partial_z \left( \frac{1}{2} \int_{-1}^1 \mu \tilde{I} d\mu \right) &= -\frac{1}{2} \partial_z \log n \cdot \int_{-1}^1 \partial_\mu \{ (1 - \mu^2) \tilde{I} \} d\mu \\ &\quad - \frac{1}{2} \kappa \int_{-1}^1 \tilde{I} d\mu + \frac{1}{2} \int_{-1}^1 \kappa_a \tilde{B}_\nu d\mu + \frac{\kappa_s}{2} \int_{-1}^1 \tilde{I} d\mu', \end{aligned}$$

because  $\int_{-1}^1 P_2(\mu) d\mu = 0$ . Now the first term on the right integrates to zero and  $\kappa - \kappa_s = \kappa_a$ .  $\square$

For the numerical simulations (3.5) is more appropriate, but to derive energy estimates (3.4) is better. The differences are in the source terms and the boundary conditions, so we can easily switch from one to the other.

#### 4. A Stratified Medium with a Discontinuous Refractive Index

Consider 3 parallel planes at  $z = 0$ ,  $z = Y > 0$  and  $z = Z > Y$ . The refractive index of the medium is  $n^-$  when  $z < Y$  and  $n^+$  when  $z > Y$ . denote, when the roots exist,

$$n_\mp = \frac{n_-}{n_+}, \quad n_\pm = \frac{n_+}{n_-}, \quad \eta(n, \mu) = \sqrt{1 - n^2(1 - \mu^2)}, \quad \mu_c(n) = \sqrt{1 - \frac{1}{n^2}}. \quad (4.1)$$

Fresnel's refraction laws are [5],

$$\begin{aligned} \tilde{\mathbf{I}}(Y^-, -\mu) &= \mathbf{X}(n_\mp, \mu) \tilde{\mathbf{I}}(Y^-, \mu) + \mathbf{Y}(n_\mp, \mu) \tilde{\mathbf{I}}(Y^+, -\eta(n_\mp, \mu)), \quad \mu \in (0, 1), \\ \tilde{\mathbf{I}}(Y^+, \mu) &= \mathbf{X}(n_\pm, \mu) \tilde{\mathbf{I}}(Y^+, -\mu) + \mathbf{Y}(n_\pm, \mu) \tilde{\mathbf{I}}(Y^-, \eta(n_\pm, \mu)), \quad \mu \in (0, 1). \end{aligned} \quad (4.2)$$

$$\mathbf{X}(n, \mu) = \begin{cases} \mathbf{G}(n, \mu), & n \leq 1, \\ \mathbf{G}(n, \mu) H[\mu - \mu_c(n)] + \mathbf{\Gamma}(n, \mu) \{1 - H[\mu - \mu_c(n)]\}, & n \geq 1, \end{cases} \quad (4.3)$$

$$\mathbf{Y}(n, \mu) = \begin{cases} \mathbf{D}(n, \mu), & n \leq 1, \\ \mathbf{D}(n, \mu) H[\mu - \mu_c(n)], & n \geq 1. \end{cases} \quad (4.4)$$

Here  $\tilde{\mathbf{I}} \in \mathbb{R}^4$ ,  $\mathbf{X}, \mathbf{Y}$  are  $4 \times 4$  matrices given in terms of  $H$ , the Heaviside function and 3 matrices  $\mathbf{G}, \mathbf{D}, \mathbf{\Gamma}$ , for which the non-zero terms are ,

$$\begin{aligned} \Gamma_{11} &= \Gamma_{22} = 1, \\ G_{11}(n, \mu) &= G_{22}(n, \mu) = \frac{1}{2} \left\{ \left[ \frac{\mu - n\eta(n, \mu)}{\mu + n\eta(n, \mu)} \right]^2 + \left[ \frac{n\mu - \eta(n, \mu)}{n\mu + \eta(n, \mu)} \right]^2 \right\} \\ G_{12}(n, \mu) &= G_{21}(n, \mu) = \frac{1}{2} \left\{ \left[ \frac{\mu - n\eta(n, \mu)}{\mu + n\eta(n, \mu)} \right]^2 - \left[ \frac{n\mu - \eta(n, \mu)}{n\mu + \eta(n, \mu)} \right]^2 \right\} \\ D_{11}(n, \mu) &= D_{22}(n, \mu) = 2n\mu\eta(n, \mu) \left\{ \frac{1}{[\mu + n\eta(n, \mu)]^2} + \frac{1}{[n\mu + \eta(n, \mu)]^2} \right\} \\ D_{12}(n, \mu) &= D_{21}(n, \mu) = 2n\mu\eta(n, \mu) \left\{ \frac{1}{[\mu + n\eta(n, \mu)]^2} - \frac{1}{[n\mu + \eta(n, \mu)]^2} \right\} \\ \Gamma_{33} &= \Gamma_{44} = \frac{2(1 - \mu^2)^2}{1 - (1 + n^{-2})\mu^2} - 1, \quad \Gamma_{43} = -\Gamma_{34} = \frac{2\mu(1 - \mu^2)(\mu_c^2 - \mu^2)^{\frac{1}{2}}}{1 - (1 + n^{-2})\mu^2} \\ G_{33} &= G_{44} = \left( \frac{\mu - n\eta(n, \mu)}{\mu + n\eta(n, \mu)} \right) \left( \frac{n\mu - \eta(n, \mu)}{n\mu + \eta(n, \mu)} \right), \end{aligned}$$

**Remark 1.** Notice that

- if  $\tilde{\mathbf{I}} = [I, Q, 0, 0]^T$  in the right side of (4.2), then the last 2 components of  $\tilde{\mathbf{I}}$  on the left will also be zero. Therefore, when the polarization is with  $U = V = 0$ , we can work with  $\tilde{\mathbf{I}} = [\tilde{I}, \tilde{Q}]^T$  and the  $2 \times 2$  matrices obtained from the left upper part of the full matrices.
- Notice that if  $n \equiv 1$  then  $\mathbf{X} = 0$  and  $\mathbf{Y} = \mathbf{1}$ .
- Finally notice also that the eigenvalues of the  $2 \times 2$  matrices  $\mathbf{X}$  and  $\mathbf{Y}$  are real and less or equal to 1.

*Proof*

$$\mathbf{X} = \begin{pmatrix} a + b & a - b \\ a - b & a + b \end{pmatrix} \quad \text{with } a = \frac{1}{2} \left[ \frac{\mu - n\eta(n, \mu)}{\mu + n\eta(n, \mu)} \right]^2, \quad b = \frac{1}{2} \left[ \frac{n\mu - \eta(n, \mu)}{n\mu + \eta(n, \mu)} \right]^2$$

The eigenvalues  $\lambda$  are solutions of

$$\lambda^2 - 2\lambda(a + b) + 4ab = 0 \quad \Rightarrow \quad \lambda_1 = 2a, \quad \lambda_2 = 2b.$$

It is similar for  $\mathbf{Y}$  with  $a = \frac{2n\mu\eta(n, \mu)}{[\mu + n\eta(n, \mu)]^2} \leq \frac{1}{2}$  and  $b = \frac{2n\mu\eta(n, \mu)}{[n\mu + \eta(n, \mu)]^2} \leq \frac{1}{2}$ .  $\square$



**Remark 2.** It may be convenient to work with the 2 orthogonal components  $\tilde{I}_l, \tilde{I}_r$  of the intensity. Then Fresnel's law written for  $\tilde{\mathbf{I}} = [\tilde{I}_l, \tilde{I}_r]^T$  have  $\mathbf{X}$  and  $\mathbf{Y}$  matrices changed to

$$\begin{pmatrix} \mathbf{X}_{11} + \mathbf{X}_{12} & 0 \\ 0 & \mathbf{X}_{11} - \mathbf{X}_{12} \end{pmatrix}, \quad \begin{pmatrix} \mathbf{Y}_{11} + \mathbf{Y}_{12} & 0 \\ 0 & \mathbf{Y}_{11} - \mathbf{Y}_{12} \end{pmatrix}.$$

**Notation 3.** From now on the tildes are dropped and  $\mathbf{I}$  etc are understood as  $\tilde{\mathbf{I}}$  etc.

## 5. Stratified VRTE with a Planar Discontinuity

Consider the partition  $(0, Z) = (0, Y] \cup [Y, Z)$ . Assume that the refractive index is  $n_z = n^-(z)$  in  $(0, Y)$  and  $n_z = n^+(z)$  in  $(Y, Z)$ . We assume that  $\{n^+, n^-\}$  are smooth functions of  $z$ . The convective part of the vector radiative transfer equations for  $\mathbf{I} = [I, Q]^T$  is (tildes are dropped),

$$\mu \partial_z \mathbf{I} + \partial_z \log n \cdot \partial_\mu \{(1 - \mu^2) \mathbf{I}\} + \kappa(z) \mathbf{I} = \mathbf{S}, \quad (5.1)$$

with the source terms  $\mathbf{S} = [S(z, \mu), S'(z, \mu)]^T$ . By the method of characteristics, one has

$$\begin{aligned} \mathbf{I}(z, \mu)|_{z < Y} = & \mathbf{1}_{\mu > 0} \left[ e^{-\int_0^z \frac{\kappa(z')}{\eta_{z'}} dz'} \mathbf{I}(0, \eta_0) + \int_0^z \frac{e^{-\int_{z'}^z \frac{\kappa(z'')}{\eta_{z''}} dz''}}{\eta_{z'}} \mathbf{S}(z', \eta_{z'}) dz' \right] \\ & + \mathbf{1}_{\mu < 0} \left[ e^{-\int_z^Y \frac{\kappa(z')}{\eta_{z'}} dz'} \mathbf{I}(Y^-, -\eta_Y) + \int_z^Y \frac{e^{-\int_z^{z'} \frac{\kappa(z'')}{\eta_{z''}} dz''}}{\eta_{z'}} \mathbf{S}(z', -\eta_{z'}) dz' \right] \end{aligned} \quad (5.2)$$

$$\begin{aligned} \mathbf{I}(z, \mu)|_{z > Y} = & \mathbf{1}_{\mu > 0} \left[ e^{-\int_Y^z \frac{\kappa(z')}{\eta_{z'}} dz'} \mathbf{I}(Y^+, \eta_Y) + \int_Y^z \frac{e^{-\int_{z'}^z \frac{\kappa(z'')}{\eta_{z''}} dz''}}{\eta_{z'}} \mathbf{S}(z', \eta_{z'}) dz' \right] \\ & + \mathbf{1}_{\mu < 0} \left[ e^{-\int_z^Z \frac{\kappa(z')}{\eta_{z'}} dz'} \mathbf{I}(Z, -\eta_Z) + \int_z^Z \frac{e^{-\int_z^{z'} \frac{\kappa(z'')}{\eta_{z''}} dz''}}{\eta_{z'}} \mathbf{S}(z', -\eta_{z'}) dz' \right] \end{aligned} \quad (5.3)$$

with  $y = 0, Y, Z, z', z''$  in  $\eta_y := \eta(\frac{n_z}{n_y}, \mu)$  defined in (4.1) for all  $z$  and  $\mu$  for which  $\eta$  is real.

**Notation 4.** Let  $\eta_{\pm}(\mu) = \eta(n_{\pm}, \mu)$  and  $\eta_{\mp}(\mu) = \eta(n_{\mp}, \mu)$ . Similarly, let

$$\mathbf{X}_{\pm} := \mathbf{X}(n_{\pm}, |\mu|), \quad \mathbf{X}_{\mp} := \mathbf{X}(n_{\mp}, |\mu|) \text{ and similarly with } \mathbf{Y}.$$

• Denote

$$\phi(z, z', \mu) = e^{-|\int_z^{z'} \frac{\kappa(z'')}{\eta_{z''}(\mu)} dz''|}.$$

**Lemma 1.** If, for some function  $\Delta(\mu)$ ,

$$\mathbf{I}(Y^+, \mu) = \mathbf{I}(Y^-, \mu) + \Delta(\mu), \quad \mu \in [-1, 1], \quad (5.4)$$

then the solution of (5.1) is

$$\begin{aligned} \mathbf{I}(z, \mu) &= \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) + \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\ &+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) - \int_z^Z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\ &+ [\mathbf{1}_{z > Y} \mathbf{1}_{\mu > 0} - \mathbf{1}_{z < Y} \mathbf{1}_{\mu < 0}] \Delta(\mu) \phi(z, Y, \mu). \end{aligned}$$

*Proof* With these simplifications (5.2) and (5.3) become

$$\begin{aligned} \mathbf{I}(z, \mu)|_{z < Y} &= \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) + \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\ &+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Y, \mu) \mathbf{I}(Y^-, \mu) - \int_z^Y \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \end{aligned} \quad (5.5)$$

$$\begin{aligned} \mathbf{I}(z, \mu)|_{z > Y} &= \mathbf{1}_{\mu > 0} \left[ \phi(z, Y, \mu) \mathbf{I}(Y^+, \mu) + \int_Y^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\ &+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) - \int_z^Z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right]. \end{aligned} \quad (5.6)$$

Using (5.4) in (5.5),

$$\begin{aligned} \mathbf{I}(z, \mu)|_{z < Y} &= \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) + \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\ &+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Y, \mu) [\mathbf{I}(Y^+, \mu) - \Delta(\mu)] - \int_z^Y \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right]. \end{aligned}$$

Now by (5.6) used with  $z = Y^+$ ,  $\mu < 0$ ,

$$\mathbf{I}(Y^+, \mu)|_{\mu < 0} = \phi(z, Y, \mu) \mathbf{I}(Z, \mu) - \int_Y^Z \phi(z', Y, \mu) \mu^{-1} \mathbf{S}(z', \mu) dz'.$$

Finally,

$$\begin{aligned}
\mathbf{I}(z, \mu)|_{z < Y} &= \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) + \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\
&+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Y, \mu) [\phi(z, Y, \mu) \mathbf{I}(Z, \mu) - \int_Y^Z \phi(z', Y, \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' - \Delta(\mu)] \right. \\
&- \left. \int_z^Y \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\
&= \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) + \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\
&+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) - \int_z^Z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' - \phi(z, Y, \mu) \Delta(\mu) \right].
\end{aligned}$$

Now when  $z > Y$  we use (5.4) in (5.6)

$$\begin{aligned}
\mathbf{I}(z, \mu)|_{z > Y} &= \mathbf{1}_{\mu > 0} \left[ \phi(z, Y, \mu) [\mathbf{I}(Y^-, \mu) + \Delta(\mu)] + \int_Y^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\
&+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) - \int_z^Z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right],
\end{aligned}$$

and (5.5) at  $z = Y$ , with  $\mu > 0$ ,

$$\mathbf{I}(Y^-, \mu)|_{\mu > 0} = \phi(0, Y, \mu) \mathbf{I}(0, \mu) + \int_0^Y \phi(z', Y, \mu) \mu^{-1} \mathbf{S}(z', \mu) dz'.$$

It shows that

$$\begin{aligned}
\mathbf{I}(z, \mu)|_{z > Y} &= \mathbf{1}_{\mu > 0} \left[ \phi(z, Y, \mu) [\phi(0, Y, \mu) \mathbf{I}(0, \mu) \right. \\
&+ \left. \int_0^Y \phi(z', Y, \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' + \Delta(\mu)] \right. \\
&+ \left. \int_Y^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\
&+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) - \int_z^Z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right] \\
&= \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) \right. \\
&+ \left. \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' + \phi(z, Y, \mu) \Delta(\mu) \right] \\
&+ \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) - \int_z^Z \phi(z, z', \mu) \mu^{-1} \mathbf{S}(z', \mu) dz' \right].
\end{aligned}$$

The additional term due to the discontinuity is

$$[\mathbf{1}_{z > Y} \mathbf{1}_{\mu > 0} - \mathbf{1}_{z < Y} \mathbf{1}_{\mu < 0}] \phi(z, Y, \mu) \Delta(\mu).$$

□

## 6. Application to Fresnel's Conditions

From (5.6) and (5.5) we obtain

$$\begin{aligned}\mathbf{I}(Y^+, \mu)|_{\mu < 0} &= \phi(Y, Z, \mu)\mathbf{I}(Z, \mu) - \int_Y^Z \phi(z', Y, \mu)\mu^{-1}\mathbf{S}(z')dz', \\ \mathbf{I}(Y^-, \mu)|_{\mu > 0} &= \phi(0, Y, \mu)\mathbf{I}(0, \mu) + \int_0^Y \phi(z', Y, \mu)\mu^{-1}\mathbf{S}(z')dz'.\end{aligned}$$

And (5.5) and (5.6) plugged in the Fresnel law (4.2) yield,

$$\begin{aligned}\mathbf{I}(Y^-, \mu)|_{\mu < 0} &= \mathbf{X}_\mp \left[ \phi(0, Y, \mu)\mathbf{I}(0, -\mu) - \int_0^Y \phi(z', Y, \mu) \frac{\mathbf{S}(z', -\mu)}{\mu} dz' \right] \\ &\quad + \mathbf{Y}_\mp \left[ \phi(Y, Z, \eta_\mp(\mu))\mathbf{I}(Z, -\eta_\mp(\mu)) \right. \\ &\quad \left. + \int_Y^Z \phi(z', Y, \eta_\mp(\mu)) \frac{\mathbf{S}(z', -\eta_\mp(\mu))}{\eta_\mp(\mu)} dz' \right], \\ \mathbf{I}(Y^+, \mu)|_{\mu > 0} &= \mathbf{X}_\pm \left[ \phi(Y, Z, \mu)\mathbf{I}(Z, -\mu) + \int_Y^Z \phi(z', Y, \mu) \frac{\mathbf{S}(z', \mu)}{\mu} dz' \right] \\ &\quad + \mathbf{Y}_\pm \left[ \phi(0, Y, \eta_\pm(\mu))\mathbf{I}(0, \eta_\pm(\mu)) \right. \\ &\quad \left. + \int_0^Y \phi(z', Y, \eta_\pm(\mu)) \frac{\mathbf{S}(z', \eta_\pm(\mu))}{\eta_\pm(\mu)} dz' \right].\end{aligned}$$

Therefore,

$$\begin{aligned}
\Delta(\mu)|_{\mu>0} &= \mathbf{I}(Y^+, \mu)|_{\mu>0} - \mathbf{I}(Y^-, \mu)|_{\mu>0} \\
&= \mathbf{X}_\pm \phi(Y, Z, \mu) \mathbf{I}(Z, -\mu) + \mathbf{Y}_\pm \phi(0, Y, \eta_\pm(\mu)) \mathbf{I}(0, \eta_\pm(\mu)) \\
&\quad - \phi(0, Y, \mu) \mathbf{I}(0, \mu) \\
&\quad + \mathbf{X}_\pm \int_Y^Z \phi(z', Y, \mu) \frac{\mathbf{S}(z', \mu)}{\mu} dz' - \int_0^Y \phi(z', Y, \mu) \frac{\mathbf{S}(z', -\mu)}{\mu} dz' \\
&\quad + \mathbf{Y}_\pm \int_0^Y \phi(z', Y, \eta_\pm(\mu)) \frac{\mathbf{S}(z', \eta_\pm(\mu))}{\eta_\pm(\mu)} dz', \\
\Delta(\mu)|_{\mu<0} &= \mathbf{I}(Y^+, \mu)|_{\mu<0} - \mathbf{I}(Y^-, \mu)|_{\mu<0} \\
&= \phi(Y, Z, \mu) \mathbf{I}(Z, -\mu) - \mathbf{X}_\mp \phi(0, Y, \mu) \mathbf{I}(0, \mu) \\
&\quad - \mathbf{Y}_\mp \phi(Y, Z, \eta_\mp(\mu)) \mathbf{I}(Z, -\eta_\mp(\mu)) \\
&\quad - \int_Y^Z \phi(z', Y, \mu) \frac{\mathbf{S}(z', \mu)}{\mu} dz' + \mathbf{X}_\mp \int_0^Y \phi(z', Y, \mu) \frac{\mathbf{S}(z', \mu)}{\mu} dz' \\
&\quad - \mathbf{Y}_\mp \int_Y^Z \phi(z', Y, \eta_\mp(\mu)) \frac{\mathbf{S}(z', -\eta_\mp(\mu))}{-\eta_\mp(\mu)} dz'. \tag{6.1}
\end{aligned}$$

## 7. Implementation

To implement the iterative algorithm with  $\mu$ -integrals and  $\mathbf{S}(z, \mu) = \mathbf{S}_0(z) + \mathbf{S}_2(z)\mu^2$ , the only functions needed to compute  $\int_{-1}^1 \mathbf{I}(z, \mu) \mu^k d\mu$ ,  $k = 0, 2$  and that includes the computation of

$$\int_0^1 \mu^k \phi(Y, z, \mu) \Delta(\mu) d\mu, \quad z > Y \quad \text{and} \quad \int_{-1}^0 \mu^k \phi(Y, z, \mu) \Delta(\mu) d\mu, \quad z < Y.$$

We could use (6.1) but it is somewhat easier to compute directly, first for  $z < Y$ ,

$$\begin{aligned}
&\int_{-1}^0 \mu^k \phi(z, Y, \mu) I(Y^+, \mu) d\mu = \\
&\quad \int_{-1}^0 \mu^k \phi(z, Y, \mu) \left[ \phi(Y, Z, \mu) \mathbf{I}(Z, \mu) - \int_Y^Z \phi(z', Y, \mu) \frac{\mathbf{S}(z')}{\mu} dz' \right] d\mu \\
&\int_{-1}^0 \mu^k \phi(z, Y, \mu) I(Y^-, \mu) d\mu = \\
&\quad \int_{-1}^0 \mu^k \phi(z, Y, \mu) \left\{ \mathbf{X}_\mp \left[ \phi(0, Y, \mu) \mathbf{I}(0, -\mu) - \int_0^Y \phi(z', Y, \mu) \frac{\mathbf{S}(z', \mu)}{\mu} dz' \right] \right. \\
&\quad \left. + \mathbf{Y}_\mp \left[ \phi(Y, Z, \eta_\mp(\mu)) \mathbf{I}(Z, -\eta_\mp(\mu)) + \int_Y^Z \phi(z', Y, \eta_\mp(\mu)) \frac{\mathbf{S}(z', -\eta_\mp(\mu))}{\eta_\mp(\mu)} dz' \right] \right\} d\mu,
\end{aligned}$$

and then for  $z > Y$ ,

$$\begin{aligned}
& \int_0^1 \mu^k \phi(z, Y, \mu) I(Y^+, \mu) d\mu = \\
& \int_0^1 \mu^k \phi(z, Y, \mu) \left\{ \mathbf{X}_\pm \left[ \phi(Y, Z, \mu) \mathbf{I}(Z, -\mu) + \int_Y^Z \phi(z', Y, \mu) \frac{\mathbf{S}(z', \mu)}{\mu} dz' \right] \right. \\
& \left. + \mathbf{Y}_\pm \left[ \phi(0, Y, \eta_\pm(\mu)) \mathbf{I}(0, \eta_\pm(\mu)) + \int_0^Y \phi(z', Y, \eta_\pm(\mu)) \frac{\mathbf{S}(z', \eta_\pm(\mu))}{\eta_\pm(\mu)} dz' \right] \right\} d\mu \\
& \int_0^1 \mu^k \phi(z, Y, \mu) \mathbf{I}(Y^-, \mu) d\mu \\
& = \int_0^1 \mu^k \phi(z, Y, \mu) \left[ \phi(0, Y, \mu) \mathbf{I}(0, \mu) + \int_0^Y \phi(z', Y, \mu) \frac{\mathbf{S}(z')}{\mu} dz' \right].
\end{aligned}$$

Consequently, with  $\mathbf{S} = \mathbf{S}_0 + \mu^2 \mathbf{S}_2$ ,

$$\begin{aligned}
& \int_{-1}^1 \mu^k \phi(Y, z, \mu) [\Delta(\mu) [\mathbf{1}_{z>Y} \mathbf{1}_{\mu>0} - \mathbf{1}_{z<Y} \mathbf{1}_{\mu<0}]] d\mu \\
& = \boldsymbol{\alpha}^k(z) + \sum_{i=0,2} \int_0^Z \mathbf{Z}^{k,i-1}(z, z') \mathbf{S}_i(z') dz', \tag{7.1}
\end{aligned}$$

with

$$\begin{aligned}
\boldsymbol{\alpha}^k(z) = & \mathbf{1}_{z>Y} \int_0^1 \mu^k \phi(Y, z, \mu) [\mathbf{X}_\pm \phi(Y, Z, \mu) \mathbf{I}(Z, -\mu) \\
& + \mathbf{Y}_\pm \phi(0, Y, \eta_\pm(\mu)) \mathbf{I}(0, \eta_\pm(\mu)) - \phi(0, Y, \mu) \mathbf{I}(0, \mu)] d\mu \\
& - \mathbf{1}_{z<Y} \int_{-1}^0 \mu^k \phi(z, Y, \mu) [\phi(Y, Z, \mu) \mathbf{I}(Z, \mu) - \mathbf{X}_\mp \phi(0, Y, \mu) \mathbf{I}(0, -\mu) \\
& - \mathbf{Y}_\mp \phi(Y, Z, \eta_\pm(\mu)) \mathbf{I}(Z, -\eta_\mp(\mu))] d\mu
\end{aligned}$$

and with the  $2 \times 2$  matrices

$$\begin{aligned}
\mathbf{Z}^{k,i}(z, z') := & \mathbf{1}_{z>Y} \int_0^1 \mu^k \phi(Y, z, \mu) \{ \mathbf{X}_\pm \phi(z', Y, \mu) \mu^i \mathbf{1}_{z'>Y} \\
& + [ \mathbf{Y}_\pm \phi(z', Y, \eta_\pm(\mu)) \eta_\pm^i(\mu) - \mathbf{1} \phi(z', Y, \mu) \mu^i ] \mathbf{1}_{z'<Y} \} d\mu, \\
& - \mathbf{1}_{z<Y} (-1)^i \int_0^1 \mu^k \phi(z, Y, \mu) [ \mathbf{X}_\mp \phi(z', Y, \mu) |\mu|^i \mathbf{1}_{z'<Y} \\
& + ( \mathbf{Y}_\mp \phi(z', Y, \eta_\mp(\mu)) \eta_\mp^i(\mu) - \mathbf{1} \phi(z', Y, \mu) |\mu|^i ) \mathbf{1}_{z'>Y} ] d\mu,
\end{aligned}$$

Let  $n_z = n_{\pm} \mathbf{1}_{z>Y} + n_{\mp} \mathbf{1}_{z<Y}$ , then

$$\begin{aligned} \mathbf{Z}^{k,i}(z, z') := & \int_0^1 \mu^k \phi(z, Y, \mu) \{ \mathbf{X}(n_z, \mu) \phi(z', Y, \mu) \mu^i [\mathbf{1}_{z'>Y} \mathbf{1}_{z>Y} + \mathbf{1}_{z'<Y} \mathbf{1}_{z<Y}] \\ & - (-1)^i [ \mathbf{Y}(n_z, \mu) \phi(z', Y, \eta(n_z, \mu)) \eta^i(n_z, \mu) \\ & - \mathbf{1} \phi(z', Y, \mu) \mu^i ] [\mathbf{1}_{z'>Y} \mathbf{1}_{z<Y} + \mathbf{1}_{z'<Y} \mathbf{1}_{z>Y}] \} d\mu. \end{aligned} \quad (7.2)$$

**Remark 3.** *Whenever feasible it is computationally advantageous to separate in  $\alpha$  the part containing  $\nu$  from the one containing  $z$ .*

For our purpose

$$\begin{aligned} \mathbf{I}(0, \mu) &= [\mu C_E B_\nu(T_E), 0]^T, \quad \mathbf{I}(Z, -\mu) = [\mu C_S B_\nu(T_S), 0]^T \\ \Rightarrow \alpha^k(z) &= [\alpha_E^k(z) B_\nu(T_E) + \alpha_S^k(z) B_\nu(T_S), 0]^T \end{aligned}$$

with

$$\begin{aligned} \alpha_E^k(z) &= C_E \int_0^1 \mu^k \phi(z, Y, \mu) [\mathbf{1}_{z>Y} (\mathbf{Y}_{11}(n_{\pm}, \mu) \phi(0, Y, \eta_{\pm}(\mu)) \eta_{\pm}(\mu)) \\ & \quad - \phi(0, Y, \mu) \mu + \mathbf{1}_{z<Y} \mathbf{X}_{11}(n_{\mp}, \mu) \phi(0, Y, \mu) \mu] d\mu \\ \alpha_S^k(z) &= C_S \int_0^1 \mu^k \phi(z, Y, \mu) [\mathbf{1}_{z<Y} (\mathbf{Y}_{11}(n_{\mp}, \mu) \phi(Y, Z, \eta_{\mp}(\mu)) \eta_{\mp}(\mu)) \\ & \quad - \phi(Y, Z, \mu) \mu + \mathbf{1}_{z>Y} \mathbf{X}_{11}(n_{\pm}, \mu) \phi(Y, Z, \mu) \mu] d\mu \end{aligned}$$

## 8. Integral representation of the Problem

Denote

$$J_k(z) = \frac{1}{2} \int_{-1}^1 \mu^k I d\mu, \quad K_k(z) = \frac{1}{2} \int_{-1}^1 \mu^k Q d\mu. \quad k = 0, 2.$$

Consider the system for the irradiance  $I$  and the polarization  $Q$ ,

$$\begin{aligned} \mu \partial_z I + \partial_z \log n \cdot \partial_\mu \{ (1 - \mu^2) I \} + \kappa I &= \kappa_a B_\nu + \kappa_s J_0 \\ & \quad + \frac{\beta \kappa_s}{4} P_2(\mu) (3J_2 - J_0 - 3K_0 + 3K_2) \\ \mu \partial_z Q + \partial_z \log n \cdot \partial_\mu \{ (1 - \mu^2) Q \} + \kappa Q &= \\ & \quad - \frac{\beta \kappa_s}{4} (1 - P_2(\mu)) (3J_2 - J_0 - 3K_0 + 3K_2) \end{aligned}$$

where  $P_2(\mu) = \frac{1}{2}(3\mu^2 - 1)$ . Hence

$$\begin{aligned}
\mathbf{S}(z, \mu) &= [S, S']^T = [S_0 + \mu^2 S_2, S'_0 + \mu^2 S'_2]^T \text{ with} \\
S &= \kappa_a B_\nu + \kappa_s J_0 + \frac{\beta \kappa_s}{4} P_2(\mu) (3J_2 - J_0 - 3K_0 + 3K_2) \\
S' &= -\frac{\beta \kappa_s}{4} (1 - P_2(\mu)) (3J_2 - J_0 - 3K_0 + 3K_2) \\
S_0 &= \kappa_a B_\nu + \kappa_s J_0 - \frac{9\beta \kappa_s}{8} (J_2 - \frac{1}{3} J_0 - K_0 + K_2) \\
S_2 &= \frac{9\beta \kappa_s}{8} (J_2 - \frac{1}{3} J_0 - K_0 + K_2) \\
S'_0 &= \frac{9\beta \kappa_s}{8} (J_2 - \frac{1}{3} J_0 - K_0 + K_2) \\
S'_2 &= -\frac{9\beta \kappa_s}{8} (3J_2 - \frac{1}{3} J_0 - K_0 + K_2)
\end{aligned} \tag{8.1}$$

Let (5.2) be multiplied by  $\mu^k$  and integrated. Then, by (7.1),

$$\begin{aligned}
J_k(z) &= \frac{1}{2} \int_0^Z \left[ \left( \int_0^1 \mu^k \eta^{-1}(\mu) \phi(z, z', \mu) d\mu + \mathbf{Z}_{11}^{k,-1}(z, z') \right) S_0(z') \right. \\
&\quad \left. + \mathbf{Z}_{12}^{k,-1}(z, z') S'_0(z') \right] dz' \\
&\quad + \frac{1}{2} \int_0^Z \left[ \left( \int_0^1 \mu^k \eta(\mu) \phi(z, z', \mu) d\mu + \mathbf{Z}_{11}^{k,1}(z, z') \right) S_2(z') \right. \\
&\quad \left. + \mathbf{Z}_{12}^{k,1}(z, z') S'_2(z') \right] dz' \\
&\quad + \frac{1}{2} \int_0^1 \phi(0, z, \mu) \mathbf{I}(0, \eta_0) \mu^k d\mu \\
&\quad + \frac{1}{2} \int_0^1 \phi(z, Z, \mu) \mathbf{I}(Z, -\eta_Z) \mu^k d\mu
\end{aligned} \tag{8.2}$$

Similarly (recall that  $Q$  is zero at  $z = 0$ ),

$$\begin{aligned}
K_k(z) &= \frac{1}{2} \int_0^Z \left( \int_0^1 \mu^k \eta^{-1}(\mu) \phi(z, z', \mu) d\mu + \mathbf{Z}_{22}^{k,-1} \right) S'_0(z') + \mathbf{Z}_{21}^{k,-1} S_0(z') dz' \\
&\quad + \frac{1}{2} \int_0^Z \left( \int_0^1 \mu^k \eta(\mu) \phi(z, z', \mu) d\mu + \mathbf{Z}_{22}^{k,1} \right) S'_2(z') + \mathbf{Z}_{21}^{k,1} S_2(z') dz'
\end{aligned} \tag{8.3}$$

## 9. Convergence of the Iteration on the Sources

### 9.1. Principle

In earlier studies, on simpler systems [7], convergence was shown by using the monotony of operators. Here too the same arguments are used but nor



on  $[I, Q]^T$  but on  $\mathbf{I} = [I_l, I_r]^T$ . The iterative system is

$$\begin{aligned}
\mathbf{I}^{n+1}(z, \mu) &= \mathbf{1}_{z < Y} \left\{ \mathbf{1}_{\mu > 0} \left[ \phi(z, 0, \mu) \mathbf{I}(0, \mu) + \int_0^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}^n(z', \mu) dz' \right] \right. \\
&\quad \left. + \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) + \int_z^Z \phi(z, z', \mu) (-\mu^{-1}) \mathbf{S}^n(z', \mu) dz' \right] \right\} \\
&\quad + \mathbf{1}_{z > Y} \left\{ \mathbf{1}_{\mu > 0} \left[ \phi(z, Y, \mu) \mathbf{I}(Y^-, \mu) + \int_Y^z \phi(z, z', \mu) \mu^{-1} \mathbf{S}^n(z', \mu) dz' \right] \right. \\
&\quad \left. + \mathbf{1}_{\mu < 0} \left[ \phi(z, Z, \mu) \mathbf{I}(Z, \mu) + \int_z^Z \phi(z, z', \mu) (-\mu^{-1}) \mathbf{S}^n(z', \mu) dz' \right] \right\} \\
&\quad + e^{-|\frac{\kappa(Y-z)}{\mu}|} \bar{\Delta}^n(\mu, z)
\end{aligned} \tag{9.1}$$

with  $\mathbf{S}^n$  given by (8.1)(8.2)(8.3) and  $\bar{\Delta}(\mu, z) := (\mathbf{1}_{z > Z} \mathbf{1}_{\mu > 0} - \mathbf{1}_{z < Z} \mathbf{1}_{\mu < 0}) \Delta(\mu)$  with  $\Delta(\mu)$  given by (6.1). Consequently

$$\begin{aligned}
&\mathbf{I}^{n+1}(z, \mu) - \mathbf{I}^n(z, \mu) \\
&= \mathbf{1}_{z < Y} \left\{ \mathbf{1}_{\mu > 0} \int_0^z \phi(z, z', \mu) \mu^{-1} (\mathbf{S}^n(z', \mu) - \mathbf{S}^{n-1}(z', \mu)) dz' \right. \\
&\quad \left. + \mathbf{1}_{\mu < 0} \left[ + \int_z^Z \phi(z, z', \mu) (-\mu^{-1}) (\mathbf{S}^n(z', \mu) - \mathbf{S}^{n-1}(z', \mu)) dz' \right] \right\} \\
&\quad + \mathbf{1}_{z > Y} \left\{ \mathbf{1}_{\mu > 0} \int_Y^z \phi(z, z', \mu) \mu^{-1} (\mathbf{S}^n(z', \mu) - \mathbf{S}^{n-1}(z', \mu)) dz' \right. \\
&\quad \left. + \mathbf{1}_{\mu < 0} \left[ \int_z^Z \phi(z, z', \mu) (-\mu^{-1}) (\mathbf{S}^n(z', \mu) - \mathbf{S}^{n-1}(z', \mu)) dz' \right] \right\} \\
&\quad + e^{-|\kappa(Y-z)\mu^{-1}|} (\bar{\Delta}^n(\mu) - \bar{\Delta}^{n-1}(\mu)).
\end{aligned}$$

On this system it is seen that  $\mathbf{S}^n \geq \mathbf{S}^{n-1}$  and  $\bar{\Delta}^n \geq \bar{\Delta}^{n-1}$  implies  $\mathbf{I}^{n+1} \geq \mathbf{I}^n$  because  $\phi$  is always positive. Conversely if  $\mathbf{S}^n \leq \mathbf{S}^{n-1}$  and  $\bar{\Delta}^n \leq \bar{\Delta}^{n-1}$  then  $\mathbf{I}^{n+1} \leq \mathbf{I}^n$ . However the monotony is true only for the system  $[I_l, I_r]$  and for  $[I, Q]$  the monotony holds only for  $I$ .

### 9.2. Monotony

For  $\mathbf{I} = [I_l, I_r]^T$  in (3.4) the source terms are

$$\begin{aligned} S &= \frac{3\beta\kappa_s}{8} \int_{-1}^1 ([2(1-\mu'^2)(1-\mu^2) + \mu'^2\mu^2] \tilde{I}_l + \mu^2 \tilde{I}_r) d\mu' \\ &\quad + \frac{(1-\beta)\kappa_s}{4} \int_{-1}^1 [\tilde{I}_l + \tilde{I}_r] d\mu' + \frac{\kappa_a}{2} \tilde{B}_\nu(T(z)), \\ S' &= \frac{3\beta\kappa_s}{8} \int_{-1}^1 (\mu'^2 \tilde{I}_l + \tilde{I}_r) d\mu' \\ &\quad + \frac{(1-\beta)\kappa_s}{4} \int_{-1}^1 [\tilde{I}_l + \tilde{I}_r] d\mu' + \frac{\kappa_a}{2} \tilde{B}_\nu(T(z)), \end{aligned}$$

Denote  $D_{l,r}^n = I_{r,l}^n - I_{l,r}^{n-1}$ . Obviously,

$$\begin{aligned} S_l^n - S_l^{n-1} &= \frac{3\beta\kappa_s}{8} \int_{-1}^1 ([2(1-\mu'^2)(1-\mu^2) + \mu'^2\mu^2] D_l^n + \mu^2 D_r^n) d\mu' \\ &\quad + \frac{(1-\beta)\kappa_s}{4} \int_{-1}^1 [D_l^n + D_r^n] d\mu' + \frac{\kappa_a}{2} [B_\nu(T^n) - B_\nu(T^{n-1})] \\ S_r^n - S_r^{n-1} &= \frac{3\beta\kappa_s}{8} \int_{-1}^1 (\mu'^2 D_l^n + D_r^n) d\mu' \\ &\quad + \frac{(1-\beta)\kappa_s}{4} \int_{-1}^1 [D_l^n + D_r^n] d\mu' + \frac{\kappa_a}{2} [B_\nu(T^n) - B_\nu(T^{n-1})] \end{aligned}$$

The terms under the integrals are positive and  $T \rightarrow B_\nu(T)$  is monotone in the sense that  $T^n \geq T^{n-1}$  implies  $B_\nu(T^n) \geq B_\nu(T^{n-1})$ . Consequently  $T^n \geq T^{n-1}$  and  $I_{l,r}^n \geq I_{l,r}^{n-1}$  implies  $S_{l,r}^n \geq S_{l,r}^{n-1}$ .

Now we return to the problem of showing that the monotony of  $\mathbf{S}$  implies the monotony of  $\mathbf{I}$ . By looking at (7.1) and (9.1) we see that we don't need to show that  $\bar{\Delta}^n(\mu, z)$  is increasing with  $n$ , but only that  $\int_0^1 \mu^k \phi(z, Y, \mu) \bar{\Delta}^n$  is increasing with  $n$ .

Now in (7.2), with  $i$  odd, the only negative contribution to  $\mathbf{Z}_{ii}^k$  comes from

$$\int_0^1 \mu^k \eta^i(\mu) \phi(z, Y, \mu) \phi(z', Y, \mu) d\mu = \int_0^1 \mu^k \eta^i(\mu) \phi(z', z, \mu) d\mu, \text{ if } z' < Y < z.$$

Luckily this term is almost equal to another term in (7.2):  $\int_0^1 \phi(z', z, \mu) \mu^{k+i} d\mu$ .

$$\text{Hence it compensates the negative term in } \mathbf{Z}_{ii}^k, \text{ when } n_\pm \approx 1. \quad (9.2)$$

Finally the temperature equation implies

$$\int_{\mathbb{R}_+} \kappa_a B_\nu(T^{m+1}) d\nu = \int_{\mathbb{R}_+} \kappa_a J_0^n d\nu \geq \int_{\mathbb{R}_+} \kappa_a J_0^{n-1} d\nu = \int_{\mathbb{R}_+} \kappa_a B_\nu(T^{m+1}) d\nu.$$

which implies that  $T^{n+1} \geq T^{n+1}$ . Let us apply this argument to  $\{T^{n-1}, I_{i,r}^{n-1}\}$  instead of  $\{T^n, I_{i,r}^n\}$ . It shows that

$$T^n \geq T^{n-1}, I_{l,r}^n \geq I_{i,r}^{n-1} \Rightarrow T^{n+1} \geq T^n, I_{l,r}^{n+1} \geq I_{i,r}^n.$$

To start the iterations appropriately, simply set  $T^0 = 0, I_{l,r}^0 = 0$ , then by the positivity of the coefficients  $I_{l,r}^1 \geq 0$  and  $T^1 \geq 0$ .

The same argument works with  $T^n \leq T^n, I_{l,r}^n \leq I_{l,r}^n$  implying that  $I_{l,r}^{n+1} \leq I_{l,r}^{n+1}$  and then  $T^{n+1} \leq T^{n+1}$ . Hence starting with  $T^1 < T^0, I_{l,r}^1 \leq I_{l,r}^0$  leads to a decreasing sequence toward the solution. For the scalar model, it is shown that it suffices to take  $T^0(z) > T_M, \forall z$  where  $T_M$  is the solution of  $B_\nu(T_M) = P_E B_\nu(T_E)$ . For the present vector model it is not clear that it is sufficient.

Note that the decreasing solution is bounded by zero. Consequently a solution exists.

The above results are summarized in the following proposition.

**Proposition 2.** *Subject to (9.2), if the solution  $T^*, I_{l,r}^*$  exists, then it can be reached numerically from above or below by iterations (9.1) and these are monotone increasing and decreasing respectively. If There is an initial guess such that  $T^0 \geq T^1, I_{l,r}^0 \geq I_{l,r}^1$ , then a solution exists.*

## 10. Numerical Results

The computer program is written in C++ and opensource. The functions  $\mathbf{E}$ ,  $\mathbf{Z}$  and  $\alpha$  are tabulated to speed up the runtime which is around 2 seconds on a high end Apple Macbook.

We investigated 2 cases:

- Case 1: Visible light coming from the Sun through the top of the troposphere at  $z = Z$ :  $I(0, \mu) = 0, I(Z, -\mu) = c_S B_\nu(T_S)\mu, \mu > 0$ .
- Case 2: Infrared light coming from Earth and escaping freely at  $z = Z$  with and without CO<sub>2</sub> effects modeled by a change in  $\kappa_\nu$  taken from the Gemini experiment <sup>2</sup>:  $I(0, \mu) = c_E B_\nu(T_E)\mu, I(Z, -\mu) = 0, \mu > 0$ .

In both cases there is a change of refractive index at  $z = Y := Z/2$ .

For all tests the following is used:

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<sup>2</sup>[www.gemini.edu/observing/telescopes-and-sites/sites#Transmission](http://www.gemini.edu/observing/telescopes-and-sites/sites#Transmission)

- $n(z) = 1 + \epsilon \mathbf{1}_{z>Y}$ ,
- $a_s = a_1 \mathbf{1}_{z \in (z_1, z_2)} + a_2 \mathbf{1}_{z > z_2} \mathbf{1}_{\nu \in (\nu_1, \nu_2)} \left( \frac{\nu}{\nu_2} \right)^4$ ,
- $\epsilon = -0.01$  or  $-0.3$ ,  $a_1 = 0.7$ ,  $a_2 = 0.3$ ,  $z_1 = 0.4$ ,  $z_2 = 0.8$ ,  $\nu_1 = 0.6$ ,  $\nu_2 = 1.5$ .
- $c_S = 2.0e - 5$ ,  $T_S = 5700/4798$ ,  $c_E = 2.5$ ,  $T_E = 300./4798$ .

According to [2] the variation of the refractive index in the atmosphere is quite small  $\sim 0.003$ . To enhance the effect we use 3 times this value.

The monotony of the iterative process is displayed in Figure 2. It is clear that by starting below (resp. above) the solution the values of the temperature at  $z = 300\text{m}$  are increasing (resp. decreasing). Note that 15 iterations are sufficient to obtain a 3 digit precision.

To study the effect of  $n$  on a simple case we ran the program with  $\kappa = 0.5$ ,  $n$  as above, with  $\epsilon = 0.01$  and the data of Case 2. The temperatures are shown in Figure 3 in red. The computations are done with and without Fresnel conditions at  $z = Y$ .

A similar computation is done for Case 1 with  $\kappa = 0.5$ ,  $\epsilon = -0.3$  with and without Fresnel conditions. The temperatures are displayed in blue in Figure 5. The average light and polarization intensities are shown on Figure 4.

Finally, Case 2 was run with  $\epsilon = -0.3$  with  $\kappa_\nu$  read from the Gemini website and shown on Figure 1. Then this  $\kappa_\nu$  was increased in the frequency range where  $\text{CO}_2$  is absorbent, shown in red in Figure 1. The corresponding temperatures and average light intensities are shown in Figures 5 and 6.

The main points are

- For Case 1 (Visible light crossing the atmosphere downward and passing through a refractive medium for  $z < Y$ ) Fresnel's conditions have a drastic effect on the results.
- For Case 2 (IR light coming from Earth and the refractive index decreases when  $z > Y$ ) the refraction makes the medium much more absorbing. Furthermore, with a Fresnel interface, an increase in  $\text{CO}_2$  decreases the temperature at high altitude.

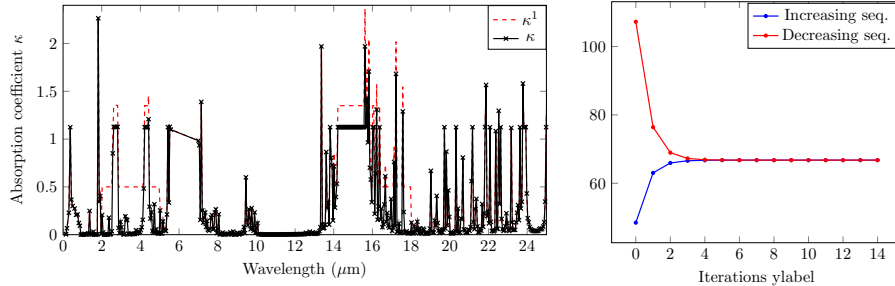


Figure 1: Absorption  $\kappa$  from the Gemini experiment, versus wavenumber ( $3/\nu$ ). In dotted lines, the modification to construct  $\kappa_1$  to account for the opacity of  $\text{CO}_2$ .

Figure 2: Convergence of the temperature at altitude 300m during the iterations. In solid line when it is started with  $T^0 = 0$ , in dashed line when the initial temperature is  $180^\circ\text{C}$ . Notice the monotonicity of both curves.

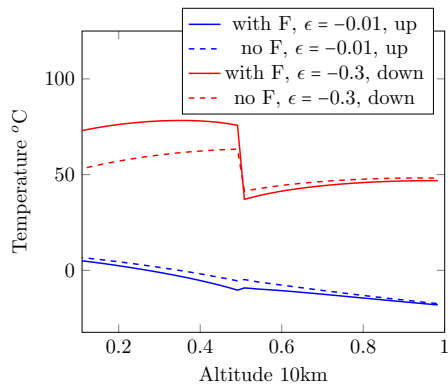


Figure 3: Temperatures versus altitude with  $\kappa = 0.5$ . In blue with  $\epsilon = -0.01$  for **Case 2** and in red with  $\epsilon = -0.3$  for **Case 1**. The solid curves are computed with Fresnel's conditions at  $z = Y = 0.5$  and the dashed curves are computed without them.

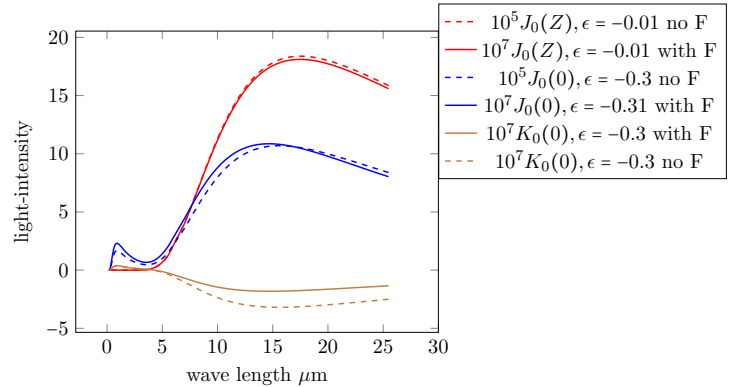


Figure 4: Total light intensity  $J_0$  and polarized  $K_0$  versus wave length at ground level or at altitude  $Z=10\text{km}$  for **Case 2** with  $\epsilon = -0.01$  and for **Case 1** with  $\epsilon = -0.3$ . The solid curves are computed with Fresnel's conditions and the dashed one without.

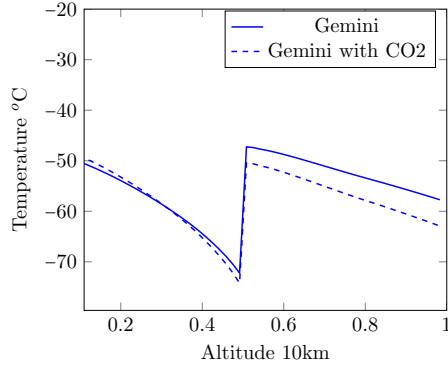


Figure 5: **Case 2.** Effect of CO<sub>2</sub> on the temperature in the presence of a Fresnel interface with  $\epsilon = -0.3$ .

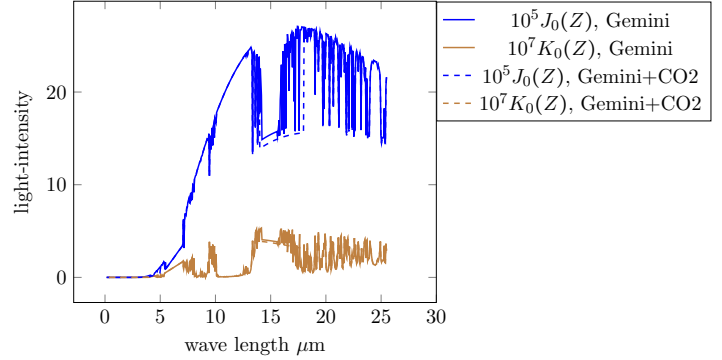


Figure 6: **Case 2.** Total light intensity  $J_0$  and polarized  $K_0$  versus wave length at altitude  $Z=10\text{km}$ .

## 11. Conclusion

In this article the methodology developed in [7] for the numerical solution of the RTE has been extended to include the Fresnel laws at an interface of discontinuity of the refractive index.

In principle the method is not hard to program (500 lines of C++ and the execution time is a few seconds; however the formulas are complex and the probability of having a bug cannot be ruled out. The effect of a change on the diffusion due to CO<sub>2</sub> is analyzed numerically.

Generalization to 3D as in [6]) and [11] for a non-stratified atmosphere looks possible.

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