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- Handling Refractive Index Discontinuities

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FAST AND STABLE SOLUTION METHOD FOR ANGLE-RESOLVED LIGHT SCATTERING SIMULATION III – HANDLING REFRACTIVE INDEX DISCONTINUITIES

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ABSTRACT

The change in refractive index that occurs at the interface between air and an ink-paper substrate causes effects such as refraction and total reflection. This report uses radiative transfer theory to account for these effects exactly, and for any measurement geometry, without approximations and without unknown constants. This is in contrast with Kubelka-Munk and the Saunderson correction, which is only an approximation and only for integrating sphere geometry, and which requires non-trivial determination of unknown constants.

This report continues previous work, and extends the solution procedure of DORT2002 to handle a discontinuous change in refractive index at the interface between two perfectly flat layers. The result of a large number of consistency and accuracy tests are presented, and they are all positive.

Some comments on planned and suggested future work are given regarding direct and inverse model development, but also for comparative studies. Comments are also given on the benefit of this work for the paper and printing industries. It is suggested that the Kubelka-Munk model should be replaced with DORT2002 in most applications.

SAMMANDRAG

Den ändring i brytningsindex som sker vid gränsen mellan luft och ett bläck-papper substrat orsakar effekter som brytning och totalreflektion. I denna rapport används radiative transfer teori för att ta hänsyn till dessa effekter exakt, och för varje mätgeometri, utan approximationer och utan okända konstanter. Det är i motsats till Kubelka-Munk och Saundersons korrektion, som bara är en approximation och bara för integrerande sfär geometri, och som kräver icke-trivial bestämning av okända konstanter.

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Denna rapport fortsätter tidigare arbete, och bygger ut lösningsmetoden i DORT2002 för att hantera en diskontinuerlig ändring i brytningsindex vid gränsen mellan två släta ytor. Resultatet av ett stort antal konsistens- och noggrannhetstester redovisas, och de är alla positiva.

Några kommentarer ges på planerat och föreslaget framtida arbete avseende utveckling av den direkta och inversa modellen, men även för jämförande studier. Kommentarer ges också om nyttan av detta arbete för pappers- och tryckindustrin. Det föreslås att Kubelka-Munk modellen ersätts med DORT2002 i de flesta tillämpningar.

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1. INTRODUCTION

When light is incident on a medium with different refractive index, a fraction is specularly reflected according to Fresnel's formula, and the remainder enters the medium but is refracted according to Snell's formula. Some of the light scattered inside the medium will also suffer from total reflection when striking the boundary from the inside. These effects are substantial in changing both the amount of light entering the medium, and the angular distribution of the light. The well-known Kubelka-Munk theory [1-3] cannot handle these changes, and is thus not adequate for media where the refractive index changes. Unfortunately, most media have a different refractive index than the surrounding air, which means that Kubelka-Munk would most often fail. However, Saunderson [4] presented a surface correction to account for this. The so called Saunderson correction was developed for integrating sphere geometry only, although corrections for other measurement geometries have been devised by using the same line of reasoning. Nevertheless, the situation is not free from problems. First, the Saunderson correction is only an approximation. Second, the use of the Saunderson correction requires determination of some constants, which is not trivial and has brought about some debate. On top of this, the Kubelka-Munk theory is itself just an approximation of the light scattering problem.

Radiative transfer theory (of which Kubelka-Munk is the simplest special case – a two-flux solution method) is no approximation, but treats the light scattering problem with any desired resolution. The angular resolution of the theory makes it possible to account for the effects of refraction and total reflection at refractive index boundaries in an exact way. The newly developed radiative transfer solution method DORT2002 by Edström [5], which is adapted to light scattering in paper and print, now includes methods for this. Thus, the problem of discontinuous changes in refractive index, e.g. light incident from air on a printed paper, can now be treated exactly, and in any measurement geometry, without approximations and without unknown constants.

Stamnes and coworkers [6-8] described a method to account for the phenomena that occur at the border between atmosphere and ocean due to change in refractive index, e.g. refraction and total reflection. This report is a detailed examination of that work, including more detailed derivations and corrections of several errors, but also adaptation and inclusion of the method into DORT2002. Tests of consistency and accuracy are also presented.

Section 1 begins with some notes and references, in section 2 the problem is stated in mathematical terms, and in section 3 the solution method is worked out in some detail, with interpolation formulas given in section 4. Section 5 covers some performance and consistency tests, suggestions for future work are given in section 6, and section 7 discusses the results in general, and the impact on the paper and printing industries in particular.

1.1. Some Comments on This Presentation

This report is not meant to be read on its own. It is, as the title suggests, the direct continuation of two previous reports by Edström [9-10]. This report, as its two predecessors, is very mathematical. It is so because the model development involves a large amount of mathematical deduction and many ideas from scientific computing. However, continuously ongoing work also presents the DORT2002 tool and its use to an applied audience in the paper and printing industry. This includes results and findings from the application of DORT2002 [11-13], but also a manual [14] to the DORT2002 Graphical User Interface [15], a tool developed to provide users with a fast and easy way of performing DORT2002 simulations. It works as a shell that encapsulates the parameters and the function calls, and offers powerful simulations through a mouse click.

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This presentation owes much to that of Yan and Stamnes [8], and the same outline and methods, and some of the notation, have been used where applicable. However, some adaptation from atmospheric applications to the field of paper and print has been done. Also, several errors have been corrected, and the implementation in MATLAB is entirely new. It uses the same textbook ideas in many cases, but has been implemented from scratch, and many parts are entirely differently implemented. Numerical stability has been improved by reformulation of certain formulas, and some effort has been made to use matrix formulations, not only for the parts naturally expressed as matrices. This has been done to make use of MATLAB's excellent matrix handling.

All necessary definitions are given in the previous reports [9-10]. Also, frequent references are done to equations in those previous reports. In fact, these three reports should be seen as one unit. Therefore, the equation numbering in this report starts from where the previous report ended. This facilitates easy references within this report, as well as references to these three reports from other sources.

2. PROBLEM STATEMENT

The solutions found in the previous reports can handle a medium that is constructed as several discrete and vertically homogenous layers placed on top of each other. With a sufficiently large number of homogeneous layers, an inhomogeneous medium can be approximated. However, changes in refractive index have not yet been considered, such as that occurring at the interface between air and an ink-paper substrate. The treatment below extends the solution procedure to handle a discontinuous change in refractive index at the interface between two perfectly flat layers.

As before, if the optical properties of the medium are a function of optical depth, the medium can be divided into a number of adjacent layers, each of which having constant optical properties. In addition to this, the medium is now allowed to have a discontinuous change in refractive index at the interface between two layers. The part of the medium above this interface is hereafter called A, and the part below this interface is called B. All use of A or B as sub- or superscripts relates to these two parts of the medium. The refractive indices are denoted n_A and n_B, respectively, where it is assumed that $n_A < n_B$, so that $n_{rel} = n_B / n_A > 1$.

At τ_A, the optical depth where part A of the medium ends, i.e. where the change in refractive index occurs, there will be refraction and total reflection. Light in the direction $(-\mu_A, \varphi)$ will be reflected into the direction $(\mu_A, \varphi + \pi)$ or refracted into the direction $(-\mu_B, \varphi)$, where, according to Snell's law

$$\mu_B = \sqrt{1 - \left(1 - \mu_A^2\right) / n_{rel}^2} \; . \tag{284}$$

Assuming unpolarized light, Fresnel's formulas give the amount of reflected and transmitted (refracted) intensity through the interface at τ_A as

$$\mathrm{Refl}(-\mu_A; n_{rel}) = \frac{1}{2}\left(\left(\frac{\mu_A - n_{rel}\mu_B}{\mu_A + n_{rel}\mu_B}\right)^2 + \left(\frac{\mu_B - n_{rel}\mu_A}{\mu_B + n_{rel}\mu_A}\right)^2\right), \tag{285}$$

$$\mathrm{Trans}(-\mu_A; n_{rel}) = 2 n_{rel}\mu_A\mu_B\left(\left(\frac{1}{\mu_A + n_{rel}\mu_B}\right)^2 + \left(\frac{1}{\mu_B + n_{rel}\mu_A}\right)^2\right), \tag{286}$$

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and of reciprocity reasons it holds that

$$\mathrm{Refl}\left(+\mu_B;1/n_{rel}\right)=\mathrm{Refl}\left(-\mu_A;n_{rel}\right), \tag{287}$$

$$\mathrm{Trans}\left(+\mu_B;1/n_{rel}\right)=\mathrm{Trans}\left(-\mu_A;n_{rel}\right). \tag{288}$$

A slight generalization of equation (69) now gives equations for each Fourier component (where the superscript m as before has been dropped) in each layer of part A and B, respectively, as

$$\begin{cases} \mu_i^A \dfrac{dI^+\left(\tau,\mu_i^A\right)}{d\tau} = I^+\left(\tau,\mu_i^A\right) - \dfrac{a}{2}\sum_{j=1}^{N_A}\omega_j^A p\left(\mu_j^A,\mu_i^A\right)I^+\left(\tau,\mu_j^A\right) \\ \qquad -\dfrac{a}{2}\sum_{j=1}^{N_A}\omega_j^A p\left(-\mu_j^A,\mu_i^A\right)I^-\left(\tau,\mu_j^A\right) - S^A\left(\tau,\mu_i^A\right) \\ -\mu_i^A \dfrac{dI^-\left(\tau,\mu_i^A\right)}{d\tau} = I^-\left(\tau,\mu_i^A\right) - \dfrac{a}{2}\sum_{j=1}^{N_A}\omega_j^A p\left(\mu_j^A,-\mu_i^A\right)I^+\left(\tau,\mu_j^A\right) \\ \qquad -\dfrac{a}{2}\sum_{j=1}^{N_A}\omega_j^A p\left(-\mu_j^A,-\mu_i^A\right)I^-\left(\tau,\mu_j^A\right) - S^A\left(\tau,-\mu_i^A\right) \end{cases}, \tag{289}$$

$$i=1,2,\ldots,N_A,$$

$$\begin{cases} \mu_i^B \dfrac{dI^+\left(\tau,\mu_i^B\right)}{d\tau} = I^+\left(\tau,\mu_i^B\right) - \dfrac{a}{2}\sum_{j=1}^{N_B}\omega_j^B p\left(\mu_j^B,\mu_i^B\right)I^+\left(\tau,\mu_j^B\right) \\ \qquad -\dfrac{a}{2}\sum_{j=1}^{N_B}\omega_j^B p\left(-\mu_j^B,\mu_i^B\right)I^-\left(\tau,\mu_j^B\right) - S^B\left(\tau,\mu_i^B\right) \\ -\mu_i^B \dfrac{dI^-\left(\tau,\mu_i^B\right)}{d\tau} = I^-\left(\tau,\mu_i^B\right) - \dfrac{a}{2}\sum_{j=1}^{N_B}\omega_j^B p\left(\mu_j^B,-\mu_i^B\right)I^+\left(\tau,\mu_j^B\right) \\ \qquad -\dfrac{a}{2}\sum_{j=1}^{N_B}\omega_j^B p\left(-\mu_j^B,-\mu_i^B\right)I^-\left(\tau,\mu_j^B\right) - S^B\left(\tau,-\mu_i^B\right) \end{cases}, \tag{290}$$

$$i=1,2,\ldots,N_B.$$

The source terms are

$$S^A\left(\tau,\pm\mu\right)=X_0\left(\tau,\pm\mu\right)e^{-\tau/\mu_0}+X_{0A}\left(\tau,\pm\mu\right)e^{-(2\tau_A-\tau)/\mu_0}, \tag{291}$$

$$S^B\left(\tau,\pm\mu\right)=X_{0B}\left(\tau,\pm\mu\right)e^{-\left(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n}\right)}, \tag{292}$$

where

$$X_0\left(\tau,\pm\mu\right)=\frac{a(\tau)}{4\pi}\left(2-\delta_{0m}\right)p^m\left(\tau,-\mu_0,\pm\mu\right)I_{0b}, \tag{293}$$

$$X_{0A}\left(\tau,\pm\mu\right)=\frac{a(\tau)}{4\pi}\mathrm{Refl}\left(-\mu_0;n_{rel}\right)\left(2-\delta_{0m}\right)p^m\left(\tau,+\mu_0,\pm\mu\right)I_{0b}, \tag{294}$$

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$$X_{0B}(\tau,\pm\mu)=\frac{a(\tau)}{4\pi}\frac{\mu_0}{\mu_{0n}}\mathrm{Trans}(-\mu_0;n_{rel})(2-\delta_{0m})p^m(\tau,-\mu_{0n},\pm\mu)I_{0b} \quad (295)$$

and

$$\mu_{0n}=\sqrt{1-\left(1-\mu_0^2\right)/n_{rel}^2}\,, \quad (296)$$

and where μ_0 and μ_{0n} refer to the incident beam with direction $(-\mu_0,\varphi_0)$ which will be refracted into the direction $(-\mu_{0n},\varphi_0)$.

Here μ_i^A, ω_i^A and μ_i^B, ω_i^B are the quadrature points and weights for parts A and B, and as before

$$\mu_{-i}=-\mu_i\,, \quad (297)$$

$$\omega_{-i}=\omega_i\,. \quad (298)$$

For part A, μ_i^A and ω_i^A, $i=1,\ldots,N_A$, are determined with the Double-Gauss quadrature rule as before. It should be noted that more quadrature points (or, equivalently, more channels) are used in part B than in part A, i.e. $N_B > N_A$, in order to account for refraction and total reflection. The number of extra quadrature points (N_B-N_A) is not an obvious choice. However, it is reasonable to choose N_B-N_A smaller than N_A, and to increase N_B-N_A when N_A increases.

Part B can be divided into two regions, I and II, separated by the critical angle

$$\mu_c=\sqrt{1-1/n_{rel}^2}\,. \quad (299)$$

In region I, light traveling upwards will undergo total reflection at the interface between parts A and B. Therefore, the only way of light in region I to reach part A is by scattering into region II. The additional N_B-N_A quadrature points in part B are invoked to accommodate the scattering interaction between regions I and II. For region I, μ_i^B and ω_i^B, $i=1,\ldots,N_B-N_A$, are determined with the Double-Gauss quadrature rule applied on the interval $[0,\mu_c]$, i.e.

$$\mu_i^B=\mu_{DG}\mu_c\,, \quad (300)$$

$$\omega_i^B=\omega_{DG}\mu_c\,, \quad (301)$$

where μ_{DG} and ω_{DG} are the points and weights for a N_B-N_A-point Double-Gauss quadrature rule on the "ordinary" interval $[0,1]$.

Region II communicates directly with part A, and the quadrature points in this region are obtained by refracting the quadrature points of part A. Hence μ_i^B, $i=N_B-N_A+1,\ldots,N_B$, are obtained by applying Snell's law as

$$\mu_i^B=\sqrt{1-\left(1-\left(\mu_{i-(N_B-N_A)}^A\right)^2\right)/n_{rel}^2}\,,\qquad i=N_B-N_A+1,\ldots,N_B\,. \quad (302)$$

This accounts for the shrinking caused by the refraction of the angular domain in part B. The corresponding weights ω_i^B, $i=N_B-N_A+1,\ldots,N_B$, are then derived as

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$$\omega_i^B = \omega_{i-(N_B-N_A)}^A \left[\frac{d\mu_B(\mu_A)}{d\mu_A} \right]_{\mu_A=\mu_{i-(N_B-N_A)}^A} = \omega_{i-(N_B-N_A)}^A \frac{\mu_{i-(N_B-N_A)}^A}{n_{rel}^2 \mu_i^B}, \qquad (303)$$

$$i = N_B - N_A + 1, \ldots, N_B .$$

This choice of quadrature scheme has several advantages. The quadrature points are denser near $\mu = 0$ both in part A and part B. They are also denser near the critical angle, μ_c, both in region I and region II. This is advantageous since the intensity will vary rapidly near these directions. This quadrature scheme will also maintain normalization of the phase function, as required by equation (70).

The quadrature scheme is illustrated in figure 1 below.

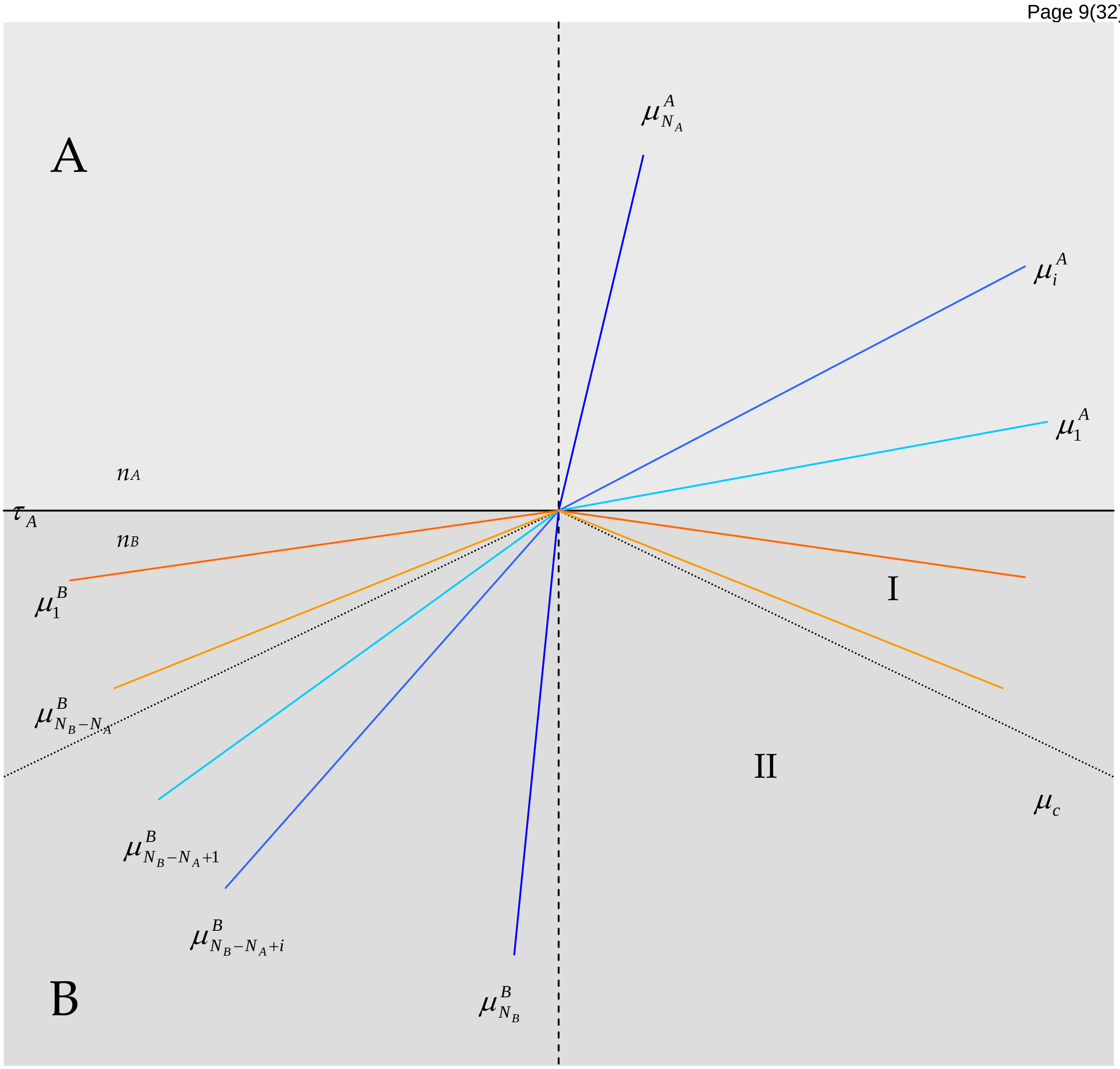

Figure 1. The medium has a discontinuous change in refractive index at the interface between two layers. The part of the medium above this interface is called A, and the part below this interface is called B. The refractive index is assumed to be larger in part B, $n_B > n_A$. At τ_A, the optical depth where part A of the medium ends, there will be refraction and total reflection, as indicated by the beams of different colors. The quadrature points for part A, μ_i^A, $i = 1,\ldots,N_A$, are determined with the Double-Gauss quadrature rule. It should be noted that more quadrature points are used in part B, i.e. $N_B > N_A$, in order to account for refraction and total reflection. Part B is divided into two regions, I and II, separated by the critical angle μ_c. In region I, light traveling upwards will undergo total reflection. For region I, μ_i^B, $i = 1,\ldots,N_B - N_A$, are determined with the Double-Gauss quadrature rule applied on the interval $[0, \mu_c]$. Region II communicates directly with part A, and the quadrature points in this region are obtained by refracting the quadrature points of part A. Hence μ_i^B, $i = N_B - N_A+1,\ldots,N_B$, are obtained by applying Snell's law.

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3. SOLUTION METHOD

Equations (289-290) can be formulated as eigenvalue problems and solved as before. The homogenous solutions can be written as a linear combination of the eigensolutions with coefficients C_j as

$$I^{\pm}\left(\tau,\mu_i^A\right)=\sum_{j=1}^{N_A}\left(C_j g_j\left(\pm\mu_i^A\right)e^{-k_j^A\tau}+C_{-j}g_{-j}\left(\pm\mu_i^A\right)e^{k_j^A\tau}\right),\ i=1,\ldots,N_A, \tag{304}$$

$$I^{\pm}\left(\tau,\mu_i^B\right)=\sum_{j=1}^{N_B}\left(C_j g_j\left(\pm\mu_i^B\right)e^{-k_j^B\tau}+C_{-j}g_{-j}\left(\pm\mu_i^B\right)e^{k_j^B\tau}\right),\ i=1,\ldots,N_B, \tag{305}$$

where the k_j and g_j are eigenvalues and eigenvectors, and C_j are constants of integration to be given by boundary and continuity conditions.

For part A, the particular solution can be expressed as

$$U^{\pm}\left(\tau,\mu_i^A\right)=Z_0\left(\pm\mu_i^A\right)e^{-\tau/\mu_0}+Z_{0A}\left(\pm\mu_i^A\right)e^{-(2\tau_A-\tau)/\mu_0},\ i=1,\ldots,N_A, \tag{306}$$

where, as can be verified by insertion, Z_0 and Z_{0A} are determined by

$$\sum_{\substack{j=-N_A\\ j\neq 0}}^{N_A}\left(\left(1+\frac{u_j^A}{\mu_0}\right)\delta_{ij}-\omega_j^A\frac{a}{2}p\left(u_j^A,u_i^A\right)\right)Z_0\left(\mu_j^A\right)=X_0\left(\mu_i^A\right), \tag{307}$$

$$\sum_{\substack{j=-N_A\\ j\neq 0}}^{N_A}\left(\left(1-\frac{u_j^A}{\mu_0}\right)\delta_{ij}-\omega_j^A\frac{a}{2}p\left(u_j^A,u_i^A\right)\right)Z_{0A}\left(\mu_j^A\right)=X_{0A}\left(\mu_i^A\right). \tag{308}$$

Similarly, the particular solution for part B can be expressed as

$$U^{\pm}\left(\tau,\mu_i^B\right)=Z_{0B}\left(\pm\mu_i^B\right)e^{-(\tau_A/\mu_0+(\tau-\tau_A)/\mu_{0n})},\ i=1,\ldots,N_B, \tag{309}$$

where Z_{0B} is determined by

$$\sum_{\substack{j=-N_B\\ j\neq 0}}^{N_B}\left(\left(1+\frac{u_j^B}{\mu_{0n}}\right)\delta_{ij}-\omega_j^B\frac{a}{2}p\left(u_j^B,u_i^B\right)\right)Z_{0B}\left(\mu_j^B\right)=X_{0B}\left(\mu_i^B\right). \tag{310}$$

Assuming there are L_A layers in part A and L_B layers in part B, the solution for the *p*th layer can in analogy with equation (154) be written as

$$I_p^{\pm}\left(\tau,\mu_i^A\right)=\sum_{j=1}^{N_A}\left(C_{jp}g_{jp}\left(\pm\mu_i^A\right)e^{-k_{jp}^A\tau}+C_{-jp}g_{-jp}\left(\pm\mu_i^A\right)e^{+k_{jp}^A\tau}\right)+U_p^{\pm}\left(\tau,\mu_i^A\right)$$
$$\text{for } i=1,\ldots,N_A \text{ and } p=1,\ldots,L_A, \tag{311}$$

$$I_p^{\pm}\left(\tau,\mu_i^B\right)=\sum_{j=1}^{N_B}\left(C_{jp}g_{jp}\left(\pm\mu_i^B\right)e^{-k_{jp}^B\tau}+C_{-jp}g_{-jp}\left(\pm\mu_i^B\right)e^{+k_{jp}^B\tau}\right)+U_p^{\pm}\left(\tau,\mu_i^B\right)$$
$$\text{for } i=1,\ldots,N_B \text{ and } p=L_A+1,\ldots,L_B, \tag{312}$$

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where as before, $k_{jp} > 0$ and $k_{-jp} = -k_{jp}$.

The solution contains in total $(2N_A \times L_A) + (2N_B \times L_B)$ constants C_{jp} to be determined. In addition to the previous boundary conditions at the top of part A and at the bottom of part B, and the continuity conditions between layers within parts A and B, the intensity must now be required to satisfy Snell's and Fresnel's equations at the interface between parts A and B. This gives the following equations to be fulfilled simultaneously. At the top of part A (and the entire medium) the boundary condition gives

$$I_1\left(0,-\mu_i^A\right) = \Upsilon\left(-\mu_i^A\right),\ i = 1,\ldots,N_A, \tag{313}$$

where $\Upsilon^m\left(-\mu_i\right)$ is the incident radiation. Continuity at the interfaces between layers in part A requires

$$I_p\left(\tau_p,\mu_i^A\right) = I_{p+1}\left(\tau_p,\mu_i^A\right),\ i = \pm 1,\ldots,\pm N_A,\ p = 1,\ldots,L_A - 1. \tag{314}$$

At the interface between parts A and B, Snell's and Fresnel's equations give

$$\begin{aligned} I_{L_A}\left(\tau_A,\mu_i^A\right) &= I_{L_A}\left(\tau_A,-\mu_i^A\right)\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right) \\ &+ \frac{I_{L_A+1}\left(\tau_A,\mu^B_{N_B-N_A+i}\right)}{n_{rel}^2}\mathrm{Trans}\left(+\mu^B_{N_B-N_A+i};1/n_{rel}\right)' \\ & i = 1,\ldots,N_A, \end{aligned} \tag{315}$$

$$\begin{aligned} \frac{I_{L_A+1}\left(\tau_A,-\mu^B_{N_B-N_A+i}\right)}{n_{rel}^2} &= \frac{I_{L_A+1}\left(\tau_A,\mu^B_{N_B-N_A+i}\right)}{n_{rel}^2}\mathrm{Refl}\left(+\mu^B_{N_B-N_A+i};1/n_{rel}\right), \\ &+ I_{L_A}\left(\tau_A,-\mu_i^A\right)\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right) \\ & i = 1,\ldots,N_A. \end{aligned} \tag{316}$$

Total reflection at the interface between parts A and B gives

$$I_{L_A+1}\left(\tau_A,-\mu_i^B\right) = I_{L_A+1}\left(\tau_A,\mu_i^B\right),\ i = 1,\ldots,N_B - N_A. \tag{317}$$

Continuity at the interfaces between layers in part B requires

$$I_p\left(\tau_p,\mu_i^B\right) = I_{p+1}\left(\tau_p,\mu_i^B\right),\ i = \pm 1,\ldots,\pm N_B,\ p = L_A + 1,\ldots,L_A + L_B - 1. \tag{318}$$

At the bottom of part B (and the entire medium) the boundary condition gives

$$\begin{aligned} I_{L_A+L_B}\left(\tau^*,+\mu_i^B\right) &= \left(1+\delta_{m0}\right)\sum_{j=1}^{N_B}\omega_j^B\mu_j^B\rho_d^m\left(-\mu_j^B,\mu_i^B\right)I_{L_A+L_B}\left(\tau^*,-\mu_j^B\right), \\ &+ \frac{\mu_{0n}}{\pi}\rho_d^m\left(-\mu_{0n},\mu_i^B\right)I_{0b}e^{-\left(\tau_A/\mu_0+\left(\tau^*-\tau_A\right)/\mu_{0n}\right)} \\ & i = 1,\ldots,N_B, \end{aligned} \tag{319}$$

where τ^* is the optical depth at the bottom, and ρ_d^m is defined in equation (120).

Substituting the solution (311-312) into these equations yields

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$$\sum_{j=1}^{N_A}\left(C_{j1}g_{j1}\left(-\mu_i^A\right)+C_{-j1}g_{-j1}\left(-\mu_i^A\right)\right)=\Upsilon\left(-\mu_i^A\right)-U_1\left(0,-\mu_i^A\right)$$ for $i=1,\ldots,N_A$,	(320)
$$\sum_{j=1}^{N_A}\left\{\left(C_{jp}g_{jp}\left(\mu_i^A\right)e^{-k_{jp}^A\tau_p}+C_{-jp}g_{-jp}\left(\mu_i^A\right)e^{+k_{jp}^A\tau_p}\right)-\left(C_{j,p+1}g_{j,p+1}\left(\mu_i^A\right)e^{-k_{j,p+1}^A\tau_p}+C_{-j,p+1}g_{-j,p+1}\left(\mu_i^A\right)e^{+k_{j,p+1}^A\tau_p}\right)\right\}=$$ $$=U_{p+1}\left(\tau_p,\mu_i^A\right)-U_p\left(\tau_p,\mu_i^A\right)$$ for $i=\pm1,\ldots,\pm N_A$ and $p=1,\ldots,L_A-1$,	(321)
$$\sum_{j=1}^{N_A}\left\{\left(C_{jL_A}g_{jL_A}\left(\mu_i^A\right)e^{-k_{jL_A}^A\tau_A}+C_{-jL_A}g_{-jL_A}\left(\mu_i^A\right)e^{+k_{jL_A}^A\tau_A}\right)-\left(C_{jL_A}g_{jL_A}\left(-\mu_i^A\right)e^{-k_{jL_A}^A\tau_A}+C_{-jL_A}g_{-jL_A}\left(-\mu_i^A\right)e^{+k_{jL_A}^A\tau_A}\right)\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right)\right\}$$ $$-\sum_{j=1}^{N_B}\left(C_{j,L_A+1}g_{j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right)e^{-k_{j,L_A+1}^B\tau_A}+C_{-j,L_A+1}g_{-j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right)e^{+k_{j,L_A+1}^B\tau_A}\right)\times\frac{1}{n_{rel}^2}\mathrm{Trans}\left(+\mu_{N_B-N_A+i}^B;1/n_{rel}\right)=$$ $$=U_{L_A}\left(\tau_A,-\mu_i^A\right)\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right)-U_{L_A}\left(\tau_A,\mu_i^A\right)+U_{L_A+1}\left(\tau_A,\mu_{N_B-N_A+i}^B\right)\frac{1}{n_{rel}^2}\mathrm{Trans}\left(+\mu_{N_B-N_A+i}^B;1/n_{rel}\right)$$ for $i=1,\ldots,N_A$,	(322)
$$\sum_{j=1}^{N_B}\left\{\left(C_{j,L_A+1}g_{j,L_A+1}\left(-\mu_{N_B-N_A+i}^B\right)e^{-k_{j,L_A+1}^B\tau_A}+C_{-j,L_A+1}g_{-j,L_A+1}\left(-\mu_{N_B-N_A+i}^B\right)e^{+k_{j,L_A+1}^B\tau_A}\right)\frac{1}{n_{rel}^2}-\left(C_{j,L_A+1}g_{j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right)e^{-k_{j,L_A+1}^B\tau_A}+C_{-j,L_A+1}g_{-j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right)e^{+k_{j,L_A+1}^B\tau_A}\right)\times\frac{1}{n_{rel}^2}\mathrm{Refl}\left(+\mu_{N_B-N_A+i}^B;1/n_{rel}\right)\right\}$$ $$-\sum_{j=1}^{N_A}\left(C_{jL_A}g_{jL_A}\left(-\mu_i^A\right)e^{-k_{jL_A}^A\tau_A}+C_{-jL_A}g_{-jL_A}\left(-\mu_i^A\right)e^{+k_{jL_A}^A\tau_A}\right)\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right)=$$ $$=U_{L_A+1}\left(\tau_A,\mu_{N_B-N_A+i}^B\right)\frac{1}{n_{rel}^2}\mathrm{Refl}\left(+\mu_{N_B-N_A+i}^B;1/n_{rel}\right)-U_{L_A+1}\left(\tau_A,-\mu_{N_B-N_A+i}^B\right)\frac{1}{n_{rel}^2}+U_{L_A}\left(\tau_A,-\mu_i^A\right)\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right)$$ for $i=1,\ldots,N_A$,	(323)

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$$\sum_{j=1}^{N_B}\left\{\left(C_{j,L_A+1}g_{j,L_A+1}\left(-\mu_i^B\right)e^{-k_{j,L_A+1}^B\tau_A}+C_{-j,L_A+1}g_{-j,L_A+1}\left(-\mu_i^B\right)e^{+k_{j,L_A+1}^B\tau_A}\right)-\left(C_{j,L_A+1}g_{j,L_A+1}\left(\mu_i^B\right)e^{-k_{j,L_A+1}^B\tau_A}+C_{-j,L_A+1}g_{-j,L_A+1}\left(\mu_i^B\right)e^{+k_{j,L_A+1}^B\tau_A}\right)\right\}=U_{L_A+1}\left(\tau_A,\mu_i^B\right)-U_{L_A+1}\left(\tau_A,-\mu_i^B\right)$$ for $i=1,\ldots,N_B-N_A$,	(324)
$$\sum_{j=1}^{N_B}\left\{\left(C_{jp}g_{jp}\left(\mu_i^B\right)e^{-k_{jp}^B\tau_p}+C_{-jp}g_{-jp}\left(\mu_i^B\right)e^{+k_{jp}^B\tau_p}\right)-\left(C_{j,p+1}g_{j,p+1}\left(\mu_i^B\right)e^{-k_{j,p+1}^B\tau_p}+C_{-j,p+1}g_{-j,p+1}\left(\mu_i^B\right)e^{+k_{j,p+1}^B\tau_p}\right)\right\}=U_{p+1}\left(\tau_p,\mu_i^B\right)-U_p\left(\tau_p,\mu_i^B\right)$$ for $i=\pm1,\ldots,\pm N_B$ and $p=L_A+1,\ldots,L_A+L_B-1$,	(325)
$$\sum_{j=1}^{N_B}\left(C_{j,L_A+L_B}r_j\left(\mu_i^B\right)e^{-k_{j,L_A+L_B}^B\tau^*}+C_{-j,L_A+L_B}r_{-j}\left(\mu_i^B\right)e^{+k_{j,L_A+L_B}^B\tau^*}\right)=\Gamma\left(\tau^*,\mu_i^B\right)$$ for $i=1,\ldots,N_B$,	(326)

where

$$r_j\left(\mu_i^B\right)=g_{j,L_A+L_B}\left(+\mu_i^B\right)-\left(1+\delta_{m0}\right)\sum_{n=1}^{N_B}\rho_d\left(-\mu_n^B,\mu_i^B\right)\omega_n^B\mu_n^B g_{j,L_A+L_B}\left(-\mu_n^B\right) \quad (327)$$

and

$$\Gamma\left(\tau^*,\mu_i^B\right)=-U_{L_A+L_B}\left(\tau^*,\mu_i^B\right)+\left(1+\delta_{m0}\right)\sum_{j=1}^{N_B}\rho_d\left(-\mu_j^B,\mu_i^B\right)\omega_j^B\mu_j^B U_{L_A+L_B}\left(\tau^*,-\mu_j^B\right)+\frac{\mu_{0n}}{\pi}\rho_d\left(-\mu_{0n},\mu_i^B\right)I_{0b}e^{-\left(\tau_A/\mu_0+(\tau^*-\tau_A)/\mu_{0n}\right)}. \quad (328)$$

This is a system of equations of size $(2N_A\times L_A)+(2N_B\times L_B)$ for the unknown coefficients C_{jp}, where $j=\pm1,\pm2,\ldots,\pm N_A$ for $p=1,\ldots,L_A$ and $j=\pm1,\pm2,\ldots,\pm N_B$ for $p=1,\ldots,L_B$. As before, the equations are ill conditioned due to the exponentials with positive arguments, but the ill conditioning can still be removed with the scaling transformation

$$C_{+jp}=C'_{+jp}e^{k_{jp}\tau_{p-1}} \text{ and } C_{-jp}=C'_{-jp}e^{-k_{jp}\tau_p}. \quad (329)$$

Using the scaling transformation and the reciprocity relations (287-288) gives the following system for the C'_{jp} (with τ_0 as the optical depth at the top)

$$\sum_{j=1}^{N_A}\left(C'_{j1}g_{j1}\left(-\mu_i^A\right)+C'_{-j1}g_{-j1}\left(-\mu_i^A\right)e^{-k_{jp}^A(\tau_1-\tau_0)}\right)=\Upsilon\left(-\mu_i^A\right)-U_1\left(\tau_0,-\mu_i^A\right)$$ for $i=1,\ldots,N_A$,	(330)

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$$
\begin{aligned}
&\sum_{j=1}^{N_A}\left\{\left(C'_{jp}\, g_{jp}\left(\mu_i^A\right) e^{-k_{jp}^A(\tau_p-\tau_{p-1})} + C'_{-jp}\, g_{-jp}\left(\mu_i^A\right)\right)\right.\\
&\qquad\left.-\left(C'_{j,p+1}\, g_{j,p+1}\left(\mu_i^A\right) + C'_{-j,p+1}\, g_{-j,p+1}\left(\mu_i^A\right) e^{-k_{j,p+1}^A(\tau_{p+1}-\tau_p)}\right)\right\}=\\
&= U_{p+1}\left(\tau_p,\mu_i^A\right) - U_p\left(\tau_p,\mu_i^A\right)\\
&\qquad\qquad \text{for } i=\pm 1,\ldots,\pm N_A \text{ and } p=1,\ldots,L_A-1,
\end{aligned}
\tag{331}
$$

$$
\begin{aligned}
&\sum_{j=1}^{N_A}\left\{\left(C'_{jL_A}\, g_{jL_A}\left(\mu_i^A\right) e^{-k_{jL_A}^A(\tau_A-\tau_{L_A-1})} + C'_{-jL_A}\, g_{-jL_A}\left(\mu_i^A\right)\right)\right.\\
&\qquad\left.-\left(C'_{jL_A}\, g_{jL_A}\left(-\mu_i^A\right) e^{-k_{jL_A}^A(\tau_A-\tau_{L_A-1})} + C'_{-jL_A}\, g_{-jL_A}\left(-\mu_i^A\right)\right)\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right)\right\}\\
&\quad-\sum_{j=1}^{N_B}\left(C'_{j,L_A+1}\, g_{j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right) + C'_{-j,L_A+1}\, g_{-j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right) e^{-k_{j,L_A+1}^B(\tau_{L_A+1}-\tau_A)}\right)\\
&\qquad\times\frac{1}{n_{rel}^2}\,\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right)=\\
&= U_{L_A}\left(\tau_A,-\mu_i^A\right)\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right) - U_{L_A}\left(\tau_A,\mu_i^A\right)\\
&\quad + U_{L_A+1}\left(\tau_A,\mu_{N_B-N_A+i}^B\right)\frac{1}{n_{rel}^2}\,\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right)\\
&\qquad\qquad \text{for } i=1,\ldots,N_A,
\end{aligned}
\tag{332}
$$

$$
\begin{aligned}
&\sum_{j=1}^{N_B}\left\{\left(C'_{j,L_A+1}\, g_{j,L_A+1}\left(-\mu_{N_B-N_A+i}^B\right) + C'_{-j,L_A+1}\, g_{-j,L_A+1}\left(-\mu_{N_B-N_A+i}^B\right) e^{-k_{j,L_A+1}^B(\tau_{L_A+1}-\tau_A)}\right)\frac{1}{n_{rel}^2}\right.\\
&\qquad-\left(C'_{j,L_A+1}\, g_{j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right) + C'_{-j,L_A+1}\, g_{-j,L_A+1}\left(\mu_{N_B-N_A+i}^B\right) e^{-k_{j,L_A+1}^B(\tau_{L_A+1}-\tau_A)}\right)\\
&\qquad\quad\left.\times\frac{1}{n_{rel}^2}\,\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right)\right\}\\
&\quad-\sum_{j=1}^{N_A}\left(C'_{jL_A}\, g_{jL_A}\left(-\mu_i^A\right) e^{-k_{jL_A}^A(\tau_A-\tau_{L_A-1})} + C'_{-jL_A}\, g_{-jL_A}\left(-\mu_i^A\right)\right)\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right)=\\
&= U_{L_A+1}\left(\tau_A,\mu_{N_B-N_A+i}^B\right)\frac{1}{n_{rel}^2}\,\mathrm{Refl}\left(-\mu_i^A;n_{rel}\right) - U_{L_A+1}\left(\tau_A,-\mu_{N_B-N_A+i}^B\right)\frac{1}{n_{rel}^2}\\
&\quad + U_{L_A}\left(\tau_A,-\mu_i^A\right)\mathrm{Trans}\left(-\mu_i^A;n_{rel}\right)\\
&\qquad\qquad \text{for } i=1,\ldots,N_A,
\end{aligned}
\tag{333}
$$

$$
\begin{aligned}
&\sum_{j=1}^{N_B}\left\{\left(C'_{j,L_A+1}\, g_{j,L_A+1}\left(-\mu_i^B\right) + C'_{-j,L_A+1}\, g_{-j,L_A+1}\left(-\mu_i^B\right) e^{-k_{j,L_A+1}^B(\tau_{L_A+1}-\tau_A)}\right)\right.\\
&\qquad\left.-\left(C'_{j,L_A+1}\, g_{j,L_A+1}\left(\mu_i^B\right) + C'_{-j,L_A+1}\, g_{-j,L_A+1}\left(\mu_i^B\right) e^{-k_{j,L_A+1}^B(\tau_{L_A+1}-\tau_A)}\right)\right\}=\\
&= U_{L_A+1}\left(\tau_A,\mu_i^B\right) - U_{L_A+1}\left(\tau_A,-\mu_i^B\right)\\
&\qquad\qquad \text{for } i=1,\ldots,N_B-N_A,
\end{aligned}
\tag{334}
$$

$$\sum_{j=1}^{N_B}\Big\{\Big(C'_{jp}g_{jp}\left(\mu_i^B\right)e^{-k_{jp}^B(\tau_p-\tau_{p-1})}+C'_{-jp}g_{-jp}\left(\mu_i^B\right)\Big) - \Big(C'_{j,p+1}g_{j,p+1}\left(\mu_i^B\right)+C'_{-j,p+1}g_{-j,p+1}\left(\mu_i^B\right)e^{-k_{jp}^B(\tau_{p+1}-\tau_p)}\Big)\Big\}= =U_{p+1}\left(\tau_p,\mu_i^B\right)-U_p\left(\tau_p,\mu_i^B\right)$$ for $i=\pm 1,\ldots,\pm N_B$ and $p=L_A+1,\ldots,L_A+L_B-1$,	(335)
$$\sum_{j=1}^{N_B}\Big(C'_{j,L_A+L_B}r_j\left(\mu_i^B\right)e^{-k_{j,L_A+L_B}^B(\tau^*-\tau_{L_A+L_B-1})}+C'_{-j,L_A+L_B}r_{-j}\left(\mu_i^B\right)\Big)=\Gamma\left(\tau^*,\mu_i^B\right)$$ for $i=1,\ldots,N_B$,	(336)

Since $k_{jp}>0$ and $\tau_p>\tau_{p-1}$, all exponentials in the system of equations for the coefficients C'_{jp} have negative arguments. Thus, the ill conditioning is avoided, and the problem of solving for the C'_{jp} is unconditionally stable.

There is a risk for overflow in the solution for the *p*th layer, but by using the same scaling, that solution becomes

$$I_p^{\pm}\left(\tau,\mu_i^A\right)=\sum_{j=1}^{N_A}\Big(C'_{jp}g_{jp}\left(\pm\mu_i^A\right)e^{-k_{jp}^A(\tau-\tau_{p-1})}+C'_{-jp}g_{-jp}\left(\pm\mu_i^A\right)e^{-k_{jp}^A(\tau_p-\tau)}\Big)+U_p^{\pm}\left(\tau,\mu_i^A\right) \tag{337}$$

for $i=1,\ldots,N_A$ and $p=1,\ldots,L_A$,

$$I_p^{\pm}\left(\tau,\mu_i^B\right)=\sum_{j=1}^{N_B}\Big(C'_{jp}g_{jp}\left(\pm\mu_i^B\right)e^{-k_{jp}^B(\tau-\tau_{p-1})}+C'_{-jp}g_{-jp}\left(\pm\mu_i^B\right)e^{-k_{jp}^B(\tau_p-\tau)}\Big)+U_p^{\pm}\left(\tau,\mu_i^B\right) \tag{338}$$

for $i=1,\ldots,N_B$ and $p=L_A+1,\ldots,L_B$.

Since $k_{jp}>0$ and $\tau_{p-1}<\tau<\tau_p$, all exponentials have negative arguments, and the risk of overflow is avoided. It should be pointed out that since DORT2002 uses the scaled coefficients in the rest of the solution procedure, it does not use any re-scaling transformation, and there is no risk of enlarging errors later.

4. INTERPOLATION FORMULAS

The solution procedure outlined so far gives the intensity at any depth, but only in the quadrature points. If the intensity in an arbitrary direction is wanted, an interpolation formula is needed. The interpolation formula is constructed as before, but the change in refractive index will make it a little more elaborate, which is considered below.

Equations (289) and (290) can be written on the form

$$\begin{cases}\mu\dfrac{dI^+(\tau,\mu)}{d\tau}=I^+(\tau,\mu)-S^+(\tau,\mu)\\[2ex] -\mu\dfrac{dI^-(\tau,\mu)}{d\tau}=I^-(\tau,\mu)-S^-(\tau,\mu)\end{cases} \tag{339}$$

for the respective parts A and B, where for part A

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$$
\begin{aligned}
S^{\pm}(\tau,\mu^A) = {} & \frac{a}{2}\sum_{j=1}^{N_A}\omega_j^A p(\mu_j^A,\pm\mu^A)I^{+}(\tau,\mu_j^A) + \frac{a}{2}\sum_{j=1}^{N_A}\omega_j^A p(-\mu_j^A,\pm\mu^A)I^{-}(\tau,\mu_j^A) \\
& + X_0(\pm\mu^A)e^{-\tau/\mu_0} + X_{0A}(\pm\mu^A)e^{-(2\tau_A-\tau)/\mu_0}
\end{aligned}, \tag{340}
$$

and for part B

$$
\begin{aligned}
S^{\pm}(\tau,\mu^B) = {} & \frac{a}{2}\sum_{j=1}^{N_B}\omega_j^B p(\mu_j^B,\pm\mu^B)I^{+}(\tau,\mu_j^B) + \frac{a}{2}\sum_{j=1}^{N_B}\omega_j^B p(-\mu_j^B,\pm\mu^B)I^{-}(\tau,\mu_j^B) \\
& + X_{0B}(\pm\mu^B)e^{-(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n})}
\end{aligned}, \tag{341}
$$

and where X_0, X_{0A}, X_{0B} and μ_{0n} are given by (293-296). Inserting the solutions (311-312) and using proper layer indexing, interpolation formulas for the source functions $S^{\pm}(\tau,\mu)$ can be written as follows.

For part A

$$
\begin{aligned}
S_p^{\pm}(\tau,\mu^A) = {} & \sum_{j=1}^{N_A} C_{jp}\tilde{g}_{jp}(\pm\mu^A)e^{-k_{jp}^A\tau} + \sum_{j=1}^{N_A} C_{-jp}\tilde{g}_{-jp}(\pm\mu^A)e^{k_{jp}^A\tau} \\
& + \tilde{Z}_{0p}(\pm\mu^A)e^{-\tau/\mu_0} + \tilde{Z}_{0Ap}(\pm\mu^A)e^{-(2\tau_A-\tau)/\mu_0}
\end{aligned}, \tag{342}
$$

where

$$
\tilde{g}_{jp}(\pm\mu^A) = \frac{a}{2}\sum_{i=1}^{N_A}\left(\omega_i^A p(-\mu_i^A,\pm\mu^A)g_{jp}(-\mu_i^A) + \omega_i^A p(+\mu_i^A,\pm\mu^A)g_{jp}(+\mu_i^A)\right), \tag{343}
$$

$$
\begin{aligned}
\tilde{Z}_{0p}(\pm\mu^A) = {} & \frac{a}{2}\sum_{i=1}^{N_A}\left(\omega_i^A p(-\mu_i^A,\pm\mu^A)Z_{0p}(-\mu_i^A) + \omega_i^A p(+\mu_i^A,\pm\mu^A)Z_{0p}(+\mu_i^A)\right) \\
& + X_{0p}(\pm\mu^A)
\end{aligned}, \tag{344}
$$

$$
\begin{aligned}
\tilde{Z}_{0Ap}(\pm\mu^A) = {} & \frac{a}{2}\sum_{i=1}^{N_A}\left(\omega_i^A p(-\mu_i^A,\pm\mu^A)Z_{0Ap}(-\mu_i^A) + \omega_i^A p(+\mu_i^A,\pm\mu^A)Z_{0Ap}(+\mu_i^A)\right) \\
& + X_{0Ap}(\pm\mu^A)
\end{aligned}. \tag{345}
$$

For part B

$$
\begin{aligned}
S_p^{\pm}(\tau,\mu^B) = {} & \sum_{j=1}^{N_B} C_{jp}\tilde{g}_{jp}(\pm\mu^B)e^{-k_{jp}^B\tau} + \sum_{j=1}^{N_B} C_{-jp}\tilde{g}_{-jp}(\pm\mu^B)e^{k_{jp}^B\tau} \\
& + \tilde{Z}_{0Bp}(\pm\mu^B)e^{-(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n})}
\end{aligned}, \tag{346}
$$

where

$$
\tilde{g}_{jp}(\pm\mu^B) = \frac{a}{2}\sum_{i=1}^{N_B}\left(\omega_i^B p(-\mu_i^B,\pm\mu^B)g_{jp}(-\mu_i^B) + \omega_i^B p(+\mu_i^B,\pm\mu^B)g_{jp}(+\mu_i^B)\right), \tag{347}
$$

$$
\begin{aligned}
\tilde{Z}_{0Bp}(\pm\mu^B) = {} & \frac{a}{2}\sum_{i=1}^{N_B}\left(\omega_i^B p(-\mu_i^B,\pm\mu^B)Z_{0Bp}(-\mu_i^B) + \omega_i^B p(+\mu_i^B,\pm\mu^B)Z_{0Bp}(+\mu_i^B)\right) \\
& + X_{0Bp}(\pm\mu^B)
\end{aligned}. \tag{348}
$$

These are analytical interpolation formulas for the source function $S_p^{\pm}(\tau,\mu)$ for each layer, expressed in the solutions of the eigenvalue problem for the respective layer. Using these interpolation formulas, equations (339) can be solved formally, and the result is the following interpolation formulas for the intensity at arbitrary depth and direction.

To find I^+ in part A, the first of equations (339) is integrated layer by layer from τ_A to τ, using $e^{-\tau/\mu^A}$ as integrating factor. This gives

$$\begin{aligned}I^+(\tau,\mu^A) &= I^+(\tau_A,\mu^A)e^{-(\tau_A-\tau)/\mu^A} \\ &+ \sum_{j=-N_A}^{N_A} C_{jp}\frac{\tilde{g}_{jp}(+\mu^A)}{1+k_{jp}^A\mu^A}\left(e^{-k_{jp}^A\tau} - e^{-\left(k_{jp}^A\tau_p+(\tau_p-\tau)/\mu^A\right)}\right) \\ &+ \frac{\tilde{Z}_{0Ap}(+\mu^A)}{1-k_{0p}^A\mu^A}\left(e^{-(2\tau_A-\tau)/\mu_0} - e^{-\left((2\tau_A-\tau_p)/\mu_0+(\tau_p-\tau)/\mu^A\right)}\right) \\ &+ \sum_{n=p+1}^{L_A}\sum_{j=-N_A}^{N_A} C_{jn}\frac{\tilde{g}_{jn}(+\mu^A)}{1+k_{jn}^A\mu^A}\left(e^{-\left(k_{jn}^A\tau_{n-1}+(\tau_{n-1}-\tau)/\mu^A\right)} - e^{-\left(k_{jn}^A\tau_n+(\tau_n-\tau)/\mu^A\right)}\right) \\ &+ \sum_{n=p+1}^{L_A}\frac{\tilde{Z}_{0An}(+\mu^A)}{1-k_{0n}^A\mu^A}\left(e^{-\left((2\tau_A-\tau_{n-1})/\mu_0+(\tau_{n-1}-\tau)/\mu^A\right)} - e^{-\left((2\tau_A-\tau_n)/\mu_0+(\tau_n-\tau)/\mu^A\right)}\right)\end{aligned}, \qquad (349)$$

where for all layers

$$C_0\tilde{g}_0(+\mu^A) \equiv \tilde{Z}_0(+\mu^A), \qquad (350)$$

$$k_{-j}^A = -k_j^A, \qquad (351)$$

$$k_0^A \equiv 1/\mu_0. \qquad (352)$$

To find I^+ in part B, the first of equations (339) is integrated layer by layer from τ^* to τ, using $e^{-\tau/\mu^B}$ as integrating factor. This gives

$$\begin{aligned}I^+(\tau,\mu^B) &= I^+(\tau^*,\mu^B)e^{-(\tau^*-\tau)/\mu^B} \\ &+ \sum_{j=-N_B}^{N_B} C_{jp}\frac{\tilde{g}_{jp}(+\mu^B)}{1+k_{jp}^B\mu^B}\left(e^{-k_{jp}^B\tau} - e^{-\left(k_{jp}^B\tau_p+(\tau_p-\tau)/\mu^B\right)}\right) \\ &+ \sum_{n=p+1}^{L_A+L_B}\sum_{j=-N_B}^{N_B} C_{jn}\frac{\tilde{g}_{jn}(+\mu^B)}{1+k_{jn}^B\mu^B}\left(e^{-\left(k_{jn}^B\tau_{n-1}+(\tau_{n-1}-\tau)/\mu^B\right)} - e^{-\left(k_{jn}^B\tau_n+(\tau_n-\tau)/\mu^B\right)}\right)\end{aligned}, \qquad (353)$$

where for all layers

$$C_0\tilde{g}_0(+\mu^B) \equiv \tilde{Z}_{0B}(+\mu^B)e^{-\tau_A(1/\mu_0-1/\mu_{0n})}, \qquad (354)$$

$$k_{-j}^B = -k_j^B, \qquad (355)$$

$$k_0^B \equiv 1/\mu_{0n}. \qquad (356)$$

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To find I^- in part A, the first of equations (339) is integrated layer by layer from τ_0 to τ, using e^{τ/μ^A} as integrating factor. This gives

$$\begin{aligned} I^-\left(\tau,\mu^A\right) &= I^-\left(\tau_0,\mu^A\right)e^{-(\tau-\tau_0)/\mu^A} \\ &+ \sum_{j=-N_A}^{N_A} C_{jp}\frac{\tilde{g}_{jp}\left(-\mu^A\right)}{1-k_{jp}^A\mu^A}\left(e^{-k_{jp}^A\tau}-e^{-\left(k_{jp}^A\tau_{p-1}+(\tau-\tau_{p-1})/\mu^A\right)}\right) \\ &+ \frac{\tilde{Z}_{0Ap}\left(-\mu^A\right)}{1+k_{0p}^A\mu^A}\left(e^{-(2\tau_A-\tau)/\mu_0}-e^{-\left((2\tau_A-\tau_{p-1})/\mu_0+(\tau-\tau_{p-1})/\mu^A\right)}\right) \\ &+ \sum_{n=1}^{p-1}\sum_{j=-N_A}^{N_A} C_{jn}\frac{\tilde{g}_{jn}\left(-\mu^A\right)}{1-k_{jn}^A\mu^A}\left(e^{-\left(k_{jn}^A\tau_n+(\tau-\tau_n)/\mu^A\right)}-e^{-\left(k_{jn}^A\tau_{n-1}+(\tau-\tau_{n-1})/\mu^A\right)}\right) \\ &+ \sum_{n=1}^{p-1}\frac{\tilde{Z}_{0An}\left(-\mu^A\right)}{1+k_{0n}^A\mu^A}\left(e^{-\left((2\tau_A-\tau_n)/\mu_0+(\tau-\tau_n)/\mu^A\right)}-e^{-\left((2\tau_A-\tau_{n-1})/\mu_0+(\tau-\tau_{n-1})/\mu^A\right)}\right) \end{aligned}, \quad (357)$$

where for all layers

$$C_0\tilde{g}_0\left(-\mu^A\right)\equiv\tilde{Z}_0\left(-\mu^A\right), \quad (358)$$

$$k_{-j}^A=-k_j^A, \quad (359)$$

$$k_0^A\equiv 1/\mu_0. \quad (360)$$

To find I^- in part B, the first of equations (339) is integrated layer by layer from τ_A to τ, using e^{τ/μ^B} as integrating factor. This gives

$$\begin{aligned} I^-\left(\tau,\mu^B\right) &= I^-\left(\tau_A,\mu^B\right)e^{-(\tau-\tau_A)/\mu^B} \\ &+ \sum_{j=-N_B}^{N_B} C_{jp}\frac{\tilde{g}_{jp}\left(-\mu^B\right)}{1-k_{jp}^B\mu^B}\left(e^{-k_{jp}^B\tau}-e^{-\left(k_{jp}^B\tau_{p-1}+(\tau-\tau_{p-1})/\mu^B\right)}\right) \\ &+ \sum_{n=L_A+1}^{p-1}\sum_{j=-N_B}^{N_B} C_{jn}\frac{\tilde{g}_{jn}\left(-\mu^B\right)}{1-k_{jn}^B\mu^B}\left(e^{-\left(k_{jn}^B\tau_n+(\tau-\tau_n)/\mu^B\right)}-e^{-\left(k_{jn}^B\tau_{n-1}+(\tau-\tau_{n-1})/\mu^B\right)}\right) \end{aligned}, \quad (361)$$

where for all layers

$$C_0\tilde{g}_0\left(-\mu^B\right)\equiv\tilde{Z}_{0B}\left(-\mu^B\right)e^{-\tau_A\left(1/\mu_0-1/\mu_{0n}\right)}, \quad (362)$$

$$k_{-j}^B=-k_j^B, \quad (363)$$

$$k_0^B\equiv 1/\mu_{0n}. \quad (364)$$

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Here, everything is known except $I^+\left(\tau_A,\mu^A\right)$, $I^+\left(\tau^*,\mu^B\right)$, $I^-\left(\tau_0,\mu^A\right)$ and $I^-\left(\tau_A,\mu^B\right)$. They can be determined by simple interpolation of the discrete solutions $I^+_{L_A}\left(\tau_A,\mu_i^A\right)$, $I^+_{L_A+L_B}\left(\tau^*,\mu_i^B\right)$, $I_1^-\left(\tau_0,\mu_i^A\right)$ and $I^-_{L_A+1}\left(\tau_A,\mu_i^B\right)$ from (337) and (338).

There is a risk for overflow in the interpolation formulas for the intensity, but by using the scaled coefficients C'_{jp}, the interpolation formulas for the intensity become as follows.

For I^+ in part A (where $\tau_A > ... > \tau_n > \tau_{n-1} > ... > \tau_p > \tau > \tau_{p-1}$),

$$\begin{aligned}
I^+\left(\tau,\mu^A\right) &= I^+\left(\tau_A,\mu^A\right)e^{-(\tau_A-\tau)/\mu^A} \\
&+ \frac{\tilde{Z}_{0p}\left(+\mu^A\right)}{1+\mu^A/\mu_0}\left(e^{-\tau/\mu_0} - e^{-\left(\tau_p/\mu_0+(\tau_p-\tau)/\mu^A\right)}\right) \\
&+ \sum_{j=1}^{N_A} C'_{jp}\frac{\tilde{g}_{jp}\left(+\mu^A\right)}{1+k^A_{jp}\mu^A}\left(e^{-k^A_{jp}(\tau-\tau_{p-1})} - e^{-\left(k^A_{jp}(\tau_p-\tau_{p-1})+(\tau_p-\tau)/\mu^A\right)}\right) \\
&+ \sum_{j=1}^{N_A} C'_{-jp}\frac{\tilde{g}_{-jp}\left(+\mu^A\right)}{1-k^A_{jp}\mu^A}\left(e^{-k^A_{jp}(\tau_p-\tau)} - e^{-(\tau_p-\tau)/\mu^A}\right) \\
&+ \frac{\tilde{Z}_{0Ap}\left(+\mu^A\right)}{1-\mu^A/\mu_0}\left(e^{-(2\tau_A-\tau)/\mu_0} - e^{-\left((2\tau_A-\tau_p)/\mu_0+(\tau_p-\tau)/\mu^A\right)}\right) \\
&+ \sum_{n=p+1}^{L_A}\Bigg\{\frac{\tilde{Z}_{0n}\left(+\mu^A\right)}{1+\mu^A/\mu_0}\left(e^{-\left(\tau_{n-1}/\mu_0+(\tau_{n-1}-\tau)/\mu^A\right)} - e^{-\left(\tau_n/\mu_0+(\tau_n-\tau)/\mu^A\right)}\right) \\
&\quad + \sum_{j=1}^{N_A} C'_{jn}\frac{\tilde{g}_{jn}\left(+\mu^A\right)}{1+k^A_{jn}\mu^A}\left(e^{-(\tau_{n-1}-\tau)/\mu^A} - e^{-\left(k^A_{jn}(\tau_n-\tau_{n-1})+(\tau_n-\tau)/\mu^A\right)}\right) \\
&\quad + \sum_{j=1}^{N_A} C'_{-jn}\frac{\tilde{g}_{-jn}\left(+\mu^A\right)}{1-k^A_{jn}\mu^A}\left(e^{-\left(k^A_{jn}(\tau_n-\tau_{n-1})+(\tau_{n-1}-\tau)/\mu^A\right)} - e^{-(\tau_n-\tau)/\mu^A}\right) \\
&\quad + \frac{\tilde{Z}_{0An}\left(+\mu^A\right)}{1-\mu^A/\mu_0}\left(e^{-\left((2\tau_A-\tau_{n-1})/\mu_0+(\tau_{n-1}-\tau)/\mu^A\right)} - e^{-\left((2\tau_A-\tau_n)/\mu_0+(\tau_n-\tau)/\mu^A\right)}\right)\Bigg\}
\end{aligned} \tag{365}$$

For I^+ in part B (where $\tau^* > ... > \tau_n > \tau_{n-1} > ... > \tau_p > \tau > \tau_{p-1} > ... > \tau_A$),

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$$
\begin{aligned}
I^{+}\left(\tau,\mu^{B}\right) &= I^{+}\left(\tau^{*},\mu^{B}\right)e^{-(\tau^{*}-\tau)/\mu^{B}} \\
&+ \frac{\tilde{Z}_{0Bp}\left(+\mu^{B}\right)}{1+\mu^{B}/\mu_{0n}}\left(e^{-(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n})} - e^{-\left((\tau_p-\tau_A)/\mu_{0n}+\tau_A/\mu_0+(\tau_p-\tau)/\mu^{B}\right)}\right) \\
&+ \sum_{j=1}^{N_B} C'_{jp}\,\frac{\tilde{g}_{jp}\left(+\mu^{B}\right)}{1+k_{jp}^{B}\mu^{B}}\left(e^{-k_{jp}^{B}(\tau-\tau_{p-1})} - e^{-\left(k_{jp}^{B}(\tau_p-\tau_{p-1})+(\tau_p-\tau)/\mu^{B}\right)}\right) \\
&+ \sum_{j=1}^{N_B} C'_{-jp}\,\frac{\tilde{g}_{-jp}\left(+\mu^{B}\right)}{1-k_{jp}^{B}\mu^{B}}\left(e^{-k_{jp}^{B}(\tau_p-\tau)} - e^{-(\tau_p-\tau)/\mu^{B}}\right) \\
&+ \sum_{n=p+1}^{L_A+L_B}\left\{\frac{\tilde{Z}_{0Bn}\left(+\mu^{B}\right)}{1+\mu^{B}/\mu_{0n}}\left(e^{-\left((\tau_{n-1}-\tau_A)/\mu_{0n}+(\tau_{n-1}-\tau)/\mu^{B}\right)} - e^{-\left((\tau_n-\tau_A)/\mu_{0n}+(\tau_n-\tau)/\mu^{B}\right)}\right)e^{-\tau_A/\mu_0}\right. \\
&\quad + \sum_{j=1}^{N_B} C'_{jn}\,\frac{\tilde{g}_{jn}\left(+\mu^{B}\right)}{1+k_{jn}^{B}\mu^{B}}\left(e^{-(\tau_{n-1}-\tau)/\mu^{B}} - e^{-\left(k_{jn}^{B}(\tau_n-\tau_{n-1})+(\tau_n-\tau)/\mu^{B}\right)}\right) \\
&\quad \left. + \sum_{j=1}^{N_B} C'_{-jn}\,\frac{\tilde{g}_{-jn}\left(+\mu^{B}\right)}{1-k_{jn}^{B}\mu^{B}}\left(e^{-\left(k_{jn}^{B}(\tau_n-\tau_{n-1})+(\tau_{n-1}-\tau)/\mu^{B}\right)} - e^{-(\tau_n-\tau)/\mu^{B}}\right)\right\}.
\end{aligned}
\tag{366}
$$

For I^{-} in part A (where $\tau_A > \ldots > \tau_p > \tau > \tau_{p-1} > \ldots > \tau_n > \tau_{n-1} > \ldots > \tau_0$),

$$
\begin{aligned}
I^{-}\left(\tau,\mu^{A}\right) &= I^{-}\left(\tau_0,\mu^{A}\right)e^{-(\tau-\tau_0)/\mu^{A}} \\
&+ \frac{\tilde{Z}_{0p}\left(-\mu^{A}\right)}{1-\mu^{A}/\mu_0}\left(e^{-\tau/\mu_0} - e^{-\left(\tau_{p-1}/\mu_0+(\tau-\tau_{p-1})/\mu^{A}\right)}\right) \\
&+ \sum_{j=1}^{N_A} C'_{jp}\,\frac{\tilde{g}_{jp}\left(-\mu^{A}\right)}{1-k_{jp}^{A}\mu^{A}}\left(e^{-k_{jp}^{A}(\tau-\tau_{p-1})} - e^{-(\tau-\tau_{p-1})/\mu^{A}}\right) \\
&+ \sum_{j=1}^{N_A} C'_{-jp}\,\frac{\tilde{g}_{-jp}\left(-\mu^{A}\right)}{1+k_{jp}^{A}\mu^{A}}\left(e^{-k_{jp}^{A}(\tau_p-\tau)} - e^{-\left(k_{jp}^{A}(\tau_p-\tau_{p-1})+(\tau-\tau_{p-1})/\mu^{A}\right)}\right) \\
&+ \frac{\tilde{Z}_{0Ap}\left(-\mu^{A}\right)}{1+\mu^{A}/\mu_0}\left(e^{-(2\tau_A-\tau)/\mu_0} - e^{-\left((2\tau_A-\tau_{p-1})/\mu_0+(\tau-\tau_{p-1})/\mu^{A}\right)}\right) \\
&+ \sum_{n=1}^{p-1}\left\{\frac{\tilde{Z}_{0n}\left(-\mu^{A}\right)}{1-\mu^{A}/\mu_0}\left(e^{-\left(\tau_n/\mu_0+(\tau-\tau_n)/\mu^{A}\right)} - e^{-\left(\tau_{n-1}/\mu_0+(\tau-\tau_{n-1})/\mu^{A}\right)}\right)\right. \\
&\quad + \sum_{j=1}^{N_A} C'_{jn}\,\frac{\tilde{g}_{jn}\left(-\mu^{A}\right)}{1-k_{jn}^{A}\mu^{A}}\left(e^{-\left(k_{jn}^{A}(\tau_n-\tau_{n-1})+(\tau-\tau_n)/\mu^{A}\right)} - e^{-(\tau-\tau_{n-1})/\mu^{A}}\right) \\
&\quad + \sum_{j=1}^{N_A} C'_{-jn}\,\frac{\tilde{g}_{-jn}\left(-\mu^{A}\right)}{1+k_{jn}^{A}\mu^{A}}\left(e^{-(\tau-\tau_n)/\mu^{A}} - e^{-\left(k_{jn}^{A}(\tau_n-\tau_{n-1})+(\tau-\tau_{n-1})/\mu^{A}\right)}\right). \\
&\quad \left. + \frac{\tilde{Z}_{0An}\left(-\mu^{A}\right)}{1+\mu^{A}/\mu_0}\left(e^{-\left((2\tau_A-\tau_n)/\mu_0+(\tau-\tau_n)/\mu^{A}\right)} - e^{-\left((2\tau_A-\tau_{n-1})/\mu_0+(\tau-\tau_{n-1})/\mu^{A}\right)}\right)\right\}
\end{aligned}
\tag{367}
$$

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For I^- in part B (where $\tau_p > \tau > \tau_{p-1} > \ldots > \tau_n > \tau_{n-1} > \ldots > \tau_A$),

$$
\begin{aligned}
I^-\left(\tau,\mu^B\right) = {} & I^-\left(\tau_A,\mu^B\right)e^{-(\tau-\tau_A)/\mu^B} \\
& + \frac{\tilde{Z}_{0Bp}\left(-\mu^B\right)}{1-\mu^B/\mu_{0n}}\left(e^{-(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n})} - e^{-\left((\tau_{p-1}-\tau_A)/\mu_{0n}+\tau_A/\mu_0+(\tau-\tau_{p-1})/\mu^B\right)}\right) \\
& + \sum_{j=1}^{N_B} C'_{jp}\,\frac{\tilde{g}_{jp}\left(-\mu^B\right)}{1-k_{jp}^B\mu^B}\left(e^{-k_{jp}^B(\tau-\tau_{p-1})} - e^{-(\tau-\tau_{p-1})/\mu^B}\right) \\
& + \sum_{j=1}^{N_B} C'_{-jp}\,\frac{\tilde{g}_{-jp}\left(-\mu^B\right)}{1+k_{jp}^B\mu^B}\left(e^{-k_{jp}^B(\tau_p-\tau)} - e^{-\left(k_{jp}^B(\tau_p-\tau_{p-1})+(\tau-\tau_{p-1})/\mu^B\right)}\right) \\
& + \sum_{n=L_A+1}^{p-1}\left\{\frac{\tilde{Z}_{0Bn}\left(-\mu^B\right)}{1-\mu^B/\mu_{0n}}\left(e^{-\left((\tau_n-\tau_A)/\mu_{0n}+(\tau-\tau_n)/\mu^B\right)} - e^{-\left((\tau_{n-1}-\tau_A)/\mu_{0n}+(\tau-\tau_{n-1})/\mu^B\right)}\right)e^{-\tau_A/\mu_0}\right. \\
& \qquad + \sum_{j=1}^{N_B} C'_{jn}\,\frac{\tilde{g}_{jn}\left(-\mu^B\right)}{1-k_{jn}^B\mu^B}\left(e^{-\left(k_{jn}^B(\tau_n-\tau_{n-1})+(\tau-\tau_n)/\mu^B\right)} - e^{-(\tau-\tau_{n-1})/\mu^B}\right) \\
& \qquad \left. + \sum_{j=1}^{N_B} C'_{-jn}\,\frac{\tilde{g}_{-jn}\left(-\mu^B\right)}{1+k_{jn}^B\mu^B}\left(e^{-(\tau-\tau_n)/\mu^B} - e^{-\left(k_{jn}^B(\tau_n-\tau_{n-1})+(\tau-\tau_{n-1})/\mu^B\right)}\right)\right\}.
\end{aligned}
\tag{368}
$$

Since all exponentials in the interpolation formulas for the intensity now have negative arguments, the risk of overflow is avoided.

As can be seen, there is also a risk that the denominators $1-\mu/\mu_0$ and $1-k_j\mu$ in the interpolation formulas for the intensity, can be close to zero. This risk can be entirely eliminated, as before, by noting that when they are close to zero, there is in fact an exponential with argument close to zero in the integral in the step before. An exponential with zero argument is a constant, and the corresponding anti-derivative does not have this denominator at all. If a denominator is close to zero, the corresponding term in the interpolation formulas is simply substituted as described below.

For I^+ in part A,

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$$\text{substitute } C'_{-jp}\frac{\tilde{g}_{-jp}\left(+\mu^A\right)}{1-k^A_{jp}\mu^A}\left(e^{-k^A_{jp}(\tau_p-\tau)}-e^{-(\tau_p-\tau)/\mu^A}\right)$$

$$\text{for } \frac{1}{\mu^A}C'_{-jp}\tilde{g}_{-jp}\left(+\mu^A\right)e^{-k^A_{jp}(\tau_p-\tau)}\left(\tau_p-\tau\right) \tag{369}$$

if $1-k^A_{jp}\mu^A$ is close to zero,

$$\text{substitute } \frac{\tilde{Z}_{0Ap}\left(+\mu^A\right)}{1-\mu^A/\mu_0}\left(e^{-(2\tau_A-\tau)/\mu_0}-e^{-\left((2\tau_A-\tau_p)/\mu_0+(\tau_p-\tau)/\mu^A\right)}\right)$$

$$\text{for } \frac{1}{\mu^A}\tilde{Z}_{0Ap}\left(+\mu^A\right)e^{-(2\tau_A-\tau)/\mu_0}\left(\tau_p-\tau\right) \tag{370}$$

if $1-\mu^A/\mu_0$ is close to zero,

$$\text{substitute } C'_{-jn}\frac{\tilde{g}_{-jn}\left(+\mu^A\right)}{1-k^A_{jn}\mu^A}\left(e^{-\left(k^A_{jn}(\tau_n-\tau_{n-1})+(\tau_{n-1}-\tau)/\mu^A\right)}-e^{-(\tau_n-\tau)/\mu^A}\right)$$

$$\text{for } \frac{1}{\mu^A}C'_{-jn}\tilde{g}_{-jn}\left(+\mu^A\right)e^{-k^A_{jn}(\tau_n-\tau)}\left(\tau_n-\tau_{n-1}\right) \tag{371}$$

if $1-k^A_{jn}\mu^A$ is close to zero,

$$\text{substitute } \frac{\tilde{Z}_{0An}\left(+\mu^A\right)}{1-\mu^A/\mu_0}\left(e^{-\left((2\tau_A-\tau_{n-1})/\mu_0+(\tau_{n-1}-\tau)/\mu^A\right)}-e^{-\left((2\tau_A-\tau_n)/\mu_0+(\tau_n-\tau)/\mu^A\right)}\right)$$

$$\text{for } \frac{1}{\mu^A}\tilde{Z}_{0Ap}\left(+\mu^A\right)e^{-(2\tau_A-\tau)/\mu_0}\left(\tau_n-\tau_{n-1}\right) \tag{372}$$

if $1-\mu^A/\mu_0$ is close to zero.

For I^+ in part B,

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$$\text{substitute } C'_{-jp}\,\frac{\tilde{g}_{-jp}\left(+\mu^B\right)}{1-k^B_{jp}\mu^B}\left(e^{-k^B_{jp}(\tau_p-\tau)}-e^{-(\tau_p-\tau)/\mu^B}\right)$$

$$\text{for } \frac{1}{\mu^B}C'_{-jp}\tilde{g}_{-jp}\left(+\mu^B\right)e^{-k^B_{jp}(\tau_p-\tau)}\left(\tau_p-\tau\right) \tag{373}$$

$$\text{if } 1-k^B_{jp}\mu^B \text{ is close to zero,}$$

$$\text{substitute } C'_{-jn}\,\frac{\tilde{g}_{-jn}\left(+\mu^B\right)}{1-k^B_{jn}\mu^B}\left(e^{-\left(k^B_{jn}(\tau_n-\tau_{n-1})+(\tau_{n-1}-\tau)/\mu^B\right)}-e^{-(\tau_n-\tau)/\mu^B}\right)$$

$$\text{for } \frac{1}{\mu^B}C'_{-jn}\tilde{g}_{-jn}\left(+\mu^B\right)e^{-k^B_{jn}(\tau_n-\tau)}\left(\tau_n-\tau_{n-1}\right) \tag{374}$$

$$\text{if } 1-k^B_{jn}\mu^B \text{ is close to zero.}$$

For I^- in part A,

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$$\text{substitute } \frac{\tilde{Z}_{0p}\left(-\mu^A\right)}{1-\mu^A/\mu_0}\left(e^{-\tau/\mu_0} - e^{-\left(\tau_{p-1}/\mu_0 + (\tau-\tau_{p-1})/\mu^A\right)}\right)$$

$$\text{for } \frac{1}{\mu_0}\tilde{Z}_{0p}\left(-\mu^A\right)e^{-\tau/\mu_0}\left(\tau-\tau_{p-1}\right) \tag{375}$$

if $1-\mu^A/\mu_0$ is close to zero,

$$\text{substitute } C'_{jp}\frac{\tilde{g}_{jp}\left(-\mu^A\right)}{1-k_{jp}^A\mu^A}\left(e^{-k_{jp}^A(\tau-\tau_{p-1})} - e^{-(\tau-\tau_{p-1})/\mu^A}\right)$$

$$\text{for } \frac{1}{\mu^A}C'_{jp}\tilde{g}_{jp}\left(-\mu^A\right)e^{-k_{jp}^A(\tau-\tau_{p-1})}\left(\tau-\tau_{p-1}\right) \tag{376}$$

if $1-k_{jp}^A\mu^A$ is close to zero,

$$\text{substitute } \frac{\tilde{Z}_{0n}\left(-\mu^A\right)}{1-\mu^A/\mu_0}\left(e^{-\left(\tau_n/\mu_0 + (\tau-\tau_n)/\mu^A\right)} - e^{-\left(\tau_{n-1}/\mu_0 + (\tau-\tau_{n-1})/\mu^A\right)}\right)$$

$$\text{for } \frac{1}{\mu_0}\tilde{Z}_{0n}\left(-\mu^A\right)e^{-\tau/\mu_0}\left(\tau_n-\tau_{n-1}\right) \tag{377}$$

if $1-\mu^A/\mu_0$ is close to zero,

$$\text{substitute } C'_{jn}\frac{\tilde{g}_{jn}\left(-\mu^A\right)}{1-k_{jn}^A\mu^A}\left(e^{-\left(k_{jn}^A(\tau_n-\tau_{n-1}) + (\tau-\tau_n)/\mu^A\right)} - e^{-(\tau-\tau_{n-1})/\mu^A}\right)$$

$$\text{for } \frac{1}{\mu^A}C'_{jn}\tilde{g}_{jn}\left(-\mu^A\right)e^{-k_{jn}^A(\tau-\tau_{n-1})}\left(\tau_n-\tau_{n-1}\right) \tag{378}$$

if $1-k_{jn}^A\mu^A$ is close to zero.

For I^- in part B,

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$$\text{substitute } \frac{\tilde{Z}_{0Bp}\left(-\mu^B\right)}{1-\mu^B/\mu_{0n}}\left(e^{-(\tau-\tau_A)/\mu_{0n}}-e^{-\left((\tau_{p-1}-\tau_A)/\mu_{0n}+(\tau-\tau_{p-1})/\mu^B\right)}\right)e^{-\tau_A/\mu_0}$$

$$\text{for } \frac{1}{\mu_{0n}}\tilde{Z}_{0Bp}\left(-\mu^B\right)e^{-\left(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n}\right)}\left(\tau-\tau_{p-1}\right) \tag{379}$$

$$\text{if } 1-\mu^B/\mu_{0n} \text{ is close to zero,}$$

$$\text{substitute } C'_{jp}\frac{\tilde{g}_{jp}\left(-\mu^B\right)}{1-k^B_{jp}\mu^B}\left(e^{-k^B_{jp}(\tau-\tau_{p-1})}-e^{-(\tau-\tau_{p-1})/\mu^B}\right)$$

$$\text{for } \frac{1}{\mu^B}C'_{jp}\tilde{g}_{jp}\left(-\mu^B\right)e^{-k^B_{jp}(\tau-\tau_{p-1})}\left(\tau-\tau_{p-1}\right) \tag{380}$$

$$\text{if } 1-k^B_{jp}\mu^B \text{ is close to zero,}$$

$$\text{substitute } \frac{\tilde{Z}_{0Bn}\left(-\mu^B\right)}{1-\mu^B/\mu_{0n}}\left(e^{-\left((\tau_n-\tau_A)/\mu_{0n}+(\tau-\tau_n)/\mu^B\right)}-e^{-\left((\tau_{n-1}-\tau_A)/\mu_{0n}+(\tau-\tau_{n-1})/\mu^B\right)}\right)e^{-\tau_A/\mu_0}$$

$$\text{for } \frac{1}{\mu_{0n}}\tilde{Z}_{0Bn}\left(-\mu^B\right)e^{-\left(\tau_A/\mu_0+(\tau-\tau_A)\mu_{0n}\right)}\left(\tau_n-\tau_{n-1}\right) \tag{381}$$

$$\text{if } 1-\mu^B/\mu_{0n} \text{ is close to zero,}$$

$$\text{substitute } C'_{jn}\frac{\tilde{g}_{jn}\left(-\mu^B\right)}{1-k^B_{jn}\mu^B}\left(e^{-\left(k^B_{jn}(\tau_n-\tau_{n-1})+(\tau-\tau_n)/\mu^B\right)}-e^{-(\tau-\tau_{n-1})/\mu^B}\right)$$

$$\text{for } \frac{1}{\mu^B}C'_{jn}\tilde{g}_{jn}\left(-\mu^B\right)e^{-k^B_{jn}(\tau-\tau_{n-1})}\left(\tau_n-\tau_{n-1}\right) \tag{382}$$

$$\text{if } 1-k^B_{jn}\mu^B \text{ is close to zero.}$$

These terms are found by setting the corresponding exponential argument to zero and integrating as in the original interpolation formula. This can in fact be seen as an application of l'Hospital's rules.

As mentioned above, and also stated in previous reports, there is a (very rare) risk of divide-by-zero in the solution procedure, but the analytically derived substitution terms above eliminate this risk. However, a bug (although extremely unlikely to occur) in the code of version 2.0 was detected when using infinite layer thickness. It turns out that the substitution terms can give rise to an error of the type inf * 0 = NaN. Here, inf comes from an integration over a now infinite interval, and 0 comes from the boundary conditions. The zero has precedence in these cases, and the problem is avoided by explicitly setting the result to zero there, which is now implemented in the solution procedure.

It is worth stating once again that this is the solution for one Fourier component of the diffuse intensity. The complete azimuthal dependence can be assembled through the Fourier cosine series expansion for the diffuse intensity (151), as stated earlier. The total intensity is the sum of the diffuse and beam components, where the diffuse component has just been calculated, and the beam component is given by a natural modification of (152) as follows.

For part A,

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$$I_b^-(\tau,\mu,\varphi) = I_{0b} e^{-\tau/\mu_0} \delta(\mu-\mu_0)\delta(\varphi-\varphi_0), \tag{383}$$

$$I_b^+(\tau,\mu,\varphi) = I_{0b}\,\mathrm{Refl}(-\mu_0;n_{rel}) e^{-(2\tau_A-\tau)/\mu_0} \delta(\mu-\mu_0)\delta(\varphi-(\varphi_0+\pi)). \tag{384}$$

For part B,

$$I_b^-(\tau,\mu,\varphi) = I_{0b}\frac{\mu_0}{\mu_{0n}}\mathrm{Trans}(-\mu_0;n_{rel}) e^{-(\tau_A/\mu_0+(\tau-\tau_A)/\mu_{0n})} \delta(\mu-\mu_{0n})\delta(\varphi-\varphi_0). \tag{385}$$

The diffuse component in part B includes reflection from any underlying surface, and the beam component is therefore in part B only present in downward directions.

The final expression for the total intensity is thus in part A given by

$$\begin{cases} I^- = I_d^- + I_b^- \\ I^+ = I_d^+ + I_b^+ \end{cases}, \tag{386}$$

and in part B by

$$\begin{cases} I^- = I_d^- + I_b^- \\ I^+ = I_d^+ \end{cases}. \tag{387}$$

5. PERFORMANCE AND CONSISTENCY TESTS

5.1. Some Comments on the Solution Procedure

The Kubelka-Munk theory has traditionally been used to derive formulas for R_∞ for multilayer structures. The formulas use total reflectance and total transmittance for the individual layers. The Kubelka-Munk equations introduce errors, however, both in the calculation of the total reflectance and total transmittance for the individual layers, and in the formation of multilayer structures where R_g is identified with the underlying layer. This is due to the inability to model the anisotropy that exists in any real material. Any angular resolved model that handles this anisotropy correctly should thus avoid the Kubelka-Munk formulas for R_∞ for multilayer structures, if it wants to maintain its accuracy. DORT2002 can calculate R_∞ exactly for single layer structures. For multilayer structures, it allows the user to choose the number of structures to approximate infinite thickness, much as in real-life measurements. In cases with refractive index changes R_∞ is not available, since the solution procedure only allows one change in refractive index. This should not be a problem, however, since this is also how the Saunderson correction is used with Kubelka-Munk today.

As stated in previous reports, the δ-*N*, TMS and IMS methods are implemented to handle strongly forward-peaked scattering with high accuracy and small *N*. These methods work in both single and multilayer structures. The solution procedure to handle a discontinuous change in refractive index developed in this report contains the δ-*N* method, but not the TMS and IMS methods. They are also possible to implement in principle, but this is not done here due to the tremendous amount of algebra that arises when integrating over the refractive index discontinuity. Should it be necessary in the future, it is straightforward but very time demanding. For asymmetry factor values close to zero, the missing TMS and IMS methods have no effect. In cases with strongly forward-peaked scattering, accuracy can be maintained by increasing *N* sufficiently, so this should not present a problem in practice. The influence of this has already been studied [16].

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The interpolation formulas for the intensity for both single and multilayer structures give exactly the same results at the quadrature points as the general solution. They also satisfy the boundary conditions for all polar angles μ, even though such conditions were imposed only at the quadrature points. However, this nice property is not inherited by the interpolation formulas in the solution procedure for refractive index discontinuity. The boundary conditions are, of course, satisfied at the quadrature points, but it is in general not possible to satisfy them in between. The error increases with increasing g, and when the illumination is not diffuse. The largest errors arise for low N and high g, but any desired accuracy can still be achieved by increasing N sufficiently as previously reported [16], so this should not present a problem in practice.

There will be a small built-in error in the new code due to that the Matlab interpolation function `interp1` had to be used to find $I^+\left(\tau_A,\mu^A\right)$, $I^+\left(\tau^*,\mu^B\right)$, $I^-\left(\tau_0,\mu^A\right)$ and $I^-\left(\tau_A,\mu^B\right)$ used in the interpolation formulas. This is due to the more complex relations imposed by the boundary conditions at the refractive index boundary. This error is dependent on the scattering distribution and the number of calculation channels, N. This means that more calculation channels should be used for strongly forward or backward scattering media. Also, since the TMS/IMS scattering correction is not implemented in the new code, more calculation channels have to be used for the same accuracy for these cases.

5.2. Tests and Results

A number of verification tests were made of the new code for refractive index changes. All tests were done for a large number of illumination conditions, different scattering properties and different number of layers. No TMS/IMS scattering correction was used in any test.

Consistency was tested by setting the relative change in refractive index to 1, i.e. no change in refractive index. Using the DORT2002 code with and without the method for handling refractive index boundaries, but otherwise with the same conditions, should then provide the same output, although with completely different methods and code.

Consistency was also tested by verifying the new code against itself with different settings describing the same conditions. Using the same medium divided in different number of calculation sub layers, but otherwise with the same conditions, should provide the same output.

The impact of using the Matlab interpolation function `interp1` instead of the strategy used in the single and multilayer solution procedures was evaluated in a number of tests with different N.

All tests showed the desired result, i.e. the new code seems have the wanted performance regarding accuracy in calculations. There are small errors due to the facts mentioned in the previous section, i.e. that the TMS/IMS scattering correction is not implemented and that parts of the interpolation are cruder. The worst case detected had a relative error in reflectance calculations around 10^{-3}. However, the errors are noticeable only for strongly forward-peaked scattering (high values of g), and always decrease when N is increased. In those cases the desired accuracy can be achieved by approximately doubling N compared to the situation without change in refractive index. In most cases, the relative error in reflectance calculations is less than 10^{-6}, often far less, even for 'normal' values of N.

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6. SUGGESTIONS FOR FUTURE WORK

6.1. A Comparative Study

A study will be performed to compare the new DORT2002 code on one hand and Kubelka-Munk with Saunderson corrections on the other hand with real measurements. This will have to include ellipsometry measurements for finding refractive index values, as well as considerations for measurement geometry. A preliminary study of Kubelka-Munk with Saunderson corrections was recently made in a masters' thesis [17], and some of its outcomes will be used. Another recent masters' thesis [13] presented interesting results on anisotropic scattering and its effects on reflectance measurements, and analyzed that using DORT2002. Those findings will also be an important part in the planned study.

6.2. Direct Model Development

Work is currently in progress to package version 3.0 of the DORT2002 tool for use in the paper and printing industry. This includes the new code for refractive index changes, but also extremely fast reflectance calculations and several types of inverse calculations that have not yet been available. This also includes a manual to the new DORT2002 Graphical User Interface, a tool developed to provide users with a fast and easy way of performing DORT2002 simulations. It works as a shell that encapsulates the parameters and the function calls, and offers powerful simulations through a mouse click. Several simulations will also be available through Excel.

The model is prepared to include fluorescence. All that is needed is to add a corresponding term in the integro-differential equation. This term is easy to fit into the discretization and the solution procedure. An outer loop over wavelengths will be needed to perform the coupling of the intensities of the different wavelengths associated with the fluorescence.

An interesting development would be to investigate better surface modeling, including gloss and scattering from rough surfaces, which in turn can be divided into diffraction from small surface irregularities, and geometrical scattering from the distribution of surface facets. A possible approach would be to combine DORT2002 with a specialized surface model.

6.3. Inverse Model Development

The inverse problem for this model will be studied thoroughly. This includes the continued study and development of fast and numerically stable algorithms for parameter estimation. The problem involves several numerical difficulties, so it will require some effort. The work is going well, and inverse solution methods have already been successfully developed for reflectance measurements. Initial inverse solution methods for angle-resolved intensity measurements have been tested. Although they work well, further improvements on accuracy and speed will be done.

The parameter estimation will be done to fit model simulations to angle-resolved light scattering measurements or to desired angle-resolved light scattering patterns. Also, studies of error estimation and sensitivity of perturbations will be performed.

In addition, it would be interesting to see studies of inverse Monte-Carlo methods. They should be evaluated with respect to accuracy and speed, and compared with the inverse model outlined above. It should also be investigated whether an inverse DORT method and an inverse Monte-Carlo method could be used together, one doing a coarse fitting, and the other doing fine-tuning.

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7. DISCUSSION

Changes in refractive index occur for example at the interface between air and an ink-paper substrate. This report uses radiative transfer theory to account for the effects of refraction and total reflection at refractive index boundaries exactly, and in any measurement geometry, without approximations and without unknown constants. This is in contrast with Kubelka-Munk and the Saunderson correction, which is only an approximation and only for integrating sphere geometry, and which requires non-trivial determination of unknown constants. This report is a detailed examination of the work by Stamnes and coworkers [6-8], including more detailed derivations and corrections of several errors. It also covers adaptation and inclusion of the method into the radiative transfer solution method DORT2002 by Edström [5], which is adapted to light scattering in paper and print.

The result of a large number of tests of consistency and accuracy of the method are presented. All tests are positive. There are some small errors due to complexities in the solution procedure, as discussed in section 5.1. However, the errors are noticeable only for strongly forward-peaked scattering (high values of g), and always decreases when N is increased. In those cases the desired accuracy can be achieved by approximately doubling N compared to the situation without change in refractive index. In most cases, the relative error in reflectance calculations is less than 10^{-6}, often far less, even for 'normal' values of N.

Some comments on planned and suggested future work are given regarding direct and inverse model development, but also for comparative studies.

7.1. The Impact of DORT2002 on the Paper and Printing Industries

There are different areas within the paper industry where one could find use for light scattering models. Among them are fine-tuning and troubleshooting in the papermaking process, designing new paper qualities, and optimization of color reproduction for a given combination of paper grades and printing techniques. Today the Kubelka-Munk model (or extended models thereof) is most widely used to cover these applications.

The change in refractive index that occurs at the interface between air and an ink-paper substrate causes effects such as refraction and total reflection. These effects are usually modeled with Kubelka-Munk and the Saunderson correction. However, this is only an approximation and only for integrating sphere geometry. Furthermore, it requires the non-trivial determination of unknown constants. In addition to this, the Kubelka-Munk model itself is just an approximation of the light scattering problem, and as has been reported [11-13, 18-25] its errors in reflectance calculations and measurements can be substantial due to its inability to model the anisotropy of the scattered light. All these problems are avoided by using DORT2002, since it models both the anisotropy of the scattered light and the effects of refractive index changes exactly for any measurement geometry, without approximations and without unknown constants.

From the view of the applied user, DORT2002 also has several other advantages compared to the Kubelka-Munk model. The angular distribution of reflection and transmission is modeled, as well as different scattering asymmetries of the bulk. DORT2002 allows the use of collimated light to analyze the optical response of a sample, and is not limited to diffuse light as the Kubelka-Munk model. Since DORT2002 handles any illumination and detection conditions, the interior of instruments otherwise closed for inspection can be simulated, and the influence of instrument geometry on measurements can be evaluated. This makes it possible to suggest measurement corrections for deviations due to instrument geometry, and to make calibration and measurements with different instrument geometries comparable. Furthermore, DORT2002 is consistent for translucent and highly absorbing

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media, and it is prepared to be combined with a surface model to handle gloss. It is also prepared for a future implementation of fluorescence, which will allow the effect of OBA (optical brightening agents) in paper and print to be modeled. The whiteness and brightness of paper cannot be designed with the Kubelka-Munk model since fluorescence phenomena are not explicitly included. With DORT2002 the accuracy for color matching for multicolor prints would possibly increase.

These improvements are important for a number of reasons. Paper can be translucent, glossy and strongly absorbing, e.g. low opacity paper, calendared paper or heavily dyed paper. This is also the case for full tone print. The standardized measurement geometries (d/0° and 45°/0°) for brightness of paper can give different ranking, which cannot be explained with the Kubelka-Munk model, but is readily given by DORT2002. Moreover, there is experimental evidence that the reflection and transmission of paper and print deviate from the Kubelka-Munk model description [18-25], which can be interpreted more accurately with DORT2002 [11-13].

DORT2002 is far more powerful than Kubelka-Munk, and still almost as fast. DORT2002 has larger range of applicability, higher accuracy, and serves to increase the understanding of light scattering in paper and print. The Graphical User Interface makes the model easy to use, and after a short introduction any desired simulation is just a button-click away. These arguments result in the following suggestion: replace Kubelka-Munk with DORT2002 for most applications.

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