

# Basic equations used in computer color matching, II. Tristimulus match, two-constant theory

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(Received 28 December 1973)

The calculation of a tristimulus match in an opaque film using two-constant theory and four colorants can proceed in two stages: first, the computation of a rough match, and second, iteration to an exact match. The same formal matrix is used for the rough solution and for the iterative calculations, but it must be recomputed and reinverted once before the iterative stage of the program.

Index Headings: Reflectance; Scattering; Absorption; Color.

In a previous paper,<sup>1</sup> which will be referred to herein after as Paper I, the problem of obtaining a tristimulus match to a sample with the use of single-constant theory<sup>2</sup> was discussed. In the present paper, we consider the problem of the extension of the algorithm to the case of two-constant theory.

We assume: (a) The familiar, simplified form of the Kubelka-Munk equation<sup>3</sup> applies:  $K/S = (1-R)^2/2R$ , where  $K$  is the Kubelka-Munk absorption coefficient,  $S$  is the Kubelka-Munk scattering coefficient, and  $R$  is the reflectance, all three quantities applying to monochromatic light. A corollary of this assumption is that the film is opaque to visible light of all wavelengths. (b) Both the absorption coefficient and the scattering coefficient of the film are separately linear functions of the concentrations of the colorants.

We will not be concerned with the problem of the refractive-index difference between the film and air, because the appropriate corrections can always be applied.

## COMPUTATION OF APPROXIMATE MATCH

We define the matrices and vectors  $\mathbf{t}$ ,  $\mathbf{T}$ ,  $\mathbf{E}$ ,  $\mathbf{r}^{(m)}$  as in Paper I. The vector that was previously denoted  $\mathbf{r}^{(s)}$ , the reflectance vector of the sample to be matched, will now be denoted  $\mathbf{r}^{(a)}$ , where  $a$  stands for aim. The condition for a tristimulus match, given by Eq. (1) in Paper I, is now expressed as

$$\mathbf{t} = \mathbf{T}\mathbf{E}\mathbf{r}^{(a)} = \mathbf{T}\mathbf{E}\mathbf{r}^{(m)},$$

and therefore

$$\mathbf{T}\mathbf{E}[\mathbf{r}^{(a)} - \mathbf{r}^{(m)}] = \mathbf{0}. \quad (1)$$

We now postulate, as before, that the reflectance curves of sample and match are not too far different from each other. We also assume that the same is true for the absorption and scattering coefficients. We may, therefore, write with a fair degree of accuracy

$$\begin{aligned} R_i^{(a)} - R_i^{(m)} &= \Delta R_i = (\partial R / \partial K)_i \Delta K_i + (\partial R / \partial S)_i \Delta S_i \\ &= (\partial R / \partial K)_i [K_i^{(a)} - K_i^{(m)}] \\ &\quad + (\partial R / \partial S)_i [S_i^{(a)} - S_i^{(m)}], \end{aligned}$$

where  $R_i^{(a)}$  and  $R_i^{(m)}$  represent the reflectance at wave-

length  $i$  of sample and match, respectively,  $K_i^{(a)}$  represents the Kubelka-Munk absorption coefficient of the sample at wavelength  $i$ ,  $S_i^{(a)}$  represents the Kubelka-Munk scattering coefficient of the sample at wavelength  $i$ , and  $K_i^{(m)}$  and  $S_i^{(m)}$  represent the corresponding values for the match. The derivatives,  $\partial R / \partial K$  and  $\partial R / \partial S$ , can be derived from the well-known Kubelka-Munk relation

$$R = 1 + K/S - (K^2/S^2 + 2K/S)^{1/2},$$

and are given by

$$(\partial R / \partial K)_i = -2R_i^{(a)2} / [S_i^{(a)}(1 - R_i^{(a)2})]; \quad (2)$$

$$(\partial R / \partial S)_i = R_i^{(a)}[1 - R_i^{(a)}] / [S_i^{(a)}(1 + R_i^{(a)})]. \quad (3)$$

Let

$$\mathbf{k}^{(a)} = \begin{bmatrix} K_{400}^{(a)} \\ K_{420}^{(a)} \\ \vdots \\ K_{700}^{(a)} \end{bmatrix}; \quad \mathbf{s}^{(a)} = \begin{bmatrix} S_{400}^{(a)} \\ S_{420}^{(a)} \\ \vdots \\ S_{700}^{(a)} \end{bmatrix}.$$

Define  $\mathbf{k}^{(m)}$  and  $\mathbf{s}^{(m)}$  in an analogous fashion, with  $(a)$  always referring to sample and  $(m)$  to match. Let

$$\mathbf{D}_k = \begin{bmatrix} d_{k,400} & 0 & \cdots & 0 \\ 0 & d_{k,420} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & d_{k,700} \end{bmatrix}$$

and

$$\mathbf{D}_s = \begin{bmatrix} d_{s,400} & 0 & \cdots & 0 \\ 0 & d_{s,420} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & d_{s,700} \end{bmatrix},$$

where  $d_{k,i} = (\partial R / \partial K)_i$  and  $d_{s,i} = (\partial R / \partial S)_i$  are given by Eqs. (2) and (3). Then the approximation for  $R_i^{(a)} - R_i^{(m)}$  can be written for all wavelengths as

$$\mathbf{r}^{(a)} - \mathbf{r}^{(m)} = \mathbf{D}_k[\mathbf{k}^{(a)} - \mathbf{k}^{(m)}] + \mathbf{D}_s[\mathbf{s}^{(a)} - \mathbf{s}^{(m)}]. \quad (4)$$

Substituting Eq. (4) in Eq. (1) and transposing, we obtain

$$\mathbf{T}\mathbf{E}[\mathbf{D}_k\mathbf{k}^{(a)} + \mathbf{D}_s\mathbf{s}^{(a)}] = \mathbf{T}\mathbf{E}[\mathbf{D}_k\mathbf{k}^{(m)} + \mathbf{D}_s\mathbf{s}^{(m)}]. \quad (5)$$

We now assume that the opaque film contains a fraction  $\alpha$  of total colorant. We need four colorants to

obtain the three degrees of freedom necessary for matching the tristimulus values of the sample. The fractions of the four colorants are represented by  $C_1, C_2, C_3$ , and  $\alpha - C_1 - C_2 - C_3$ . According to the assumption of additivity of the Kubelka-Munk absorption and scattering coefficients, we have

$$C_1 K_i^{(1)} + C_2 K_i^{(2)} + C_3 K_i^{(3)} + (\alpha - C_1 - C_2 - C_3) K_i^{(4)} + (1 - \alpha) K_i^{(t)} = K_i^{(m)}, \quad (6)$$

where  $K_i^{(j)}$  represents the absorption coefficient of a unit amount of colorant  $j$  at wavelength  $i$ , and  $K_i^{(t)}$  represents the absorption coefficient of a unit amount of substrate. We therefore have

$$[K_i^{(1)} - K_i^{(4)}]C_1 + [K_i^{(2)} - K_i^{(4)}]C_2 + [K_i^{(3)} - K_i^{(4)}]C_3 + \alpha K_i^{(4)} + (1 - \alpha) K_i^{(t)} = K_i^{(m)}. \quad (7)$$

Similarly,

$$[S_i^{(1)} - S_i^{(4)}]C_1 + [S_i^{(2)} - S_i^{(4)}]C_2 + [S_i^{(3)} - S_i^{(4)}]C_3 + \alpha S_i^{(4)} + (1 - \alpha) S_i^{(t)} = S_i^{(m)}. \quad (8)$$

We now define

$$\Phi_k = \begin{bmatrix} K_{400}^{(1)} & K_{400}^{(2)} & K_{400}^{(3)} \\ K_{420}^{(1)} & K_{420}^{(2)} & K_{420}^{(3)} \\ \dots & \dots & \dots \\ K_{700}^{(1)} & K_{700}^{(2)} & K_{700}^{(3)} \end{bmatrix}; \quad \mathbf{k}^{(4)} = \begin{bmatrix} K_{400}^{(4)} \\ K_{420}^{(4)} \\ \vdots \\ K_{700}^{(4)} \end{bmatrix};$$

$$\Phi_s = \begin{bmatrix} S_{400}^{(1)} & S_{400}^{(2)} & S_{400}^{(3)} \\ S_{420}^{(1)} & S_{420}^{(2)} & S_{420}^{(3)} \\ \dots & \dots & \dots \\ S_{700}^{(1)} & S_{700}^{(2)} & S_{700}^{(3)} \end{bmatrix}; \quad \mathbf{s}^{(4)} = \begin{bmatrix} S_{400}^{(4)} \\ S_{420}^{(4)} \\ \vdots \\ S_{700}^{(4)} \end{bmatrix};$$

$$\mathbf{u} = [1 \quad 1 \quad 1]; \quad \mathbf{k}^{(t)} = \begin{bmatrix} K_{400}^{(t)} \\ K_{420}^{(t)} \\ \vdots \\ K_{700}^{(t)} \end{bmatrix};$$

and

$$\mathbf{c} = \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix}.$$

We can therefore write, from Eqs. (7) and (8),

$$[\Phi_k - \mathbf{k}^{(4)}\mathbf{u}]\mathbf{c} + \alpha \mathbf{k}^{(4)} + (1 - \alpha)\mathbf{k}^{(t)} = \mathbf{k}^{(m)}, \quad (9)$$

$$[\Phi_s - \mathbf{s}^{(4)}\mathbf{u}]\mathbf{c} + \alpha \mathbf{s}^{(4)} + (1 - \alpha)\mathbf{s}^{(t)} = \mathbf{s}^{(m)}. \quad (10)$$

Substituting Eqs. (9) and (10) into Eq. (5) and transposing, we have

$$\begin{aligned} \mathbf{TE}\{\mathbf{D}_k[\Phi_k - \mathbf{k}^{(4)}\mathbf{u}] + \mathbf{D}_s[\Phi_s - \mathbf{s}^{(4)}\mathbf{u}]\}\mathbf{c} \\ = \mathbf{TE}\{\mathbf{D}_k[\mathbf{k}^{(a)} - \alpha \mathbf{k}^{(4)} - (1 - \alpha)\mathbf{k}^{(t)}] \\ + \mathbf{D}_s[\mathbf{s}^{(a)} - \alpha \mathbf{s}^{(4)} - (1 - \alpha)\mathbf{s}^{(t)}]\}, \end{aligned}$$

from which

$$\begin{aligned} \mathbf{c} = (\mathbf{TE}\{\mathbf{D}_k[\Phi_k - \mathbf{k}^{(4)}\mathbf{u}] + \mathbf{D}_s[\Phi_s - \mathbf{s}^{(4)}\mathbf{u}]\})^{-1} \\ \cdot \mathbf{TE}\{\mathbf{D}_k[\mathbf{k}^{(a)} - \alpha \mathbf{k}^{(4)} - (1 - \alpha)\mathbf{k}^{(t)}] \\ + \mathbf{D}_s[\mathbf{s}^{(a)} - \alpha \mathbf{s}^{(4)} - (1 - \alpha)\mathbf{s}^{(t)}]\}. \quad (11) \end{aligned}$$

As in Paper I, Eq. (11) represents three linear simultaneous equations in three unknowns— $C_1, C_2, C_3$ .

The fraction of the fourth colorant is obtained from  $C_4 = \alpha - C_1 - C_2 - C_3$ .

We should note that to use Eq. (11) in the strict sense we should know the absorption- and scattering-coefficient vectors of the sample,  $\mathbf{k}^{(a)}$  and  $\mathbf{s}^{(a)}$ . In practice, however, we usually know only the reflectance values,  $\mathbf{r}^{(a)}$ . I have found that the assumption

$$S_i^{(a)} = 1,$$

which leads to

$$\begin{aligned} K_i^{(a)} &= [1 - R_i^{(a)}]^2 / 2R_i^{(a)}, \\ d_{k,i} &= -2R_i^{(a)2} / [1 - R_i^{(a)2}], \\ d_{s,i} &= R_i^{(a)}[1 - R_i^{(a)}] / [1 + R_i^{(a)}], \end{aligned}$$

gives good results, and always yields a rough match that is fairly close to the final calculated match.

### ITERATION TO A CLOSE MATCH

We define the matrices and vectors  $\Delta \mathbf{t}$ ,  $\Delta \mathbf{c}$ ,  $\mathbf{B}$ ,  $\mathbf{P}$ , and  $\mathbf{Q}$  as in Paper I, and find as before that

$$\Delta \mathbf{t} = \mathbf{B} \Delta \mathbf{c}, \quad (12)$$

$$\mathbf{B} = \mathbf{P} \mathbf{Q}, \quad (13)$$

$$\mathbf{P} = \mathbf{T} \mathbf{E}. \quad (14)$$

With regard to the  $\mathbf{Q}$  matrix, we have

$$\begin{aligned} \frac{\partial R_i^{(m)}}{\partial C_j} &= \left( \frac{\partial R}{\partial K} \right)_i \frac{\partial K_i^{(m)}}{\partial C_j} + \left( \frac{\partial R}{\partial S} \right)_i \frac{\partial S_i^{(m)}}{\partial C_j} \\ &= d_{k,i} \frac{\partial K_i^{(m)}}{\partial C_j} + d_{s,i} \frac{\partial S_i^{(m)}}{\partial C_j}. \end{aligned}$$

But in view of Eq. (6) and the corresponding equation for  $S_i^{(m)}$ ,

$$\partial K_i^{(m)} / \partial C_j = K_i^{(j)} - K_i^{(4)}, \quad \partial S_i^{(m)} / \partial C_j = S_i^{(j)} - S_i^{(4)},$$

and therefore

$$\partial R_i^{(m)} / \partial C_j = d_{k,i} [K_i^{(j)} - K_i^{(4)}] + d_{s,i} [S_i^{(j)} - S_i^{(4)}].$$

Accordingly,

$$\mathbf{Q} = \mathbf{D}_k[\Phi_k - \mathbf{k}^{(4)}\mathbf{u}] + \mathbf{D}_s[\Phi_s - \mathbf{s}^{(4)}\mathbf{u}]. \quad (15)$$

If we combine Eqs. (12)–(15), we see, in strict analogy to Paper I, that

$$\Delta \mathbf{c} = (\mathbf{TE}\{\mathbf{D}_k[\Phi_k - \mathbf{k}^{(4)}\mathbf{u}] + \mathbf{D}_s[\Phi_s - \mathbf{s}^{(4)}\mathbf{u}]\})^{-1} \Delta \mathbf{t}. \quad (16)$$

It might seem, as was found to be the case for single-constant theory in Paper I, that the inverted matrix used for iterative improvement of the concentrations of the colorants is the same as that used to calculate the rough match. But this statement is only true in a formal sense. If we attempt iteration with the identical numerical matrix that was used for the rough match, we do not obtain convergence. The reason is that the

first matrix was based on the assumption that the sample had a uniform scattering coefficient of unity throughout the spectrum. This assumption suffices for the rough match, but leads to trouble during the iterations. The approximation embodied in Eq. (4) is based on the supposition that the scattering coefficient of the sample at each wavelength is fairly close to that of the match, and that the same is true of the absorption coefficients. Keeping the scattering coefficient of the sample at unity throughout the spectrum violates this supposition and causes trouble in the iterative part of the calculation.

I have found that this difficulty can be avoided by resynthesizing and re-inverting the matrix once, right after the calculation of the rough match. We can calculate the scattering coefficient of the rough match by Eq. (8) [or, if we prefer, by the equation analogous to Eq. (6) applying to  $S_i^{(m)}$  instead of  $K_i^{(m)}$ ]. We then assume that  $S_i^{(a)} = S_i^{(m)}$ , and recalculate the  $d_{k,i}$  and the  $d_{s,i}$  by Eqs. (2) and (3). We are now in a position to recalculate a much more powerful matrix for Eq. (16),

based on a set of scattering coefficients for the sample very close to those of the match, which can be used all through the subsequent iterations. Because the reflectances of sample and match do not differ too greatly, the absorption coefficients of sample and match are likewise fairly close, and the approximation of Eq. (4) holds well enough to assure convergence during the iterations. I found that an alternative program, in which the matrix was recomputed after each iteration, did not give faster convergence in the cases tested.

#### REFERENCES

- <sup>1</sup>E. Allen, J. Opt. Soc. Am. **56**, 1256 (1966).  
<sup>2</sup>Single-constant theory refers to either Beer's law, in which the negative logarithm of transmittance is assumed to be linearly related to the concentrations of the colorants, or the special case of Kubelka-Munk theory for which the ratio of  $\bar{K}$  to  $S$ , not each separately, is similarly considered to be linearly related to the concentrations of the colorants.  
<sup>3</sup>A good elementary presentation of Kubelka-Munk theory is found in D. B. Judd and G. Wyszecki, *Color in Business, Science and Industry*, 2nd ed. (Wiley, New York, 1963), pp. 387-426.

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