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Kubelka-Munk Model for Imperfectly Diffuse Light Distribution in Paper

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Abstract. *Perfectly diffuse light is a fundamental assumption in the Kubelka-Munk (KM) model. This assumption is, however, seldom fulfilled by real media. In this work, we build a bridge between a weakly absorbing medium with an imperfectly diffuse light distribution and the corresponding KM model relying on a perfectly diffuse light distribution. We multiply the apparent K and S phenomenal coefficients deduced from a learning set medium by a scaling factor expressing the ratio of light diffuseness between the target medium and the learning set medium. For the target medium, thanks to this diffuseness scaling factor, theoretically predicted reflection and transmission spectra agree with the corresponding measured spectra. The illumination geometry, the optical properties and the thickness of the medium have an impact on the light diffuseness and therefore on the proposed diffuseness scaling factor. © 2008 Society for Imaging Science and Technology.*
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INTRODUCTION

The Kubelka-Munk (KM) theory is a two-flux simplified approach of the radiation transfer theory. The KM theory was originally developed for light propagation in parallel colorant layers of infinite *xy*-extension.[1,2] The KM theory assumes that light scattering in the sample is isotropic; i.e., it is independent of the angle of the incident light rays and that the light distribution inside the medium layer is perfectly diffused. Relying on these assumptions, we model light propagation in the layer by two simultaneous light fluxes traversing the layers, one traveling upwards and the other traveling downwards.

After its introduction in the 1930s, KM theory was extended by removing some of the original assumptions. Saunderson introduced a correction accounting for the Fresnel reflections at the interface between the considered medium and air.[3] Kubelka himself extended the applicability of the KM theory to stacked optically inhomogeneous diffuse layers of known reflectance and transmittance.[4]

Because of its simplicity and usefulness, the KM theory has been the most widely applied theoretical model in studying light propagation in turbid media since its introduction in the 1930s. While enjoying great success in both scientific and industrial applications,[5–9] the theory seems to have shortcomings that prevent the model from being applied to media layers containing an absorptive component,[10,11] for example, a dyed sheet,[12–16] because the light distribution is not perfectly diffuse when light absorption is strong.

The perfectly diffuse light distribution is one of the most fundamental assumptions of the KM model. Since light distribution in a real medium is often not perfectly diffuse, this topic is frequently discussed in the literature.[10–22] There are two problems. Firstly, the medium should have a strong light scattering power. This ensures that the illuminating light can be scattered a sufficient number of times, resulting in a nearly perfectly diffuse light distribution. Secondly, the medium should be only weakly absorbing in order to allow a sufficient number of scattering events to occur before light is absorbed.

In the present paper, we consider only weakly absorbing media, such as paper. Other approaches exist for dealing with the reduction of diffuseness due to absorbance.[10,23–26]

THEORY

In the KM model, light propagation in a medium layer is represented by two light fluxes through the layers, one traveling upwards and the other traveling downwards. These light fluxes are averaged representations of three-dimensional fluxes towards the upper and lower hemispheres, respectively, governed by the phenomenal coefficients of absorption K and of scattering S. For a medium layer of thickness D, the reflectance values is expressed by (see Appendix)

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$$R = Cr_0 + (1-r_0)(1-r_1) \times \frac{(R_{\infty 0}-r_1)\exp(-2\sqrt{K^2+2KS}D) - R_{\infty 0}(1-R_{\infty 0}r_1)}{(R_{\infty 0}-r_1)^2\exp(-2\sqrt{K^2+2KS}D) - (1-R_{\infty 0}r_1)^2}. \quad (1)$$

In the equation, r_0 and r_1 stand for the external and internal Fresnel reflection coefficients at the air-medium interface; C is the proportion of captured specularly reflected light, ranging from zero to unity, depending on the measurement setup; $R_{\infty 0}$ is the intrinsic (bulk) reflectance of a semi-infinitely thick medium, which is expressed by

$$R_{\infty 0} = 1 + \frac{K}{S} - \sqrt{\left(\frac{K}{S}\right)^2 + 2\frac{K}{S}}. \quad (2)$$

When D approaches infinity, Eq. (1) becomes

$$R_\infty = Cr_0 + (1-r_0)(1-r_1)\frac{R_{\infty 0}}{(1-R_{\infty 0}r_1)}. \quad (3)$$

Similarly, the transmittance of the medium layer is (see Appendix)

$$T = (1-r_0)(1-r_1) \times \frac{(1-R_{\infty 0}^2)\exp(-\sqrt{K^2+2KS}D)}{(1-r_1R_{\infty 0})^2 - (R_{\infty 0}-r_1)^2\exp(-2\sqrt{K^2+2KS}D)}. \quad (4)$$

In the KM model, the phenomenal coefficients of absorption and scattering, i.e., K and S, respectively, are linear functions of the intrinsic coefficients of absorption and scattering of the medium, i.e., a and s, respectively, according to Nobbs[10]:

$$K = \alpha a, \quad S = \frac{\alpha}{2}s, \quad (5)$$

with α being a constant ($\alpha=2$) when the light distribution is perfectly diffuse.[2] The general expression for α, for an arbitrary angular light distribution $\partial J/\partial\phi$ is[2,27]

$$\alpha = \int_0^{\pi/2} \frac{1}{J}\frac{\partial J}{\partial \phi}\frac{d\phi}{\cos\phi}. \quad (6)$$

The α factor is equal to unity for incident collimated light normal to a nondiffusing medium and equal to 2 when the light distribution is perfectly diffuse, as in the case of the original KM model.[2] For other types of light distributions, α takes a value between these two extremes, namely, $1<\alpha<2$, depending on their respective diffuseness grade. In other words, the magnitude of α can be considered as a measure of the diffuseness of the light distribution within the medium. In addition, factor α expresses the relative mean path length of light within the medium.[2]

There are a few factors that may affect the light distribution. The angular distribution of the incident light has a clear effect on the angular distribution of light in the medium. When the medium is illuminated by perfectly diffuse light, the light distribution inside the medium will also be well diffused, if the medium is not strongly absorptive. When collimated light is used as the illumination, light distribution inside the medium depends on the optical properties of the medium. Light scattering contributes positively to light diffusion. Even if the incident light is collimated, after entering the medium, light scattering makes it diffuse. The diffuseness grade, or equivalently, the mean path length of light, depends on the average number of scattering events. More scattering events induce a higher light diffuseness. On the contrary, light absorption impacts negatively on the light diffuseness as it limits the number of scattering events before absorption. Another factor that is often overlooked is the thickness (or grammage) of the medium layer. Since light may exit the medium at the medium-air interfaces, the average number of scattering events depends on the thickness of the medium. When illuminating a weakly absorbing medium with collimated light, an increase in thickness of the medium layer enhances the diffuseness of the light distribution.

MEASUREMENTS OF SPECTRAL REFLECTANCE AND TRANSMITTANCE

Spectral reflectance and transmittance values of paper (Biotop 3 from Neusiedler, 80 g/m^2, without fluorescent brighteners) have been measured by employing the Gretag MacBeth Eye One™ spectrophotometer. The spectrophotometer has a 45°/0° measurement geometry in reflection mode. The sample is illuminated by collimated light at 45° incident angle and reflected light is recorded in the direction of the paper's normal. In transmittance mode, a high quality light table (Just Normlicht Classic Line) is used as the source of illumination. The spectrophotometer works in a $D/0°$ geometry, because the light table creates the diffuse light hitting the paper samples from beneath. In order to avoid undesired reflections between the light table and the paper sample, the paper sample is placed on top of a black sheet having a transparent window of 1 cm^2, through which the incident light hits the bottom face of the paper sample. Both the paper sample and the black sheet are placed at a distance of 5 cm from the light table.

The measurements include reflection and transmission spectra of single, double, and triple paper sheets. The multiple sheets are simply laid out on top of one another. The spectra are denoted as R_1, T_1, R_2, T_2, R_3, and T_3, with the numbers in the subscript corresponding to the number of stacked paper sheets. The reflectance of many stacked paper sheets R_∞ is also measured.

THE PHENOMENAL COEFFICIENTS *K* AND *S* AND THE DIFFUSENESS FACTOR α

It is a common practice to obtain the phenomenal coefficients K and S of a medium from two measured reflection spectra (training set), by solving the set of equations (1)–(3). The deduced S and K coefficients can then be used to predict the spectral reflectance and transmittance values of medium layers of different thicknesses, using Eqs. (1) and (4).

Traditionally, the phenomenal coefficients K and S are computed from spectral measurements of a single paper sheet (R_1, measured against a black backing) and many stacked paper sheets (R_∞). We denote these deduced coefficients as K_1 and S_1. According to Eq. (5), these coefficients are related to the intrinsic absorption and scattering coefficients a and s of the medium by the diffuseness factor $\alpha_1 : K_1 = \alpha_1 a$ and $S_1 = (\alpha_1/2)s$. The reflectance of a semi-infinitely thick layer R_∞ depends only on the ratio of K_1/S_1 [see Eq. (2)] and is therefore independent of α_1. Consequently, quantity α_1 depends only on the light diffuseness; i.e., on the angular distribution of light within the single sheet of paper.

Since the paper is uncoated, we assume that its refraction index is the same as air; i.e., unity. Fresnel reflections at the air-paper and paper-air interfaces are therefore assumed to be negligible; i.e., $r_0 = r_1 = 0$.

DIFFUSENESS SCALING FACTOR IN REFLECTANCE MODE

According to the arguments given in Sec. 2, the apparent phenomenal coefficients K_1 and S_1 obtained from the spectra of a single sheet R_1 and of many sheets R_∞ as the training set cannot directly be used to predict the reflectance and transmittance values of paper of different thicknesses (e.g., two stacked sheets) because of the thickness dependence of the light distributions, when the illumination is not perfectly diffuse. Due to the thickness effect, the light diffuseness α_2 of the double sheet is greater than the light diffuseness α_1 of the single sheet. We propose to take into account the thickness effect by introducing a scaling factor describing the relative diffuseness of a target medium with respect to the training set medium. For example, for paper of double thickness (double sheet), the phenomenal coefficients can be computed as

$$K_2 = \alpha_2 a = \frac{\alpha_2}{\alpha_1} K_1, \quad S_2 = \frac{\alpha_2}{2} s = \frac{\alpha_2}{\alpha_1} S_1. \tag{7}$$

In these equations, the ratio α_2/α_1 is the scaling factor that describes the relative light diffuseness of the double-sheet layer with respect to the single-sheet layer. Since the light distribution in the double sheet is more diffuse than in the single sheet, the scaling factor is greater than unity; i.e., $\alpha_2/\alpha_1 > 1$. The scaling factor may be a scalar (independent of wavelength) when the ratio of α_2 and α_1 exhibits no spectral dependence, as is approximately the case with white papers. In the present study, in order to match measured and calculated spectra, the scaling factors of the double and triple sheets are $\alpha_2/\alpha_1 = 1.06$, and $\alpha_3/\alpha_1 = 1.14$, respectively (see Comparison of Reflection Spectra).

If the exact scattering behavior of a medium would be known, one might consider calculating the α value (light diffuseness) as a function of the illumination geometry, the optical properties, and the thickness of that medium. In the present contribution, we use the concept of scaling factor to account for the ratio of diffuseness or equivalently, of mean path length, between the medium used as the training set and the target medium whose reflection or transmission spectra are predicted. This is a way of establishing a bridge between a medium having an imperfectly diffuse light distribution and a medium with a perfectly diffuse light distribution, as required by the KM model. We give an example showing how the α value may be estimated by combining spectra measured according to different measurement geometries (see Comparison of Transmission Spectra) and also discuss related issues in the conclusions.

DIFFUSENESS SCALING FACTOR IN TRANSMITTANCE MODE

Since a perfectly diffuse illumination is used in measuring the transmittance spectra, the light distributions in single-, double-, and triple-sheet systems are identical; namely, perfectly diffuse. Their α factors (denoted as α_T to avoid confusion with those for reflection) are all equal to $\alpha_T = 2$. Consequently, when computing the transmittance values of the samples, identical phenomenal coefficients should be used for all the considered layer thicknesses, namely,

$$K_T = \alpha_T a = \frac{\alpha_T}{\alpha_1} K_1, \quad S_T = \frac{\alpha_T}{2} s = \frac{\alpha_T}{\alpha_1} S_1. \tag{8}$$

In the current study, the scaling factor $\alpha_T/\alpha_1 = 1.21$ is used for the calculation of the transmittance spectra of single-, double-, and triple-sheet layers (see the beginning of the next section).

COMPARING PREDICTED AND MEASURED REFLECTION AND TRANSMISSION SPECTRA

To illustrate the impact of the light diffuseness, we consider different illumination geometries as well as different thicknesses. Corresponding reflection and transmission spectra are predicted by calculations and compared with the corresponding measured spectra.

The reflection and transmission spectra of single-, double-, and triple-sheet layers are calculated with Eqs. (1) and (4). The apparent phenomenal coefficients of scattering and absorption of the single sheet, S_1 and K_1, are shown by solid lines in Figure 1. They are obtained by solving the set of equations (1)–(3), using the reflection spectra pair R_∞ and R_1 as the training set. These values depend solely on the light diffuseness α_1 of a single sheet, because R_∞ depends only on the ratio of K_1/S_1 [see Eq. (2)] and is therefore independent of α. For verification purpose, the S_1 and K_1 values are compared with the values (dots) computed from the transmittances of a single sheet T_1 and of two stacked sheets T_2, by dividing the obtained S_T and K_T values by the ratio $\alpha_T/\alpha_1 = 1.21$, according to Eq. (8).

Comparison of Reflection Spectra

Let us first assume, as in the KM model, that light distribution is identical (i.e., perfectly diffuse) and independent of the paper thickness. The coefficients of scattering and absorption of the double and triple sheet are assumed to be identical to the ones obtained from the single sheet, i.e.,

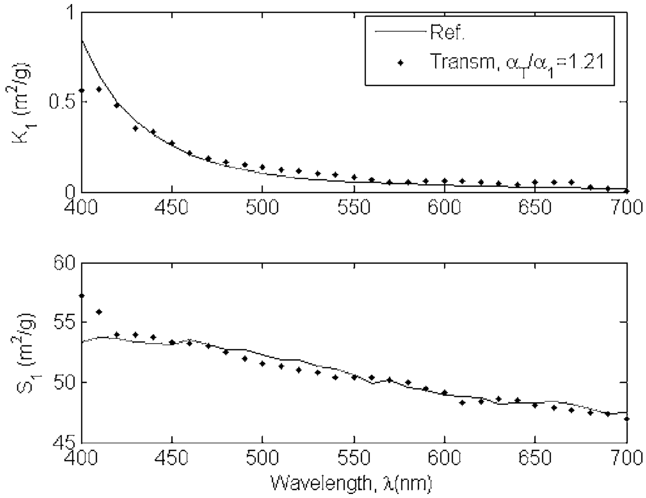

Figure 1. The apparent phenomenal coefficients of absorption K_1 and scattering S_1 (solid lines) obtained from spectra pair R_∞ and R_1. For verification purpose, the S_1 and K_1 values (dots) are also computed from the transmittances of a single sheet T_1 and of two stacked sheets T_2, by dividing the obtained S_T and K_T values by $\alpha_T/\alpha_1 = 1.21$, according to Eq. (8).

$$K_3 = K_2 = K_1 \quad \text{and} \quad S_3 = S_2 = S_1, \tag{9}$$

with the subscripts denoting the number of paper sheets.

Figure 2 shows the comparison between predicted and measured reflection spectra of paper. The abbreviations "Meas." and "Cal." denote the measured and calculated spectra, respectively, for single- (P1), double- (P2), and triple-sheet (P3) layers, respectively. Since the reflection spectrum of the single sheet is used as the training set, the comparisons are made for the double- and triple-sheet media, calculated versus measured. Figure 2 reveals systematic deviations at wavelengths longer than 450 nm, where there is nearly no light absorption. The deviations increase with decreasing light absorption.

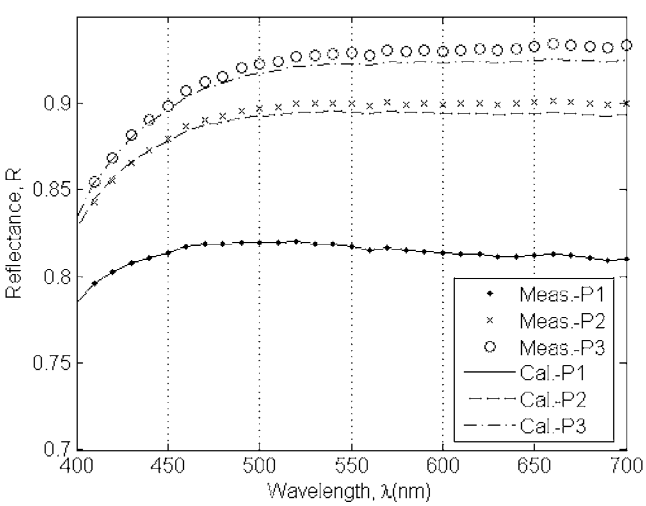

Figure 2. The calculated spectral reflectance values of double (dashed line) and triple (dash-dotted line) sheet layers of paper. The double- and triple-sheet reflection spectra are calculated with the KM model, assuming that the phenomenal coefficients are identical at different thicknesses. The phenomenal coefficients of the single sheet are deduced from reflectance values R_∞ and R_1.

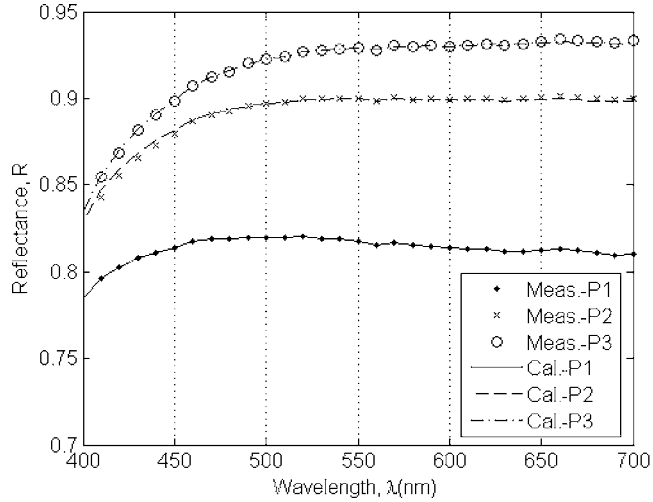

Figure 3. The spectral reflectance values of single (solid), double (dashed), and triple (dash-dotted) sheet layers. The spectra are calculated by accounting for the thickness effect. The scaling factors $\alpha_2/\alpha_1 = 1.06$ and $\alpha_3/\alpha_1 = 1.14$ were chosen for calculating the spectra of the double- and triple-sheet layers.

The deviations can easily be understood in light of the thickness effect. As pointed out in the preceding section, when a medium is illuminated by nondiffuse light (here, 45°/0°), light diffuseness in the medium layer depends on the average number of photon scattering events. This number increases with the layer's thickness (thickness effect). In contrast, light absorption in the medium limits the number of scattering events and thus reduces the thickness effect. In other words, Fig. 2 confirms that the thickness effect is more pronounced in the nonabsorbing region than in the absorbing one.

Let us now calculate the spectra again, by taking into account the thickness effect. The light distribution in the single sheet is only partially diffuse and the diffuseness of the double- and triple-sheet media increases with increasing paper thickness. The thickness effect is accounted for by using the following fitted scaling factors in Eq. (8) for, respectively, the double- and the triple-sheet media:

$$\frac{\alpha_2}{\alpha_1} = 1.06 \quad \text{and} \quad \frac{\alpha_3}{\alpha_1} = 1.14. \tag{10}$$

These factors are fitted by minimizing the sum of square differences between computed and measured reflectance spectra. As shown in Figure 3, the computed spectra are in excellent agreement with the measured spectra, over the whole spectral range. This is the first evidence that supports our argument in respect to the thickness effect. Below we also compare calculated and measured transmission spectra in order to verify the presence of the thickness effect.

Comparison of Transmission Spectra

Comparative calculations of transmission spectra are made, with the conventional KM model and with the proposed method accounting for the light diffuseness in the media as a function of thickness. Figure 4 shows the transmission

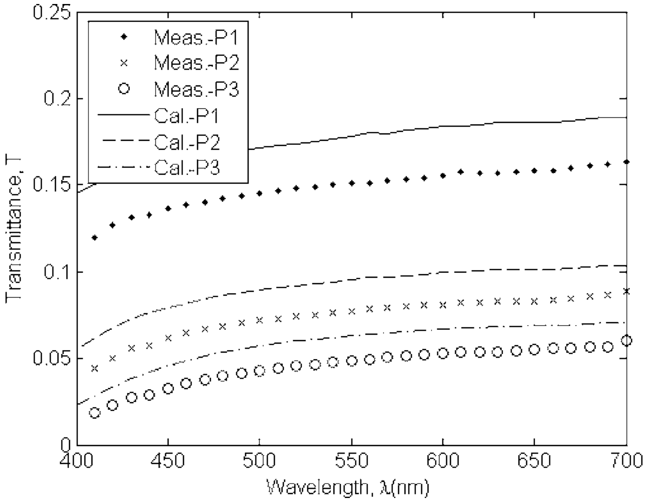

Figure 4. The spectral transmittance values of single (solid line), double (dashed line), and triple (dash-dotted line) layers of paper. The spectra are calculated using the KM model, in which the phenomenal coefficients of scattering and absorption (K_1 and S_1), derived from the reflectance values R_∞ and R_1, are directly used in all of the calculations.

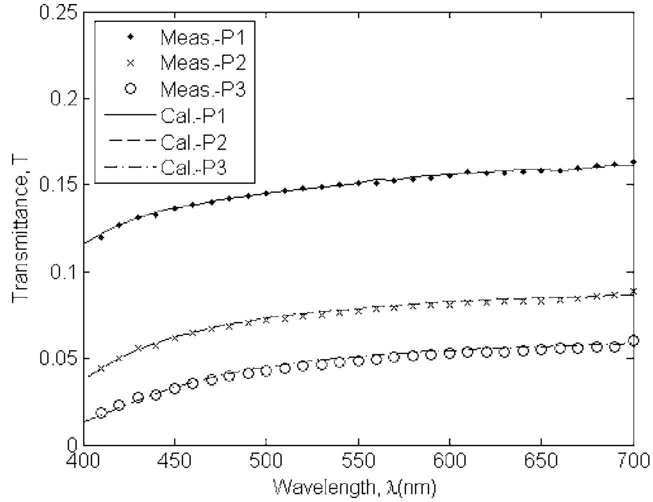

Figure 5. The transmission spectra of single (solid), double (dashed), and triple (dash-dotted) sheet layers. The phenomenal coefficients are obtained using reflectance values R_∞ and R_1 as training set. The ratio between the perfect diffuseness of light in the transmission measurements and the non-perfect diffuseness of light in the reflection measurements of the learning set is expressed by a diffuseness scaling factor of $\alpha_T/\alpha_1 = 1.21$.

spectra, directly calculated with the phenomenal coefficients of absorption and scattering (the conventional way), derived from the reflectance spectra pair (R_∞, R_1), for single-, double-, and triple-sheet samples according to Eq. (9). Clearly, for all of the samples, the calculated spectra differ significantly from the measured spectra.

Due to the difference in the measurement geometries of the reflectance $(45°/0°)$ and the transmittance $(D/0°)$ measurements, resulting in different light distributions in reflection and transmission modes, the significant discrepancy between calculated spectra and measured spectra is not a surprise. Since the reflection spectra that are used as training sets were measured with a $45°/0°$ geometry, the light diffuseness is not perfect. The transmission spectra are obtained with a $D/0°$ measuring geometry, which induces a perfectly diffuse light distribution $(\alpha_T = 2)$ identical in all the paper samples (single-, double-, and triple-sheet layers).

In order to account for the difference in measurement geometries or more exactly for the difference in light diffuseness within the media, a scaling factor $(\alpha_T/\alpha_1 = 1.21)$ is used for calculating the transmittance spectra [Eq. (8)]. Figure 5 depicts the transmittance spectra, calculated by accounting for the different light diffuseness induced by the different measuring geometries. The calculated spectra are in excellent agreement with the measured spectra, indicating the soundness as well as the practical applicability of the proposed method. Moreover, from the scaling factor $(\alpha_T/\alpha_1 = 1.21)$ and the known value of $\alpha_T = 2$ (the light distribution is perfectly diffuse in the transmittance measurements), one may obtain an estimation of the light diffuseness in the single-sheet system when it is illuminated according to a $45°/0°$ geometry (reflective measurement); i.e., $\alpha_1 = 1.65$. This demonstrates the possibility of estimating the light diffuseness in media by combining spectra measured with different measurement geometries, where at least one of the geometries relies on diffuse illumination.

CONCLUSIONS

Even though the Kubelka-Munk model was originally developed for ideal optical systems in which light distribution is perfectly diffuse, some of its elements can be adapted to the situation where light distribution is only partially diffuse. For nonabsorbing media such as paper, one may adapt the so-called α factor whose value depends on light diffuseness within the medium. The light distribution in the medium depends on the specific illumination geometry used for measurement purposes, on the intrinsic coefficients of scattering and absorption s and a, as well as on the layer thickness D.

For nonabsorbing or slightly absorbing media such as paper, we propose to account for a difference in light diffuseness between the learning set and the target medium by introducing a diffuseness scaling factor expressing the ratio of corresponding α factors. Conceptually, this diffuseness scaling factor can also be conceived as a ratio between respective mean path lengths of light. Thanks to this diffuseness scaling factor, we establish a bridge between a medium having a non-perfectly diffuse light distribution and the original Kubelka-Munk model that requires a perfectly diffuse light distribution.

APPENDIX: REFLECTANCE AND TRANSMITTANCE EXPRESSED ACCORDING TO THE KM THEORY

Assume that the light fluxes towards the lower and upper hemispheres are I and J, respectively. These fluxes fulfil the differential equations; i.e.,

$$-\frac{dI}{dz} = -(S+K)I + SJ, \quad \frac{dJ}{dz} = -(S+K)J + SI. \quad \text{(A1)}$$

General solutions of these differential equations can be expressed as

$$I = a_1 \exp(\sqrt{K^2 + 2KSz}) + a_2 \exp(-\sqrt{K^2 + 2KSz}),$$

$$J = b_1 \exp(\sqrt{K^2 + 2KSz}) + b_2 \exp(-\sqrt{K^2 + 2KSz}). \tag{A2}$$

Inserting the solutions into the Eqs. (A1), one obtains the following relations between the unknown coefficients:

$$b_1 = R_{\infty 0} a_1, \quad b_2 = \frac{1}{R_{\infty 0}} a_2, \tag{A3}$$

with $R_{\infty 0} = 1 + K/S - \sqrt{(K/S)^2 + 2K/S}$. Hence, there are only two unknown coefficients which can, in turn, be determined by applying boundary conditions at $z=0$ and $z=D$, respectively.

Considering the fluxes' continuation at the $z=D$ interface, one receives the following boundary conditions:

$$I(D) = I_0(1 - r_0) + J(D) r_1, \tag{A4}$$

$$I_0 R = I_0 r_0 + J(D)(1 - r_1). \tag{A5}$$

Similarly, at $z=0$, there is

$$J(0) = I(0) R_g, \tag{A6}$$

with R_g being the reflectance of the backing. Combining Eqs. (A3)–(A6), one obtains the expressions for the reflectance:

$$R = C r_0 + (1 - r_0)(1 - r_1) \times \frac{(R_{\infty 0} - r_1)\exp(-2\sqrt{K^2 + 2KSD}) - R_{\infty 0}(1 - R_{\infty 0} r_1)}{(R_{\infty 0} - r_1)^2 \exp(-2\sqrt{K^2 + 2KSD}) - (1 - R_{\infty 0} r_1)^2}. \tag{A7}$$

In the equation, the contribution of the Fresnel reflection at the air/paper interface is regulated by the factor C. The quantity C ranges between 0 and 1, depending on the illumination-measurement geometry.

For a free suspended medium layer ($R_g = r_1$), the reflection at $z=0$ interface is purely due to the internal medium-air surface reflectance, r_1. Consequently, the boundary condition given in Eq. (A6) should be replaced, accounting for Eq. (A3), by

$$R_{\infty 0} a_1 + \frac{1}{R_{\infty 0}} a_2 = r_1(a_1 + a_2). \tag{A8}$$

From the continuity of the light stream (propagating downward), one may obtain an extra boundary condition beneath the $(z=0)$ interface,

$$I_0 T = (1 - r_1)(a_1 + a_2). \tag{A9}$$

Combining Eqs. (A3) and (A4) with Eqs. (A8) and (A9), one obtains the expression for the transmittance of the medium layer:

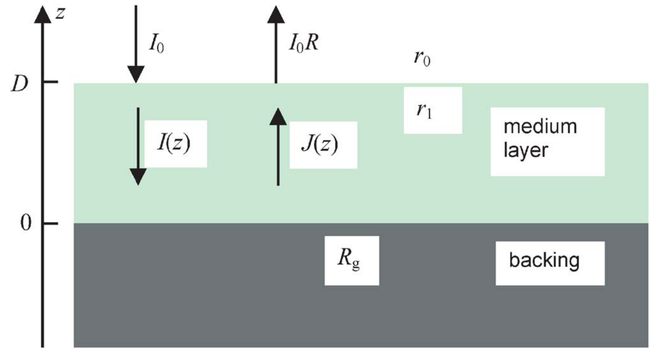

Figure A1. The schematic diagram of light propagation in the media.

$$T = (1 - r_0)(1 - r_1) \times \frac{(1 - R_{\infty 0}^2)\exp(-\sqrt{K^2 + 2KSD})}{(1 - r_1 R_{\infty 0})^2 - (R_{\infty 0} - r_1)^2 \exp(-2\sqrt{K^2 + 2KSD})}. \tag{A10}$$

Detailed information for deriving the formulas can be found in Ref. 28.

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