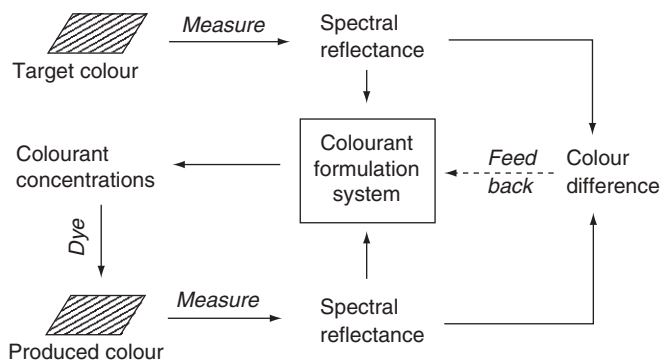

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8.1 Introduction

Formulating colourant recipes to match target colours is not an easy task. Manual colour prediction often uses a trial and error method, for which the experience of the colourist is essential. The majority of colour matches also require colours to be matched not only under daylight, but also under other artificial light sources, typically cool white fluorescent (CWF) and incandescent sources. A previous recipe archive is very useful for manual colour matching. A colourist would firstly search the previous recipe archive to find out the closest colour matching the target (or standard) and then make some adjustment to the recipe if the recipe colour is not the exact match to the target. However, this trial and error process can be lengthy and arduous even for a professional colourist.

Computer colourant formulation is an alternative method. The commercial application of computer colour recipe formulation in textiles was first disclosed by Alderson *et al.* in 1961.¹ The most well-known algorithms for colour recipe formulation are the two proposed by Allen, one for the single-constant and the other for two-constant formulation.^{2,3} In recent years, computer colourant formulation has been widely applied, especially when supplying the coloured articles to companies with global sourcing practice, thanks to the formidable advance of the digital computer, especially the personal computer. This greatly improves the lead-time for the colour matching, especially when experienced colourists are not available. It has become a necessity for a modern dyehouse to install a computer colourant formulation system.

The flowchart of the coloured goods production process employing a colourant formulation system is illustrated in Fig. 8.1. The spectral reflectance of a target colour is first measured using a spectrophotometer, and the colourant concentrations are computed using the colourant formulation system. These concentrations are used in the colouration process to produce the matching coloured goods. If the colour difference between the target



8.1 Flow chart of colour production process using colour recipe prediction.

and the produced colour is too large to be accepted, the recipe should be corrected. As the dyeing and colour quality control processes are usually costly and time consuming, it is important and still very challenging for any colourant formulation system to be 'right first time' in colour matching with a generally acceptable colour difference.

8.2 Colourant recipe formulation

Colour matching to a target depends not only on the formulation system but also on the accuracy of the recipe preparation, the repeatability of the dyeing process and the colour measurement process. There is a need for quality control at each step in the colouration and measuring processes. The core of the formulation system is based on the theory developed by Kubelka and Munk (K–M theory).^{4,5} As the theory involves quite a few assumptions that are necessary for the prediction of the colourant concentrations, the real dyes and pigments do not ideally conform to these assumptions. Therefore, the K–M theory is only an approximation to the real pigmented systems. Nevertheless, methods to improve the prediction accuracy are available in certain commercial colourant formulation systems. In addition, methods based on artificial intelligence can also be employed in recipe formulation. The scope of this chapter is delimited to the colourant formulation of the textile materials. The colourant formulation for plastics and paints can be found elsewhere.⁹

8.2.1 Kubelka–Munk Theory

When light passes through a pigmented layer, two things will happen: part of the light is absorbed by the pigments and the medium in which pigments

are dispersed; part of the light is scattered by the pigments. K–M theory is based on earlier research by Schuster,⁶ who studied the weakening of light from the stars by scattering and absorption before reaching the observer. However, pigmented systems are more complicated because of the interaction between pigments, especially when the pigment loading is high. Therefore, K–M theory has to simplify the real situation in order to derive any useful mathematical equations. In practical colourant formulation, we are restricted to the following assumptions:

1. diffuse illumination and diffuse viewing without polarisation of the light,
2. a plane parallel surface of the object without light losses at the edges,
3. the unit layers of the material are homogeneous and isotropic,
4. the theory does not account for the presence of large particles, agglomeration or orientation of the particle in the layer, and
5. optical contact with the next layer.

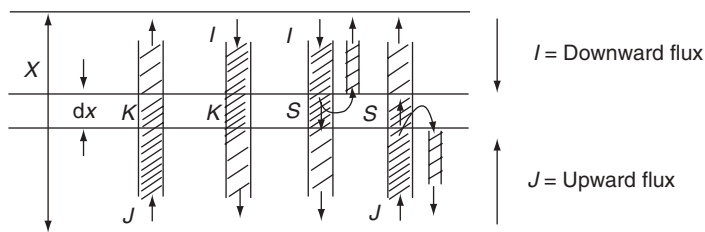
Figure 8.2 shows a simplified case of light passing through a very thin layer of thickness dx . We consider the downwards and upwards components of the incident light separately, and assume that the absorption coefficient is denoted by K and the scattering coefficient by S . Then, the downward flux (intensity I) is given as

$$dI = -KI \, dx - SI \, dx + SJ \, dx \quad [8.1]$$

and the upward flux (intensity J) is given as

$$dJ = -KJ \, dx - SJ \, dx + SI \, dx \quad [8.2]$$

We note that light loss through the edges is neglected. The internal reflection that exists when leaving an optically denser medium, e.g. light leaving from textile fibres, which is optically denser than air, is also neglected by the theory. Other assumptions such as uniform distribution of the pigments, etc., may also differ from the real situation.



8.2 Schematic diagram of the simplified version of light passing through a finite colourant layer used in K–M theory.

A series of the solutions can be obtained by solving the differential equations (eqn 8.1) and (eqn 8.2). These solutions and the examples of how they can be used are given by Judd and Wyszecki.⁸ In textile formulation, the solution can be even more simplified. Firstly, textile fabrics can be considered opaque because the measurements are made at sufficient thickness of the fabric swatches. Secondly, the scattering coefficients of the textile dyes are negligible when compared with the substrate in which they are dissolved, so that only the scattering coefficient of the substrate needs to be considered. Thirdly, it can be assumed that the total absorption and scattering is the summation of those from each individual colourant, i.e. the absorption and scattering are additive. Hence, we obtain the following equation:

$$R_{\infty} = 1 + (K/S) - [(K/S)^2 + 2(K/S)]^{1/2} \quad [8.3]$$

and its inverse

$$K/S = \frac{(1 - R_{\infty})^2}{2R_{\infty}} \quad [8.4]$$

where R_{∞} is the reflectance of a colour sample of optically infinite thickness.

In K–M theory, the absorption and scattering coefficients of a colour sample can be further represented using absorption and scattering coefficients of the individual pigments or dyes:

$$\begin{aligned} (K/S)_{\text{mixture}} &= (K/S)_1 + \dots + (K/S)_n \\ &= K_1/S_{\text{sub}} + \dots + K_n/S_{\text{sub}} + K_{\text{sub}}/S_{\text{sub}} \end{aligned} \quad [8.5]$$

where K_1 to K_n are the absorption coefficients of the dyes, K_{sub} and S_{sub} are the absorption and scattering coefficients of the substrate, respectively.

From (eqn 8.3)–(eqn 8.5), it can be seen that, for a dye system, the reflectance of the coloured sample can be predicted from only the ratio of the absorption coefficient of each dye in the mixture and the scattering coefficient of the substrate, i.e. K_n/S_{sub} . The various K/S_{sub} ratios may be considered as a single constant, which are commonly called ‘absorption coefficients’ in textile dye formulation, and the theory is therefore known as single-constant K–M theory.²

The absorption coefficient for a colourant is related to its concentration and, in many cases, the relationship is a non-linear one with the exhaustion decreasing with an increase in dye concentration. In practice, a range of concentrations will be used to obtain a so-called calibration database by dyeing, and an absorption coefficient is correlated to the corresponding dye concentration in the dye bath. Using this calibration database, the absorption coefficient at a given concentration can easily be found.

8.2.2 Calibration database

As described above, a calibration database is necessary for a formulation system to establish the relation between the K/S values and the concentrations for each dye. Because formulations are based on the database, its preparation should be carried out using exactly the same substrate and dyeing conditions as those of the formulated recipes to be subsequently used. For example, if in the calibration database, plain woven cotton fabric is used as the substrate, the formulated recipe should be used only for the dyeing of the plain woven cotton fabric. Any change in substrate, whether it is the reflectance or the absorbance property, would be expected to give inaccurate results. The same is true for other conditions such as dyebath pH, temperature, liquor ratio, etc. One difficulty in that aspect is that laboratory dyeings that are used for preparing the database do not always represent the bulk production dyeings and there is often no clear relation between laboratory and bulk dyeings.

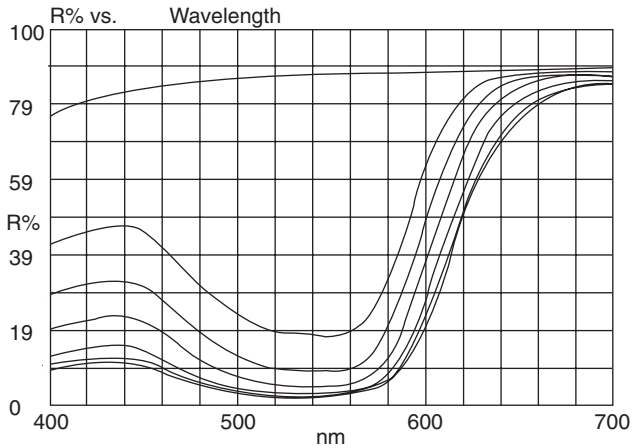
Since colour matching relies on the calibration database, accurate preparation of the database is essential. Any error in the database can subsequently affect the formulation. Good computer formulation systems should be able to detect abnormal points in the database preparation only if these points are scarce in comparison with the rest of the normal points.

The database consists of the calibration dyeings of each dye used in the system. Usually, six or more calibration dyeings are required for each dye in order to cover the concentration level of, say, from 0.05% to 2.0% of the weight of the fabric. The highest concentration level should comply with the recommendations of the dyestuff manufacturer. Additional errors may be introduced if a formulated recipe uses a dye at much below or much above the concentration range of its calibration dyeing.

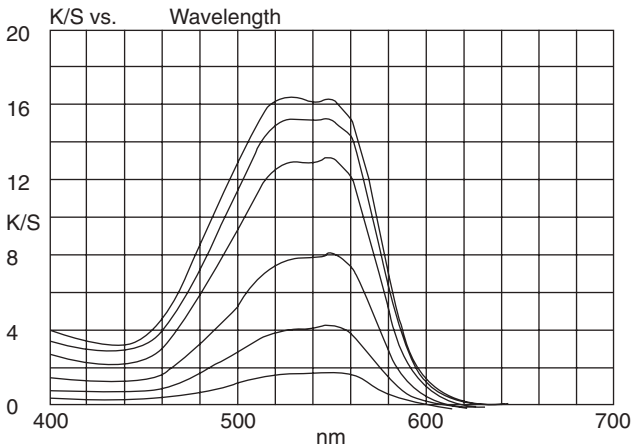
An example of the acid dye on wool is given below. Figure 8.3 is the reflectance data of calibration samples at different concentrations plotted against wavelength. The K/S value of each calibration sample can be calculated according to (eqn 8.4), and its distribution against wavelength is plotted in Fig. 8.4. The K/S values against concentration at a maximum absorption wavelength of 520 nm are shown in Fig. 8.5. A non-linear relationship exists between the K/S value and the concentration of the colour sample.

In commercial computer colourant formulation systems, the K/S values and their corresponding concentrations for all calibration dyeings are stored. The recipe formulation function uses these values for linear interpolation.^{8,9} For example, at a concentration c_{target} , the K/S value of the target is given by:

$$(K/S)_{\text{target}} = (K/S)_{\text{low}} + B[(K/S)_{\text{high}} - (K/S)_{\text{low}}] \quad [8.6]$$



8.3 Reflectance of dye Ramazol Red 3BS at different concentrations plotted against wavelength.



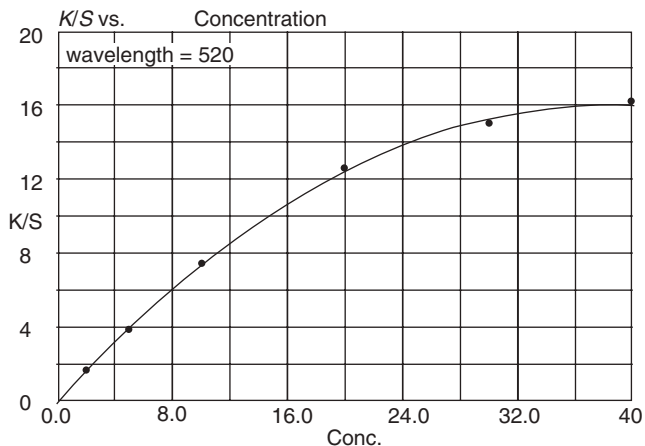
8.4 K/S values of dye Ramazol Red 3BS at different concentrations plotted against wavelength.

where

$$B = (c_{\text{target}} - c_{\text{low}}) / (c_{\text{high}} - c_{\text{low}}) \quad [8.7]$$

and c is the dye concentration and the subscripts low and high denote the two neighbouring points in the calibration data.

In some cases, the use of second-order or third-order polynomial equations and curve-fitting techniques to find the correlation between the K/S



8.5 K/S values of the six Ramazol Red 3BS calibration data plotted against the dye concentration (g/l) at 520 nm.

values and concentration can smooth out certain fluctuation of the calibration dyeings to overcome dyeing errors, without the need for re-dyeing. However, if a calibration dyeing sample is far from the trend of the rest of the calibration samples, it should be re-dyed. Equation (8.8) below is an example of a third-order polynomial equation:

$$(K/S)_{\text{target}} = a_1c + a_2c^2 + a_3c^3 + K_{\text{sub}}/S_{\text{sub}} \quad [8.8]$$

where a_1 , a_2 and a_3 are the coefficients. The coefficients are optimised from the calibration database and are stored by the system for use in recipe formulation. The K/S value for a given concentration can be found using (eqn 8.8).

Some early commercial systems may have taken the physical–chemical approach, which models the relationship between K/S and dye-in-fibre using the Langmuir isotherm for dye absorption, which results in a relationship with two coefficients.¹⁰

8.2.3 Recipe formulation

In this section, we discuss the colour recipe formulation of non-fluorescent textile samples, as the K–M theory cannot be applied to fluorescent materials. It is known that recipe formulation can be carried out using colorimetric and spectrophotometric matching algorithms.⁹ Spectrophotometric matching algorithms minimise the reflectance difference between the target and prediction:

$$\sum_{\lambda} [R_{\lambda,\text{target}} - R_{\lambda,\text{prediction}}]^2 \rightarrow \min \quad [8.9]$$

where λ represents wavelengths from 400 to 700 nm with a 20 nm interval. According to (eqn 8.4) and (eqn 8.9), we have the equation at wavelength λ :

$$(K/S)_{\lambda,\text{target}} = (K/S)_{\text{sub},\lambda} + (K/S)_{1,\lambda} + \dots + (K/S)_{n,\lambda} \quad [8.10]$$

where n is the number of colourants in a mixture, which is usually equal to 3. In the case of a 20 nm interval, there are 16 simultaneous equations. This over-determined system can be solved using the least-squares method.

Though the spectrophotometric algorithm is very straightforward, it is restricted to a non-metameric match. In other words, the optical properties of the substrate and the dyes used by both the target and the match should be spectrally very similar, otherwise the algorithm will often give poor matching results. Another drawback is that human eyes are more sensitive to lights at certain wavelengths than at others in the visual spectrum. Thus, the reflectance differences at the wavelengths that are more sensitive to human eyes are more important in colour matching than others. The spectrophotometric curve matching does not take this into consideration. Attempts can be made to give carefully selected weights at different wavelengths¹¹:

$$\sum_{\lambda} w_{\lambda}^2 [R_{\lambda,\text{target}} - R_{\lambda,\text{prediction}}]^2 \rightarrow \min \quad [8.11]$$

where weights w_{λ} reflect the importance of different wavelengths for visual perception. It is reported that the spectrophotometric strategy is not as successful in diminishing colour difference for a particular illuminant as the colorimetric strategy.¹¹ Nevertheless, the spectrophotometric strategy does produce more ‘balanced’ colour differences between different illuminants, and can therefore be used to reduce metamerism.

In most commercial systems, the colorimetric matching algorithm to minimise ΔX , ΔY , and ΔZ has now been universally adopted. This algorithm is based on the strategy

$$(\Delta X, \Delta Y, \Delta Z) \rightarrow (0, 0, 0) \quad [8.12]$$

Colorimetric matching is very effective because it minimises the colour difference directly. Smaller differences in ΔX , ΔY and ΔZ result in closer colour match. The drawback of colorimetric matching is that a match achieved under a particular illuminant (e.g. D65) may not be a match under another illuminant (e.g. A), especially when different types of dyes are involved. This type of match is the so-called metameric match, i.e. the reflectance curve of the predicted sample is very likely different from that

of the standard and, when plotted, these two reflectance curves have at least three cross-over points.

We show below how a three-dye recipe is formulated using colorimetric matching according to the following steps.

1. Select the starting concentrations c_1 , c_2 and c_3 .
2. Use (eqn 8.6) or (eqn 8.8) (depending on how the system establishes the relation between K/S values and the concentrations) to obtain the K/S of each colourant in the mixture.
3. Use (eqn 8.5) to obtain the K/S value of the mixture assuming these colourants are additive.
4. Use (eqn 8.3) to calculate the reflectance of the predicted sample. The tristimulus values X , Y and Z can, thus, be obtained using the illuminant required for the matching.
5. Calculate the colour difference between the standard and the match and if the colour difference is smaller than the tolerance, the recipe is found.
6. If the colour difference is larger than the tolerance, the following matrix is devised:

$$\begin{bmatrix} \Delta X \\ \Delta Y \\ \Delta Z \end{bmatrix} = \begin{bmatrix} \frac{\partial X}{\partial c_1} & \frac{\partial X}{\partial c_2} & \frac{\partial X}{\partial c_3} \\ \frac{\partial Y}{\partial c_1} & \frac{\partial Y}{\partial c_2} & \frac{\partial Y}{\partial c_3} \\ \frac{\partial Z}{\partial c_1} & \frac{\partial Z}{\partial c_2} & \frac{\partial Z}{\partial c_3} \end{bmatrix} \begin{bmatrix} \Delta c_1 \\ \Delta c_2 \\ \Delta c_3 \end{bmatrix} \quad [8.13]$$

where

$$\begin{aligned} \frac{\partial X}{\partial c_i} &= \sum E_\lambda \bar{x}_\lambda \frac{\partial R_\lambda}{\partial c_i}, \\ \frac{\partial Y}{\partial c_i} &= \sum E_\lambda \bar{y}_\lambda \frac{\partial R_\lambda}{\partial c_i}, \\ \frac{\partial Z}{\partial c_i} &= \sum E_\lambda \bar{z}_\lambda \frac{\partial R_\lambda}{\partial c_i} \end{aligned} \quad [8.14]$$

and in (eqn 8.14):

$$\frac{\partial R_\lambda}{\partial c_i} = \frac{dR_\lambda}{d[(K/S)_\lambda]} \frac{\partial [(K/S)_\lambda]}{\partial c_i} \quad [8.15]$$

where E_λ is the illuminant spectral power distribution, \bar{x}_λ , \bar{y}_λ , and \bar{z}_λ are the CIE standard observer functions, and $\partial[(K/S)_\lambda]/\partial c_i$ can be obtained from (eqn 8.8) or by linear interpolation using (eqn 8.6), and

$$\frac{d[(K/S)_\lambda]}{dR_\lambda} = \frac{R_\lambda^2 - 1}{2R_\lambda^2} \quad [8.16]$$

and thus

$$\frac{dR_\lambda}{d[(K/S)_\lambda]} = \frac{2R_\lambda^2}{R_\lambda^2 - 1} \quad [8.17]$$

Hence, in (eqn 8.13) all the items are known and the differences for each colourant can be calculated by matrix inversion:

$$\begin{bmatrix} \Delta c_1 \\ \Delta c_2 \\ \Delta c_3 \end{bmatrix} = \begin{bmatrix} \frac{\partial c_1}{\partial X} & \frac{\partial c_1}{\partial Y} & \frac{\partial c_1}{\partial Z} \\ \frac{\partial c_2}{\partial X} & \frac{\partial c_2}{\partial Y} & \frac{\partial c_2}{\partial Z} \\ \frac{\partial c_3}{\partial X} & \frac{\partial c_3}{\partial Y} & \frac{\partial c_3}{\partial Z} \end{bmatrix} \begin{bmatrix} \Delta X \\ \Delta Y \\ \Delta Z \end{bmatrix} \quad [8.18]$$

The new corrected recipe is then

$$\begin{aligned} c_{1,\text{new}} &= c_{1,\text{original}} + \Delta c_1 \\ c_{2,\text{new}} &= c_{2,\text{original}} + \Delta c_2 \\ c_{3,\text{new}} &= c_{3,\text{original}} + \Delta c_3 \end{aligned} \quad [8.19]$$

Steps 1 to 6 are repeated until the colour difference between the standard and the prediction is within the tolerance limit.

The number of iterations required to obtain the desired recipe depends on the effectiveness of the starting concentration provided in Step 1. If the reflectance of the target is known, the starting recipe can be determined by Allen's² method, where the matrix expression of the starting recipe is given as

$$C = (TEDA)^{-1} TED(F - S) \quad [8.20]$$

where C is the concentration matrix, T is the matrix composed of CIE standard observer functions, E is composed of the spectral power distribution of the matching illuminant, D is composed of the element $dR_\lambda/d[(K/S)_\lambda]$, A is composed of $\partial[(K/S)_\lambda]/\partial c_i$ for each colourant, F is com-

posed of the K/S values of the target and S is composed of the K/S values of the substrate.

The starting concentration determined by this method is often very close to the target. Usually, only several iterations are required to bring the colour difference within the tolerance limit. Commercial recipe formulation systems have the option to sort the predicted recipes according to the cost and the metamerism under a secondary illuminant.

8.2.4 Recipe correction

After recipe formulation, a new colour sample can be produced according to the colourant concentrations suggested. Because of the influence of various variables in the dyeing process, the produced sample may not be acceptable and a recipe correction process may be needed.

Laboratory correction

Laboratory correction gives a fresh recipe according to what was obtained by previous dyeing. The new concentration calculation is as follows:

$$C_{\text{new}} = C_{\text{predicted}} \times C_{\text{used}}/C_{\text{batch}} \quad [8.21]$$

or

$$C_{\text{new}} = C_{\text{predicted}} + C_{\text{use}} - C_{\text{batch}} \quad [8.22]$$

where C_{new} is the corrected recipe, $C_{\text{predicted}}$ is the predicted recipe for the standard, C_{used} is the recipe used in dyeing, which may be equal to $C_{\text{predicted}}$, and C_{batch} is the recipe back-predicted for the batch dyeing result. Correction method (eqn 8.21) is called weighted (or ratio) correction and method (eqn 8.22) is called additive correction.

We note that the use of (eqn 8.21) and (eqn 8.22) above would give relatively similar results for correcting small colour differences. However, for a large colour difference, (eqn 8.22) may give wrong results and the use of (eqn 8.21) is recommended. If a large colour difference exists between standard and batch, correction accuracy is limited. On the other hand, for a small colour difference, the correction accuracy is limited by the repeatability of the dyeing process.

Production correction

Production correction predicts the additional amount of dyes to be added to the dyeing bath:

$$C_{\text{add}} = C_{\text{new}} - C_{\text{used}} \quad [8.23]$$

where C_{new} is calculated according to the laboratory correction via either weighted or additive methods. There is no 'bleed-off' included in the calculation. It may be added if bleeding is a problem.

If a batch is already too dark compared with a standard, this correction for exhaustion dyeing will fail, meaning that the absorbed dyes should be stripped before correction. For continuous dyeing, diluents need to be added to dilute the dye liquor. However, for a slight dark colour, the production correction for exhaustion dyeing should correct hue difference and try to reduce the overall colour difference.

8.3 Improvement of the formulation accuracy

In most current colour formulation systems, K–M theory is applied for recipe prediction. However, there are many situations in which the K–M recipe prediction cannot be used successfully. For example, the prediction result of fluorescent colourants is rather poor. This is mainly due to a breakdown of the K–M assumptions and the failure of the model to describe the optical behaviour of the colourants accurately. Moreover, it is necessary to prepare an accurate calibration database, which would greatly affect the prediction performance. However, sometimes an accurate database cannot be achieved because the samples prepared in the laboratory may not correlate well with the actual dyehouse production samples. Even if the accurate samples can be prepared, a new calibration database will need to be produced if there are changes in dyes and substrates, but for many dye-houses this is prohibitively costly and time consuming.

Consequently, the K–M model has many limitations, which make the prediction unreliable in some cases. Drawbacks of the K–M model have motivated the colourists to develop other methods for recipe formulation. As we know, it is possible for a professional colourist to predict the colourant concentrations with high accuracy even for fairly complex situations without being aware of the K–M theory. Colourists accumulate experience of the behaviour of colourants and have the ability to predict the recipe of a new colour shade from previous ones. Therefore, it is possible to use artificial intelligence techniques such as neural networks to mimic the behaviour of professional colourists.

8.3.1 Artificial neural network¹²

The human brain is a neural network itself. The basic unit of the brain is the neuron, which is a special nerve cell and, although simple creatures may only possess a few thousand neurons, the human brain contains approximately 10^{12} neuron cells. What makes neurons different from other cells in the body is the way in which they are connected to each other. A neuron receives information from other neurons using its dendrites and sends information to other neurons using its axons. The synapse is the point where the axon of one cell meets the dendrite of another. One of the most impor-

tant properties of the brain that we would like to mimic in computer systems is its ability to learn.

The neural network can be considered as a black box that is connected to the world by a series of inputs, which interacts with the world via a series of outputs. Inside the black box, a network system performs a mapping function between its input and output. The units of the neural network are connected by weights that can be modified and they perform a similar function to the connection structure in the brain. Figure 8.6 shows a schematic diagram of the function of a single unit. The unit receives input I_i from n other units. The total input to the unit is the weighted sum of n inputs, that is the sum of each of the n inputs multiplied by the respective value of the weighted connections w_i . The output O of the unit is then given by some transfer function $f(\cdot)$ of its weighted input. Thus, mathematically it can be written as

$$O = f\left(\sum_{i=1}^n I_i w_i\right) \quad [8.24]$$

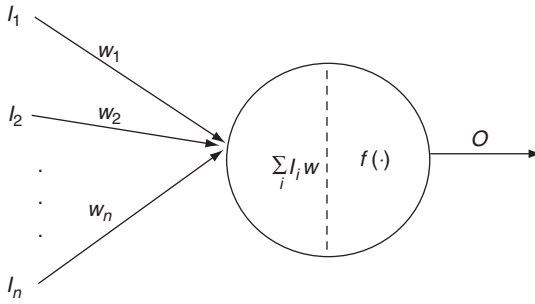
A typical non-linear transfer function is the sigmoid function

$$f(x) = \frac{1}{1+e^{-x}} \quad [8.25]$$

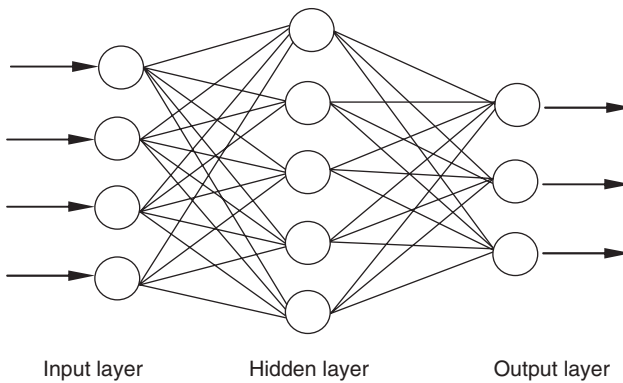
where x is the input of the unit. Non-linear transfer functions are usually due to the function's ability to approximate complex mapping between input and output vectors, while linear transfer functions are sometimes used for units in the output layer.

There are many types of neural networks. The complexity of the neural network is determined by the problem to be solved. One of the simplest and most successful networks is the multi-layer perception (MLP). The MLP consists of simple processing units in layers. Each neuron receives an input and modifies it in a simple way to produce an output. The neural network will contain one or more hidden layers between the input and output layers, and the number of units in each layer also depends on the complexity of the problem. A simple structure of a neural network is shown in Fig. 8.7, which consists of an input layer, a hidden layer, and an output layer.

Before a neural network can be used to solve a given task, it must first be trained using known pairs of input and output vectors. The training process consists of adjusting the weights in the network so that, when a certain input is presented in the input layer, the output layer will produce



8.6 The generalised unit of a neural network.



8.7 A simplified structure of a neural network.

the desired output. Samples of input–output pairs are presented to the input and output layers of the network, respectively. The input vector is used to generate an output for each unit in the network, layer by layer, until an output is produced in the output layer. The error between the target output and the actual output is then calculated, and the network adjusts the weights to reduce this error. This is repeated until the network can accurately predict the correct output vectors for all the training samples. The process of presenting all training pairs to the network and assessing its accuracy of prediction is called an epoch. To reach a desired prediction accuracy, the training process may need several thousand or more epochs. There are several kinds of learning strategies in a neural network for error minimisation, among which back-propagation of the generalised delta rule may be the most well known. The trained network can then be used to calculate the output for given input vectors.

After the training process, a set of testing samples needs to be presented to the neural network in order to test its prediction accuracy. Input vectors of the test samples are presented to the neural network and the output vectors are then calculated. If the neural network is appropriately designed, the testing error should be comparable to the training error; otherwise, the neural network should be restructured and trained again. A common problem with MLPs is that they may be over-fitting the training data, i.e. producing a very small training error but a very large testing error. This problem arises when there are too many hidden units such that the network actually memorises the training samples rather than learns rules from them. In practice, the training and testing samples are drawn from the same population, and the set of training samples is larger than that of the testing samples.

Previous publications on the use of artificial neural networks in colour recipe formulation of textile fabrics can be obtained from references 16 and 17. As claimed by the authors,^{16,17} the use of neural networks offers several advantages over conventional recipe prediction using K–M theory.

1. It is not necessary to prepare a special calibration database in order to use the neural network method. The network can be trained with real known production samples.
2. The neural network can continue to learn after the initial training period, since future data for the production sample can be fed back into the system and this knowledge incorporated into the network. This gives the network the potential to adapt to changes in important factors such as water supply, substrate properties or colourant strengths.
3. The network may be able to learn the behaviour of colourant systems for which the mathematical descriptions are complex. For example, fluorescent dyes are currently difficult to treat using standard K–M theory.

8.3.2 Fluorescent colourant formulation using a neural network

A sample is said to be fluorescent if it contains electrons that can be excited by radiation at a low wavelength and emit radiation at a high wavelength. As the fluorescent colours can considerably enhance the whiteness and extend the colour gamut, they are widely utilised in fashion items. However, the K–M theory will break down in the colourant formulation of fluorescent dyes due to their anomalous optical behaviour. This section introduces fluorescent colourant formulation by the use of a neural network.

For a fluorescent sample, some of the light incident on it is re-emitted with a change of wavelength. At each wavelength, the total re-emitted is

the sum of the reflection and the fluorescence emission components. In discussing the effects of fluorescence, three spectral radiance factor (SRF) terms need to be defined.^{9,13} The first one is the reflected SRF $\beta_s(\lambda)$, which is a ratio of the radiance produced by reflection by a sample to that produced by the perfect reflecting diffuser identically irradiated. The second one is the luminescent SRF $\beta_L(\lambda)$, which is also a ratio of the radiance produced by luminescence by a sample to that produced by reflection by the perfect reflecting diffuser identically irradiated. The third is the total SRF $\beta_T(\lambda)$, which is the sum of the reflected SRF $\beta_s(\lambda)$ and the luminescent SRF $\beta_L(\lambda)$:

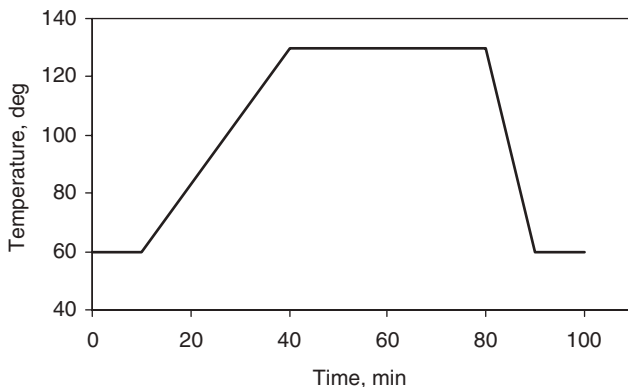
$$\beta_T(\lambda) = \beta_s(\lambda) + \beta_L(\lambda) \quad [8.26]$$

In the above definition the term radiance factor is used instead of the reflectance factor, because the latter applies only to reflected light and not to fluorescent light.

According to the ASTM standard,¹⁴ the colour of fluorescent samples should be measured as they would be perceived when illuminated by daylight. The recommended measurement geometry is the 45/0 (or equivalent 0/45) illuminating and viewing geometry. In practice, the fluorescent colour is always measured using a spectrophotometer which employs polychromatic illumination of the sample and monochromatic detection of the radiant energy. Since fluorescent emission is related to the spectral energy distribution of the illuminant, usually a light source similar to D65 such as a xenon lamp is used in the spectrophotometer. The coating on the integrating sphere has an effect on the measurement as the fluorescent sample itself generates light at a long wavelength. Therefore, in measurement practice, the sample apertures on the integrating sphere should be as small as possible.

In the following, an experimental example will be presented for better understanding of the fluorescent colour recipe formulation based on a neural network. In the experiment, 86 samples, which are polyesters dyed with disperse dyestuffs, are used. Three dyes used were Palanil Brilliant Yellow GN, Palanil Red FD-BFY 200 and Dispersol Navy C-VS 300. The samples were dyed using the three-dye mixture with different concentrations. The dyeing process was done in an Ahiba Nuance laboratory dyeing machine. The dyeing parameters are given in Fig. 8.8. The samples were measured using a Datacolor SF-600 spectrophotometer under the condition of illuminant D65 and 1964 10° observers according to the ASTM standard.¹⁴ The spectral range of the measurement is from 400 to 700 nm with a 10 nm interval.

The recipe formulation is to predict the colourant concentrations based on the colour measurement results. Therefore, the input layer of the neural network was presented with the measured SRF $\beta_T(\lambda)$, and the output layer



8.8 Dyeing parameters adopted in the experiment.

was fed with the concentrations of the three dyestuffs. In the investigation, 60 samples were used for training, and the other 26 samples were used for testing. Neural networks with different hidden layers and hence different hidden units were constructed and their performances were compared. It was found that the network with a single hidden layer and 31 hidden units performed well. The relative prediction error of the network was calculated using the following equation:

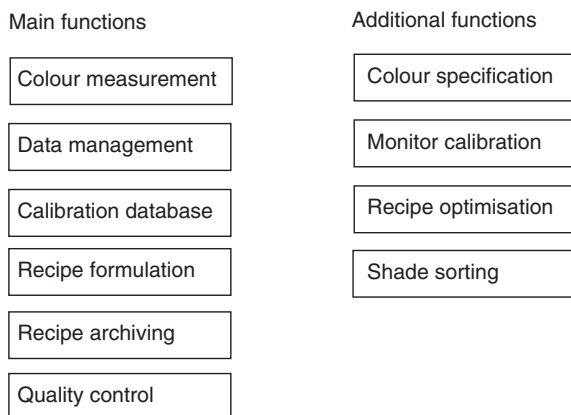
$$\frac{\text{predicted conc.} - \text{target conc.}}{\text{target conc.}} \times 100\% \quad [8.27]$$

For the 86 samples used in the experiment, the training error was 2.3%, and the testing error was 4.2%.

In addition to predicting colourant concentrations from SRF, the neural network can also be used to predict SRF from colourant concentrations. Bezerra and Hawkyard¹⁵ reported such research. They found that the predicted SRF curve was very close to the target SRF curve, with a mean CIELAB colour difference of 7.38.

8.4 A case study for matching a target using a commercial colour recipe formulation system

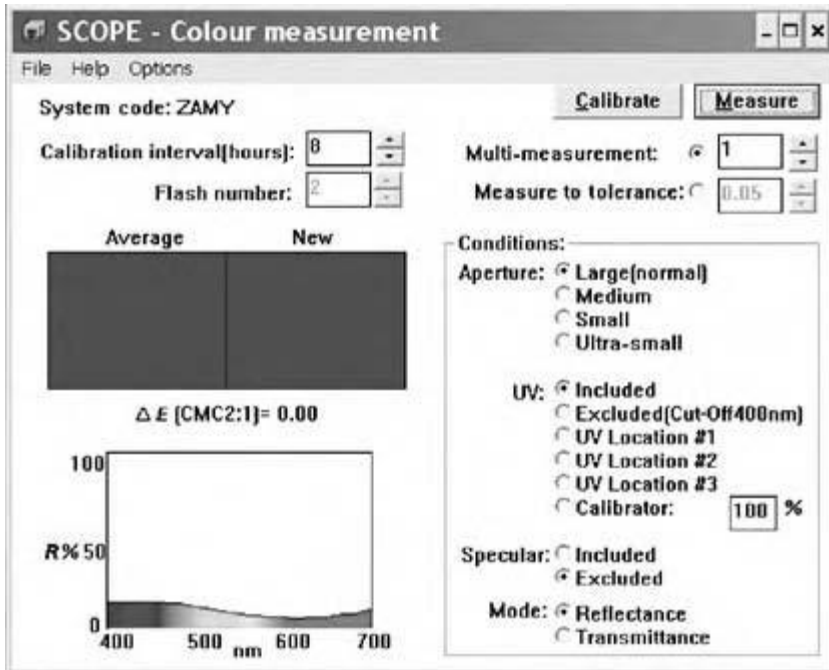
Figure 8.9 shows the main and additional functions often provided by modern commercial colour formulation systems. In these systems, colour can be measured using various types of spectrophotometers and stored in the system. The measured colours can be reviewed or edited using a house-



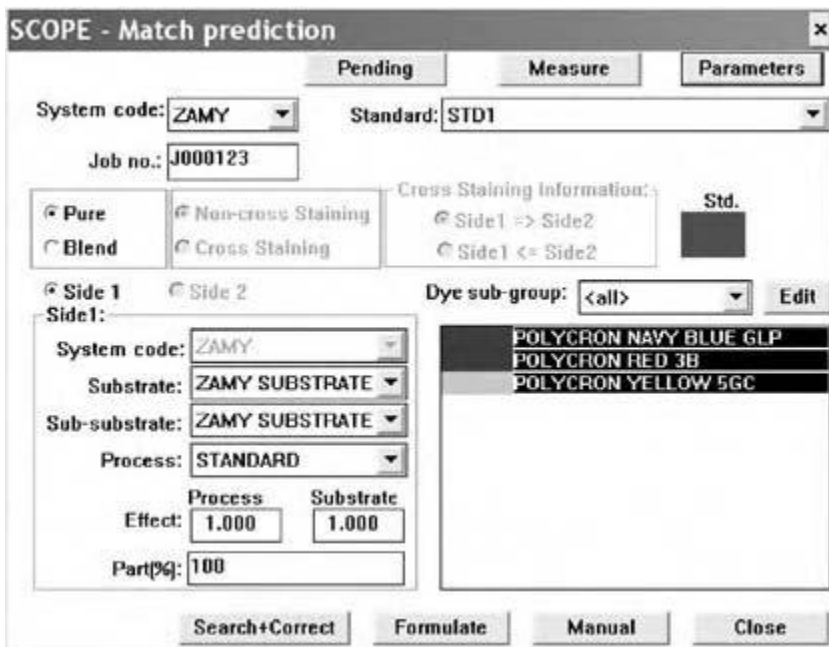
8.9 Functions integrated in commercial colour formulation systems.

keeping function, e.g. the data management functions in Fig. 8.9. The colour specifications including reflectance, transmittance, CIEXYZ, and CIELAB can be evaluated. Colour quality evaluations including colour difference, whiteness, grey-scale rating, yellowness, etc. are performed in a quality control function. In some systems, the colour difference evaluation or visualisation can be performed on a calibrated monitor screen in ‘what you see is what you get’ (WYSIWYG) manner, and the physical samples may not be needed. The method of monitor calibration can be found in Chapter 6. Some commercial systems are equipped with recipe optimisation functions using historical dyeing data. Shade sorting,¹⁸ a process to sort different batches with small colour differences into groups so that all batches within a group are an acceptable match to each other, may also be provided by a commercial colour formulation system.

In this section, we show the workflow of predicting the dye concentrations to match a target colour (or standard) using the SCOPE[®] system¹⁹ developed by Gain Associates Inc., Taiwan. The first step is to measure the target colour using a spectrophotometer, as shown in Fig. 8.10. Then, dye combinations are selected from a list of dyes for which the calibration database has been established as shown in Fig. 8.11. The parameters such as illumination/observer, colour formula and matching criteria can be defined as shown in Fig. 8.12. The colour formulation results given in Fig. 8.13 show the predicted dyestuff concentrations, as well as the predicted colour differences under various illuminations. The predicted concentrations are then used to produce an actual batch sample, which is then measured into the system before using the colour quality control function to determine if the batch is a satisfactory match to the target. Figure 8.14 shows



8.10 Colour measurement.



8.11 Selection of dyestuff combination.

Match Prediction - Parameters

Illums./Observer:

C
D50
D55
D75
DLE 7

=>

Delete

D65
A
CWF_2

2 ?
 10 ?

Formula:

CIEL*a*b*
 CIEL*u*v*
 ANLAB
 Hunter Lab
 FMC2
 JPC79
 CMC i: 2.0
 BFD
 CIE94

Matching criteria:

ΔE (Normal match): 0.000
 ΔE (Accept match): 0.500
 ΔE (Shade search): 0.500
Dye Combination: 3
Max.no.of recipe: 10

Correction:

Additive
 Weighted
 Both

Use expert match?

Yes
 No

Output sort:

Metamerism
 Cost

Close

8.12 Parameter setting for colour formulation.

Match prediction - recipes

Close Print Save recipe reflectance curve Options

Job No.: J000123 Standard: STD1 Side 1 Side 2

Output Sort: Meta Cost ΔE ZANY/ZANY SUBSTRATE:1.00/STANDARD:1.00/100%

CNC(2 0:1)

No.	Cost	MI	Dyestuff (unit: % f)	Conc
1	0.00	0.93	POLYCRON NAVY BLUE G1P	1.11042
			POLYCRON RED 3B	0.06595
			POLYCRON YELLOW 5GC	0.12211

Original

Illums/obs.	D65/10	A/10CWF_2/10
ΔE :	0.00	1.40 0.45
ΔL :	0.00	0.04 -0.19
ΔC :	0.00	-0.34 0.40
ΔH :	-0.00	1.36 -0.07
Cost:	0.00	

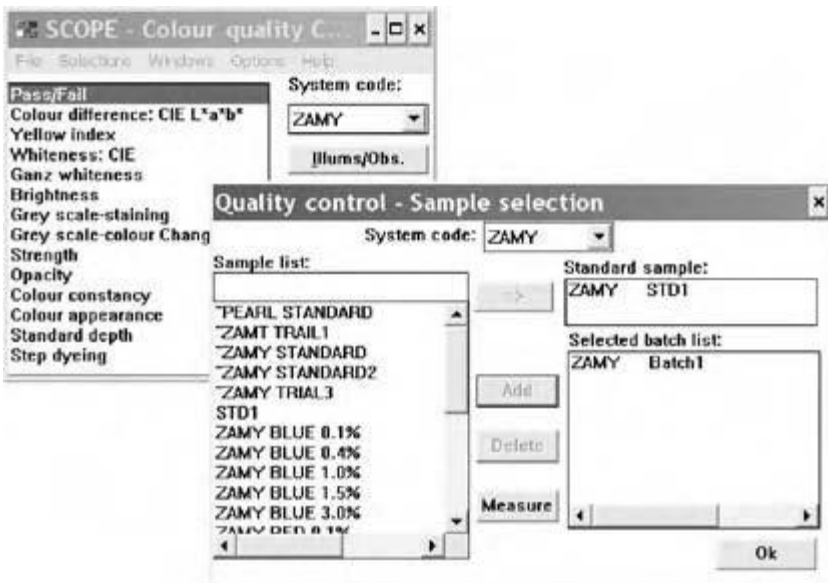
8.13 Colour formulation results.

the process of selecting a standard sample and a batch sample. Figure 8.15 shows the colour difference results between the standard and the batch sample under various illuminations. The results indicate that the batch colour matches the standard colour well under the predefined colour tolerance (e.g. $0.7 \Delta E_{CMC(2:1)}$ unit). If the colour quality of the batch is unacceptable, i.e. if the colour difference is larger than $0.7 \Delta E_{CMC(2:1)}$ unit, further recipe corrections will be needed.

8.5 Sources of further information and future trends

The colourant recipe formulation using a computer system is widely adopted in the textile industry and in other colour-related industries. In this chapter, we introduced the widely used K–M theory and the alternative method of using an artificial neural network for colourant formulation.

In the literature, various optimisation strategies have been presented for the K–M theory-based approach. For example, Sluban proposed a modified colorimetric algorithm to minimise the colour differences under several different illuminants.^{11,20} He also investigated colour sensitivity and correctness of colour-matching recipes.^{21,22} In the artificial neural network



8.14 Selection of standard and batch colours for quality control.

SCOPE - Colour quality control

File Selections Windows Options Help

Save Batch

Pass/fail results

Standard: ZANV/STD1 IAV::SCE::UWI
 Batch: ZANV/Batch1 IAV::SCE::UWI
 Formula: CMC(2,0.1)

Illums/obs.	ΔL	ΔC	ΔH	ΔE	PASS	Lr	Vr	Gr	Yr
D65/10	0.392	-0.325	-0.236	0.561	PASS	Lr	Vr	Gr	(Yr)
A/10	0.433	-0.349	-0.035	0.557	PASS	Lr	Vr	Gr	(Yr)
CWF_2/10	0.413	-0.363	-0.175	0.577	PASS	Lr	Vr	Gr	(Yr)

8.15 Colour quality control.

approach, Mizutani *et al.* proposed a comprehensive evolutionary computing system integrating a neural network, fuzzy classification and a genetic algorithm.²³ It is noted that both the K–M theory based and the neural network-based approaches only consider the optimisation problem from a mathematical viewpoint. In practice, however, the accuracy of recipe formulation is not only affected by optimisation strategies, but also by the whole colouration process. Chen *et al.*^{24,25} studied the effects of simultaneous and separate changes of several dyeing parameters on the colours. In the colour industry, one of the major objectives is to reproduce colour samples with high right-first-time rate. To improve the prediction accuracy considerably, the complex interaction between dyestuffs and materials needs to be studied further, with the various parameters under close control. In some commercial systems, historic recipes are stored in a database and can then be used to improve the accuracy of new predictions. Recipe optimisation in these cases may use numerical methods. However, to improve the prediction accuracy further, more intelligent algorithms need to be investigated.

8.6 References

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