What Has Been Overlooked in Kubelka-Munk Theory?

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Abstract

A general theory describing light propagation in turbid media is presented, taking into account the effect of scattering on the path length of light propagation. This leads to new relationships between the K-M scattering (S) and absorbing (K) coefficients and the intrinsic scattering (s) and absorbing (a) coefficients of material. It is shown that experimental findings of dyed paper, typical examples that the original K-M theory failed to explain can clearly be understood and accommodated by the theory.

Introduction

The original theory of Kubelka-Munk (K-M) is a two-flux approach to the general Radiation Transfer Theory, developed for light propagation in parallel colorant layers of infinite xy-extension.[1] In the theory, the downward (-z direction) flux, *I*, is an average representation of all rays traveling towards the lower hemisphere. Likewise, the upward flux (+z direction), *J*, is an average of all rays traveling towards the upper hemisphere. The propagation of the up- and down-ward fluxes are characterized by so-called K-M scattering and absorption coefficients, denoted as *S* and *K*, respectively, i.e.,

$$-\frac{dI}{dz} = -(S+K)I + SJ, \quad \frac{dJ}{dz} = -(S+K)J + SI \tag{1}$$

Quantities *S* and *K* have no direct physical meaning on their own, even though they appear as if they represent portions of light scattered and absorbed, respectively, per unit vertical length. In the case of diffuse light distribution, the average path length for a light ray passing through a layer of Δz is $2\Delta z$. Therefore, *K* is twice the intrinsic absorption coefficient.[2] *S* is subject to the same change as *K* due to the average path length, but additionally, in the formulation of Eqs (1), *S* addresses only the portion of the scattered light that changes direction from upward and downward, or vice versa. For isotropic scattering, this is exactly half of the actually scattered light. Thus, Kubelka and Munk suggested the following relationships

$$K=2a, \quad S=s, \tag{2}$$

where *a* and *s* are the intrinsic absorbing and scattering coefficients of the media. Unlike *K* and *S*, quantities *a* and *s* are the physical properties of the material, representing the probabilities of light being absorbed (*a*) and scattered (*s*) per unit path length isotropically.

The K-M theory has enjoyed great successes in both scientific and industrial applications, since introduction in the 1930's. In present day paper-making and color-using industries, it remains as one of the most widely used theories. Nevertheless, this theory has, at the same time, been over-shadowed by experimental findings suggesting non-linear relationships between *S* and *K*, and *a* and *s*.[3,4] Here, we use an example, a dyed-paper sheet,[5] to illustrate the difficulties encountered in the paper-related applications.

Let K_i and S_i, and K_p and S_p be the K-M coefficients of absorption and scattering of ink (i) and paper (p), respectively. If the ink is mixed homogeneously with the paper and if the linearity given in Eq. (2) holds, the K-M scattering and absorbing powers of this dyed sheet may be computed by,[6]

$$K_{ip}(w_p + w_i) = K_i w_i + K_p w_p, \quad S_{ip}(w_p + w_i) = S_i w_i + S_p w_p, \tag{3}$$

where w_i and w_p are the grammages of the ink and paper, respectively. Because the ink is almost purely absorptive and the paper is mainly scattering, one would anticipate that an ink-dyed sheet has a similar K-M absorbing power to that of the ink and, at the same time, a similar K-M scattering power to that of the paper. Unfortunately, inverse calculations[5] based on measured spectra for a dyed (paper) sheet giving its K-M powers, $S_{ip}(w_p+w_i)$ and $K_{ip}(w_p+w_i)$, reveal that the light absorption power is remarkably nonlinear to dye concentration.[5] Scattering power, on the other hand, is dramatically decreased with respect to increasing ink concentration in the absorbing band of the ink, compared with that of the pure paper.[7] These observations do not at all agree with the K-M expectations, which has contributed to the long standing debate on the applicability of the K-M theory.

Understanding the origin of the shortcomings of K-M theory have attracted continuing interests of researchers in decades.[3,4,8-11] To overcome the difficulties, different approaches have been proposed, aiming at compensating these shortcomings by expressing *K* and *S* as sophisticated functions of the intrinsic coefficients, *a* and *s*, of the materials. However, they have proved not to be transferable to applications in other contexts.

This report presents a revision on the K-M theory, taking into account effects of light scattering on path length, overlooked in the original K-M theory. The revised theory is then illustrated by applications to dye-dispersed paper.

The Revised K-M Theory

For clarity and simplicity of the descriptions, assumptions used in this presentation are summarized as follows. First, the sample is a plane layer (perpendicular to the z-axis) whose size in the xy-extension is much larger than its thickness. Edge effects are therefore negligible. Second, the sample is optically homogeneous. Third, the scattering in the sample is random and isotropic, i.e., it is independent of the angle between the incident and scattering directions. Finally, the light is incoherent or light interference is negligible. Here, we only report studies on a media system in which light distribution is diffuse. More general theoretical descriptions may be found elsewhere.[12]

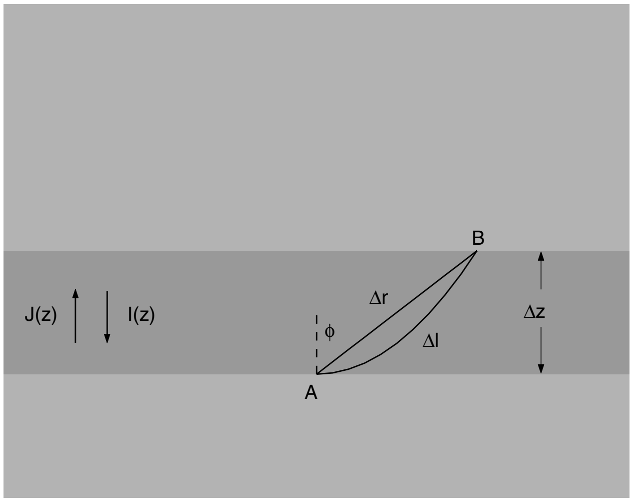

Figure 1. The schematic diagram of light propagation in turbid media.

Figure 1 is a schematic presentation for a photon that transverses the medium layer of thickness Δz, from A to B. The length of the displacement between the incident and the exiting points is Δr. Because of light scattering, the photon propagates in the media in a zigzag fashion rather than straight forward towards the exiting point. As a consequence, the photon takes a longer path (represented by Δl) than it seems to be. We define μ as the ratio between the real path length, Δl, and the nominal one, Δr, i.e,

$$\mu = \Delta l / \Delta r \qquad (4)$$

Then, the real path length corresponding to the displacement equals $\Delta l = \mu \Delta r$. Consequently, the possibility for a photon being absorbed and/or scattered, which is proportional to the real path length, becomes μ times enlarged. Since the media is homogeneous and light scattering is isotropic, quantity μ is hence directionally independent. Therefore, the average path length for a light ray passing through a layer of Δz becomes $2\Delta z$. Consequently, Eq. (2) should be replaced by:

$$K = 2\mu a, \quad S = \mu s. \qquad (5)$$

Based on fundamental principles of physics, the mathematic expression for μ has been worked out,[12] i.e.,

$$\mu = 2sD, \qquad (6)$$

where the quantity, D, has the meaning of the average depth of photons that undergo reflection and exit from the upper surface and is expressed as:

$$D = \frac{1}{A} \frac{1 - 2Aw\exp(-Aw) - \exp(2Aw)}{1 - 2\exp(-Aw) + \exp(-2Aw)}, \qquad (7)$$

with $A = (K^2 + 2KS)^{1/2}$.

As the quantity, μ, depends on both light scattering and absorption, as well as the grammage (or equivalently thickness) of the medium layer, w, K-M coefficients K and S are generally nonlinear functions of a and s, which is in contrast with what were suggested in the original K-M theory (Eq. (2)). In other words, the original K-M theory is only a special case of the revised theory *(μ=const.)*.

Equations (5)-(7) are the principle results of the revised model.

Applications and Discussions

This section has the intention of demonstrating the powerfulness of the revised theory, applying to dyed paper sheets. At the same time it also intends to provide an understanding of experimental observations unsatisfactorily represented by the original K-M theory.

Experimental Observations

The optical properties of paper, a_p and s_p, can be computed from the corresponding K-M coefficients of absorption and scattering of paper K_p and S_p, using Eqs. (5-7). The latter can be determined from spectral reflectance values of a paper sheet measured with white and black backings, respectively.[13] Similarly, one obtains the intrinsic properties of the ink, a_i and s_i.

Assuming the validity of the superposition principle, the total absorption and scattering coefficients of the dyed paper, a_{ip} and s_{ip}, are weight summations of those of the ink and the paper, i.e.

$$a_{ip} = \frac{w_i}{w_i + w_p} a_i + \frac{w_p}{w_i + w_p} a_p$$
$$s_{ip} = \frac{w_i}{w_i + w_p} s_i + \frac{w_p}{w_i + w_p} s_p \qquad (8)$$

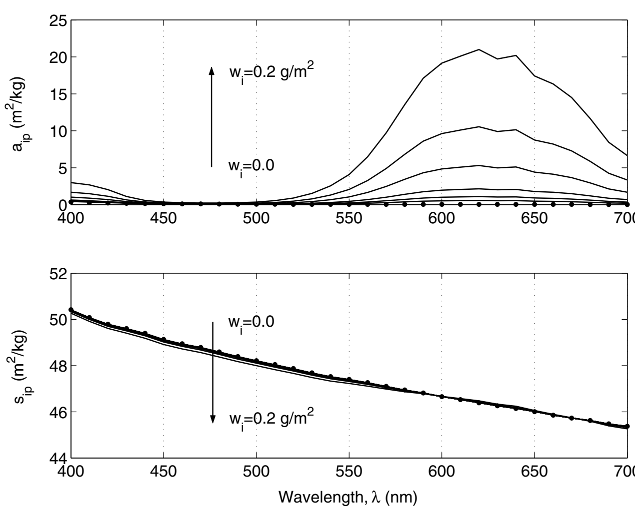

Figure 2. The intrinsic absorption and scattering coefficients of the cyan-dyed sheets, a_{ip} and s_{ip}, computed with w_p = 40g/m^2 and w_i = [0, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2] g/m^2. The results in the case of white paper are denoted by the dots.

Figure 2 depicts the intrinsic coefficients of the cyan-dyed sheets, a_{ip} and s_{ip}, computed with w_p = 40 g/m^2 and with varying amounts of dye: w_i = 0.0-0.2 g/m^2. The behavior depicted by the curves in these figures is straightforward to explain. Since $w_i a_i << w_p a_p$ and $w_i s_i << w_p s_p$, the physically meaningful coefficient of absorption, a_{ip}, is dominated by the dye component. Hence, the greater the amount of dye, the stronger the absorption, in the absorption band of the dye. On the other hand, as we have already argued, the scattering property of the mixture is dominated by the paper component and thus the total scattering coefficient, s_{ip}, is approximately independent of dyeing.

Figure 3 shows typical examples of K-M coefficients, K_{ip} and S_{ip}, computed from experimental spectra for paper sheets (*p*) dyed with different amounts of cyan ink (*i*). In the case shown, the grammage of the white paper was w_p=*40.51g/m*^{2}. With ink-dye present, the grammage for the dyed sheets varied from 40.16 to 41.73*g/m*^{2}. The K-M absorption coefficient, K_{ip}, shows a clear response to increases in dye, even for very small amounts. On the other hand, the scattering coefficient, S_{ip}, exhibits a less remarkable variation upon dyeing, unless the amount of ink is significantly high. More precisely, S_{ip} decreases in the absorption band of dye, when the amount of dye is sufficiently large, but is little changed elsewhere. Such behavior in S_{ip} is completely unexpected from K-M theory,[7] as the following argument will show. According Eq. (2), $K_{ip}=2a_{ip}$ and $S_{ip}=s_{ip}$. Since the scattering and mass properties of the ink-paper mixture are dominated by the paper material, $s_p >> s_i$ and $w_p >> w_i$, one deduces from Eqs. (8) that $S_{ip}=s_{ip} \approx s_p=S_p$. That is, S_{ip} is approximately constant, independent of the amount of dye. This is clearly in contradictory to the experimental findings demonstrated in Fig. 3.

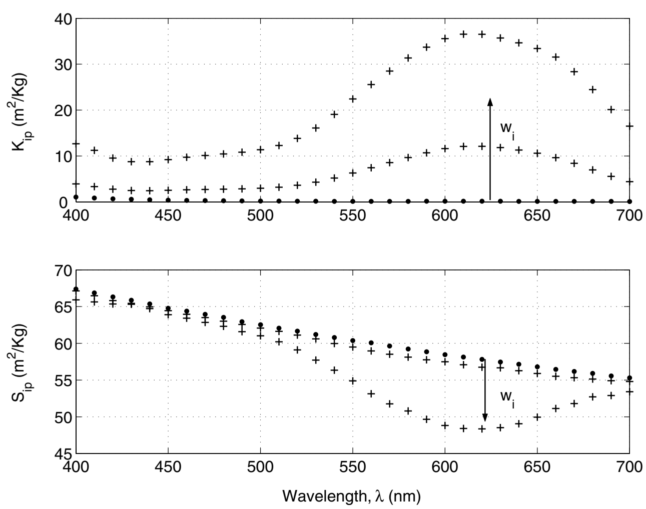

Figure 3. The K-M coefficients of absorption and scattering of the cyan-dyed sheets having nominal grammages 40.16-41.73g/m^2, computed from experimental spectra.[13] The results in the case of white paper are denoted by the dots.

Explanations with the Revised Theory

In the revised theory, the K-M coefficients of absorption and scattering of the dyed paper, K_{ip} and S_{ip}, relate nonlinearly to the intrinsic coefficients, a_{ip} and s_{ip}, i.e.,

$$K_{ip} = 2\mu_{ip} a_{ip}, \quad S_{ip} = \mu_{ip} a_{ip}. \tag{9}$$

The quantity μ_{ip} that reflects the effect of light scattering on the real path length in the dyed paper, can be computed iteratively employing Eqs. (5-7), starting with μ_{ip} = 1.

Figure 4 depicts the factor, μ_{ip}, computed with w_i = *0.0-0.2g/m*^{2} and w_p=*40g/m*^{2}. It shows clear dependence on the amount of dye. When w_i is small, for example, μ_{ip} is little changed, which results in essentially linear relationships between K_{ip} and S_{ip} and, a_{ip} and s_{ip}. Consequently, K_{ip} increases linearly with the amount of dye, while S_{ip} is little changed. In such a case, the original K-M theory applies well as been known for some time. However, when the dye amount further increases, the factor μ_{ip} significantly decreases upon dyeing in the absorption band of the dye, while changes little elsewhere. Such a nonlinear dependency of μ_{ip} on the amount of dyeing is responsible for the failure of the original theory, when applied to such a medium system as heavily dyed paper.

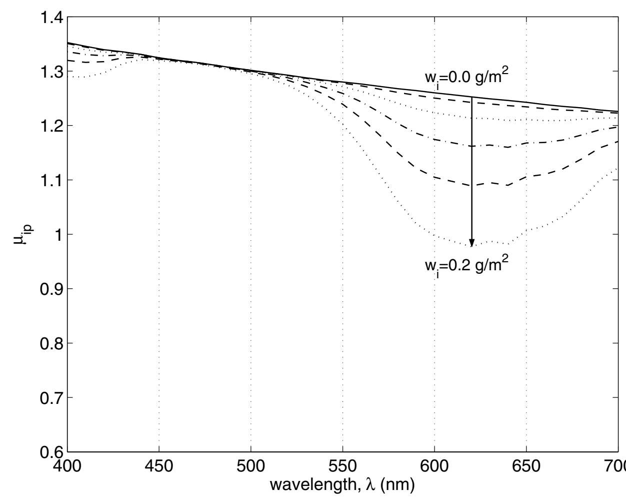

Figure 4. The quantity μ_{ip} computed with w_p=40g/m^2 and w_i=[0, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2] g/m^2.

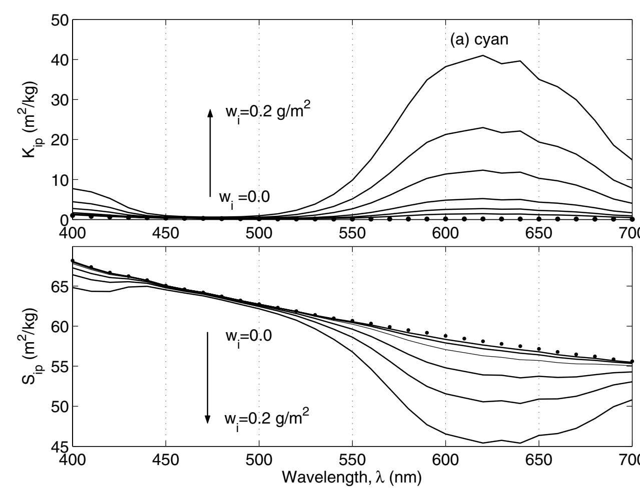

Figure 5. The KM coefficients of absorption and scattering for the cyan-dyed paper sheets computed with w_p=40g/m^2 and w_i =[0, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2] g/m^2.

Figure 5 shows the computed K_{ip} and S_{ip} values of the cyan-dyed paper. As seen, the experimental features shown in Fig. 3 are very well reproduced, indicating the applicability of the revised theory to systems of various absorption powers. Simulations to dyed paper sheets with magenta and yellow dyes[14] further confirm the nonlinear relationships between the K-M coefficients of absorption and scattering, K_{ip} and S_{ip}, and their intrinsic count parts, a_{ip} and s_{ip}, respectively, which are compared very favorably with experimental observations.

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