

Correspondence between continuous and discrete two-flux models for reflectance and transmittance of diffusing layers

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Abstract

This paper provides a theoretical connection between two different mathematical models dedicated to the reflectance and the transmittance of diffusing layers. The Kubelka–Munk model proposes a continuous description of scattering and absorption for two opposite diffuse fluxes in a homogeneous layer (continuous two-flux model). On the other hand, Kubelka's layering model describes the multiple reflections and transmissions of light taking place between various superposed diffusing layers (discrete two-flux model). The compatibility of these two models is shown. In particular, the Kubelka–Munk reflectance and transmittance expressions are retrieved, using Kubelka's layering model, with mathematical arguments using infinitely thin sublayers. A new approach to the Kubelka–Munk expressions is thus obtained, giving, moreover, new details for physical interpretation of the Kubelka–Munk theory.

Keywords: Kubelka–Munk model, Kubelka model, light scattering, reflectance, transmittance, matrix exponential, diffusing layer

1. Introduction

Modelization is an essential part of scientific activity. Rather often, the mathematical apparatus of a model can be as important as, for example, the physical properties it sustains. Indeed, the core of the mathematical part can convey by itself a large part of the general meaning of the model. Such will be the case, in this article, for the exponential of a matrix, that gives a key for understanding the relationship between continuous and discrete two-flux models, a role that has not been noticed until now.

The continuous two-flux model results from the well-known Kubelka–Munk theory [1, 2], used in an extremely wide range of applications. The discrete two-flux model was introduced later by Kubelka [3]. Both continuous and discrete two-flux models describe the evolution of two oppositely directed light fluxes, assumed perfectly diffused, as functions of their depth within the diffusing medium. They indirectly encapsulate into equations the three complementary phenomena taking place in elementary layers of the medium, i.e. reflection (also called backscattering), transmission and/or

absorption. Their main difference lies in the assumptions made on the diffusing medium. The continuous model requires a homogeneous scattering medium, i.e. with the same scattering and absorption properties whatever the depth. Selecting an infinitesimally thin sublayer located at an arbitrary depth, the variation of the upward flux and of the downward flux is described by the famous Kubelka–Munk differential equation system (3). The solutions of this system are analytical expressions for the reflectance and the transmittance of a layer as functions of its thickness. In the discrete model, the medium is assimilated to superposed diffusing layers, without concern about their thickness or their homogeneity in depth. The superposed layers may be different, with their own reflectance and transmittance at their upper and lower sides. The upward and the downward fluxes are determined by an analysis of the multiple reflections and transmissions taking place between the layers. Therefore, choosing between Kubelka–Munk and Kubelka models fundamentally depends on the nature of the considered specimen. Due to their simplicity, the two-flux models should be restricted to highly scattering media [4]. Various attempts have been made recently to improve the

Kubelka–Munk model, especially in the description of the lateral propagation of light. They rely on extended continuous models [5, 6] and/or use discrete approaches such as random walks [7], and Markov chains [8]. In this context, studying the interconnection of the classical two-flux models may be helpful.

Our study is concentrated on homogeneous diffusing layers satisfying the applicability conditions of both the Kubelka–Munk and the Kubelka models. On the one hand, the Kubelka–Munk model gives directly analytical expressions for the layers reflectance and transmittance, being given the scattering and absorption coefficients. On the other hand, there exists a relationship between these scattering and absorption coefficients and the reflectance and transmittance of infinitely thin sublayers. Then, a thick layer is modeled as a pile of these sublayers. Its reflectance and transmittance are given by Kubelka’s model. Our aim is to show that they are identical to those given by the Kubelka–Munk model. For this purpose, a new matrix formalism will be introduced.

The present paper is structured as follows. The Kubelka–Munk model and the Kubelka model are first recalled in sections 2 and 3 respectively. In section 4, we show how the Kubelka–Munk expressions can be combined according to Kubelka’s discrete model. Then, we treat the special case of infinitely thin layers in section 5 and model a superposition of infinitely thin layers according to the discrete model in section 6. Section 7 deals specifically with reflectance, for which the Kubelka–Munk expression is obtained using continued fractions. As a matter of conclusion, in section 8, the proposed mathematical developments are given a physical interpretation.

2. The Kubelka–Munk model

Let us consider a homogeneous layer with thickness h characterized by its absorption coefficient K and its scattering coefficient S , and considered without its interfaces with the surrounding medium. In this layer, the diffuse irradiance i_r propagates upward and the diffuse irradiance i_t propagates downward. Both i_r and i_t are functions of their depth x in the layer. Depth 0 corresponds to the layer’s boundary receiving the incident irradiance I_0 . Depth h indicates the other substrate layer’s boundary. We consider at an arbitrary depth x a sublayer of infinitesimal thickness dx (figure 1). It receives the downward irradiance $i_t(x)$ on one side and the upward irradiance $i_r(x + dx)$ on the other side. In the sublayer, at position x , a fraction Sdx from both irradiances $i_r(x)$ and $i_t(x)$ is backscattered, leading to an exchange of light, and a fraction Kdx is absorbed.

While crossing the sublayer, the upward irradiance $i_r(x + dx)$ loses both the absorbed irradiance $Ki_r(x)dx$ and the backscattered irradiance $Si_r(x)dx$ and gains the backscattered irradiance $Si_t(x)dx$. The irradiance $i_r(x)$ leaving the sublayer is therefore

$$i_r(x) = i_r(x + dx) - (K + S)i_r(x)dx + Si_t(x)dx. \quad (1)$$

Likewise, the downward irradiance $i_t(x)$ loses the absorbed irradiance $Ki_t(x)dx$ and the backscattered irradiance

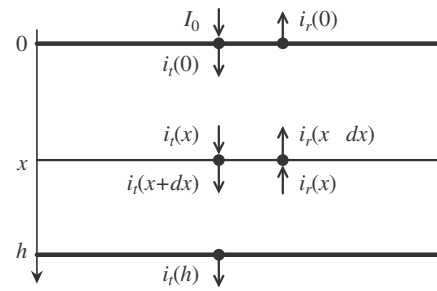


Figure 1. Upward and downward irradiances crossing an infinitesimal sublayer in the diffusing layer.

$Si_t(x)dx$ and gains the backscattered irradiance $Si_r(x)dx$. The irradiance $i_t(x + dx)$ leaving the sublayer is

$$i_t(x + dx) = i_t(x) - (K + S)i_t(x)dx + Si_r(x)dx. \quad (2)$$

The Kubelka–Munk differential equation system [1, 2] is obtained by giving equations (1) and (2) another form:

$$\begin{aligned} \frac{d}{dx}i_r(x) &= (K + S)i_r(x) - Si_t(x) \\ \frac{d}{dx}i_t(x) &= Si_r(x) - (K + S)i_t(x). \end{aligned} \quad (3)$$

The solutions $i_r(x)$ and $i_t(x)$ of (3) can be easily determined using the Laplace transform [9]. Another solving method, introduced by Emmel [10], uses a matrix representation $\frac{d}{dx}\mathbf{V} = \Omega\mathbf{V}$ for (3) and a matrix exponential for expressing $\mathbf{V} = \exp(x\Omega) \cdot \mathbf{V}_0$. The reflectance $r(h)$ of the layer with thickness h , corresponding to the ratio $i_r(0)/I_0$ of incident light emerging at depth 0, is [2]

$$r(h) = \frac{\sinh(bSh)}{b \cosh(bSh) + a \sinh(bSh)} \quad (4)$$

with

$$a = \frac{K + S}{S} \quad \text{and} \quad b = \sqrt{a^2 - 1}. \quad (5)$$

The transmittance of the layer with thickness h , corresponding to the ratio $i_t(h)/I_0$ of incident light emerging at depth h , is [2]

$$t(h) = \frac{b}{b \cosh(bSh) + a \sinh(bSh)}. \quad (6)$$

3. Kubelka’s layering model

When various layers with identical refractive indices are superposed, their global reflectance and transmittance can be computed according to Kubelka’s layering model [3] and expressed as functions of the individual layer reflectances and transmittances. Let us consider a ‘bilayer’, formed by two layers with upper reflectance R_1 for the top layer, resp. R_2 for the bottom layer, with lower reflectance R'_1 , resp. R'_2 , with upper transmittance T_1 , resp. T_2 , and with lower transmittance T'_1 , resp. T'_2 . Figure 2 shows the multiple reflection–transmission process of light within the bilayer for a top illumination.

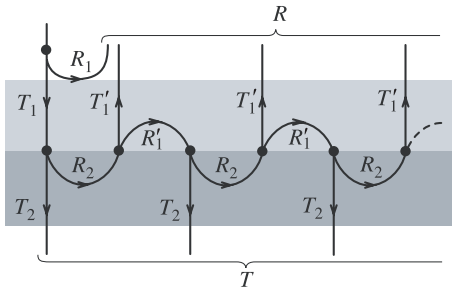


Figure 2. Multiple reflection–transmission of light within two superposed nonsymmetrical layers.

Summing the different fractions of light emerging at the upper side, we obtain a geometric series expressing the bilayer’s global reflectance:

$$R = R_1 + T_1 R_2 T'_1 + T_1 R_2 R'_1 R_2 T'_1 + T_1 R_2 (R'_1 R_2)^2 T'_1 + \dots,$$

whose sum is

$$R = R_1 + T_1 T'_1 R_2 \frac{1}{1 - R'_1 R_2}. \quad (7)$$

The fractions of light emerging at the lower side also form a geometric series, expressing the bilayer’s global transmittance:

$$T = T_1 T_2 + T_1 R_2 R'_1 T_2 + T_1 (R_2 R'_1)^2 T_2 + \dots$$

which can be given the form

$$T = T_1 T_2 \frac{1}{1 - R'_1 R_2}. \quad (8)$$

Each layer may be represented by a 3×3 matrix, called the *layering matrix*, whose top-left entry is 1 and where the upper and lower reflectances and transmittances are arranged as follows:

$$\mathbf{M}_k = \begin{pmatrix} 1 & -R'_k & 0 \\ R_k & A_k & 0 \\ 0 & 0 & T_k \end{pmatrix} \quad (9)$$

with $A_k = T_k T'_k - R_k R'_k$. A superposition of layers is represented by the multiplication of their layering matrices. In order to have its top-left entry equal to 1, the product matrix is divided by its own top-left entry. This ‘normalization’ operation is written with a double underlining:

$$\underline{\underline{\mathbf{M}}} = \frac{1}{m_{11}} \mathbf{M}. \quad (10)$$

Let us consider the bilayer presented in figure 2. Its layering matrix \mathbf{M} is the normalized product of the layering matrices \mathbf{M}_1 and \mathbf{M}_2 :

$$\mathbf{M} = \underline{\underline{\mathbf{M}_1 \mathbf{M}_2}} = \frac{\mathbf{M}_1 \mathbf{M}_2}{1 - R'_1 R_2}, \quad (11)$$

using notations as in (9).

Note that the layering matrix corresponding to the upper layer is placed at the left.

One may verify that the entries of \mathbf{M} are consistent with Kubelka’s formulae: the upper reflectance, resp. transmittance, corresponding to the entry m_{21} of \mathbf{M} , resp. the entry m_{33} , is expressed as (7), resp. as (8). Relation (11) can be generalized to the superposition of N layers, i.e.,

$$\mathbf{M} = \underline{\underline{\mathbf{M}_1 \mathbf{M}_2 \mathbf{M}_3 \dots \mathbf{M}_N}}. \quad (12)$$

4. Combination of the continuous and the discrete models

In the special case where two layers of a same diffusing medium are superposed, both the Kubelka–Munk model and Kubelka’s model apply. Since the layers are homogeneous, their upper and lower reflectances, as well as their upper and lower transmittances, are equal. Let us denote h_1 and h_2 as the thicknesses of the upper layer and the lower layer respectively. Their reflectances according to the Kubelka–Munk model, respectively $r(h_1)$ and $r(h_2)$, are given by (4) and their transmittances, respectively $t(h_1)$ and $t(h_2)$, are given by (6). The superposed layers form a homogeneous layer with thickness $h_1 + h_2$, whose reflectance $r(h_1 + h_2)$ is again given by equation (4). We may verify that the same reflectance expression is obtained using Kubelka’s reflectance formula (7), i.e.

$$r(h_1 + h_2) = r(h_1) + \frac{t(h_1)^2 r(h_2)}{1 - r(h_1) r(h_2)}. \quad (13)$$

Likewise, the transmittance $t(h_1 + h_2)$, given by (6), can be equivalently obtained by combining the layers’ reflectance and transmittance according to Kubelka’s transmittance formula (8).

According to the matrix formalism introduced in section 3, we have

$$\mathbf{M}(h_1 + h_2) = \underline{\underline{\mathbf{M}(h_1) \mathbf{M}(h_2)}}} \quad (14)$$

where $\mathbf{M}(h_1 + h_2)$, $\mathbf{M}(h_1)$ and $\mathbf{M}(h_2)$ represent the layering matrices of the bilayer, the upper layer and the lower layer respectively, with entries expressed according to the Kubelka–Munk model.

Equation (14) is also valid for a subdivision of a layer. Let us consider a homogeneous layer with thickness h whose Kubelka–Munk reflectance $r(h)$ and transmittance $t(h)$ are given respectively by equation (4) and equation (6). Its layering matrix is

$$\mathbf{M}(h) = \begin{pmatrix} 1 & -r(h) & 0 \\ r(h) & A(h) & 0 \\ 0 & 0 & t(h) \end{pmatrix} \quad (15)$$

with $A(h) = t^2(h) - r^2(h)$. The layer is subdivided into n identical sublayers with thickness h/n . Their reflectance $r(h/n)$, transmittance $t(h/n)$ and layering matrix $\mathbf{M}(h/n)$ are given respectively by equations (4), (6) and (15) with h replaced by h/n . According to relations (12) and (14), we have

$$\mathbf{M}(h) = \underline{\underline{\mathbf{M}(h/n)^n}}. \quad (16)$$

5. Infinitesimally thin sublayers

As in equation (16) n may be arbitrary large, we have

$$\mathbf{M}(h) = \lim_{n \rightarrow \infty} \mathbf{M}(h/n)^n. \quad (17)$$

The sublayer becomes infinitesimally thin. According to the Kubelka–Munk model, the reflectance of such an infinitesimal sublayer is proportional to its thickness, where the scattering coefficient S of the diffusing medium is the coefficient of proportionality. Hence, the Kubelka–Munk reflectance function $r(x)$ tends to Sx as x tends to 0. This is shown by the Taylor expansion of (4):

$$\frac{\sinh(bSx)}{a \sinh(bSx) + b \cosh(bSx)} = Sx + O(x^2) \quad (18)$$

where $O(x^2)$ means ‘terms of degree 2 or more’. Likewise, the transmittance of the sublayer is the fraction of light that is neither backscattered nor absorbed, i.e., $1 - Sdx - Kdx$. The Kubelka–Munk transmittance function $t(x)$ tends to $1 - Sx - Kx$ as x tends to 0, which is shown by the Taylor expansion of (6):

$$\begin{aligned} \frac{b}{b \cosh(bSx) + a \sinh(bSx)} &= 1 - aSx + O(x^2) \\ &= 1 - (K + S)x + O(x^2). \end{aligned} \quad (19)$$

Therefore, the reflectance of the sublayer with infinitesimal thickness h/n becomes

$$r(h/n) = S \frac{h}{n}, \quad (20)$$

its transmittance becomes

$$t(h/n) = 1 - aS \frac{h}{n} = 1 - (K + S) \frac{h}{n}, \quad (21)$$

and its layering matrix becomes

$$\mathbf{M}(h/n) = \begin{pmatrix} 1 & -Sh/n & 0 \\ Sh/n & A(h/n) & 0 \\ 0 & 0 & 1 - aSh/n \end{pmatrix} \quad (22)$$

with

$$A(h/n) = 1 - 2aSh/n - (bSh/n)^2. \quad (23)$$

6. Kubelka–Munk expressions obtained from the discrete model

Let us now verify that the layering matrix $\mathbf{M}(h/n)$ of infinitesimal sublayers expressed by (22) still satisfies equation (17). By showing this, we also show that continuous Kubelka–Munk expressions of reflectance and transmittance for a thick layer can be obtained from the reflectance and the transmittance of infinitesimally thin layers according to Kubelka’s discrete model.

Equation (22) can be reformulated in the following way:

$$\mathbf{M}(h/n) = \mathbf{I}_3 + \frac{1}{n} \mathbf{A} \quad (24)$$

with \mathbf{I}_3 the 3×3 identity matrix and

$$\mathbf{A} = \begin{pmatrix} 0 & -Sh & 0 \\ Sh & -2aSh + \varepsilon & 0 \\ 0 & 0 & -aSh \end{pmatrix}. \quad (25)$$

From a physical point of view, the term $\varepsilon = b^2 S^2 h^2 / n$ in equation (25) corresponds to the second-order scattering within the sublayer, i.e., the portion of light that is scattered twice before being reflected, transmitted or absorbed. This term tends to 0 as n tends to infinity. Thus, at an infinitesimal scale, only the first-order scattering is relevant, which means that at most one scattering event takes place in average within the sublayer. Moreover, the reflectance of the infinitesimal sublayer being proportional to its thickness according to equation (20), we may conclude that the medium is almost non-scattering at the scale at which the Kubelka–Munk differential equations system describes scattering and absorption. This is not in contradiction with the fact that the medium is strongly scattering, because at the macroscopic scale a high number of scattering events occur.

According to a classical limit of the (numerical) exponent function that can be extended to the matrix exponential [11],

$$\lim_{n \rightarrow \infty} \mathbf{M}(h/n)^n = \lim_{n \rightarrow \infty} \left(\mathbf{I}_3 + \frac{1}{n} \mathbf{A} \right)^n = \exp(\mathbf{A}). \quad (26)$$

The diagonalization of matrix $\exp(\mathbf{A})$ is obtained through the diagonalization of \mathbf{A} [11]:

$$\exp(\mathbf{A}) = \mathbf{E}^{-1} \cdot \Delta \cdot \mathbf{E} \quad (27)$$

with

$$\mathbf{E} = \begin{pmatrix} a - b & 1 & 0 \\ a + b & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (28)$$

and

$$\Delta = \text{diag}(e^{-(a+b)Sh}, e^{-(a-b)Sh}, e^{-aSh}). \quad (29)$$

According to (26), we have

$$\lim_{n \rightarrow \infty} \mathbf{M}(h/n)^n = \frac{e^{-aSh}}{b} \begin{pmatrix} bc + as & -s & 0 \\ s & bc - as & 0 \\ 0 & 0 & b \end{pmatrix} \quad (30)$$

with $c = \cosh(bSh)$ and $s = \sinh(bSh)$. This matrix, divided by its top-left entry, corresponds to the layering matrix of the superposed sublayers:

$$\underline{\underline{\lim_{n \rightarrow \infty} \mathbf{M}(h/n)^n}} = \begin{pmatrix} 1 & -\frac{s}{bc+as} & 0 \\ \frac{s}{bc+as} & \frac{bc-as}{bc+as} & 0 \\ 0 & 0 & \frac{b}{bc+as} \end{pmatrix}. \quad (31)$$

As desired, we retrieve the layering matrix $\mathbf{M}(h)$ given by equation (15), particularly the Kubelka–Munk expression (4) for the reflectance (entry m_{21} and negative of entry m_{12}) and (6) for the transmittance (entry m_{33}).

7. Kubelka–Munk reflectance expressed as a continued fraction

A layer with thickness h is decomposed into n sublayers, for which the reflectance formula (7) is used instead of the matrix formalism of the previous section. Let r_k be the reflectance of k superposed sublayers. According to equation (7), we have for every $k \geq 1$

$$r_{k+1} = r(h/n) + \frac{t^2(h/n)}{-r(h/n) + \frac{1}{r_k}} \quad (32)$$

with functions r and t given by (4) and (6) respectively, and $r_1 = r(h/n)$. Using $n - 1$ times recursion (32), we obtain a continued fraction expressing the reflectance $r_n = r(h)$ of the whole layer.

It is known [12] that every finite continued fraction

$$q_0 + \frac{p_1}{q_1 + \frac{p_2}{q_2 + \dots + \frac{p_k}{q_k}}} \quad (33)$$

can be reduced to a simple fraction P/Q , where P and Q are obtained as the second column entries of the following matrix product:

$$\begin{pmatrix} \dots & P \\ \dots & Q \end{pmatrix} = \begin{pmatrix} 1 & q_0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & p_1 \\ 1 & q_1 \end{pmatrix} \begin{pmatrix} 0 & p_2 \\ 1 & q_2 \end{pmatrix} \dots \begin{pmatrix} 0 & p_k \\ 1 & q_k \end{pmatrix}. \quad (34)$$

In the case of equation (32), a 2-period appears for coefficients p_k and q_k . Thus, equation (32) becomes

$$\mathbf{C}_n = \mathbf{U}_n (\mathbf{V}_n \mathbf{W}_n)^{n-1} = \mathbf{U}_n \mathbf{V}_n (\mathbf{W}_n \mathbf{V}_n)^{n-2} \mathbf{W}_n \quad (35)$$

where \mathbf{U}_n , \mathbf{V}_n and \mathbf{W}_n designate respectively the matrices

$$\begin{pmatrix} 1 & r(h/n) \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & t(h/n)^2 \\ 1 & -r(h/n) \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & r(h/n) \end{pmatrix}. \quad (36)$$

As n tends to infinity, $r(h/n)$ and $t(h/n)$ are reduced to expressions (20) and (21), and thus tend to 0 and 1 respectively, with the consequence that both $(\mathbf{U}_n \mathbf{V}_n)$ and \mathbf{W}_n tend to

$$\mathbf{J} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (37)$$

Hence, using equation (35) and the fact that, for taking the limit, an $n - 2$ exponent is the same as an n exponent, matrix \mathbf{C}_n tends to

$$\mathbf{C}_\infty = \mathbf{J} \cdot \lim_{n \rightarrow \infty} \begin{pmatrix} 1 & -Sh/n \\ Sh/n & A(h/n) \end{pmatrix}^n \cdot \mathbf{J} \quad (38)$$

with $A(h/n)$ as in equation (23). The matrix to the power n is exactly the top-left 2×2 block of $\mathbf{M}(h/n)$ given by equation (22). Using for this matrix the same line of reasoning as in the previous section for matrix $\mathbf{M}(h/n)$, the central matrix in equation (38) is the top-left 2×2 block of the matrix

in equation (30). Finally, by straightforward computations, equation (38) becomes

$$\mathbf{C}_\infty = \frac{e^{-aSh}}{b} \begin{pmatrix} bc - as & s \\ -s & bc + as \end{pmatrix} \quad (39)$$

with $c = \cosh(bSh)$ and $s = \sinh(bSh)$. As expected, the right column of \mathbf{C}_∞ gives the numerator (upper term) and the denominator (lower term) of the layer reflectance $r(h)$ expressed according to the Kubelka–Munk model.

8. Conclusion

A correspondence has been established between the Kubelka–Munk model (continuous two-flux model) and the Kubelka layering model (discrete two-flux model), with a mathematical equivalence achieved in the case of a homogeneous diffusing layer. The transition from a discrete to a continuous model relies on a new matrix formalism and the use of a matrix exponential. The notion of layering matrix characterizes the reflectance and transmittance of layers, incorporating the limit case of infinitesimally thin layers. The equations of Kubelka’s layering model, used to model the reflectance and the transmittance of a pile of infinitesimally thin layers, lead naturally to a matrix exponential, like in the work of Emmel, although the ‘exponentialized’ matrix is slightly different [10]. The present contribution is a step forward in our interconnection attempt, initiated in previous works, of various classical models in the domain of color reproduction [8–10].

From a physical point of view, the use of infinitesimally thin sublayers for obtaining Kubelka–Munk expressions needs some comments. Usually, scattering is due to heterogeneities in the medium, e.g. particles, whose size cannot be assumed as infinitesimally small. According to the intrinsic properties of the diffusing medium, a model should be chosen for the description of the scattering of light by a single particle (single scattering model, such as Mie’s theory [13]) or by collections of particles (multiple scattering model). It is possible to determine first the reflectance and the transmittance of an elementary sublayer made of this diffusing medium and, afterwards, use the discrete two-flux model to consider various superposed sublayers, like in Melamed’s model for powers [14]. The discrete two-flux model should be used when the sublayer behaves as a perfect diffuser, with the assumption that the medium is intensely diffusing and that the sublayer has a minimal thickness, at least the size of an average particle. The upward and downward fluxes are evaluated at discrete depths only, corresponding to multiples of the sublayer thickness. However, the equivalence that has been established between the continuous and the discrete models allows one to associate to the real diffusing medium an ‘imaginary’ medium; this medium is characterized by a scattering coefficient and an absorption coefficient such that the Kubelka–Munk model gives the same values for upward and downward fluxes at the discrete depths considered in the discrete model. At the intermediate depths, the value given by the continuous model corresponds to a mathematical interpolation.

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