Kubelka-Munk model of full-gamut oil colour mixing

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Kubelka-Munk theory (K-M) describes the spectral interaction of light with thin permeable media such as paint [1]. It has found widespread use as an accurate model of colour mixing. Usage often involves characterising a set of base paints[1] by measuring the concentrations and reflectance spectra of standardised mix samples, deriving absorption and scattering spectra for each base paint, and using these spectra to predict the colour of new mixes. This paper demonstrates an efficient, accurate application of K-M to a limited palette of five Winsor & Newton oil paints applied in an opaque or *alla prima*[2] method, achieving an average error of 1.49 ΔE_{00} with 33 mixes. A mix sampling technique is proposed such that the mixed colours comprising the K-M dataset are minimal in quantity, and well-distributed throughout the colour gamut accessible with the base paints, or "full-gamut". K-M concentration is specified by proxy of base paint mass; accounting for the different oil absorptions and mass densities of the base paints was not found to give any improvement. Model generality was confirmed by holdout cross-validation.

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Introduction

K-M holds that light incident on a paint film is absorbed by, and scattered between, individual pigment particles. These microscopic phenomena are denoted with the macroscopic quantities K and S respectively. For fully opaque paints such as are considered herein, the reflectance R of a paint film simplifies to a function of K/S, or the ratio of absorption to scattering, at each wavelength λ. The perceived colour of a paint film is a function of its reflectance spectrum $R(\lambda)$, along with models of the illuminant and observer.

[1] "Base paints" here refers to any set of pure, unmixed paints directly from manufacturer's tubes, from which other colours may be mixed.

[2] *Alla prima* refers to a technique in which a painting is completed "all at once" or "at first attempt" with an opaque application of paint, rather than gradually with transparent layers, as is also common.

There is no known method for directly measuring the absorption and scattering spectra, *K* and *S*. Instead, various indirect methods have been demonstrated using standardised mix samples. Haase and Meyer created tints of their base paints that were 95% white by mass, and idealised white as having S=1 for all wavelengths λ,[3] allowing direct calculation of *K* and *S* from a single mix [2]. Similarly, Kirchner tinted with 50% and 10% white, while adding shades of 99% and 97% black, as well as measuring pure base paints [3]. The spectra developed from these two datasets (Haase and Meyer; Kirchner) were shown to accurately reproduce the associated colour measurements. However, these methods based on tinting and shading do not produce a full-gamut set of colours, particularly for a limited palette. For example, yellow and blue are known to produce green, but conventional sampling methods would generate no samples of this hue, leading to larger model extrapolations in this region of the colour gamut.

An alternate method of mix sampling is described by painter Richard Schmid, having earlier been advanced by Bill Mosby [4, p.212-225]. Schmid's method entails mixing every base paint with every other base paint, in both a dominant and non-dominant capacity, at five levels of tinting including zero percent. In contrast to conventional methods, Schmid's method is designed to be full-gamut, and was therefore hypothesised to confer benefit in K-M. This paper is believed to be the first application of Schmid's method to K-M.

This remainder of this paper is organised into several sections that collectively describe an investigation of Schmid's method within the K-M framework. First, a set of base paints is identified, and Schmid's method is adapted to create a set of mix samples. Then, *K* and *S* spectra are derived for each base paint using the reflectance spectra of the mix samples, and validated by simulating the measured colours of the mix samples. Last, the base paint compositions are analysed for potential benefit to model accuracy, and the model is cross-validated using various holdout schemes.

Paint selection

Five base paints are used: burnt umber (BU), cadmium red deep hue (CR), cadmium yellow pale hue (CY), cobalt blue hue (CB), and titanium white (TW). These constitute a conventional limited palette from which most other colours of interest can be produced as mixes. All paints are from Winsor & Newton's Winton Oil Colour line, and are rated as opaque, permanent, and lightfast [5]. The binder is linseed oil, except titanium white which is bound with safflower oil.

Sample method

Since Schmid's method was originally developed as a tool for painters, it lacks the technical definition that is required for use in K-M. It was therefore formalised by introducing several new parameters so that it was fully defined. The original method as applied to this set of five base paints would have yielded 81 samples (20 samples per non-white base paint, plus pure white) which was considered impractical and excessive for a K-M application. The specifications of the mix dataset were chosen as follows.

Dominance fraction here refers to the fraction of the dominant (i.e. greater in mass) non-white base paint to the total non-white paint mass. A value of 0.75 was taken by bisecting the limiting range of 0.5

[3] As shown later, this is approximately equivalent to assuming $K = 0$, since $R(\lambda) \approx 1$, given the white colour.

to 1.0. Two tinting levels were taken so that the average number of mixes per base paint was comparable to Kirchner's method.

A *tinting fraction*, or fraction of non-white to white paint by mass, of 0.50 was chosen on the basis that colour saturation is maximised at intermediate value. A target mass of 1.000 g of paint per sample was found to be sufficient to opaquely[4] cover a square region measuring about 19 mm wide. An ingredient tolerance of ± 0.050 g was chosen based on the level of precision that could be practically achieved with a manual process. These base paint masses were then converted to concentrations by dividing them by the total mass of the mix.

In total, 33 samples were produced according to these specifications, of which 5 were masstones (i.e. pure base paints) and 28 were mixes. Of these mixes, 16 had two ingredients, and 12 had three ingredients, the third being titanium white. These samples are shown in Figure 1.

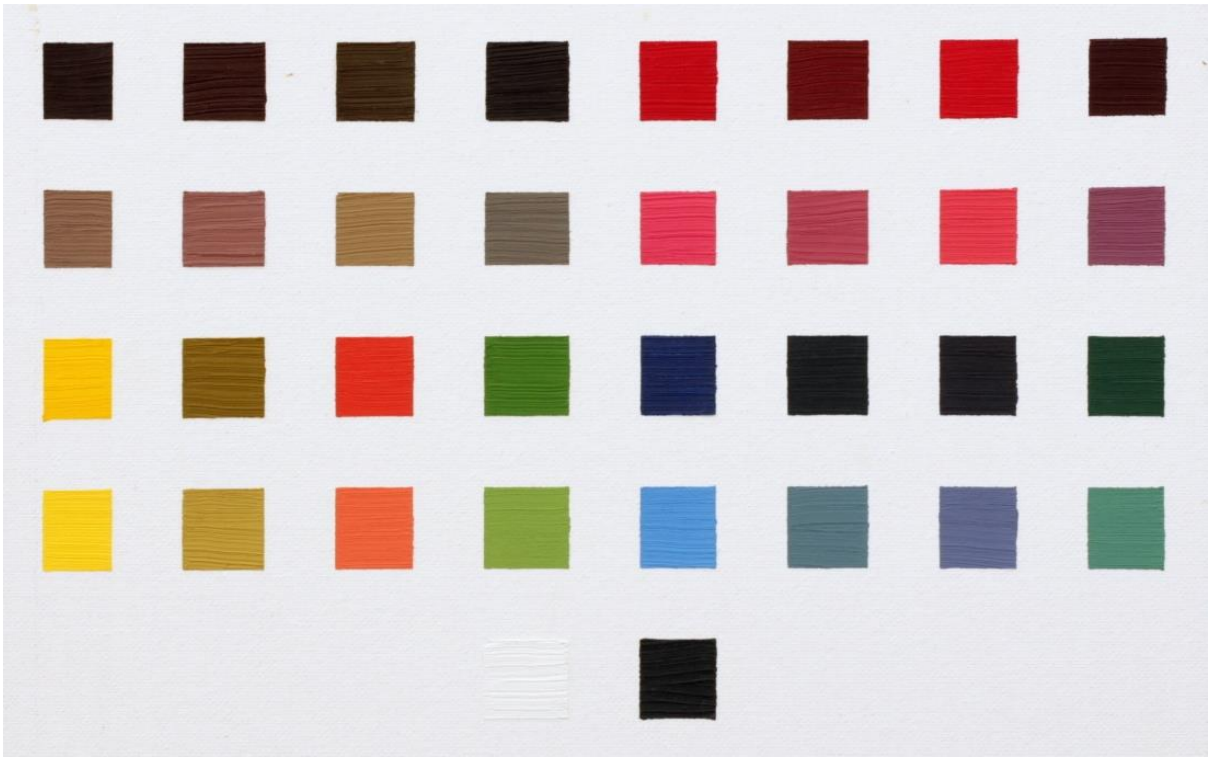

Figure 1: Colour samples according to an adaptation of Schmid's method with five base paints and two tinting levels. Each square measures about 19 mm wide. An additional sample of pure ivory black was included for image calibration (bottom row, right).

Each sample was scanned with a calibrated Variable Spectro 1 spectrophotometer, measuring the fraction of light reflected at each wavelength from 400 to 700 nm with 10 nm spectral resolution. These reflectance spectra are shown in Figure 2. Base paint concentrations were measured by mass using a consumer-grade scale with 0.001 g precision, calibrated with a 200 g weight. These concentrations are shown in Figure 3, further ahead in the text after supporting discussion.

[4] Opaque application enables use of the "infinitely thick" formulation of K-M, and was verified by visual inspection.

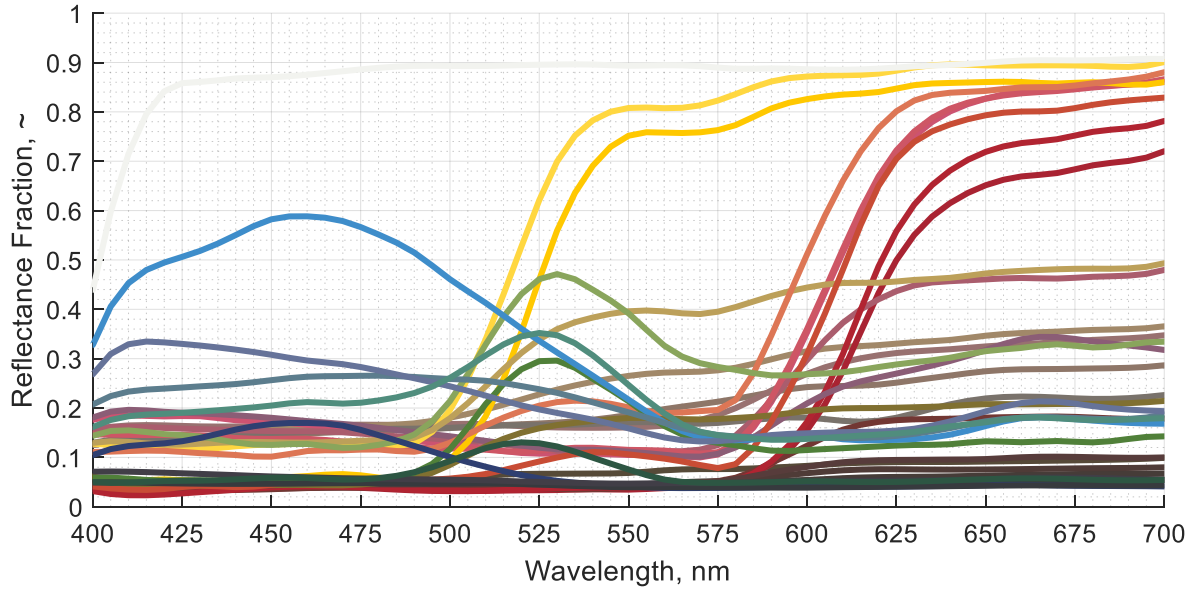

Figure 2: Reflectance spectrum and colour as measured by spectrophotometer for each sample.

Calculating spectra

Walowit *et al.* (WMB) solve a system of linear equations containing base paint concentrations and K/S values at each wavelength λ to find $K(\lambda)$ and $S(\lambda)$ using a linear least-squares method [6]. This method is flexible, as it makes no stipulations about the quantity or composition of the samples, provided that the system is mathematically well-posed. Centore observed that the residuals in WMB are implicitly unweighted, and improved this method by introducing "perceptual reflectance weighting" [7]. Centore's method was found to outperform WMB and is used herein [8].

Simulating mixes

The absorption and scattering spectra of a colour mix, $K_m(\lambda)$ and $S_m(\lambda)$, are linear combinations of the ingredient spectra $K_i(\lambda)$ and $S_i(\lambda)$, in proportion to their concentrations c_i, with the ingredient index i from 1 to n, the number of ingredients:

$$K_m = \sum_{i=1}^{n} K_i c_i \quad (1)$$

$$S_m = \sum_{i=1}^{n} S_i c_i \quad (2)$$

By definition, the concentrations of the ingredients in a mix sum to unity:

$$\sum_{i=1}^{n} c_i = 1 \quad (3)$$

The opaque formulation of K-M states that at each wavelength λ, reflectance R(λ) is given by:

$$R = 1 + \frac{K}{S} - \sqrt{\left(\frac{K}{S}\right)^2 + 2\frac{K}{S}} \quad (4)$$

This can be rearranged to solve for the ratio K/S:

$$\frac{K}{S} = \frac{(1-R)^2}{2R} \quad (5)$$

Tristimulus colour *XYZ* is calculated using the CIE 1931 2° observer functions $\bar{x}, \bar{y}, \bar{z}$, and the CIE D65 illuminant representing natural midday light [9-10]. This colour is then converted to sRGB for display, and to CIELAB for colour difference calculation.

Model validation

These spectra were validated together with concentration data by simulating the colour of each mix, and comparing it against the measured colour reported by the spectrophotometer. This colour difference, or error, is quantified using ΔE_{00} in CIELAB, while the sRGB colours are superimposed for qualitative comparison. The average colour error for all samples was 1.49 ΔE_{00}, which is slightly higher than the expected range from literature of 0.9-1.1 ΔE_{00} [3, 11]. This may be attributable to the exclusion of black mixes, which can be useful for improving estimation of S spectra. Results are shown in Figure 3.

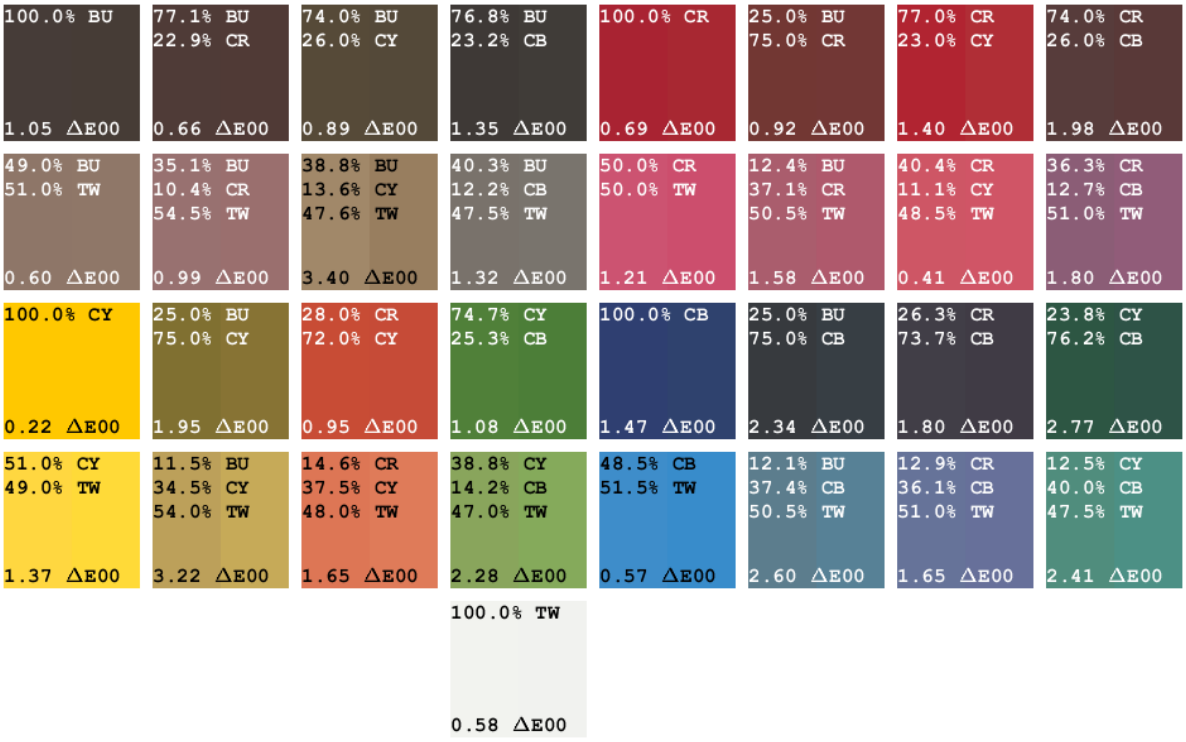

Figure 3: Comparison of measurement and model. Each of the 33 squares corresponds to a single sample, and shows the ingredient concentrations (top), measured colour (left half), simulated colour (right half), and colour difference (bottom).[5]

[5] These colours are accurate reproductions of the calculated sRGB values, but their appearance may vary depending on the device and conditions with which they are viewed.

Specifying concentration

Paint mass is often taken as a convenient proxy for the relative amount or concentration of the ingredient in a K-M sample, because it can be easily and accurately measured with a scale. In its simplest form, oil paint consists of dry pigment powder suspended in a natural oil binder. Its colours derive from its pigments, which vary in their mass density and oil absorption. Accordingly, it was hypothesised that specifying concentration using pigment mass or pigment volume could improve the model's accuracy. For completeness, paint volume was also considered. In total, four proxies for concentration were considered: paint mass, paint volume, pigment mass, and pigment volume.

The composition of the commercial paint used here is not publicly known, but the pigments are reported. As such, the oil absorption ratios (OAR) were estimated by lookup [12]. Using these quantities, the approximate density of oil at 0.95 g/mL, and the measured mass of paint in each of the 200 mL tubes, approximate values were produced for the physical properties of the paints used [13]. A summary is given in Table 1.

Paint Name	**Source**	**Burnt Umber**	**Cad. Red Deep Hue**	**Cad. Yellow Pale Hue**	**Cobalt Blue Hue**	**Titanium White**
Pigment(s)	Vendor	PBr7	PR170, PO36	PY74	PW5, PB29, PB15:1	PW6, PW4
OAR, g Oil/100 g Pig.[6]	Lookup	20.0	59.3	52.5	34.3	20.0
Full Tube Mass, g	Meas.	271.870	322.310	321.290	355.655	410.980
Full Tube Paint Mass, g	Meas.	236.810	287.250	286.230	320.595	375.920
Pigment Mass Frac., ~	Derived	0.83	0.63	0.66	0.74	0.83
Paint Density, g/mL	Derived	1.18	1.44	1.43	1.60	1.88
Pigment Density, g/mL	Derived	1.25	2.06	1.95	2.10	2.34

Table 1: Approximate physical properties of paints used.

Using dimensional analysis, the measured paint masses were converted to estimated paint volumes, pigment masses, and pigment volumes. The K and S spectra were separately calculated and validated for each of these four concentration proxies. It was found that paint mass (1.49 ΔE_{00}) did not significantly outperform paint volume (1.49 ΔE_{00}), pigment mass (1.51 ΔE_{00}), or pigment volume (1.53 ΔE_{00}). This suggests that accounting for paint composition does not significantly improve or affect model accuracy. This could be determined more conclusively with manufacturer data, or with direct control of the mulling process by which the pigment is suspended in the binder.

[6] Taken as an average of all OAR ranges for all constituent pigments.

Cross-validation

The model was cross-validated by a holdout method, partitioning the mix dataset into training and testing subsets. This statistical technique verifies that the model is detailed enough to reproduce known measurements (training), while also being general enough to reproduce unknown measurements (testing). Several permutations were analysed. A summary is shown in Table 2.

			Error, ΔE_{00}			
No.	**Training Subset**	**Testing Subset**	**Training, Average**	**Training, Max**	**Testing, Average**	**Testing, Max**
1	All mixes (33)	No mixes (0)	1.49	3.40	-	-
2	LOOCV (32)	LOOCV, skipping masstones (28 × 1)	-	-	2.11	4.85
3	Remainder (17)	Non-white masstones, three-ingredient (16)	1.18	3.56	2.26	3.96
4	Remainder (21)	Three-ingredient mixes (12)	1.25	2.69	2.37	4.24
5	Remainder (29)	Non-white masstones (4)	1.46	3.33	2.15	4.41

Table 2: Summary of cross-validation results.

It was found that the non-white masstones (4 total) and all three-ingredient mixes (12 total) could be withheld from the training dataset with only minor penalty. This result is shown in Figures 4 and 5. Leave-one-out (LOOCV)[7] was also performed, skipping masstones, which showed only a minor increase in average error to 2.11 ΔE_{00}, which is consistent with the average error of 2.22 ΔE_{00} reported by Kirchner for unseen samples [3]. Several additional permutations were attempted, but were found to produce errors in Centore's method.

Figure 4: Holdout cross-validation training dataset, 1.18 ΔE_{00}.

[7] In LOOCV, the model is first trained on all samples except one, then tested on the single withheld sample. This process is then repeated for all samples of interest.

Figure 5: Holdout cross-validation testing dataset, 2.26 ΔE_{00}.

The ability of the model to withstand substantial and variable losses in training data confirms its generality and the absence of overfitting. These findings suggest a quantitative benefit of Schmid's method compared to conventional methods, though a direct comparison with equal sample quantities could not be produced from this dataset. Although model accuracy improves with sample quantity, diminishing returns are observed around five to seven samples per base paint, where colour errors become mostly imperceptible. For practical purposes, the sample quantity proposed herein was found to be minimised to its approximate natural limit.

Conclusions

This paper demonstrates an accurate model of colour mixing for a limited palette of five commercially available opaque oil paints. The average error was found to be 1.49 ΔE_{00} for the training dataset, and 2.11 ΔE_{00} for an independent dataset simulated by means of LOOCV. Schmid's method was adapted to produce 33 samples that were well distributed throughout the colour gamut that is accessible with the base paints. Centore's method of spectral derivation was used to minimise perceptual colour error. Specifying K-M concentration using estimates for pigment mass, pigment volume, and paint volume gave no significant improvement compared to the more convenient proxy of paint mass. By holdout cross-validation, the model was shown to retain accuracy for unseen samples, confirming its generality, while suggesting that the sample quantity had been minimised to its approximate natural limit. Accordingly, this method is both accurate in minimising colour error, and efficient in minimizing sample quantity.

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