

Mathematical and empirical evaluation of accuracy of the Kubelka–Munk model for color match prediction of opaque and translucent surface coatings

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Abstract Attempts were made to evaluate mathematically and empirically the accuracy of the Kubelka–Munk model for color match prediction of opaque and translucent surface coatings in the color using industries. To this end, an innovative inversed mathematical evaluation procedure was concocted which comprised of plotting the absorption and scattering constants of the Kubelka–Munk model or any of its various modified form or replacements theories against the intrinsic optical coefficients of the respective exact radiation transfer theories, namely Chandrasekhar for opaque and van de Hulst for translucent media. The results prove mathematically that the Kubelka–Munk model for opaque media is a sound theory and its various suggested modifications or replacements do not improve the color match prediction of opaque surface coating media. This mathematical conclusion was further confirmed by color match prediction of actual opaque paint samples. On the other hand, the mathematical prediction for translucent media illustrated a completely different picture, depicting nonlinearity between the optical constants and the respective concentrations of colorants. This implies that much further work has to be carried out to derive invertible new equations to enforce linearity to such situations or

make use of alternative artificial intelligent procedures which are designed especially for nonlinearity.

Keywords Kubelka–Munk model, Color match prediction, Opaque, Translucent, Exact radiation transfer theories

Introduction

The well-known Kubelka–Munk model, depicted in equation (1), is based on the work of Schuster who in 1905¹ modeled the radiation of an opaque-dust cloud surrounding a star. Kubelka and Munk² completed their model for translucent systems denoted by equation (2). This model is applicable to many industries such as surface coatings,^{3–11} textiles,^{12–14} printing of paper^{15,16} and color matching of dental systems.^{17–19} There are several reasons for the acceptance of Kubelka–Munk equations worldwide:

1. The analytical equations are simple and easily understood by nonspecialists.^{20–23}
2. The Kubelka–Munk equations can be used to predict the reflectance of a specimen with reasonable accuracy. This advantage among others has made the Kubelka–Munk model more preferable compared to other more complicated models.²⁰
3. Comparing the Kubelka–Munk equations with other complicated models such as the “van de Hulst” equations shows that generally, the reflectance and transmittance of these equations seem to be of the same form. Because calculating Kubelka–Munk coefficients is easy, the Kubelka–Munk equation is still being used.²⁴
4. Kubelka–Munk model is among the first attempts to relate the reflectance (or transmittance) of colored media to the concentration of dyes or pigments present in such media.²

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$$R_{\infty} = \left(1 + K/S\right) - \left(\left(1 + K/S\right)^2 - 1\right)^{1/2} \quad (1)$$

$$R = \frac{1 - R_g(a - b\text{Coth}(bSX))}{a - R_g + b\text{Coth}(bSX)} \quad (2)$$

$$a = 1 + K/S$$

$$b = \sqrt{a^2 - 1}$$

where R , R_g , X , R_{∞} , K , S are the respective translucent reflectance, background reflectance, thickness of the layer, infinite reflectance, absorbance coefficient, and scattering coefficient.

Ultimately, a relationship between the concentration of each colorant and the reflectance of a colored media having a mixture of colorants is sought after. However, the Kubelka–Munk model only provides a relationship between the reflectance and the optical coefficients (i.e., absorption and scattering coefficients). Therefore, complementary equations are needed to signify the relationship between optical coefficients and concentrations of colorants. In 1940, Duncan²⁵ put forward the concept of “additivity” in a mixture of colorants. Such introduction made provisions for the concepts of “linearity” and “additivity” between the optical coefficients of the Kubelka–Munk model and the concentrations of colorants as illustrated in equations (3a) and (3b). Duncan’s complementary equations have been referred to in the literature with different names such as the “additivity of Duncan”²⁶ or “the usual mixing law.”^{27,28}

$$K = \sum_{i=1}^n c_i k_i = c_1 k_1 + c_2 k_2 + \cdots + c_n k_n \quad (3a)$$

$$S = \sum_{i=1}^n c_i s_i = c_1 s_1 + c_2 s_2 + \cdots + c_n s_n \quad (3b)$$

where k_i , s_i and c_i are absorption, scattering constants (optical constants), and concentration of pigments, respectively.

Generally, the Kubelka–Munk model has been successful in various scientific and industrial applications.^{5,6,29–31} However, certain articles have tried to demonstrate some of the theory’s shortcomings and have attempted to modify the Kubelka–Munk model to overcome such shortcomings.^{20,23}

In the present study, attempts were made to clarify mathematically and empirically whether the Kubelka–Munk model needs to be modified firstly for opaque media and secondly for translucent media.

Theoretical background

The Kubelka–Munk model is, in essence, a two flux hypothesis with numerous assumptions. Some of such assumptions are as follows:

1. Ideally diffuse radiation distribution is present on the irradiation side^{22,32}; however, it has been shown that good results are obtained for parallel radiation in semi-infinite layers.³³
2. Ideally diffuse radiation distribution is present in the interior of the layer.^{22,32}
3. Surface phenomena resulting from the discontinuity in refractive index is not considered.³²
4. Scattering is isotropic inside the layer and scattering angles distribute light according to the Lambert’s law.^{22,34}
5. A colored layer is homogenous and sufficient in extent for there to be no light lost from the edges of the layer.²⁰ However, Kubelka published an article for nonhomogenous layers in 1954.³⁵
6. Radiation is incoherent and there is no interference.³³

In addition to the initial assumptions listed above, in order to reach a simple final equation, further simplifications are carried out that could lead to additional inaccuracies. For instance, Kubelka–Munk equation assumes that radiation will be ideally diffuse in the colored layer but absorption causes this not to remain diffuse¹ or the Schuster–Schwartzchild assumption claims that optical coefficients are the same in the forward and reverse direction of flux,³⁶ which is inherent to the Kubelka–Munk model but is in no way correct, similarly, it is almost impossible to predict the pathway of light in the actual layer due to complex multi-scattering.^{23,33,37–39} Such inaccuracies can lead to nonlinear relationships between optical coefficients of the Kubelka–Munk equation and the concentrations of pigments. Many articles have attempted to modify the Kubelka–Munk model either by modifying the basic equations or by modifying the relationship between optical coefficients and concentration of pigments. In general, there are two basic procedures available to modify the Kubelka–Munk hypothesis, namely, mathematical and empirical modifications which are discussed below:

Mathematical modification: In this procedure, modification is carried out by two methods: First, by correcting for the assumptions and simplifications which were used to derive the Kubelka–Munk equations as described in previous section and second, by correction through comparison^{20,38} with more exact equations,^{34,40–42} for instance, mathematically more exact equations proposed by Chandrasekhar for opaque media,^{41,43} which modeled angular propagation of materials, or van de Hulst for translucent media.⁴⁴

In astronomy, such exact equations are derived for the interaction of light and matter and are referred to as exact radiative transfer theories (exact RTT) to describe the transfer of radiation from stars and planets.³⁴ Exact RTT theories completely describe radiation transfer of light and the angular scattering of light by colorants in the color layer; therefore, these theories are complete exact equations and do not entail any simplifications; however, the mathematics is too complex (i.e., integral differential equations) making them practically inappropriate to be employed in the color industries.²⁴ Basic equations of these theories are for spherical space as a function of cosine of the angle of view, azimuthal angle and the optical depth and have a phase function parameter (which describes the directions and amounts of light which are scattered by a pigment).³⁴ Optical coefficients of exact RTTs which are referred to as the intrinsic optical coefficients are fundamental properties of materials and should have linear relationships equations (4a) and (4b) with concentrations of scattering/absorbing materials (e.g., pigments).²⁰

$$\mu_a = \sum_{i=1}^n c_i \mu_{ai} = c_1 \mu_{a1} + c_2 \mu_{a2} + \cdots + c_n \mu_{an} \quad (4a)$$

$$\mu_s = \sum_{i=1}^n c_i \mu_{si} = c_1 \mu_{s1} + c_2 \mu_{s2} + \cdots + c_n \mu_{sn} \quad (4b)$$

On the other hand, the Kubelka–Munk optical coefficients in contrast to exact RTTs coefficients do not have any electrodynamic²⁴ or direct physical³³ meaning of their own and their calculation from first principles of exact RTTs is almost impossible.²⁴ Therefore, the initial assumptions of the Kubelka–Munk model must be enforced on exact RTTs to make the comparison of the two models viable. These modified equations can be tabled as below:

- a. Linear univariate ($K = x\mu_a$ and $S = y\mu_s$): where K and S are Kubelka–Munk absorption and scattering coefficients, respectively, μ_a and μ_s are intrinsic absorption and scattering coefficients per unit path length of the layer, x and y are constants. The first relationship was proposed by Kubelka³⁷ where $K = 2 * \mu_a$ and $S = \mu_s$. Other authors have proposed various other relationships.^{45,46} These equations use different averaging logic to reach their equations. For example, Blevin and Brown⁴⁵ corrected Kubelka–Munk model for $R = 0.5$ (for opaque media) and used them for all reflectances.
- b. Linear bivariate ($K = x\mu_a + y\mu_s$ or $S = x'\mu_a + y'\mu_s$): where x, y, x', y' are constants. Some researchers^{36,47–50} have shown that the Kubelka–Munk optical coefficients are not independent of each other. So practically any changes in absorption of the layer can change the Kubelka–Munk scattering coefficients and vice versa. The

Mudgett–Richards³⁶ model is one example of this group. This model is made to remove the Schuster–Schwartzchild assumption by comparing the Kubelka–Munk equation with photon diffusion model,^{40,42} which is a more exact model and it works for $\mu_a/\mu_s = 10^{-2} - 10^{-6}$.

$$K = 2 * \mu_a \quad (5a)$$

$$S = 3/4\mu_s - 1/4\mu_a \quad (5b)$$

- c. *Nonlinear group 1* ($K = f(\mu_a, \mu_s)$ or $S = g(\mu_a, \mu_s)$ and $K/S = x\mu_a/\mu_s$): where f and g are nonlinear functions and x is a constant. Nonlinearity in these equations are in such a way that K/S has a linear relationship with μ_a/μ_s .^{23,33} The Yang–Kruse³³ model is an example of this group which modified Kubelka–Munk equation by taking into account the effect of scattering on the path length of light propagation equations (6a) and (6b).

$$K = 2 * \mu * \mu_a \quad (6a)$$

$$S = \mu * \mu_s \quad (6b)$$

$$\mu = \begin{cases} (\mu_s/\mu_a)^{1/2} & \mu_s \geq \mu_a \\ 1 & \text{otherwise} \end{cases}$$

- d. *Nonlinear group 2* ($K = f(\mu_a, \mu_s)$ or $S = g(\mu_a, \mu_s)$): where f and g are nonlinear equations. Some researchers have reached nonlinear relationships between the Kubelka–Munk optical coefficients and the intrinsic optical coefficients.^{22,23,33,38,51–56} The Graaff³⁸ model is one example of this group which resulted in equations (7a) and (7b) as compared with exact RTT models.

$$K/\mu_a = 1 + (C'')^{B_k} \quad (7a)$$

$$S/\mu_s = 0.25 + 0.5C'' + B_s(1 - C'')^{2.3} \quad (7b)$$

$$C'' = \frac{\mu_s''}{\mu_a + \mu_s''}$$

$$\mu_s'' = \mu_s * A$$

where in isotropic state: $B_s = 0.0$, $B_k = 1.22$ and $A = 1.19$.

- e. *Nonlinear group 3* ($K/S = f(R, \frac{\mu_a}{\mu_s})$): where R is the reflectance of the layer. This equation was proposed by Nobbs²⁰ and is applicable only for opaque layers equations (8a) and (8b). Nobbs believed that the basic error of the Kubelka–Munk model is due to the wrong assumption of a uniform diffuse flux throughout the layer and derived the

following expression as compared with the RTT exact equations.

$$\frac{K}{S} = \beta_{\infty} \frac{2\mu_a}{\mu_s} \quad (8a)$$

$$\beta_{\infty} = 1.22743 + 0.11291R_{\infty} \quad (8b)$$

where R_{∞} is reflectance of the opaque media.

Many such models have been studied in astronomy or scattering sciences and some are applicable in the color industries. On the other hand, some of the models above were defined for a range of absorptions or scattering (for example, low absorptions) and consequently are of no use in the color industries.

The main reason for employing such equations (especially the Kubelka–Munk equation) in color industries is the relationship between the concentrations of pigments and the spectrophotometrically measured reflectance or color attributes of the colored medium. According to equations (1)–(3), in order to predict the reflectance of a colored material from the concentration of pigments present, it is imperative to initially calculate the Kubelka–Munk optical constants (k and s). There are various experimental procedures to calculate such constants for opaque^{52,57–61} and translucent³³ media. These procedures make use of the inverse matrix of equations (1) and (2) (equation (10) for opaque² and equation (11) for translucent media at the same thickness.⁴ Therefore, it is obligatory that any modified equation must also be available in its inverse form. Finally, for color matching systems, the concentration of pigments will be calculated by the aid of equations (3) and (9) (for opaque) or (3) and (10) (for translucent) media by the trial and error method^{60–67} or by some sophisticated procedures.^{64,68}

$$K/S = \frac{(1 - R_{\infty})^2}{2R_{\infty}} \quad (9)$$

$$SX = \frac{1}{b} \left(\coth^{-1} \left(\frac{a - R_k}{b} \right) - \coth^{-1} \left(\frac{a - R_{gk}}{b} \right) \right) \quad (10)$$

$$KX = SX(a - 1)$$

$$a = \frac{(R_w - R_k)(1 + R_{gw}R_{gk}) - (R_{gw} - R_{gk})(1 + R_wR_k)}{2(R_wR_{gk} - R_kR_{gw})}$$

where R_w , R_k , R_{gw} , R_{gk} and X are reflectance on white background, reflectance on black background, white and black background reflectance and thickness, respectively.

In general, for a nonabsorbing media and discarding all surface phenomena, the reflectance of a transparent layer would be only one point (equating to zero), and that of an opaque layer would also be a point (equating

to one). However, for the same supposition, the reflectance of a translucent layer would be a range of points (equating to a range of values between zero to one). So it is logical that the shortcomings of equations be more apparent for translucent media. Reflectance in exact RTTs is related to optical thickness (equation 11a) and albedo (equation 11b).⁴⁴ Optical thickness (ot) is a parameter which can describe the extent of translucency. Fortunately, if physical thickness is known, intrinsic optical thickness can be calculated by optical thickness and albedo or vice versa.

$$ot = \sqrt{\mu_a(\mu_a + \mu_s)}X \quad (11 - a)$$

$$\text{albedo} = \frac{\mu_s}{\mu_a + \mu_s} \quad (11 - b)$$

Equation (11a) shows that the optical thickness is related to optical coefficients and physical thickness (x) of the layer. For a transparent layer with no absorption, the value of optical thickness is zero and for an opaque layer it is infinite.

Mathematical evaluation

Evaluation of accuracy of the Kubelka–Munk model purely based on experimental data is difficult, because such data do not follow the assumptions made in deriving the Kubelka–Munk model. So many articles evaluate the degree of accuracy of Kubelka–Munk model or its modified forms by comparing them with an exact RTT.^{20,34} There are several methods to calculate reflectance from the intrinsic optical coefficients, for example, Monte Carlo,⁷⁷ adding doubling,⁸⁰ or various other analytical methods based on Twer-sky's work.⁸¹ These methods are rather complicated; therefore, in the present study use was made of published data in some references to obtain the required data for opaque media.^{20,41} Table 1 is created here by calculating from data published in the literature to show the percentage error of the Kubelka–Munk model and some of its modified forms for opaque media (one experimental evaluations and five mathematical modifications of the Kubelka–Munk model) compared to the exact Chandrasekhar RTT models⁴³ for opaque media.

The Mudgett–Richards model works only for low absorptions; however, for high absorptions, the model predicts unrealistic negative reflectance. For opaque media, reflectance has a ratio relationship of absorption coefficient to scattering coefficient; therefore, models in group (d) presented in section “Theoretical background” work like group (a). Table 1 illustrates that when the absorption to scattering ratio is high (i.e., low reflectance), the Kubelka–Munk equation suffers from systematic errors. Several models have optimized the Kubelka–Munk equation for high reflectances

where absorption is low. Some of these equations may not be accurate all over the spectrum. However, the Nobbs' modified equation²⁰ as seen in Table 1 has more chance of being accurate.

In translucent media, the reflectance has a relationship with each optical coefficient individually or, as shown in equation (2), it can also be seen that the relationship is with S and R_∞ (or K/S). This illustrates that reflectance does not depend on K alone. Figures 1 and 2 are created in this study by calculating from published data to show the reflectance value of exact RTT model and the percent errors of the Kubelka–Munk model in comparison with the exact RTT model for translucent media (i.e., van de Hulst theory) for background of 0.8 (White) and 0 (Black) at a thickness = 1. Figure 1 and 2 are created here to show exact RTT reflectance and the percentage errors of the Kubelka–Munk model for translucent media, respectively, showing a more complicated behavior than for opaque media, especially at low absorption and scattering coefficients on the black background.

Tables 2 and 3 show the percentage errors of some models in comparison with the exact RTT model for

translucent media (van de Hulst) for background of 0.8 and 0, respectively, at a constant thickness. (The reflectance and transmittance data for exact RTT where there is no background were extracted from Table 15 of reference (44). These were then recalculated and converted to the reflectance on white and black backgrounds by the use of Stokes equation.²⁰) The errors are dependent on optical coefficients as well as the background reflectance. But generally, the percentage error increases for high absorption and low scattering coefficients as well as low background reflectance. Percentage errors can even be > 400% for translucent samples on a black background which is 20 times bigger than for opaque samples. Berns⁴ has demonstrated practically that the Kubelka–Munk predictions result in higher errors on black background than on white background.

Optical coefficients defined in exact RTTs would have linear relationships with concentrations if the initial assumptions were correct. The aim of all modifications of Kubelka–Munk is to simulate the result of the exact RTTs. In Tables 1, 2 and 3, the inputs are the intrinsic optical coefficients and the

Table 1: The percentage error ($\%Error = \frac{|R_{pre} - R_{exact}|}{R_{exact}} \times 100$) of the modified Kubelka–Munk model (group a) compared to the Chandrasekhar model (Gate⁶⁹ which is an experimental evaluation, Mudgett–Richards³⁶ is for group (b), Graff³⁸ is for group (d) and Nobbs²⁰ is for group (e) discussed in the section theoretical background)

Models	μ_a / μ_s									
	9	1.5	1	0.429	0.25	0.053	0.026	0.01	0.005	0.001
Kubelka–Munk ³⁷	21.36	18.33	17.09	13.9	11.73	6.34	4.6	2.97	2.13	0.97
Gate	6.87	5.08	4.39	2.86	1.99	0.47	0.2	0.04	0	0.02
Mudgett–Richards	–	48.08	31.06	12.24	6.71	1.19	0.54	0.2	0.1	0.02
Graaff	23.43	11.66	9.09	4.99	3.25	0.82	0.42	0.17	0.09	0.02
Nobbs	0.37	0.15	0.07	0.02	0.04	0	0.01	0.02	0.02	0.01

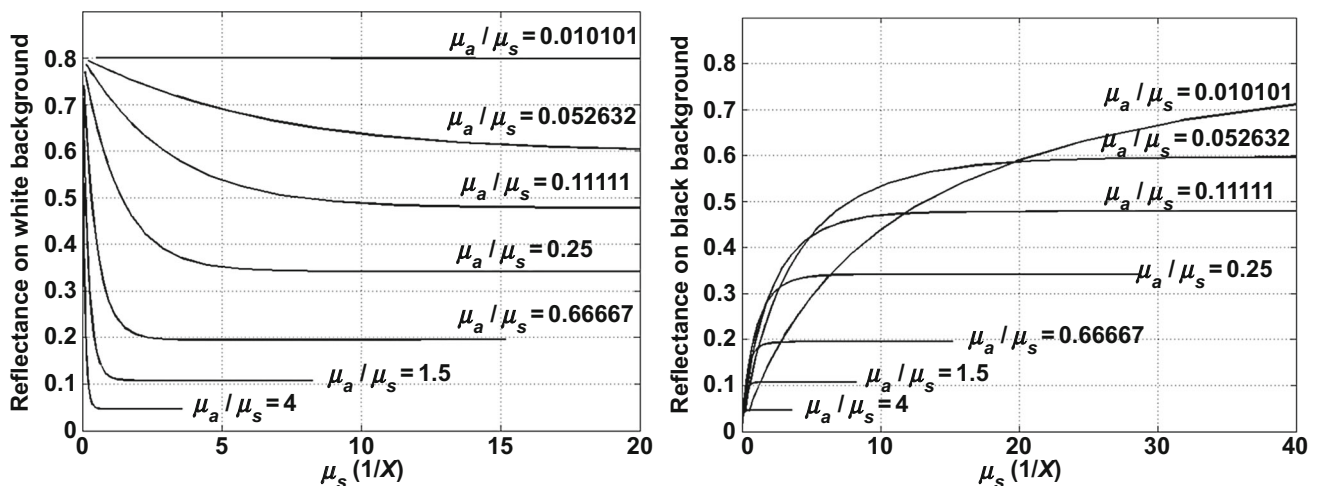


Fig. 1: Exact RTT reflectance on White ($R_g = 0.8$) and Black ($R_g = 0$) background

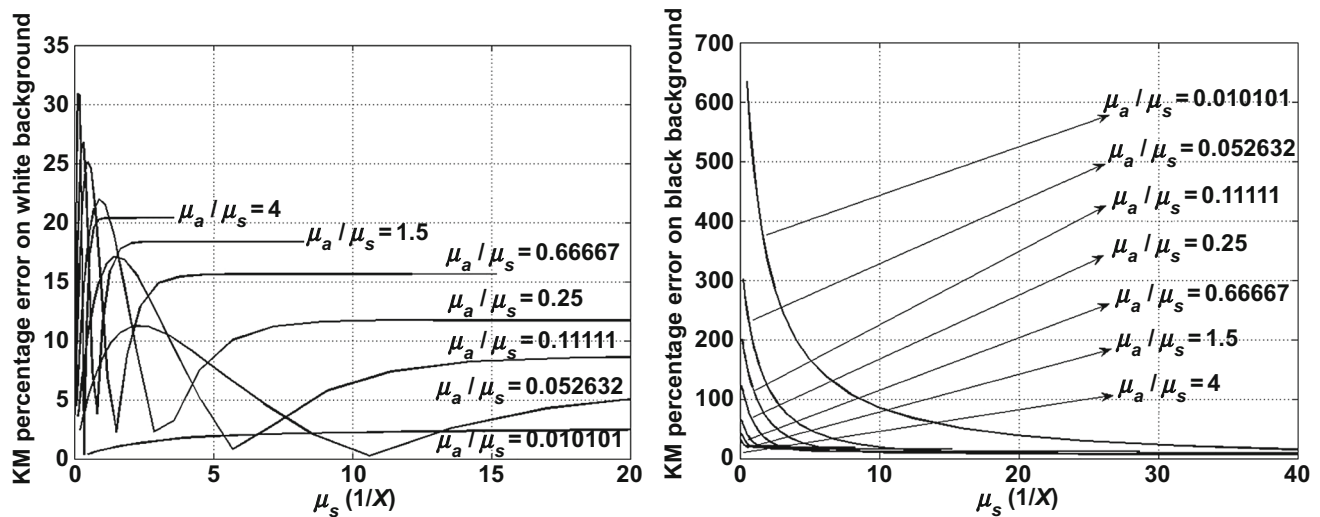


Fig. 2: Percentage error ($\%Error = \frac{|R_{pre} - R_{exact}|}{R_{exact}} * 100$) of the Kubelka–Munk model as compared to the van de Hulst model on White ($R_g = 0.8$) and Black ($R_g = 0$) background

Table 2: Percentage error ($\%Error = \frac{|R_{pre} - R_{exact}|}{R_{exact}} * 100$) of the modified Kubelka–Munk model as compared to the van de Hulst model for $R_g = 0.8$ and $X = 1$ (Gate is experimental, Mudgett–Richards is for group (b), Yang–Kruse³³ is for group (c) and Graff is for group (d))

Models	μ_a, μ_s								
	$(\mu_a/\mu_s = 4)$			$(\mu_a/\mu_s = 0.67)$			$(\mu_a/\mu_s = 0.01)$		
	0.04, 0.01	0.36, 0.09	5.72, 1.43	0.03, 0.05	0.25, 0.38	1.58, 2.37	0.01, 0.99	0.16, 15.84	0.4, 39.6
Kubelka–Munk	2.53	24.05	20.36	4.53	23.94	12.87	0.72	2.37	2.72
Gate	1.69	21.02	6.37	4.04	24.53	5.92	0.26	0.62	0.29
Mudgett–Richards	2.67	33.09	134.84	4.69	29.27	21.81	0.31	0.77	0.45
Yang–Kruse	2.53	24.05	20.36	7.08	32.17	12.85	2.18	2.38	2.72
Graaff	5.04	28.04	18.59	2.02	15.13	8.86	0.30	0.74	0.42

Table 3: Percentage error ($\%Error = \frac{|R_{pre} - R_{exact}|}{R_{exact}} * 100$) of the modified Kubelka–Munk model as compared to the van de Hulst model for $R_g = 0$ and $X = 1$

Models	μ_a, μ_s								
	$(\mu_a/\mu_s = 4)$			$(\mu_a/\mu_s = 0.67)$			$(\mu_a/\mu_s = 0.01)$		
	0.04, 0.01	0.36, 0.09	5.72, 1.43	0.03, 0.05	0.25, 0.38	1.58, 2.37	0.01, 0.99	0.16, 15.84	0.4, 39.6
Kubelka–Munk	22.02	30.51	20.36	63.77	48.57	16.29	487.40	51.26	15.29
Gate	11.50	1.69	6.37	19.76	16.86	3.12	391.52	46.65	11.91
Mudgett–Richards	130.92	135.48	134.84	2.67	3.77	19.50	401.90	46.47	11.73
Yang–Kruse	22.02	30.51	20.36	95.91	59.42	16.30	876.07	51.35	15.29
Graaff	52.10	34.80	18.59	4.87	1.86	6.45	401.12	46.51	11.77

outputs are the reflectances. However, in match prediction systems, the aim is predicting the inverse of this, in other words there is a need for obtaining the concentrations of various mixed colorants to give a certain color. Therefore, in the present study, compar-

ison of Kubelka–Munk model and its various modified forms have been verified differently:

1. Linear univariate ($K = x\mu_a, S = y\mu_s$): Intrinsic optical coefficients have a linear relationship with

concentrations of pigments, so the model can be rewritten in the form of equation (12).

$$P = x \sum_{i=1}^n c_i \mu_{xi} = \sum_{i=1}^n c_i (x \mu_{xi}) \quad (12)$$

where x for absorption (or y for scattering) is a constant, P is the Kubelka–Munk absorbance (K) or scattering (S) coefficient and μ_{xi} is the intrinsic absorbance (μ_{ai}) or scattering (μ_{si}) coefficients, respectively. Equations (12) and (3a) show that $k_i = x \mu_{ai}$ where x is a constant (or $s_i = y \mu_{si}$ where y is a constant). In other words, the Kubelka–Munk absorption coefficient has a linear relationship with concentrations of mixed pigments and, therefore, these kinds of modified equations can under no circumstance improve the Kubelka–Munk equation and in fact are useless in color match prediction systems.

2. Linear bivariate ($K = x \mu_a + y \mu_s$, $S = x' \mu_a + y' \mu_s$): equation can be rewritten in the form of equation (13).

$$P = x \sum_{i=1}^n c_i \mu_{ai} + y \sum_{i=1}^n c_i \mu_{si} = \sum_{i=1}^n c_i (x \mu_{ai} + y \mu_{si}) \quad (13)$$

where μ_{ai} and μ_{si} are the respective absorption and scattering constants for each of the pigments and x and y are constants. Comparing equations (13) and (3a) results that $k_i = x \mu_{ai} + y \mu_{si}$ or $s_i = x' \mu_{ai} + y' \mu_{si}$ where the sum of all variables has a linear relationship. This again means using such modified equations of the Kubelka–Munk would have no effect on the color matching results since the sum of the absorption and scattering coefficients has a linear relationship with concentrations of absorbing pigments in the modified equations. However, these modified equations imply that the Kubelka–Munk absorption and scattering constants may depend on each other.

3. Nonlinear: Intrinsic optical coefficients utilized in modified equations which have nonlinear relationship with the Kubelka–Munk optical coefficients. As was mentioned previously, in some of these equations, the ratio of the Kubelka–Munk coefficients and the intrinsic optical coefficients remain linear. Consequently, for opaque media, they act just like the Kubelka–Munk equation. Additionally, some of these equations cannot be inverted^{22,38} and therefore could not be employed for obtaining the optical constants. Other equations such as the Nobbs models are reversible but are defined only for opaque media.²⁰ Therefore, different procedures are needed to evaluate the performance of Kubelka–Munk and its various modification equations, as is described below:

Mathematical evaluation of the Kubelka–Munk model for opaque media

As was mentioned previously, the intrinsic optical coefficients in the exact RTTs have a perfect linear relationship with concentrations.²⁰

Therefore, in the present study, an innovative procedure was envisaged for the first time in order to predict mathematically the performance of the Kubelka–Munk model or any attributed claims of improvements of its various modified forms in color match prediction systems as compared to the appropriate radiation transfer theories (RTTs).

Such innovative procedures entail the plot of the absorption and scattering constants (or their ratio) of the Kubelka–Munk or any of its various modifications against (vs) the appropriate intrinsic optical coefficients of exact RTTs, namely Chandrasekhar for opaque and van de Hulst for translucent media. A linear plot of Kubelka–Munk constants against intrinsic optical coefficients of the RTTs would predict mathematically that no modification of the Kubelka–Munk model is necessary. Furthermore, a linear plot of any of the Kubelka–Munk's modified constants against the equivalent RTTs coefficients would predict mathematically that no improvement would be realized in actual color match prediction systems.

It is previously illustrated in Table 1, that for opaque media, the Nobbs' theory had the best performance among other listed theories bestowing the least percentage error values of at most 0.37%. Consequently, the Kubelka–Munk constants as well as the Nobbs' model were plotted against the intrinsic optical coefficients of the Chandrasekhar exact RTT, as shown in Fig. 3.

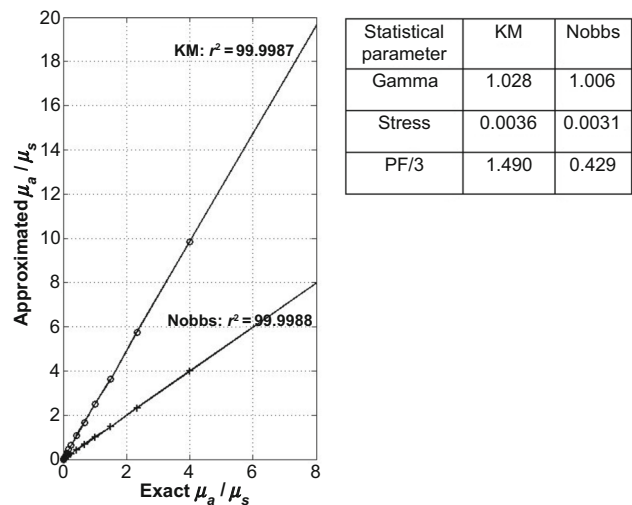


Fig. 3: Plot of the ratios of the Kubelka–Munk (o) as well as the Nobbs (+) optical coefficients vs the ratio of the intrinsic optical coefficients of the Chandrasekhar exact RTT model

The plot of Fig. 3 depicts almost perfect linearity (i.e., $r^2 = 99.99$) for both Kubelka–Munk as well as for the Nobbs' model. Figure 3 illustrates that other well-known statistical parameters also confirm a near perfect linearity (Kubelka–Munk model: $K/S = 2.46\mu_a/\mu_s$ and for Nobbs model: $K/S = 0.99\mu_a/\mu_s$).

This proves mathematically that for opaque media, the Kubelka–Munk model does not need any modification. Furthermore, the Nobbs model which is the best of a series of suggestions for improvements cannot improve Kubelka–Munk model in color match prediction systems.

Therefore, up to the present time, researchers have attempted to modify the model mainly for opaque media. However, contrary to common belief and as shown mathematically for the first time in this study there is no need to modify the Kubelka–Munk model for color match prediction of opaque media. Furthermore, the Kubelka–Munk model could be considered as a sound and reliable model for the color match prediction of opaque media and any deviation from linearity or additivity arisen from experimentation could be on-line corrected by the aid of the calculated partial differentials (correction factors).

Mathematical evaluation of the Kubelka–Munk model for translucent media

In translucent media, as was mentioned previously, reflectance is believed to vary with scattering, ratio of the optical coefficients, the thickness of the translucent

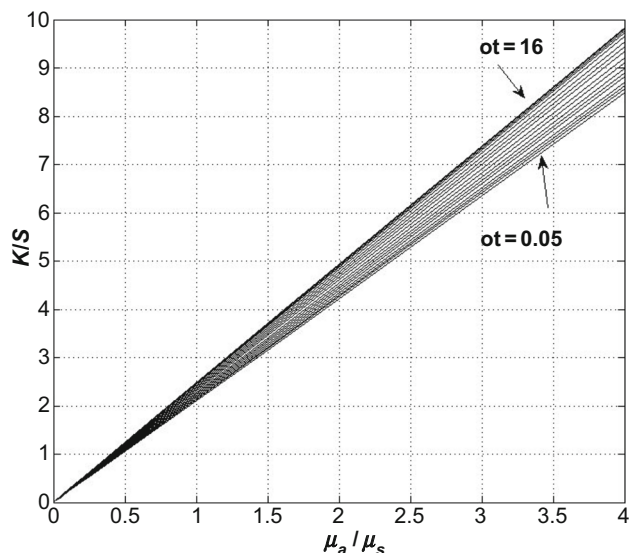


Fig. 4: Plot of the ratio of the Kubelka–Munk optical coefficients vs the ratio of the intrinsic optical coefficients of the van de Hulst model at various optical thicknesses

layer as well as the background reflectance. So, at least two equations are needed for the calculation of the optical coefficients. These two equations can be obtained by positioning the translucent colored layer separately on black and white backgrounds. Figure 4 depicts the relationship between the ratio of the Kubelka–Munk optical coefficients to that of the ratio of the intrinsic optical coefficients of van de Hulst at various optical thicknesses (not necessarily equal to the physical thicknesses). The Kubelka–Munk's optical coefficients are calculated on the white ($R = 0.8$) or black ($R = 0$) backgrounds.

It is apparent from Fig. 4 that for each specific optical thickness a linear relationship exists between the ratio of the Kubelka–Munk optical coefficients and that of the optical coefficients of the van de Hulst model for translucent media. However, such linear relationship does not hold as optical thickness is varied. Furthermore, Fig. 5 illustrates a linear relationship between the Kubelka–Munk scattering coefficients and the intrinsic optical coefficients of van de Hulst at various K/S ratios, the physical thickness (X) being constant.

Figure 5 clearly illustrates that the Kubelka–Munk scattering coefficients are related not only to the intrinsic scattering coefficients but also on the K/S ratios. Figures 4 and 5 demonstrate that, unlike the opaque media, there exist no linear relationships between the above-mentioned parameters and this means that using the Kubelka–Munk equation for color match predictions of translucent media contain an inherent error. In other words, it has been proven mathematically that the Kubelka–Munk model is not reliable for color match prediction of translucent media as it stands.

Empirical modification

In this procedure, the Kubelka–Munk predictions are compared to real experimental data and modified accordingly. Modifying procedures can be carried out

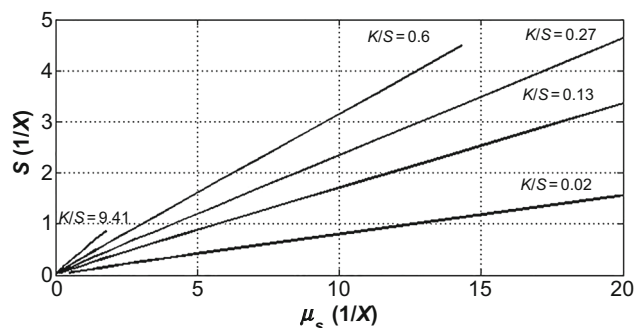
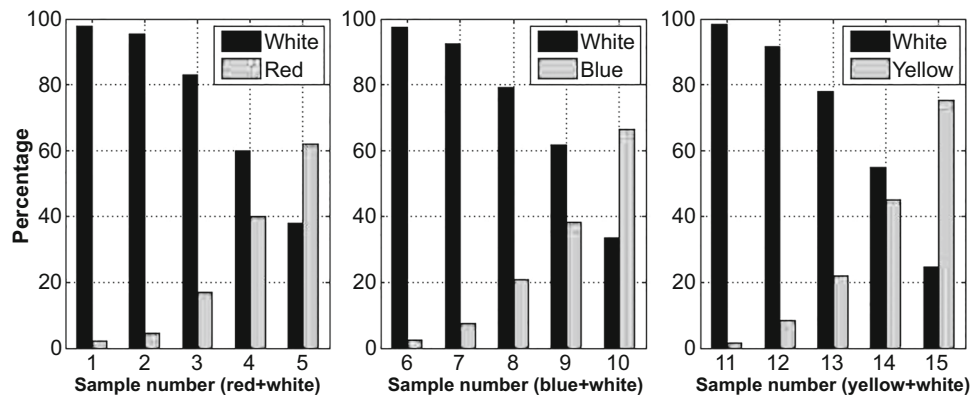


Fig. 5: Relationship between the Kubelka–Munk scattering coefficients and the intrinsic scattering coefficients at various K/S ratios and constant thickness

Table 4: The used pigments and their CI specifications

Trade name	CI Name	CI number
Hansa yellow opaque	PY 74	11741
Naphthol red medium	PR 5	12490
Phthalo blue (green shade)	PB 15:4	74160
Titanium white	PW6	77891

**Fig. 6: Percentage of used chromatic pigment to all pigments**

by correcting the Kubelka–Munk equation,⁷⁰ finding a modified relationship between the Kubelka–Munk optical coefficients and concentrations, or finding completely new optical coefficients which have a more closer linear relationship with concentrations.^{69,71} It must be noted that modification by experimental procedure has an inherent disadvantage of limited applicability to the experimental conditions under which the modifying procedure was carried out. Equations (14a) and (14b) show the Gate,⁶⁹ empirical correction for optical coefficients of the Kubelka–Munk model.

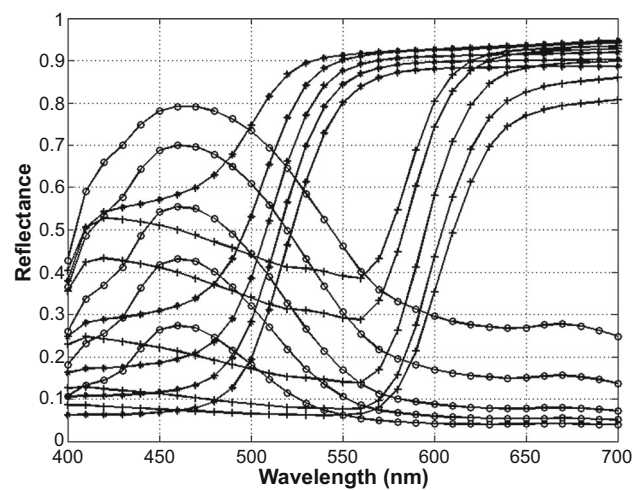
$$K/\mu_a = 1.9 \quad (14a)$$

$$S/\mu_s = 0.72 \quad (14b)$$

where μ_a and μ_s are valid absorption and scattering optical coefficients claimed to have a linear relationship with concentrations.

Materials and methods

In general, there are three methods for color formulation⁵⁸: blending finished paints, tinting base paints and full formulation. In this article, the performance of Kubelka–Munk model was checked experimentally for opaque media by tinting base paints. This means predispersions (primaries) of chromatic pigments were mixed into achromatic base paint (which was white in

**Fig. 7: Reflectance of samples listed in Table 4 (—○: blue + white, —*: yellow + white, —+: red + white)**

this article). Gloss alkyd paint together with three different pigment primaries and a white pigment dispersion base (Table 4) were employed in varying amounts in order to prepare the paint samples. Titanium white base was utilized not only to ensure complete opacity of the opaque samples at all visible wavelengths, but also to calibrate the pigment primaries in order to calculate optical coefficients. Varying amounts of pigment primaries were used to ensure the widest coverage of the color gamut.

Samples were tested for opacity and ensured to be opaque at the utilized thickness. The reflectance values

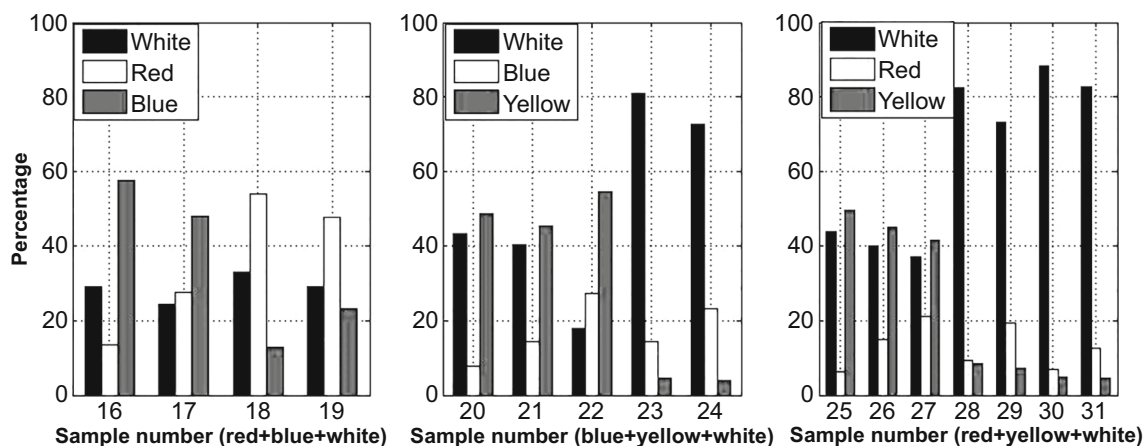


Fig. 8: The percentage of the used chromatic pigments (two chromatic pigments and titanium white) to test models

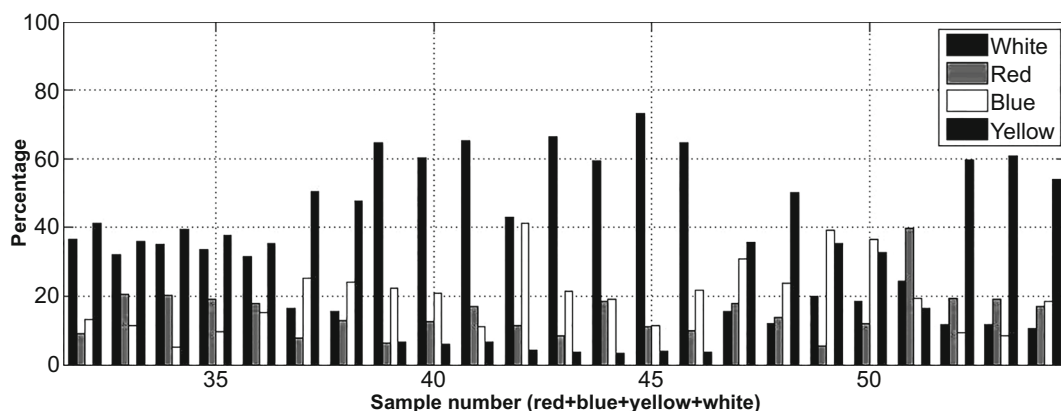


Fig. 9: The percentage of the used chromatic pigments (three chromatic pigments and titanium white) to test models

of all dried paint samples were measured on a Gretag Macbeth Color-Eye 7000 A integrating sphere spectrophotometer with a $d/8$ geometry and the specular reflection included. The average of these measurements was used in all calculations.

Each pigment primary (i.e., a dispersion of one chromatic pigment listed in Table 4) was mixed with the base paint (i.e., a dispersion of achromatic titanium white) in various proportions and applied onto black and white Leneta paper (to make sure they were opaque) and left to dry. Reflectance on black background to reflectance on white background at all wavelengths for all samples was a larger value than 0.98 demonstrating that all samples were opaque according to TAPPI (Technical Association of the Pulp and Paper Industry) opacity (T425 om-06). The reflectances of the dried samples were measured from which the absorption and scattering of the dried paint samples were calculated using the Nichols-Orchard

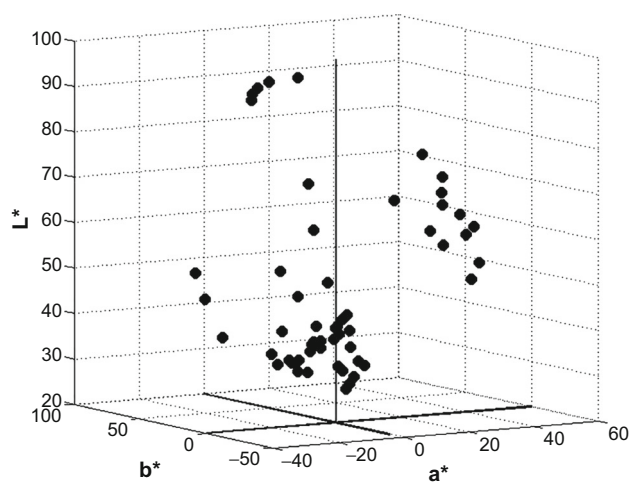


Fig. 10: Placement of samples in a 3D image of CIELAB 1976

ladder method²⁶ for both the Kubelka–Munk and the Nobbs method. The percentage of each pigment primary and white base paint is shown in Fig. 6. The reflectances of the dried final films are shown in Fig. 7. Samples concentrations and their 3D gamut in the CIELAB 1976 are listed in Figs. 6, 8, 9 and 10, respectively. All concentrations are kept below CPVC (critical pigment volume concentration) since above CPVC, most chemical, physical and optical properties will diminish tremendously.

Experimental results and discussion

In order to verify the precision and accuracy of the mathematically reached conclusion that, for opaque media, there is no need to modify the Kubelka–Munk model, the Kubelka–Munk and the Nobbs models were compared. It must be noted that exact RTT models are very complicated and not applicable in

color match prediction systems. Additionally, the Nobbs model is a near exact solution to the exact RTTs with errors of < 0.5 percent. As mentioned previously, the ratios of the optical coefficients for these two models should have the same trend, as depicted in Fig. 11.

Absorption and scattering constants for primaries were calculated for opaque media for both Kubelka–Munk and Nobbs methods. These constants are used to predict the reflectance or the color attributes of a sample, if concentrations of primaries are known or vice versa (which is more appropriate in color match predictions). Figure 12 shows reflectance differences (DR) (average of all wavelengths) between measured reflectance, and as predicted by Kubelka–Munk and Nobbs models. Figure 13 shows color differences DE_{00}^* (as calculated by the CIE color difference ΔE_{00}^* , the constants taken to be one) between the actual measured color attributes and as predicted by both Kubelka–Munk and Nobbs models. Figure 14 shows

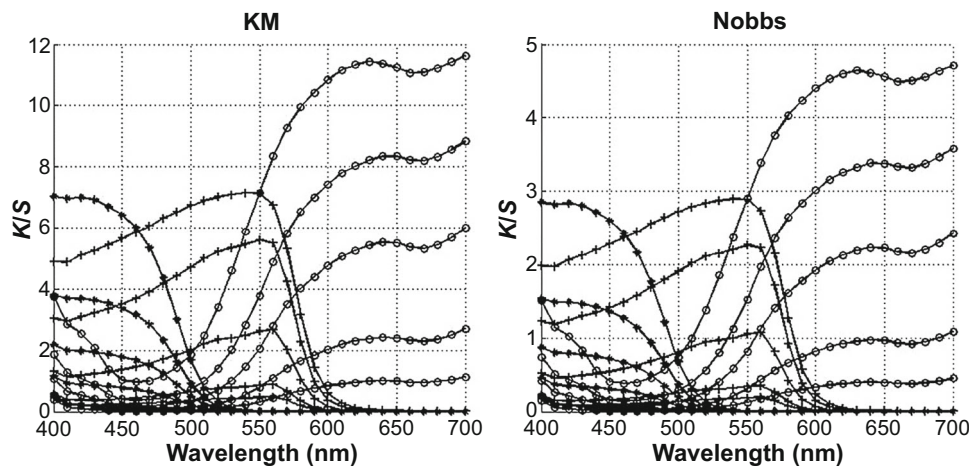


Fig. 11: Ratios of the optical coefficients for the Kubelka–Munk and the Nobbs models (–* is YW, –o is BW and –+ is RW)

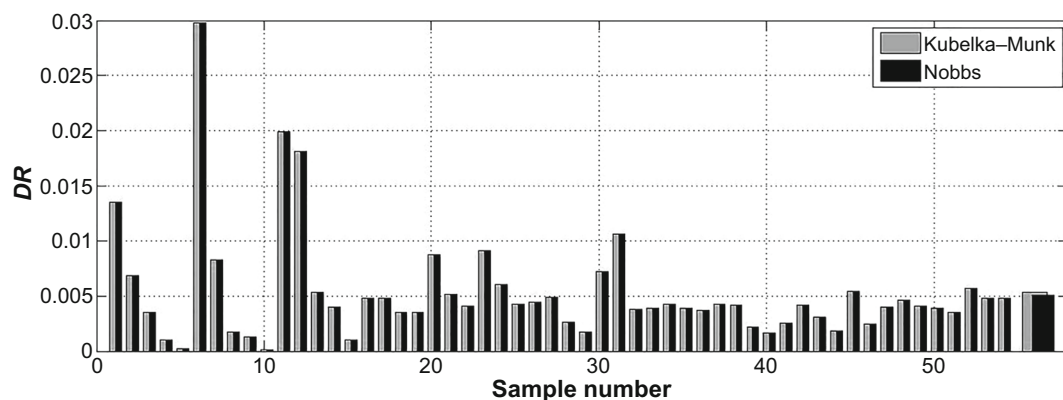


Fig. 12: Reflectance difference errors (DR) which are involved in the prediction of reflectance by the Kubelka–Munk and the Nobbs models. The average reflectance error for all samples are also given to be approximately $DR = 0.005$

concentration differences (DC) between the actual concentrations of primaries used (average for each recipe) to make the film and those predicted by the pseudo inverse method⁷² for both Kubelka–Munk and Nobbs model.

Figures 12, 13 and 14 confirm that modifications made by the Nobbs equation has in fact little effect on the final outcome compared to what is predicted by the Kubelka–Munk model. Therefore, the experimental evaluation also shows, as the mathematical evaluation did, that there is no need to modify the Kubelka–Munk model for opaque media.

However, although the Kubelka–Munk and the Nobbs models have the same trend as the exact RTT, the results show that predictions are not perfect. There are certain reasons for this:

1. Surface corrections are not considered. Because of the difference between air and the color layer, a fraction of the incident light is reflected. Kubelka–Munk and similar equations do not consider this

phenomenon.^{5,20,21,73–75} Taking this reflected light into consideration results in better predictions.

2. In the isotropic state, it is assumed that the reflected light is actually reflected in the same way in all directions but, in reality, and a phase function has to be introduced to determine the degree of reflection in each direction. For some particles like blood components⁷⁶ or white pigments and red dyes,⁷⁷ appropriate phase functions have been developed. Deviation from the isotropic scattering state^{78,79} obviously leads to errors in color match predictions.
3. Assumptions of these equations are that illumination/observed lighting is diffuse (i.e., d/d). Any practical deviation from this leads to unwanted errors. There are certain equations for compensating or minimizing such errors for $d/8$ geometry.³⁴

Reviewed modification equations for the translucent media, where the optical coefficients have a nonlinear relationship with Kubelka–Munk optical coefficients,

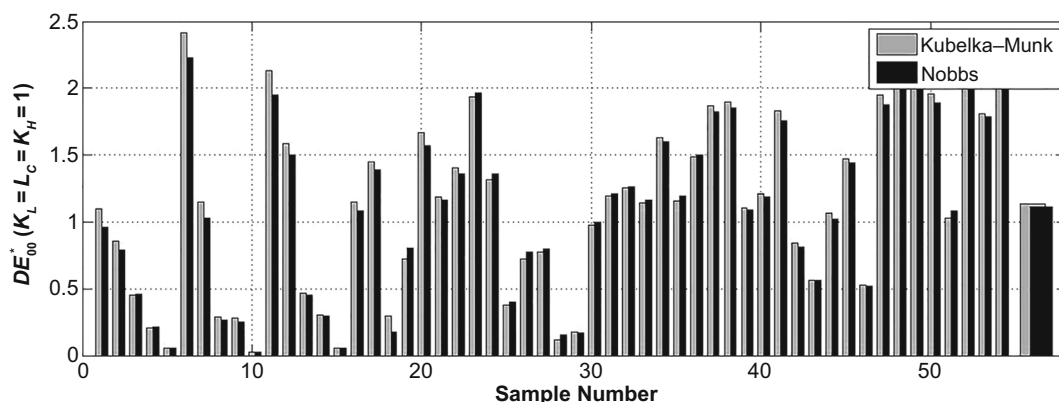


Fig. 13: Color difference errors (DE_{00}) which are involved in the prediction of color attributes by the Kubelka–Munk and the Nobbs models. The average color difference error for all samples are also given to be approximately $DE_{00} = 1$

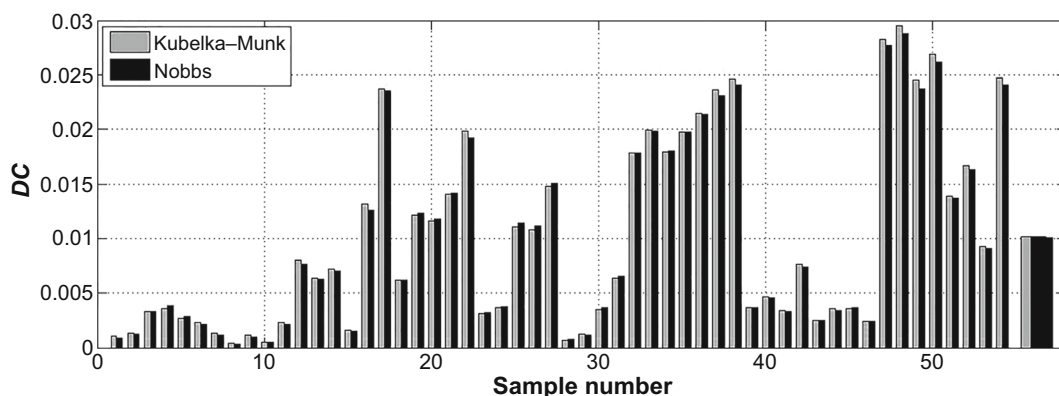


Fig. 14: Concentration difference (DC) errors which are involved in the prediction by the Kubelka–Munk and the Nobbs model. The average concentration error for all samples are also given to be approximately $DC = 0.01$

are very complicated and, more importantly, their matrices cannot be inversed (the relationships cannot be conversed). Therefore, it is very difficult to calculate their optical constants and consequently they cannot be used in color match prediction systems.

Conclusion

This study was set out to evaluate mathematically and empirically whether there is a need to modify the Kubelka–Munk model, first for opaque media and second for translucent media. To this end, an innovative inversed procedure was utilized to evaluate the performance of Kubelka–Munk model compared to an exact radiation transfer theory. As a start, a preliminary study was carried out to evaluate mathematically which of the proposed procedures put forward by various authors for modified exact radiation transfer theory had the smallest errors compared to the actual exact radiation transfer theory for opaque media. For opaque media, the calculated minimum error was attributed to the Nobbs model. Plotting the optical constants of Kubelka–Munk and Nobbs theories against the modified Chandrasekhar exact radiation transfer theory showed that a linear relationship exists for both Kubelka–Munk model and Nobbs theory. This illustrated that Nobbs theory in essence is no improvement to the Kubelka–Munk model. In other words, the Kubelka–Munk model does not need to be modified mathematically. This mathematically reached conclusion was further proved empirically by comparing the results of color match predictions of Kubelka–Munk model and Nobbs theory experimentally. From the results of mathematical and empirical evaluations, it can unequivocally be stated that there is no need to modify the Kubelka–Munk model for opaque media.

For translucent media, however, a different situation exists. It was proven mathematically that the Kubelka–Munk optical constant and the intrinsic optical coefficients of the van de Hulst relate linearly only at constant optical thickness. Therefore, the true relationship is nonlinear and the Kubelka–Munk model cannot be used in color match prediction systems and must be corrected for such nonlinearity. Since the matrices of the van de Hulst cannot be inversed and consequently the optical constants cannot be calculated; therefore, empirical evaluation is impossible. Due to nonlinearity, the best option for color match prediction systems would be an intelligent system comprising of neural network, fussy logic and genetics in future works.

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