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Evaluating Single- and Two-Constant Kubelka-Munk Turbid Media Theory for Instrumental-Based Inpainting

Roy S. Berns and Mahnaz Mohammadi

Instrumental-based color matching using non-destructive reflection spectrophotometry can be used as an aid in pigment selection for inpainting. This is useful when metamerism is of concern, particularly in modern art where the number of colorants available to artists and conservators is quite large. Simplified methods have been developed for art conservation where a single tint of each pigment mixed with white is required to define a pigment's optical properties based on the single-constant form of Kubelka-Munk (K-M) turbid media theory. Theoretically, this simplification can lead to errors in pigment selection for dark colors and colors not containing a white pigment. Instead, the two-constant form of K-M theory can be used where the model assumptions more closely match the optics of inpainting materials. The two methods were compared using four acrylic emulsion paints with a range of pigment absorption and scattering properties. It was found that the simplified method was inadequate for paints with appreciable and spectrally selective scattering, and as a consequence, pigment selection may result in a greater number of pigments than actually required. It was also found that only two samples per pigment were required to implement the two-constant technique: the mass tone and a tint.

INTRODUCTION

Instrumental-based color matching consists of creating a database of colorant optical properties based on reflection spectrophotometry, measuring the reflectance spectrum of a sample to be matched using the same spectrophotometer, and computer processing to both select the least metameric set of colorants ('colorant selection') and determine their concentrations ('recipe prediction') based on an optical model of color mixing [1]. The goal is a close spectral match and exact colorimetric (visual) match under a defined set of viewing conditions. This technique is used routinely in the coloration of paints, plastics and textiles in industry. Berns et al. used instrumental-based color matching to identify pigments that would result in minimal metamerism when used for inpainting [2]. They tested the technique for Barnett Newman's *Dionysius* and Sanford Robinson Gifford's *Siout, Egypt*, two oil paintings that are part of the permanent collection of the National Gallery of Art, Washington DC (NGA). In both cases, the areas

requiring inpainting had minimal image detail and it was known that the gallery lighting was tungsten while the conservation studio lighting was a combination of natural and artificial daylight. Thus metamerism, a well-known potential problem [3], was one of the concerns because any color mismatch would be quite obvious. Both test cases were successful.

The most common optical mixing model is the opaque form of Kubelka-Munk (K–M) turbid media theory. Industrial color matching using K–M theory has been described extensively [1, 4–7]. Johnston–Feller has described the use of K–M theory in art conservation science, including evaluating colorant changes due to ageing and light exposure and colorant identification based on curve-shape analysis and instrumental-based color matching [8]. Most of the practical examples are based on using the single-constant simplification where, for each colorant, an absorption and scattering ratio defines a colorant's optical properties. In addition, refractive index discontinuities are ignored. The Berns et al. implementation also used the single-constant simplification and ignored refractive index effects [2]. The main advantages of these simplifications are that

a colorant's optical properties are determined using a single tint and the mathematics are very straightforward.

As a general solution, it is well known that higher accuracy is achieved using two-constant K-M theory, where for each colorant, both absorption and scattering as a function of wavelength are used to define optical properties as well as accounting for refractive index discontinuities [1, 4–8]. However, sample preparation and the mathematics become considerably more complex in implementing the two-constant approach. Samples may include a mass tone, one or more tints mixed with white, and a mixture of the colorant with black. All the concentrations are weighed carefully for mixtures. Optimization and using different sample combinations for different spectral regions are required to develop the optical coefficients. This complexity has led to commercial software, often sold by spectrophotometer manufacturers, which automatically creates the colorant optical database and predicts recipes for user-defined matching criteria. However, the price is prohibitive for most conservation studios. In theory, it is possible to reduce the number of samples to two, a mass tone and a single tint mixed with white at any ratio without weighing. Eliminating weighing is possible because for inpainting, only colorant selection is required. Color mixing is determined visually by the conservator. A recipe has little value in most cases.

The Berns et al. simple implementation used a pigment database where each pigment was characterized based on a single tint at moderate lightness (between Munsell values 7 and 8). This lightness level ensured that each pigment's absorption spectrum had appreciable variability as a function of wavelength. (This is analogous to blue pigments appearing nearly indistinguishable as mass tones and quite different in hue when mixed with white.) It also minimized the influence of measurement imprecision when characterizing optical constants [7]. Because the areas requiring inpainting for both paintings were of medium-to-high lightness, the pigment database was somewhat optimal for the two paintings. In other words, the optical properties were defined at similar concentrations to the retouched areas. However, if the paintings were very dark, it would have been a concern whether the optical properties would scale accurately. Poor accuracy might lead to improper colorant selection, yielding a poor inpainting match. One of the goals of this research was to test whether a single tint could effectively represent the pigment over a range of concentrations including its mass tone form. If the single tint proved not to be scalable, then the two-constant approach would be preferred. Accordingly, the

second goal was to explore developing a two-constant technique appropriate for conservators that did not require commercial software. The results described in this publication are a portion of a comprehensive evaluation defining the optical properties of artists' paints using Kubelka-Munk theory [9–12].

THEORY

A given opaque material, such as a retouching paint or a dry pigment dispersed in an appropriate medium, is defined by two optical constants, an absorption coefficient k_λ and a scattering coefficient s_λ, each a function of wavelength, λ. When considered across a spectral range of interest, usually the visible range, two distinct spectra define the optical properties of the material (examples are shown in the Results and Discussion section). Retouching paints that are opaque (e.g. cadmium-based paints) have scattering spectra with appreciable values that are spectrally varying, whereas transparent retouching paints (e.g. ultramarine blue) have spectra that have small values and are largely spectrally invariant.

The optical constants are normalized for a unit amount of material, designated by lower-case variables [1, 5]. (This is analogous to an extinction coefficient when using Beer's law.) When the materials are mixed together, the mixture's optical properties are estimated by the summation of each material's optical properties, scaled by their concentrations:

$$\left(\frac{K}{S}\right)_{\lambda,mixture} = \frac{c_1 k_{\lambda,1} + c_2 k_{\lambda,2} + ... + c_n k_{\lambda,n}}{c_1 s_{\lambda,1} + c_2 s_{\lambda,2} + ... + c_n s_{\lambda,n}} . \qquad (1)$$

where K/S is the ratio of absorption and scattering, c is concentration expressed as a ratio to the total amount of material, n defines the number of materials, and λ is wavelength. Upper-case variables, K and S, designate that the coefficients are not normalized to a unit amount. Each material is defined by two independent coefficients, hence the term 'two-constant Kubelka-Munk'.

In some cases, one of the materials in a colorant system has appreciable scattering, and relative to this strong scatterer, the other materials' scattering properties are negligible. Examples include colored paper, dyed textiles, pastel paints, and paint mixtures where the chromatic pigments are nearly transparent. In the paint examples, the strong scatterer would be a white pigment. In this case, Equation 1 can be simplified:

$$\left(\frac{K}{S}\right)_{\lambda,mixture} = \frac{c_1 k_{\lambda,1} + c_2 k_{\lambda,2} + ... + c_w k_{\lambda,w}}{c_w s_{\lambda,w}}$$

$$= \frac{c_1}{c_w}\left(\frac{k}{s_w}\right)_{\lambda,1} + \frac{c_2}{c_w}\left(\frac{k}{s_w}\right)_{\lambda,2} + ... + \left(\frac{k}{s_w}\right)_{\lambda,w}, \qquad (2)$$

where the *w* subscript represents white. At each wavelength, each material is defined as a single constant, the ratio of absorption and scattering, referred to as 'unit *k* over *s*':

$$\left(\frac{k}{s}\right)_{\lambda,i} = \left(\frac{k_i}{s_w}\right)_\lambda. \qquad (3)$$

Mixtures are defined as a summation of each material's $(k/s)_\lambda$ suitably scaled:

$$\left(\frac{K}{S}\right)_{\lambda,mixture} = \frac{c_1}{c_w}\left(\frac{k}{s}\right)_{\lambda,1} + \frac{c_2}{c_w}\left(\frac{k}{s}\right)_{\lambda,2} + ...$$

$$+ \frac{c_{n-1}}{c_w}\left(\frac{k}{s}\right)_{\lambda,n-1} + \left(\frac{k}{s}\right)_{\lambda,w} \qquad (4)$$

Equation 4 is the single-constant simplification of the two-constant equation for paint mixtures. Transforming reflectance factor to the ratio of absorption and scattering enables the use of algebra when color matching using materials that both absorb and scatter light [13]. (This is analogous to Beer's law where a colored liquid's spectral absorbance is predicted from the absorbances of the individual dyes. Rather than absorbance, *K/S* is used.) The ratio, $(k/s)_\lambda$, is calculated from a tint of the material mixed with white:

$$\left(\frac{k}{s}\right)_{\lambda,paint} = \frac{\left(\frac{K}{S}\right)_{\lambda,tint} - \left(\frac{k}{s}\right)_{\lambda,w}}{\frac{C_{tint}}{C_w}}, \qquad (5)^1$$

---

[1]*Equation 5 differs from Johnston-Feller [8]. Berns and Mohammadi [14] have compared three different equations used to calculate $(k/s)_\lambda$; the Johnston-Feller equation is equivalent to the 'hybrid' approach, also used by Berns [1] in a numerical example for recipe prediction. These differences only affect recipe prediction, not colorant selection.*

where

$$\left(\frac{k}{s}\right)_{\lambda,w} = \left(\frac{K}{S}\right)_{\lambda,w} \qquad (6)$$

and

$$c_{tint} + c_w = 1. \qquad (7)$$

For simplicity, the subscript '*paint*' will be used to define either a retouching paint or a dry pigment dispersed in a medium. The subscript '*tint*' defines a mixture of a chromatic paint with white. (Equation 5 is analogous to defining a dye's extinction coefficient with a single dilution.) A tint is required because of the single-constant simplification in which all of the scattering is attributed to the white. When the retouching paint is transparent, the tint directly reveals the absorption spectrum because most whites have negligible absorption beyond their natural region of strong absorption at very short visible wavelengths. When the retouching paint is opaque, the absorption spectrum revealed by the tint is an approximation, often varying with concentration because the scattering of the paint is appreciable, described below.

In the Berns et al. technique [2], the concentration ratio was assumed to be unity since the specific amounts of chromatic and white paints were not measured and visual inspection during mixing was used to achieve a recommended lightness. A step-by-step procedure for using the single-constant approach for colorant selection when inpainting was provided. This approach assumed that the unit absorption and scattering coefficient of a paint, $(k/s)_{\lambda,paint}$, was invariant to the relative proportions of the chromatic and white paints and that $(k/s)_{\lambda,paint}$ determined using a tint would approximate a $(k/s)_{\lambda,paint}$ based on a mass tone. (Again using the Beer's law analogy, the line fit of a dilution series to determine the extinction coefficient of a dye would be perfectly linear passing through the origin at each wavelength. Under this condition, any dilution would result in the identical extinction coefficient.) Strictly, both assumptions are false if a chromatic paint has appreciable wavelength-dependent scattering, a common occurrence for many paints used for inpainting, hence their range of opacities. This assumption did not adversely impact the results because the unit absorption and scattering coefficients of each paint were determined at similar concentrations to those used for the retouched areas, as stated above.

It was also assumed that ignoring the refractive index discontinuity between the paint film and air did not affect this invariance. Because bi-directional geometry was used, specular reflections were excluded from any measurements resulting in an approximation to account for the refractive index discontinuity. The approximation would break down for reflectance factors below about 0.1, which did not occur in their research.

When using the two-constant approach, a minimum of two samples is required to calculate k_λ and s_λ for a pigment, shown in Equations 8–12 using a mass tone and single tint. Two simultaneous equations must be solved, hence the requirement of having at least two samples. The derivation of Equations 8–10 from Equation 1, basically an algebraic rearrangement to solve simultaneous equations, is shown in Zhao and Berns [12]. The step-by-step procedure to implement the two-constant approach is given in the Appendix.

$$k_{\lambda,paint} = \frac{1 - c_{tint}}{c_{tint}} s_{\lambda,0} \left(\frac{K}{S} \right)_{\lambda,masstone}, \tag{8}$$

$$s_{\lambda paint} = \frac{1 - c_{tint}}{c_{tint}} s_{\lambda,0}, \tag{9}$$

$$s_{\lambda,0} = \frac{\left(\left(\frac{K}{S} \right)_{\lambda,tint} \times s_{\lambda,w} \right) - k_{\lambda,w}}{\left(\frac{K}{S} \right)_{\lambda,masstone} - \left(\frac{K}{S} \right)_{\lambda,tint}}, \tag{10}$$

where

$$s_{\lambda,w} = 1, \tag{11}$$

and

$$k_{\lambda,w} = \left(\frac{K}{S} \right)_{\lambda,w}. \tag{12}$$

Variable $s_{\lambda,0}$ is an intermediate value required to solve these two simultaneous equations. (The Beer's law analogy is that two independent extinction coefficients are estimated for each dye. Solving two simultaneous equations requires two dilutions.)

In this implementation of K-M theory, the scattering of white is not determined on an absolute basis; rather it is assumed to be unity at all wavelengths (Equation 11), referred to as relative-two-constant [5]. The algebraic solution is shown in this manner to reveal that the magnitudes of k_λ and s_λ depend on the same scaling of the tint concentration: $(1-c_{tint})/c_{tint}$ (Equations 8 and 9). For

Thus, if the tint is not weighed, only recipe prediction will be affected adversely; the absorption and scattering spectra are not affected. In other words, this assumes that both spectra are invariant to the proportions of chromatic and white paints in the tint, and when using two-constant K-M theory for colorant selection, a mass tone and unweighed tint are sufficient.

When using two-constant K-M theory, it is common to account for refractive index discontinuities using the so-called 'Saunderson equations' [15], although the equations were derived by Ryde [16]. Berns and de la Rie have studied the effects of refractive index on the appearance of varnished oil paintings [17]. It is necessary to calculate the reflectance of a paint film 'on the inside', shown in Equation 13 for integrating sphere geometry with the specular component included:

$$R_{\lambda,i} = \frac{R_{\lambda,m} - K_1}{1 - K_1 - K_2 + K_2 R_{\lambda,m}}, \tag{13}$$

where $R_{\lambda,m}$ and $R_{\lambda,i}$ are the measured and the internal reflectance, respectively, K_1 is the decimal fraction of the amount of first-surface collimated light based on the refractive indices of the paint film's surface and air, and K_2 is the decimal fraction of the amount of diffused light inside the paint film. Because the relationship between measured and internal reflectance is nonlinear (see Johnston-Feller [8] for a plot), the unit absorption and scattering spectra will be slightly different when including or ignoring the refractive index discontinuity. This may improve the accuracy of colorant selection. The Saunderson correction for other common spectrophotometer geometries is given in the Appendix; the equations for any set of geometries and refractive indices are given in reference [17].

EXPERIMENTAL

Sample preparation and measurements

A comprehensive evaluation of the optical properties of artists' acrylic emulsion paints was carried out by Mohammadi and Berns [9] and Okumura [10]. Four of these were evaluated in this research: cobalt blue (PB 28) and cadmium yellow medium (PY 37) from Liquitex® Artist Materials and green gold (PY 150, PG 36, PY3) and phthalocyanine green (blue shade) (PG 7) from Golden® Artist Colors. Acrylics were selected because of their ease of use. These particular colors were selected to have a range of scattering and absorption properties. For

each paint, a tint ladder was prepared at four different concentrations with titanium white (titanium dioxide (PW 6) from Golden® Artist Colors) along with a mass tone. A drawdown bar was used to apply the paint uniformly on Lenetta opacity charts. The white and black sections of these charts enabled the verification of opacity. A notation for each mixture was defined in this experiment as H/L/C, where H represents the colorant, L represents CIELAB lightness, and C represents CIELAB chroma. A cobalt blue tint would have the notation CB/76/28. The tint concentrations are listed in Table 1.

Spectral reflectance factor was measured using a GretagMacbeth Color Eye XTH integrating sphere spectrophotometer with the specular component included. Measurements were collected from 360 to 750 nm in 10 nm intervals (Figure 1). Titanium white has the greatest reflectance throughout the majority of

Table 1 *Colorimetric designations and tint concentrations*

	Tint 1	Tint 2	Tint 3	Tint 4	Mass tone
Cobalt blue (PB 28)					
Designation	CB/76/28	CB/65/40	CB/54/48	CB/47/51	CB/33/50
Concentration tint	0.20	0.49	0.76	0.87	1.00
Cadmium yellow medium (PY 37)					
Designation	CY/94/41	CY/92/55	CY/89/71	CY/87/82	CY/82/94
Concentration tint	0.07	0.16	0.37	0.60	1.00
Green gold (PY 150, PG 36, PY3)					
Designation	GG/86/55	GG/81/62	GG/76/63	GG/68/61	GG/50/42
Concentration tint	0.20	0.40	0.60	0.80	1.00
Phtalocyanine green (PG 7)					
Designation	PG/75/38	PG/62/47	PG/55/47	PG/46/42	PG/26/8
Concentration tint	0.10	0.40	0.60	0.80	1.00
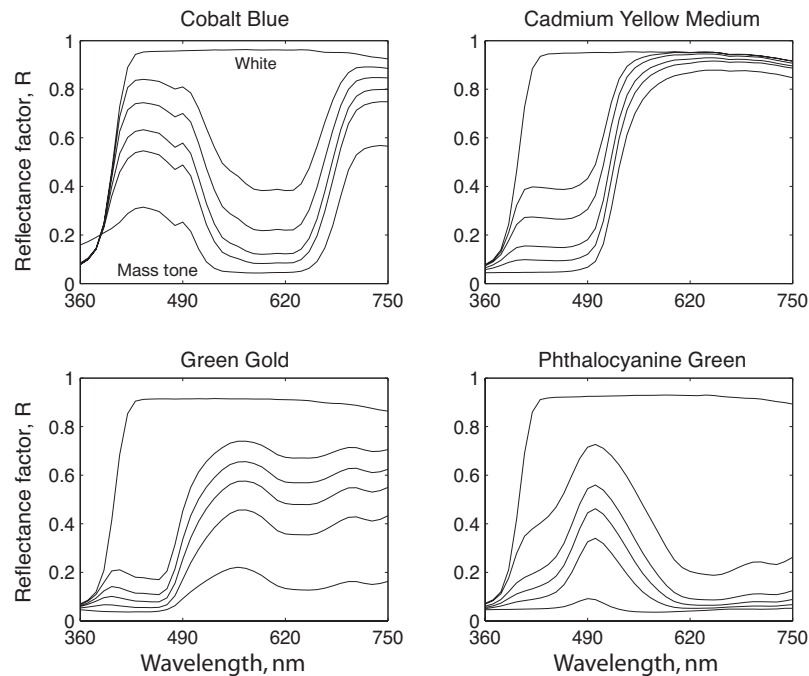
Figure 1 *Spectrophotometric curves of titanium white, tints, and mass tones for each listed paint.*

the visible spectrum and strongly absorbs light at short wavelengths, obscuring pigment absorptions in tints. The cobalt blue mass tone spectrum reflects more light than the white at these short wavelengths. With increasing concentration, reflectance decreased. The colorimetric data are plotted in Figure 2 as CIE L★ versus CIE C★$_{ab}$ (CIE illuminant D65 and the 1931 standard observer). The lightness of the mass tone of the selected paints varied in the range of between 25 and 84. The darkest sample was phthalocyanine green and the lightest was cadmium yellow medium. The range of lightnesses results from differences in each pigment's absorption, scattering and pigment volume-concentration within the acrylic-emulsion medium. The relationship between concentration and colorimetry was nonlinear and unique for each paint. The tint concentration at maximum chroma varied between 0.60 for the two greens and 1.0 for cadmium yellow medium.

Computations

Each tint was used to calculate a $(k/s)_\lambda$ using Equations 5 and 13 in order to evaluate single-constant K-M theory. For the mass tone, it was assumed that $(k/s)_\lambda$ was equal to $(K/S)_\lambda$. For the Saunderson equations, K_1 = 0.03 and K_2 = 0.65 were selected, based on previous analyses [10]. Each $(k/s)_\lambda$ was used to predict the spectral reflectance factor of the tints and mass tone for each pigment. Constrained nonlinear optimization was used where concentration was constrained between zero and unity. Concentration was estimated such that the RMS spectral reflectance factor was minimized between a tint's measured values and its estimate. The spectral reflectance factor error was minimized rather than the absorption and scattering ratio in order to relate these results to current practices of colorant selection for inpainting where minimizing reflectance is preferred when the match will be slightly metameric. If a unit absorption and scattering ratio is not scalable, the resulting reflectance spectrum is slightly metameric compared with the measured spectrum.

The mass tone and each tint were used to calculate sets of k_λ and s_λ using Equations 8–13 in order to evaluate two-constant K-M theory. Each k_λ and s_λ was used to predict the spectral reflectance factor of the tints for each pigment, using the same nonlinear optimization as for the single-constant approach.
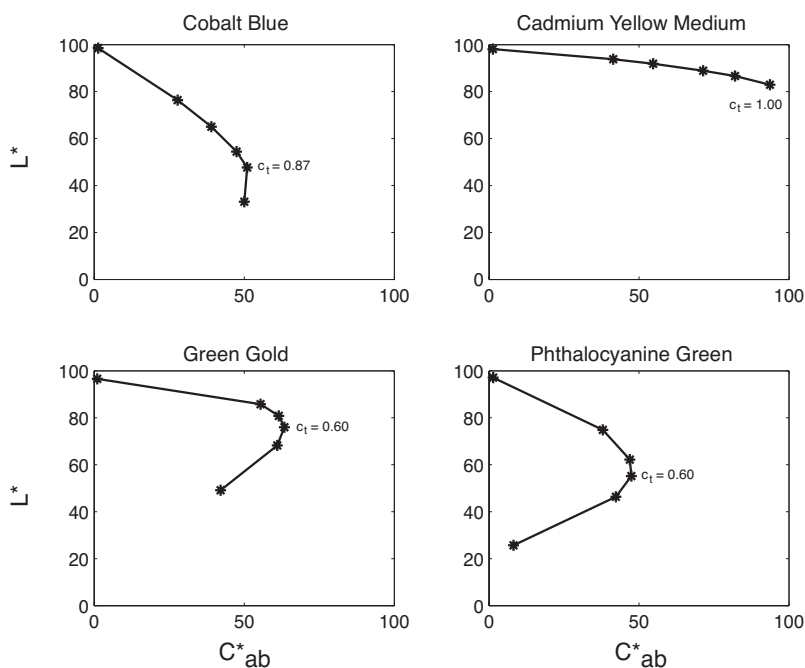

Figure 2   *Colorimetric plots of each paint's tint ladder including white and mass tone samples (CIE illuminant D65 and the 1931 standard observer).*

As described in the introduction, a number of paint-outs can be used to determine optical properties, for example a tint ladder. In this case, there are more samples than unknowns (over-determined) and linear regression can be used to calculate $(k/s)_\lambda$ or k_λ and s_λ [18]. This approach should be an improvement over any single tint. The four tints were used to calculate $(k/s)_\lambda$ and the four tints and the mass tone were used to calculate k_λ and s_λ.

RESULTS AND DISCUSSION

For single-constant K-M theory, the spectral matching results, expressed as %RMS error, are plotted in Figure 3. The average performance for the over-determined approach ('all tints') was within the range of that achieved using any single tint. There was no advantage to using the more complex over-determined method. For each paint there was a weak minimum in which one of the tints had marginally better average performance. This was in the region of maximum chroma. However, given the spread in the data, this difference was insignificant.

Thus, when preparing a tint, the specific concentration is not a factor as long as there is a sufficient amount of chromatic paint to obtain a reasonable range of spectral reflectance factor, that is, not a light pastel. All of the tints evaluated in this research had this property, seen in Figure 1. For cadmium yellow medium, the lightest tint resulted in much greater average error and a larger standard deviation compared with the other tints. For yellows, it is always problematic to separate the optical properties from white at long wavelengths, the region where yellows reflect nearly as much light as white. As the tint lightens, this problem increases. Thus, using the yellow mass tone to calculate (k/s) resulted in reasonable performance. The cobalt blue mass tone also resulted in reasonable performance, particularly given that it would poorly predict the wavelengths where titanium white was highly absorbing. For the green paints, the mass tone samples had poor performance in estimating the spectral properties of each tint. These results are better understood by plotting spectra as $\mathrm{Log}(K/S)_\lambda$, shown in Figure 4. The use of the logarithm of $(K/S)_\lambda$ results
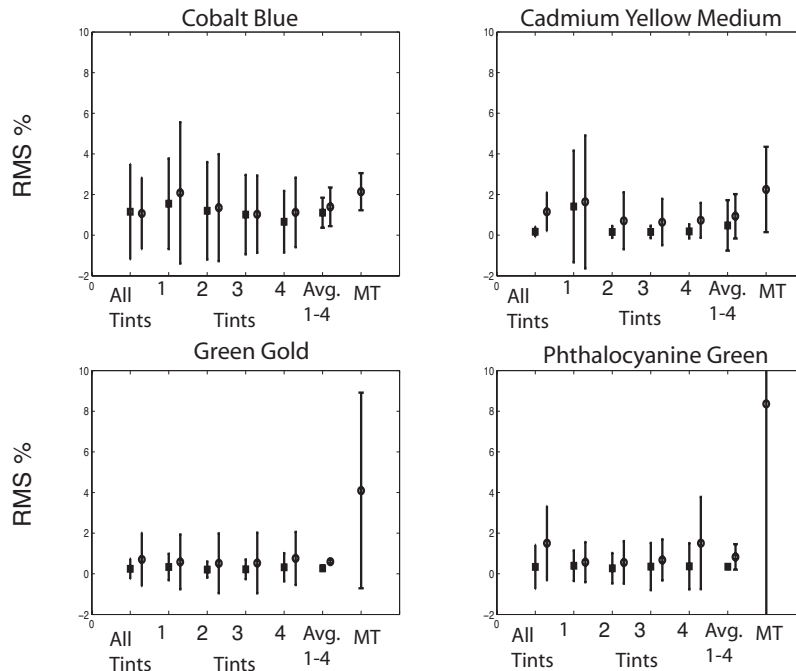
Figure 3 *Spectral reflectance %RMS performance of single- (circles) and two-constant (squares) K-M for each listed sample or set of samples predicting the entire tint ladder and mass tone. Vertical lines span ±2 standard deviations. 'All Tints': the over-determined approach using all four tints; tints 1–4: the four tints in increasing order of tint concentration; 'Avg. 1–4': the average results of tints 1–4; 'MT': mass tone.*
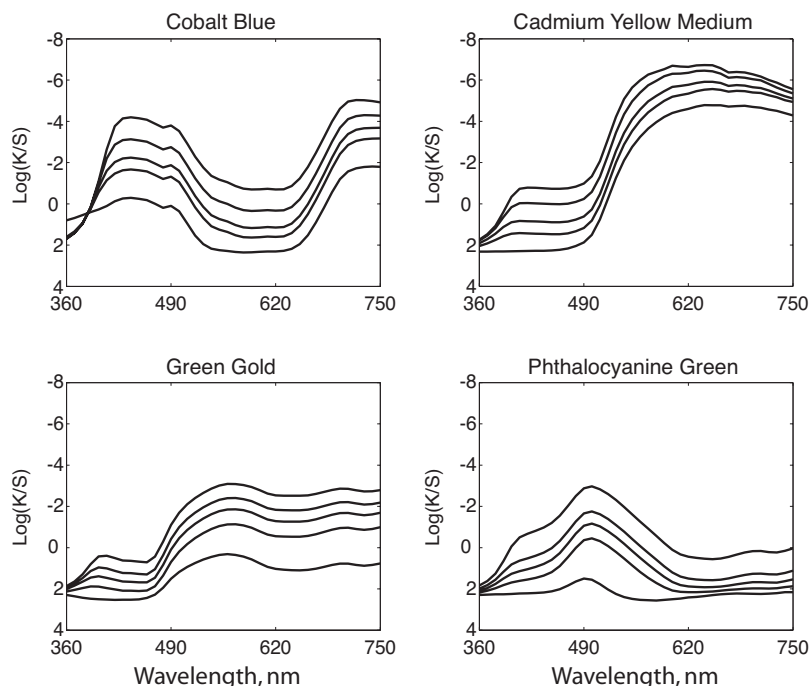
Figure 4   *Spectrophotometric curves of each tint ladder and mass tone where the ordinate is Log* (K/S).

in spectra that are the most invariant with changes in concentration [19], providing a qualitative way to evaluate the assumption of spectral invariance with changes in concentration. The evaluation should be limited to the region where the titanium white paint did not absorb, beyond 430 nm. When single-constant K-M theory predicts optical behavior accurately, the spectra have nearly identical shape. For the blue and yellow paints, all the spectra were very similar, including the mass tones. For the green mass tone spectra (lowest curves), the spectra were quite different from the tints. For phthalocyanine green, two standard deviations spanned to nearly 20%. Scaling these spectra predicted the tint spectra poorly. In fact for green gold, the use of single-constant K-M theory resulted in a metameric spectrum to the mass tone. Thus single-constant K-M theory did not describe the optical properties of these pigments over their full concentration range.

The consequence of this result was explored by using a database of 30 artists' acrylics [9, 10] in order to select a set of paints resulting in the best spectral match to the green gold mass tone. The single-constant approach including the Saunderson correction was used to characterize each paint. In this case, a bi-directional spectrophotometer was used with a wavelength range of 380–730 nm. All combinations of one, two, or three paints plus ivory black and titanium white were evaluated using the same optimization approach as described above. The closest spectral match is plotted in Figure 5. The set of paints included phthalocyanine green (chlorinated), cadmium yellow light, transparent earth red (red iron oxide) and carbon black. Although green gold was in the database, its inclusion did not result in a closer match. In this case, the single-constant simplification resulted in a much more complex recipe, four paints, compared with the actual single paint. Granted, green gold is a mixture containing brominated copper phthalocyanine and two yellows. Thus the single-constant approach was effective enough to decompose this mixture, an indicator that the general approach can be a powerful aid in colorant selection for inpainting. Nonetheless, green gold was not selected. This points out a practical limitation using the single-constant approach: more complex recipes than necessary may result.
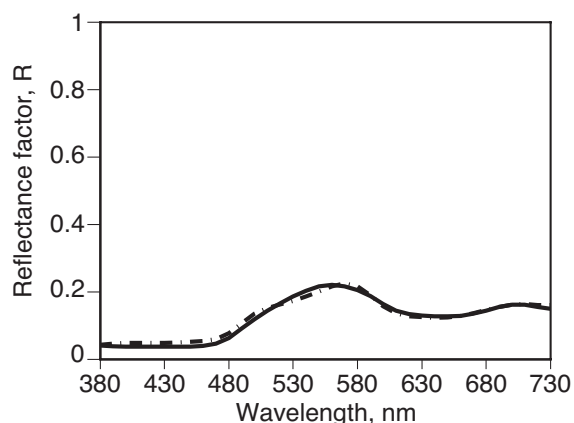
Figure 5   *Comparison between the measured spectrum of the green gold mass tone (solid line) and its color-match prediction (dotted/dashed line) using the single-constant approach and a database of 30 artists' acrylic paints.*

The two-constant performance is also plotted in Figure 3. For each tint and for 'all tints', the mass tone was used to calculate k_λ and s_λ. Therefore, there was not a two-constant result for the mass tone sample, since a single paint-out cannot determine the two constants. In similar fashion to the single-constant results, the over-determined approach did not result in marked improvement. When comparing single- and two-constant K-M theory, there was a slight improvement using the two-constant approach, seen in the averages. Since the standard deviations of the average results for green gold do not overlap, this improvement was statistically significant. For the other paints, these differences were not significant. The differences between single-constant K-M theory and two-constant K-M theory were negligible, on average. There was a difference in the range of errors; the standard deviations for the two-constant results for cadmium yellow medium and green gold were smaller. These results are clarified by evaluating each paint's predicted unit absorption and scattering spectra, plotted in Figure 6. These spectra were calculated using the mass tone and the tint resulting in the best single-constant average performance: CB/47/51, CY/89/71, GG/81/62 and PG/62/47. Recalling that the scattering coefficients were calculated relative to the scattering of white, defined as unity, the cobalt blue scattering was nearly zero. Scaling this spectrum would have a negligible effect on a tint's spectrum. Also, the scattering spectrum was nearly featureless. For cobalt blue, separating absorption and scattering

did not improve performance. In fact, the two-constant approach added error because the differences in absorption between titanium white and cobalt blue at short wavelengths resulted in inaccurate k and s at these wavelengths. The slight spike at 390 nm corresponds to the crossover point where white has stronger absorption than blue, seen in Figure 1. For the other pigments, there was appreciable scattering and the spectra varied with wavelength; thus, the more rigorous approach resulted in improvement, particularly for green gold. The improvement was due mainly to the use of separate k and s_λ. With two unique wavelength-dependent spectra per paint, changes in concentration enabled changes in the absorption and scattering spectrum of each tint. (Using the Beer's law analogy, scattering often leads to Beer's law failure and two constants enable a reduction in failures.) The two-constant K-M theory predicted the concentration-dependent spectral changes observed in the Log(K/S) spectra (Figure 4), particularly for green gold and, to a lesser degree, phthalocyanine green.

The mass tone predictions were analyzed separately, plotted in Figure 7. The two-constant approach was much more effective in predicting the mass tone spectra, by definition the expected result since the mass tone was used to create the optical database. With the exception of cobalt blue and the lightest tint for cadmium yellow medium, the choice of tint did not affect the prediction accuracy. The single-constant approach was noticeably poor for green gold and phthalocyanine green. There was also a trend where the single-constant performance improved as tint concentration increased. As white reduced, the optical properties became more similar to the mass tone. The over-determined approach proved useful for cadmium yellow medium; the single- and two-constant approaches were similar. The increase in the number of samples improved the $(k/s)_\lambda$ accuracy at long wavelengths.

The measured and predicted reflectance spectra of the lightest tint and the mass tone for each pigment are plotted in Figure 8. For the single-constant predictions, the tint resulting in the best average %RMS performance was used to define the $(k/s)_\lambda$: CB/47/51, CY/89/71, GG/81/62 and PG/62/47. These tints and the mass tone were used to define k_λ and s_λ. Acceptable performance was defined by predicted spectra that did not appear metameric. That is, by looking at these spectra, it would be clear that the two spectra were composed of paints with nearly identical spectral features. This was true for all of these light tints. Both approaches generated spectra that were unambiguous. Although the two-constant spectra were more coincident with the measured spectra,
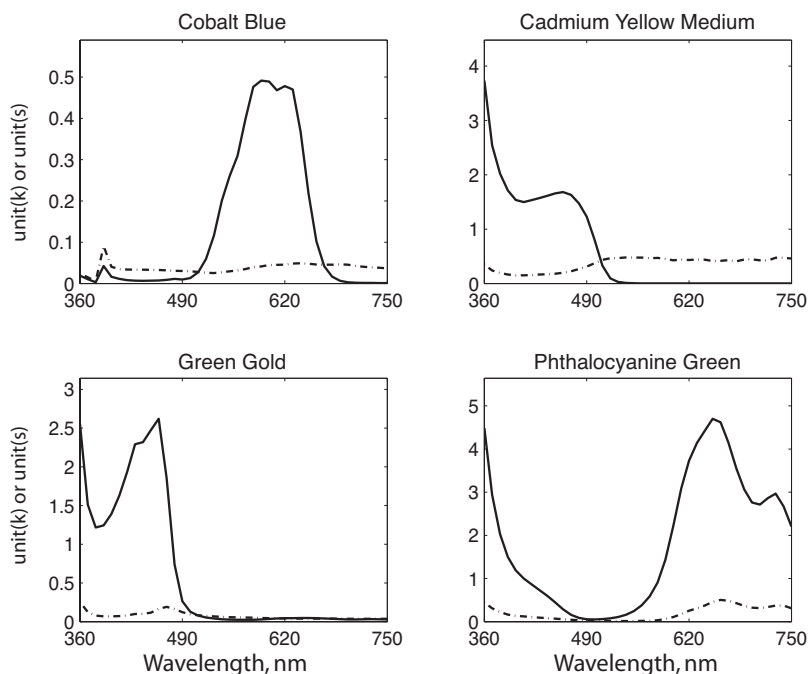
Figure 6 *Absorption (solid line) and scattering (dotted-dashed line) spectra at unit concentration predicted using CB/47/51, CY/89/71, GG/81/62, PG/62/47 and each mass tone.*

these differences were inconsequential. For the mass tone samples, the single-constant approach resulted in a metameric spectrum to green gold. There was a slight shift in the wavelength of maximum reflectance resulting in a shift in the spectrum on the left-hand side of the peak centered near 550 nm. This was a result of not accounting for this pigment's wavelength-dependent scattering.

CONCLUSIONS

One of the goals of this research was to determine whether the single-constant simplification based on a single tint would be applicable for colorant selection over the full concentration range from pastel to mass tone. In three out of four test paints, it was effective. For one of the paints, green gold, the use of single-constant K-M theory resulted in a metameric spectrum to the mass tone. As a consequence, the colorant selection may be in error, either by choosing the wrong colorant, or selecting a greater number of colorants than necessary. As the number of colorants increases, obtaining a visual match becomes more difficult.

As stated in the introduction, it was expected that the two-constant approach would be more generally applicable since this approach more closely matches the optics of paint systems where most pigments have appreciable scattering. Berns, Krueger and Swicklik were aware of the limitations of the single-constant simplification [2]. Their decision to use this method was based on three factors. First, the time and effort required to create the single-constant colorant database was considerably less than the first-listed author's experiences in creating a two-constant database, where tint ladders with at least five different concentrations, a mixture with black, and a mass tone, all carefully weighed, were used, followed by weighted nonlinear optimization to calculate k_λ and s_λ, the weighting both wavelength and sample dependent. Second, the spectral reflectance factor of the Newman painting, the first painting tested, was quite distinctive; it was clear that the single-constant approach would not limit an effective colorant selection. Third, the single-constant approach enabled the use of multiple-linear regression where the spectrum to be matched was the dependent variable and each colorant's $(k/s)_\lambda$ was the independent variable. Although multiple-
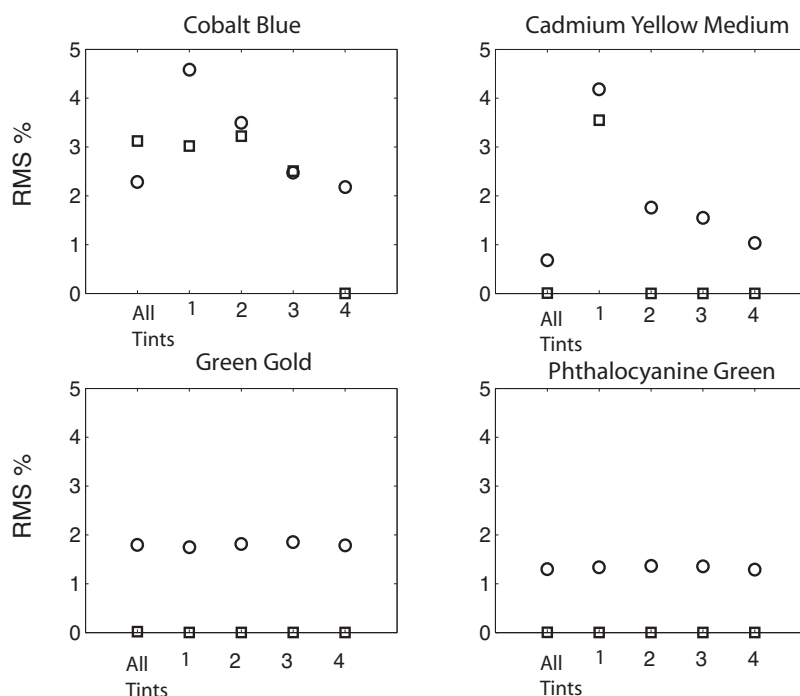
Figure 7   *Spectral reflectance %RMS performance of single- (open circles) and two-constant (open squares) K-M for each listed sample or set of samples predicting the mass tone.*

linear regression can be used with two-constant K-M theory [20], the regression is ill posed because the dependent variable is zero with a unity constraint rather than a spectral curve.

As described in these experiments, it was possible to create a two-constant database for colorant selection where each pigment was characterized with two samples, a mass tone and a tint. Although the tint concentrations were determined in these experiments, this is not required. Thus, the time and effort required to create a two-constant database is only slightly greater than for the single-constant approach. This is the time to make and measure a paint-out of the mass tone. Furthermore, by not determining tint concentrations, the mathematics required to determine k_λ and s_λ are only slightly more complex than $(k/s)_\lambda$. A step-by-step procedure is given in the Appendix.

Given that the usual approach to develop a two-constant database is quite involved, as outlined above and described in detail by Johnston-Feller [8], why do these experimental results lead to the conclusion that only two

samples are required? The answer is found by separating instrumental-based color matching into two tasks: colorant selection and recipe prediction. In industry, both are equally important. Colorant selection deals principally with minimizing or eliminating metamerism and ultimately defines match quality since all lighting conditions cannot be anticipated and individual variations in color vision are large. Recipe prediction reduces manufacturing costs by reducing the number of iterations required to achieve an acceptable color match. The complex sample preparation and mathematics are required to achieve accurate recipe prediction. If only colorant selection is required, as in inpainting, only one or two samples are required.

Having developed a practical method to develop a two-constant database, how is this database used for colorant selection? The first-listed author has continued to aid the conservation department at NGA. These experiences have resulted in a better understanding of the limitations in the Berns et al. approach. In addition to those described in this research, stepwise-multiple-
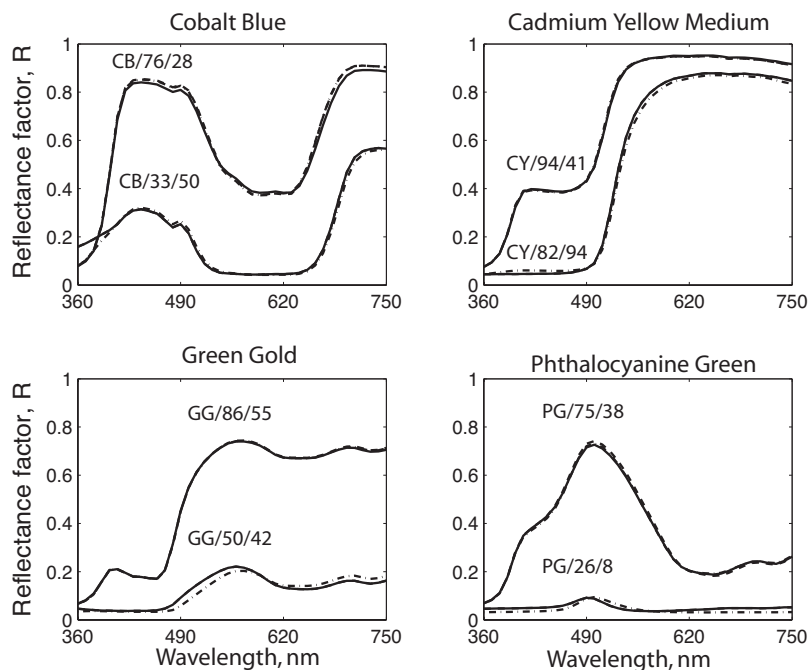
Figure 8   *Comparisons between measured (solid line) and estimated spectra using the single-constant (dotted-dashed line) and two-constant (dashed) approaches.*

linear regression, the method used to select paints, has proven problematic as a general approach. By definition, concentrations cannot be constrained between zero and unity. That means that the unit absorption and scattering ratio can be scaled positively or negatively. When scaled negatively, this is equivalent to a complementary spectrum, a paint that does not exist. The recommended practice was to remove any paint resulting in a negative concentration and repeat the regression. However, experience was required to converge to an optimal set of paints because removing and adding candidate paints became subjective. Two practitioners may select a different set of paints for the same spectrum. Furthermore, when paints cannot be found resulting in nearly identical matches in $(K/S)_\lambda$, minimizing %RMS $(K/S)_\lambda$ error does not lead to the best spectral reflectance or visual match. Both limitations are alleviated by using constrained nonlinear optimization where %RMS spectral reflectance factor error, colorimetric error, or a weighting of the two is minimized while concentration is constrained between zero and unity. In this research, %RMS spectral reflectance factor error was minimized. Once multiple-

linear regression is replaced with nonlinear optimization, using the two-constant database is straightforward. This can be implemented using spreadsheet software such as Microsoft® Excel® and its embedded optimization package, Solver. (Spreadsheets that calculate k_λ and s_λ and use Solver for colorant selection using either the single-constant or two-constant approach are available from the first-listed author.)

The opaque form of K-M theory was used in this research, where the paint-outs were opaque and the measured area adjacent to the paint loss would also be assumed to be opaque. It is unclear whether the general form of K-M theory is required for colorant selection when the inpainting must be composed of multiple layers that may be either transparent or translucent in order to match the optical properties as a function of depth in addition to wavelength. This is a current area of research [21]. However, this technique was quite effective for inpainting that required an opaque ground and a stippled translucent top layer [2]. More experiences are required to test this technique with a range of optical complexity including *tratteggio*. It seems likely that selecting the set of

pigments that minimizes metamerism can be very useful, irrespective of how the pigments are applied.

In conclusion, when creating an optical database for instrumental-based inpainting, two paint-outs should be prepared, a mass tone and a tint. The single tint can be used to implement the single-constant approach while both samples are used to implement the two-constant approach. Our recommendation is to use the more rigorous two-constant approach including accounting for refractive index discontinuities. If this seems prohibitively complex, one can gain experience using the single-constant approach as described by Berns et al. [2] and implement the two-constant approach at a later time. Either approach is preferred compared to selecting candidate paints using trial and error. Research is underway to improve the efficiency of selecting paints from a large set of candidates.

APPENDIX: RECOMMENDATIONS FOR DEVELOPING A TWO-CONSTANT K-M DATABASE

The following is a list of procedures and recommendations for creating a pigment database.

1   Obtain a reflectance spectrophotometer with a wavelength range of at least 400–700 nm. Increasing the wavelength range towards the infrared is desirable as is a 10 nm bandwidth and sampling interval. The choice of measurement geometry is not a factor but must be known.
2   Obtain pigments that will form the database. These can be dry pigments or dispersed in an appropriate medium.
3   Create paint-outs of each pigment as a mass tone and a tint mixed with titanium white in an appropriate medium. The white should be the same white used for inpainting. The paint-outs should be opaque. The tint concentration is not critical. It is reasonable to have equal proportions of the pigment and white or to achieve a color that is near the maximum chroma achievable as a tint. Be sure to prepare a paint-out of only the titanium white.
4   Measure each sample three times with replacement. That is, reposition the sample (or instrument) before each measurement. Plot the spectral reflectance as a function of wavelength. The three curves should be nearly identical in shape. If one of the curves seems different in curve shape, repeat the measurement procedure. When three consistent curves have been obtained, calculate their average.
5   Create the k_λ and s_λ database:

A. Convert reflectance factor, $R_{\lambda,m}$, to internal reflectance, $R_{\lambda,i}$. Be sure that reflectance factor is a fraction and not a percentage. For integrating sphere geometry with the specular component included:

$$R_{\lambda,i} = \frac{R_{\lambda,m} - K_1}{1 - K_1 - K_2 + K_2 R_{\lambda,m}}$$

For either integrating sphere geometry with the specular component excluded or bi-directional geometry:

$$R_{\lambda,i} = \frac{R_{\lambda,m}}{1 - K_1 - K_2 + K_2 R_{\lambda,m}}$$

The values of K_1 and K_2 are not critical as long as $R_{\lambda,i}$ is bounded by 0 and 1. Since most media have refractive indices near 1.5, set K_1 to 0.04. It is common to set K_2 to 0.4.

B. Calculate K/S for each spectrum:

$$(K/S)_\lambda = (1 - R_{\lambda,i})^2 / 2R_{\lambda,i}$$

C. Calculate k_λ and s_λ for the white:

$$k_{\lambda,w} = \left(\frac{K}{S}\right)_{\lambda,w} \text{ and } s_{\lambda,w} = 1 \, .$$

D. If the tint was weighed, calculate k_λ and s_λ using the (K/S) spectra of the tint and mass tone for each pigment using Equation 10, then Equation 8, then Equation 9. If the tint was not weighed, use the following equations where tint concentration is assumed to be 0.5:

$$s_\lambda = \frac{\left(\left(\frac{K}{S}\right)_{\lambda,\text{tint}} \times s_{\lambda,w}\right) - k_{\lambda,w}}{\left(\frac{K}{S}\right)_{\lambda,masstone} - \left(\frac{K}{S}\right)_{\lambda,\text{tint}}} \text{ and}$$

$$k_\lambda = s_\lambda \left(\frac{K}{S}\right)_{\lambda,masstone}$$

ACKNOWLEDGMENTS

SUPPLIERS

Spectrophotometer: GretagMacbeth Color Eye XTH, Gretag-Macbeth AG, www.gretagmacbeth.com.

Film applicator: drawdown bar with 10 mils thickness (one mil is equal to 1/1000 of an inch, or 25.4 μm), BYK-Gardner, www.byk-gardner.de.

Matte fluid acrylic paints: Golden Artist Colors, Inc., www.goldenpaints.com.

High viscosity acrylic artist colors: Liquitex Artist Acrylic, www.liquitex.com.

Paper: Leneta opacity charts, Form 3B (7⅝ × 11⅜ inch, 19.4 × 28.9 cm), The Leneta Company, www.leneta.com.

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Résumé — *Une méthode de reproduction des couleurs basée sur les données instrumentales acquises par spectrophotométrie en réflexion non destructive peut être utilisée pour sélectionner un pigment pour la retouche. Ceci est utile quand on a affaire à du métamérisme, particulièrement en art moderne, où le nombre de colorants à la disposition des artistes et des restaurateurs est considérable. Des méthodes simplifiées ont été développées pour la conservation, dans lesquelles une teinte unique de chaque pigment mélangé à du blanc est requise pour définir les propriétés optiques d'un pigment en se basant sur la forme de la constante simple de Kubelka-Munk (K-M) de la théorie des milieux turbides. Théoriquement, cette simplification peut conduire à des erreurs dans la sélection du pigment pour les couleurs sombres et pour les couleurs ne contenant pas de blanc. Dans ce cas, la forme de la constante double de K-M peut être utilisée, pour laquelle les hypothèses du modèle se rapprochent beaucoup des propriétés optiques des matériaux de retouche. On a comparé les deux formes en utilisant quatre peintures acryliques en émulsion ayant des propriétés d'absorption et de diffusion différentes. On a trouvé ainsi que la méthode simplifiée était inadéquate pour les peintures ayant un pouvoir de diffusion appréciable qui variait selon le spectre, et que conséquemment la sélection du pigment pouvait résulter en un nombre plus élevé de pigments que celui réellement nécessaire. On a également montré que seulement deux échantillons par pigment sont nécessaires pour utiliser la forme de la constante double : la pleine couleur et une nuance.*

Zusammenfassung — *Instrumentenbasierter Farbabgleich mit Hilfe zerstörungsfreier Spektrophotometie kann bei Retouchen bei der Auswahl von Pigmenten hilfreich sein. Dies ist besonders bei starken Metamerieeffekten nützlich, insbesondere in moderner Kunst, wo eine Vielzahl von Farbmitteln für Künstler und Konservatoren verfügbar ist. Vereinfachte Methoden für die Konservierung, bei denen eine einfach mit weiß gemischte Farbe zur Definition der Pigmenteigenschaften gewählt wird, sind auf Basis der Ein-Konstanten Kubelka-Munk (K-M) – Theorie für trübe Medien entwickelt worden. Theoretisch kann diese Vereinfachung bei dunklen Farben und Farben, die nicht mit Weiß ausgemischt sind, zur Auswahl falscher Pigmente führen. Die Zwei-Konstanten K-M-Theorie kann bei der Wahl von Retouchiermaterial zu einem Model mit stärker an der Wirklichkeit orientierten Annahmen führen. Beide Modelle werden anhand von Acrylemulsionen einer Reihe von Pigmenten bezüglich ihrer Absorptions- und Streueigenschaften verglichen. Es konnte gezeigt werden, dass die vereinfachte Methode bei Farben mit nennenswerter, wellenlängenabhängiger Streuung nicht adäquat war und als Konsequenz eine größere Auswahl an Pigmenten verwendet wurde, als benötigt. Für die Einführung einer Zwei-Konstanten Technik wurden pro Pigment nur zwei Untersuchungen benötigt: Der mass tone und der Farbton.*

Resumen — *La imitación del color por medios instrumentales utilizando espectrofotometría no-destructiva de reflexión puede ser usada como método de ayuda a la hora de seleccionar los pigmentos en la reintegración pictórica. Tal técnica es especialmente útil cuando nos enfrentamos a la problemática del metamerismo, especialmente en arte moderno, en el que el número de colorantes disponibles para los artistas es muy amplio. Ciertos métodos simplificados han sido desarrollados para la restauración de arte, en los que la coloración de cada pigmento mezclado con blanco se precisa para definir las propiedades ópticas basadas en una constante sencilla: la teoría del medio túrbido de Kubelka-Munk (K-M). Teóricamente esta simplificación puede conducir a errores en la selección de pigmentos para las zonas oscuras que no contengan blanco. Por el contrario, la forma de doble constante de la teoría K-M puede ser usada cuando las suposiciones del modelo se igualan más a las características ópticas de los materiales de retoque. Se compararon los dos métodos utilizando cuatro emulsiones acrílicas con variedad de valores absorción de pigmento y de propiedades de dispersión de la luz. Se observó que el método simplificado era inadecuado para pinturas con apreciables dispersión de la luz y*

selectividad espectral, y, como consecuencia, el proceso de selección de pigmentos podía resultar en un número mayor de pigmentos de los que realmente se necesitaban. Se llegó a la conclusión de que solo dos muestras por pigmento se requerían para llevar a efecto la técnica de las dos constantes: el tono de masa y la coloración.