DATABASE PREPARATION FOR SUCCESSFUL COMPUTER COLOR MATCHING

"What You See is What You Get!"

Ken Butts
Datacolor International
Charlotte, NC

Introduction

The basis of visual and computerized processes for determining the dye concentrations to use in color matching is a series of colorant dyeings commonly known as "primaries". The accurate production and evaluation of these primaries are essential parts of ensuring accurate results from the color matching process selected. Utilization of poorly developed primaries, especially in computer color matching, will lead to dyeings that do not match the desired target, hence, "What you see is what you get!" This paper will present basic guidelines for preparing and evaluating dye primaries that will lead to success in computer color matching.

Dye Process Variables

The first step in preparing a set of dye primaries is to identify and evaluate the variables used in the production of the dyeings. These variables include the equipment used, the dyeing process, dye and chemical selection, fabric selection, and weighing technique. Before preparing the first set of primaries, test each of these items to ensure repeatability. If the process of dyeing the primaries is not consistent, generating accurate formulas from a computer color matching system will be difficult at best.

Dyeing Equipment

Most primary dyeings will be prepared on lab-scale equipment heated by glycol, infrared energy, glass beads, or some other heating medium. Equipment problems that can lead to dyeing variability if not resolved include: leaking gaskets, uneven heating in the case of IR equipment, glycol diluted with water from leaking beakers or water lines, and poor temperature calibration. Dye contamination from previous cycles will also lead to poor quality primaries and can be controlled by proper cleaning of the dye beakers. Evaluation of various designs and suppliers is always recommended before any equipment purchase to ensure compatibility with the processes and materials used.

Dyeing Process

Regardless of the equipment used, the actual dyeing process must produce samples that correlate well with production equipment. Colors approved from lab dyeings that can be dyed in production with minimal variation will mean fewer adds on new shades. Correlation can be increased by proper control of temperature, liquor ratio, heating and cooling cycles, auxiliary selection, and sample size. It may be necessary to modify one or more of these factors to increase lab to production correlation as well as to ensure day to day repeatability. In cases where correlation is not possible, special compensation factors can be used to increase the accuracy of the software's shade predictions.

In many dyeing facilities, dyes will be used by more than one process. Examples would be high and low temperature dyeing processes and atmospheric and pressure equipment. A question that many computer users have is whether or not primaries must be redyed on each type of equipment. If the only effect of the secondary process is a change in the depth of the colors produced, then the primaries do not have to be redyed. Many software systems provide a factor that can be used to compensate for the differences in dyeability between the two processes.

In today's market, a variety of lab dyeing machines are available that range from simple, one or two step process control, to complex, multi-step programmability with auxiliary dosing. An informed investment in the beginning that allows for the flexibility required to increase lab to production correlation will lead to greater savings in the end.

Dye and Chemical Selection

As mentioned previously, chemical selection and the amounts used in the lab should be based upon the processes required to ensure good repeatability and lab to production correlation. This means that there may be occasions where lab and production formulas use different amounts of some auxiliaries. A program of quality checks for incoming chemicals should be established to minimize strength variability. Dye selection typically depends upon the type of material being dyed and on end-use requirements.

After a set of primaries has been dyed, strength variability of future lots of dye can have a significant effect on the performance of the computer color matching system. One of the most important facts to remember about a computer color matching system is that it calculates new dye formulas based on the lots of dye that were used to dye the primaries. If a new lot of dye is brought into the dyeing facility and it is ten percent stronger than the original lot, the samples produced from the software's formula prediction will have ten percent more of this color than is required. If several dyes vary in strength, significant shade variation will occur. For this reason, it is essential to develop a program of strength evaluation of new lots of dye before releasing them for use in production or the lab. Many software packages provide a factor that can be modified to compensate for variations in dye strength. This factor will not, however, compensate for differences in the hue -- or color -- of new lots of dye. If the hue of a new lot of dye is significantly different, the primary set must be dyed again and reentered into the software.

Fabric Selection

The initial set of primaries must all be done on the same type of material to ensure continuity. Select a material that is used often in the dyeing facility and has exhibited good shade repeatability. If a common material is not available, select an alternative material with sufficient quantity available to dye all primaries that are to be loaded into the software.

It is usually not necessary to redye primaries on all materials in use in a dyeing facility, especially if the only difference between the materials is denier or yarn count. Use the following technique to determine whether or not primaries should be redyed on other materials:

1 - Generate dye formulas for a beige, a medium gray, and a rose color using the same three dyes. Use dyes that are in common use and round the formulas to the nearest tenth.
2 - Use the "split bath" technique to produce a series of dyeings on all materials to be tested. As an example, assume that nine alternative materials are to be compared to the material used for the dye primaries. If the weight of each sample is ten grams, then the total weight of all material will be one hundred grams. If the bath volume is 200ml, then the total volume for all baths will be 2000ml. Using the formulas from step one, mix a 2000ml solution based on one hundred grams of fabric. After mixing the solution, divide it equally among ten beakers and perform the dyeing with the technique normally used to dye each material.
3 - Use the computer software's strength calculation option to determine the strength of each material relative to the standard material.
4 - Use the calculated strength as a factor to adjust the computer's shade prediction when a formula is required on one of the alternate materials. Again, many software systems allow the entry of a factor based on strength to automatically compensate for differences in depth of shade. If several materials exhibit the same relative strength, they may be grouped together during the formulation process.

In addition to calculating the strength difference mentioned above, be sure to visually evaluate each material to be sure there is no hue variation between the alternate material and the material used to dye the primaries. If there is a noticeable hue difference, then the formulas generated by the software will vary from the target color. It may be necessary to redye primaries on one of the alternative materials if the hue difference is significant. Hue differences between nylon 6 and nylon 6,6 would be an example of significant hue difference requiring redyeing of the primaries.

Of special note are materials that differ in color from the material used to produce the primaries, as is the case for bleached and scoured cotton. If the only difference between the two materials is their base color, and their dyeabilities are the same, then it is not necessary to redye the primaries on the alternative material. The alternative material can be measured into the software's database and the computer will modify its formula prediction to compensate for the color that is already present on the material.

Weighing Technique

Precision in weighing of fabric, dyes, and chemicals is essential in producing accurate, repeatable dye primaries. Calibrated scales that measure to two or three decimal places for fabric and analytical scales for weighing of powdered dye are required.

The most accurate technique for weighing dyes and chemicals is to pipette from a stock solution using calibrated glassware. Flasks and graduated cylinders are not accurate enough to ensure repeatable lab dyeings and should be avoided. For dye primaries, it is recommended that volumetric pipettes with a 10ml or greater volume be used with weak stock solutions. An alternative to manual pipetting is automatic dispensing using a modern lab dispensing machine and stock solution machine if available.

Preparing the Primaries

After the process variables have been defined and modified to produce repeatable and accurate dyeings, colorant primaries can be prepared for all dyes to be used in the formulation system.

Blank Dyeing

An essential part of developing a colorant database is the blank dyeing. A blank dyeing -- or mock dyeing as it is often called -- is simply a piece of the material used to dye the primaries that has been exposed to a complete dyeing process without any dye. The blank dyeing should include the same auxiliaries, dye cycle, and finish process if used. Any color change that results from the process can then be accounted for when the blank dyeing is entered into the database.

Selection of Dye Concentrations

There are a few guidelines to follow when determining the concentrations to select when preparing dye primaries, but there are no specific rules. Typically, eight to twelve levels are selected that accurately characterize the build behavior of each dye, or at least cover the range used in production. The number of samples dyed will also be dependent upon the number of primaries the software will accept.

A recommended method of determining the concentrations to use would be to multiply the largest useable concentration of each dye by a series of factors that would produce eight to twelve samples. As an example, assume that a dye is used in the range of 0% to 3%. Multiply the highest concentration -- 3% -- by the factors 1.1, 1.0, 0.8, 0.6, 0.5, 0.3, 0.2, 0.1, 0.05, and 0.025. This will produce the concentrations: 3.3%, 3.0%, 2.4%, 1.8%, 1.5%, 0.9%, 0.6%, 0.3%, 0.15%, and 0.075%. The concentrations may be modified slightly for ease of dyeing and concentrations below 0.05% are not recommended due to higher potential for error. The same technique can be used for units other than percent as well. After evaluation of the samples, it may be necessary to delete some levels to allow additional dyeings in areas where the dye behavior has not been characterized accurately.

Storing the Primary Data

After the primaries have been prepared, the next step is to store them into the color system's database. Proper techniques in sample measurement must be used or all of the effort put into accurately dyeing the primaries will be lost.

Instrument Considerations

Before measuring samples on the spectrophotometer, perform diagnostic tests to check the accuracy of the measurements. These tests should include a drift test to check for read to read repeatability, a diagnostic tile test to ensure long term repeatability, and a standardization -- or calibration -- with a white tile. Only the white tile calibration is required daily while the other diagnostic tests can be performed on a weekly basis. Any poor test results should be resolved prior to measuring any of the primary samples. Long term stability of the instrument is critical due to the fact that primaries are often used for many years.

Spectrophotometers make use of one of two light sources -- a tungsten filament bulb or a xenon flash bulb. Certain guidelines should be followed depending on the type of bulb being used. Because tungsten filament bulbs burn continuously and generate a considerable amount of heat, heat and light sensitive samples should not be placed at the instrument port until immediately prior to measurement of the sample. Extended exposure of some samples to the heat and light from the tungsten filament bulb will cause a dramatic change in the color of the sample. Xenon flash bulbs do not generate heat, but they are very rich in ultraviolet energy. This ultraviolet energy will excite any fluorescing chemicals, additives, or dyes present in the samples and will lead to inaccurate match predictions, especially in the blue area of the visible spectrum. Filters are usually available to minimize the effect of ultraviolet energy.

Measurement Technique

All samples should be measured multiple times with the largest area view available on the spectrophotometer being used. A repeatable measurement technique based on the number of layers of material used and sample rotation should be developed prior to measuring the primaries.

Two to four layers will be sufficient for most knitted and woven materials to achieve an opaque sample for presentation to the instrument. Lightweight and translucent materials will often require so many layers to become opaque that the material is forced into the interior of the instrument when measuring, causing inaccurate measurement. For these types of materials, repeatable results can be obtained by measuring only a few layers of material backed with a white ceramic tile similar to the instrument's calibration tile. Other presentation techniques would include yarn wrapped onto a card, loose fiber measured in a compression cell, and pile fabric measurement behind an optically clear glass plate.

Sample rotation and repositioning will reduce measurement variability due to fabric construction, directionality of yarns, and unlevel dyeings. A common practice in sample measurement is to leave the sample on the same position and simply rotate the sample for four or more measurements. This technique will not account for variations due to unlevel dyeing and should be avoided. A better technique is to remove the sample from the instrument and refold or reposition it before additional readings.

An optimum measurement technique has been established when a sample can be measured, removed from the instrument, and remeasured with a variation of less than 0.15 DE (CMC) units. Higher variation will decrease the confidence level in the quality of the stored data and lead to less accurate match predictions.

Evaluation of Primary Data

Once the primaries are accurately measured and stored in the database, the data must be evaluated for consistency using specialized numeric and graphic calculations.

The Mathematics of Computer Color Matching

For a computer formulation program to work effectively there must be a mathematical relationship between the concentrations of each dye used to produce a sample and the sample's color. It is not the purpose of this paper to discuss in complete detail the mathematics of color matching, but a brief description will follow. More detailed information may be obtained from a large assortment of textbooks and articles.

The mathematical basis for all color matching software is the Kubelka-Munk series of equations. These equations state that for opaque samples such as textile materials, the ratio of total light absorbed and scattered by a mixture of dyes is equal to the sum of the ratios of light absorbed and scattered by the dyes measured separately. Where absorption is defined as "K" and scattering is defined as "S", Kubelka-Munk states that [1]:

$$\mathbf{(K/S)\ mixture = (K/S)\ dye_1 + (K/S)\ dye_2 + (K/S)\ dye_3 + \ldots}$$

K/S is not a readily measurable quantity, but it can be calculated from the reflectance of a sample -- "R" -- by the Kubelka-Munk equation that states [2]:

$$\mathbf{K/S = (1 - R)^2 / 2R}$$

As an example, if a sample has a reflectance of 20% at a wavelength of 500nm, then the K/S can be calculated as:

$$\mathbf{K/S = (1 - 0.2)^2 / 2(0.2) = 1.6}$$

If the K/S of a target color is measured at several wavelengths, the concentrations of each dye can be calculated by trial and error from primary dyeings to achieve the closest match. A computer color-matching program is capable of performing hundreds of iterations in a short period of time to produce the initial dye concentrations.

Graphical Analysis of Primaries Using K/S

K/S calculations are invaluable in evaluating the build characteristics of dyestuffs because there is a direct relationship between K/S and dye concentration. In Figure 1, the K/S values of several samples are plotted versus the sample concentrations.

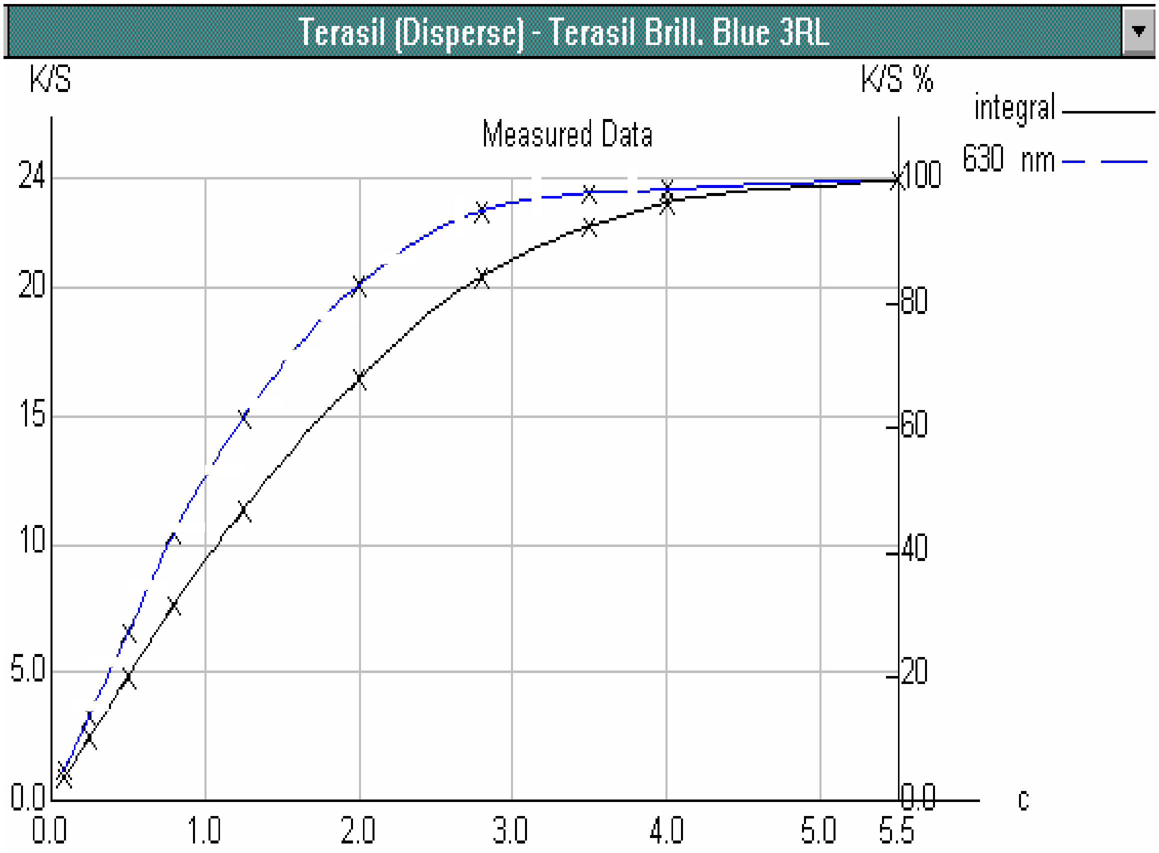

Figure 1: K/S vs. Dye Concentration

The uniformity of this curve will determine the software's ability to accurately generate new formulas, especially in the unknown areas between the known concentrations. Two curves are displayed, one based on K/S for each dye at the wavelength of maximum light absorbence and one based on K/S integrated over the range of 400-700nm. The shapes of these curves may differ due to hue changes as dye concentration increases.

The quality of the dye primaries is indicated by the smoothness of the K/S curves. Most dyes will exhibit linear behavior in the lower concentrations and will begin to flatten as the dye saturation point is approached. The point at which the K/S curve stops increasing corresponds to the maximum achievable depth of shade for a dye, approximately 5% for the dye pictured, and the concentration used should not exceed this amount in shade matching. It is often the case that, due to physical properties such as light fastness and wash fastness, the practical use range of a dye is well below its saturation concentration.

A graph of log K/S versus concentration (Figure 2) is useful for evaluating the linearity of lighter concentrations.

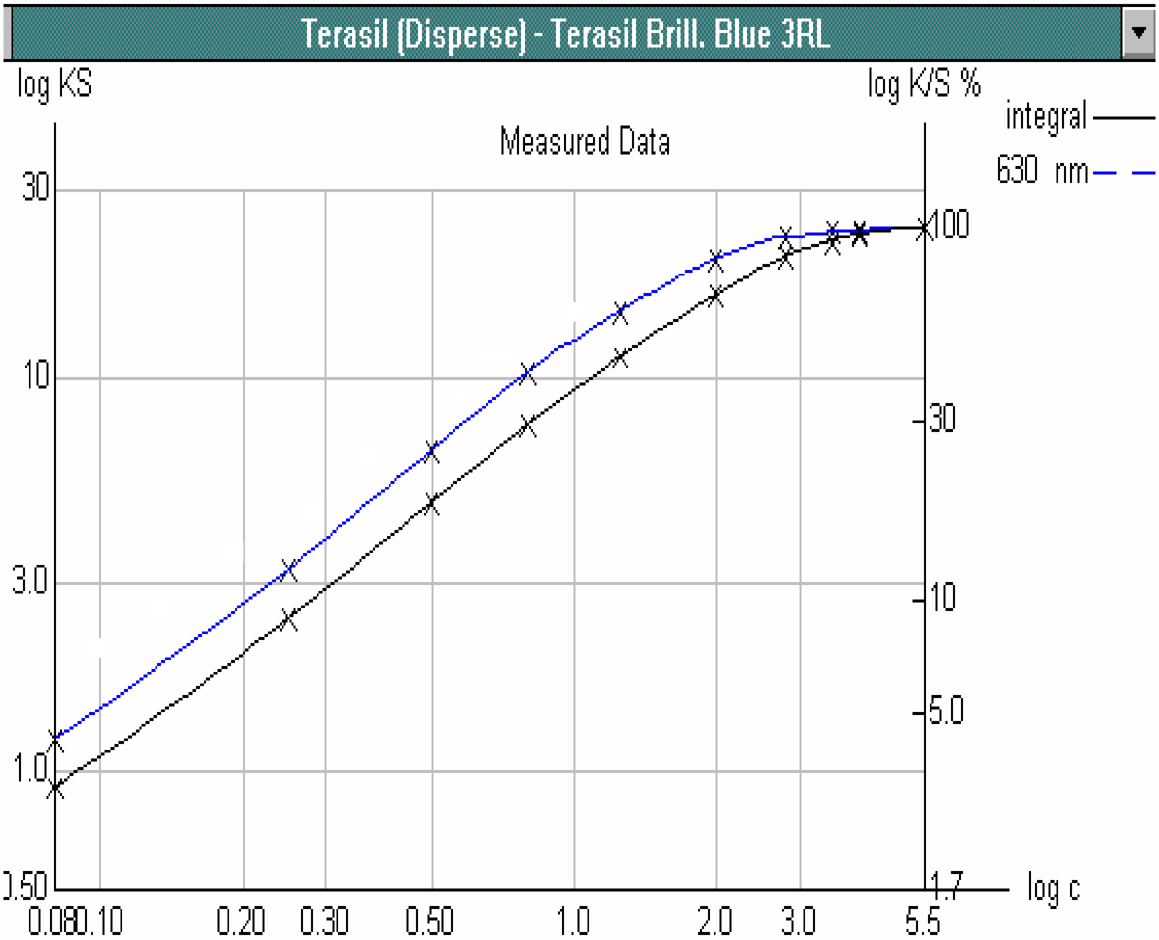

Figure 2: log K/S vs. Dye Concentration

Any samples that appear to deviate from the linearity of the majority of data points should be remeasured for confirmation and redyed if proven to be in error. It is acceptable to delete as many as two points if eight or more concentrations have been dyed as long as they are in the linear portion of the graph and are not one of the two strongest concentrations. If three or more points appear questionable, it is preferable to redye the entire set of primaries for best results from the formulation software. Small variations as indicated in Figure 3 can be corrected using mathematical smoothing techniques to produce the modified curve in Figure 4, but only if the changes are less than 10%.

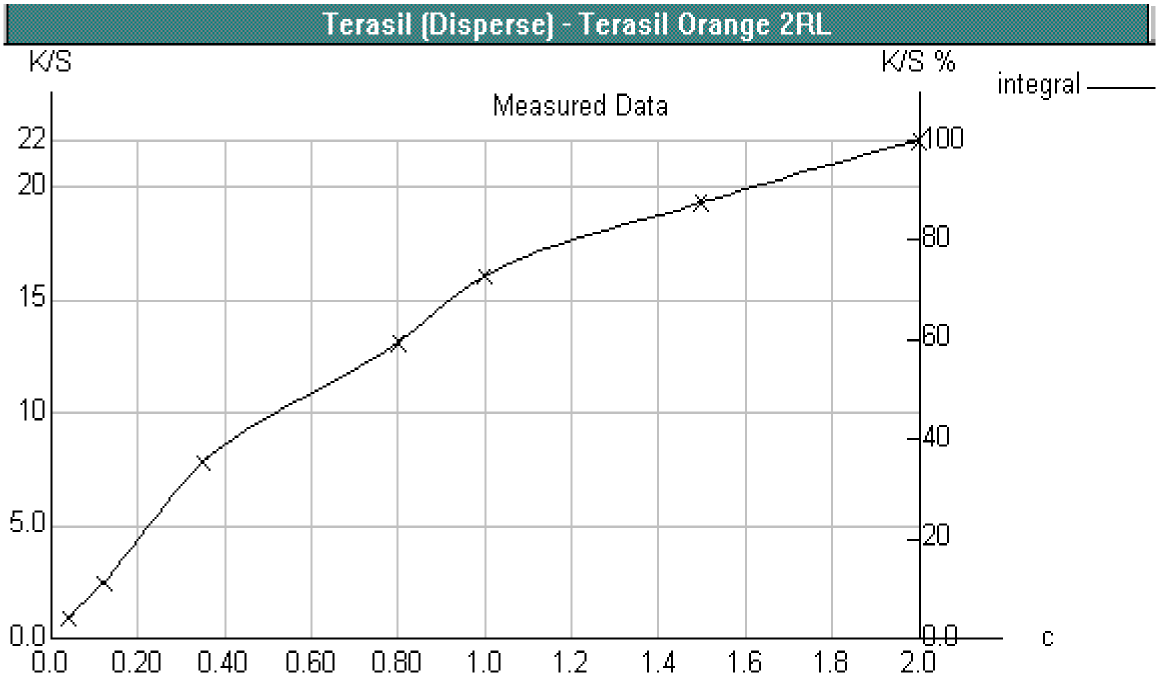

Figure 3: K/S vs. Dye Concentration - Measured Data

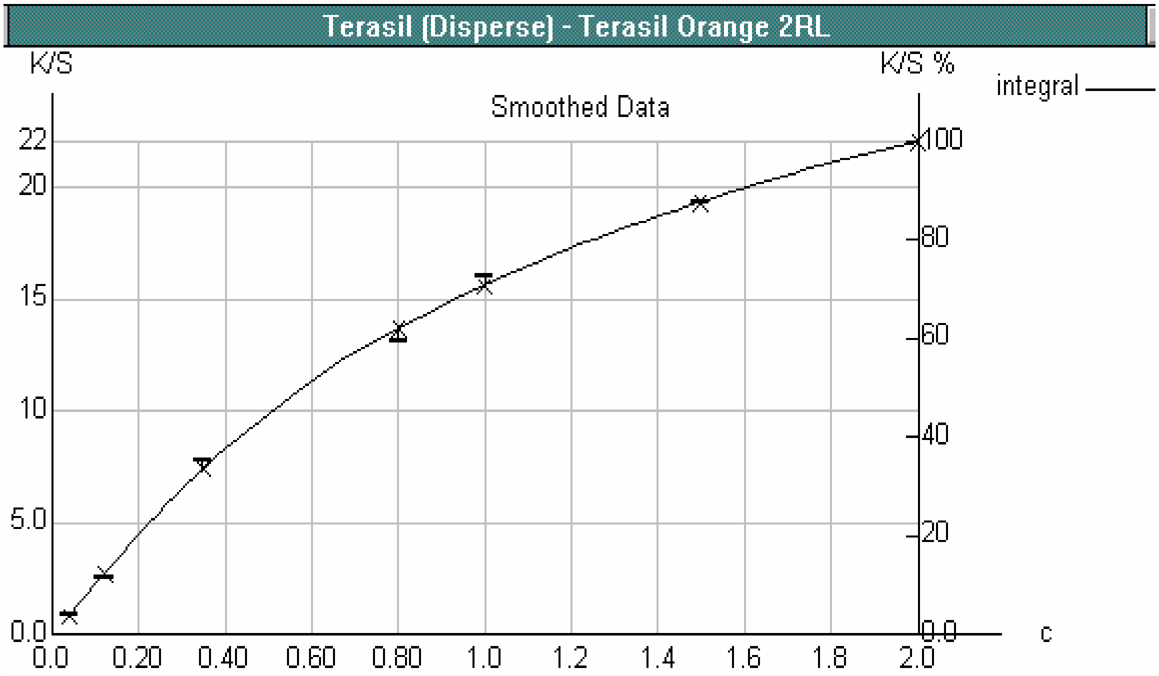

Figure 4: K/S vs. Concentration - Smoothed Data

At first glance, the K/S curve for the black dye in Figure 5 appears to be acceptable. If the formulation program were asked to generate a concentration of this dye corresponding to a sample K/S value of 17, it would predict approximately 2.4%. Notice, however, the large gap in the concentration levels between 1% and 4%. If an additional point was dyed at 2.5% and added to the database, the computer's predicted concentration would change to approximately 1.6%.

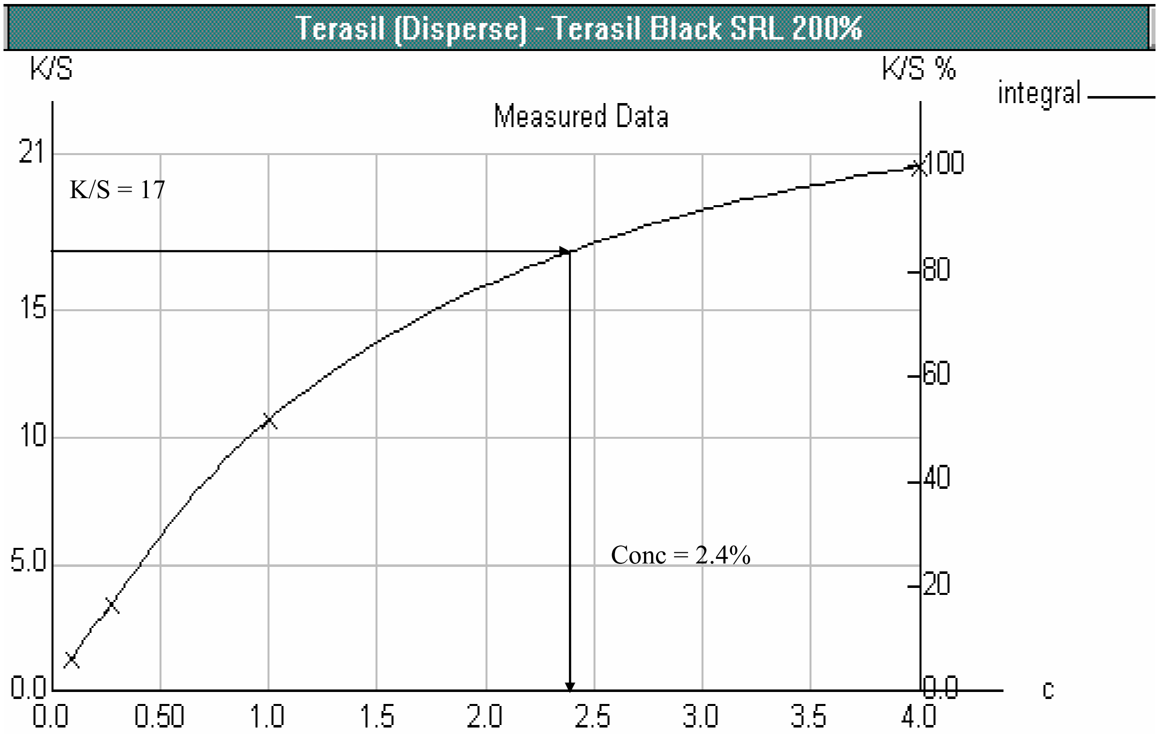

Figure 5: K/S vs. Dye Concentration for Black SRL

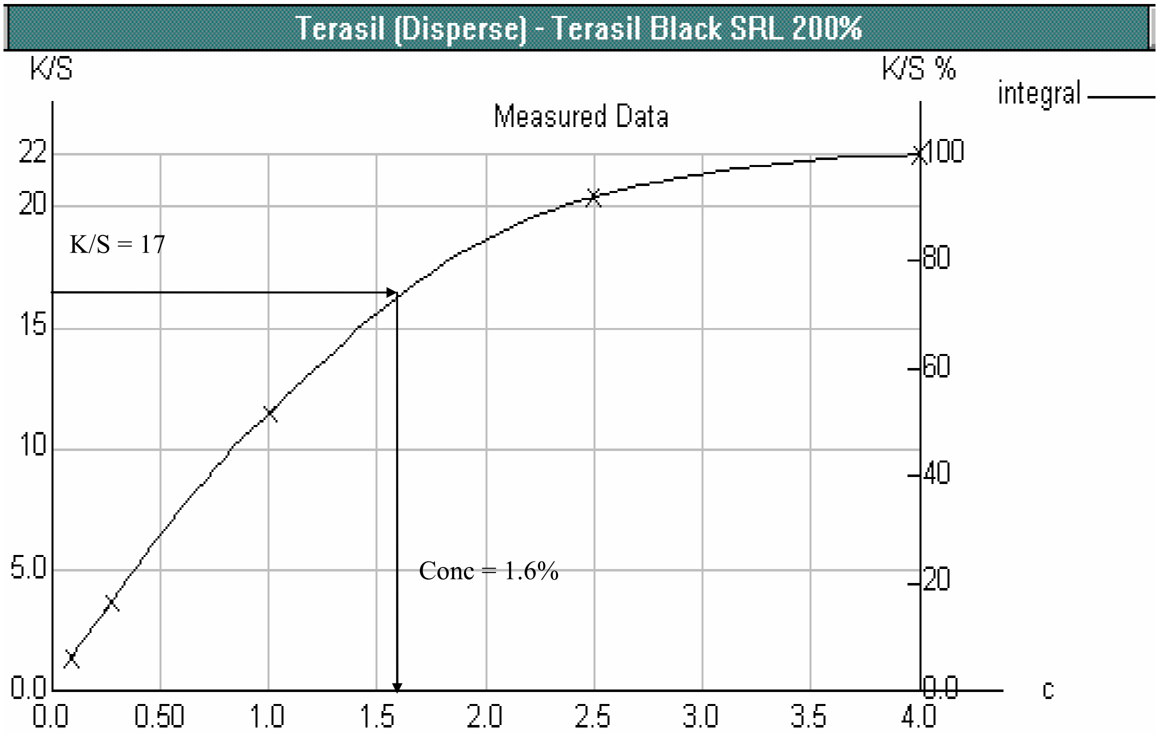

Figure 6: K/S vs. Dye Concentration for Black SRL - Modified

As a rule, it is best not to leave gaps of more than 1.0% between primary dyeings. This will be helpful in preventing the highly variable concentrations predicted in the previous example.

Graphical Analysis of Primaries Using Reflectance

Graphs of percent light reflectance (%R) versus wavelength for a set of primaries are useful in detecting the presence of contamination, especially in the lighter samples. Figure 7 is a graph of %R versus wavelength for a set of violet primaries:

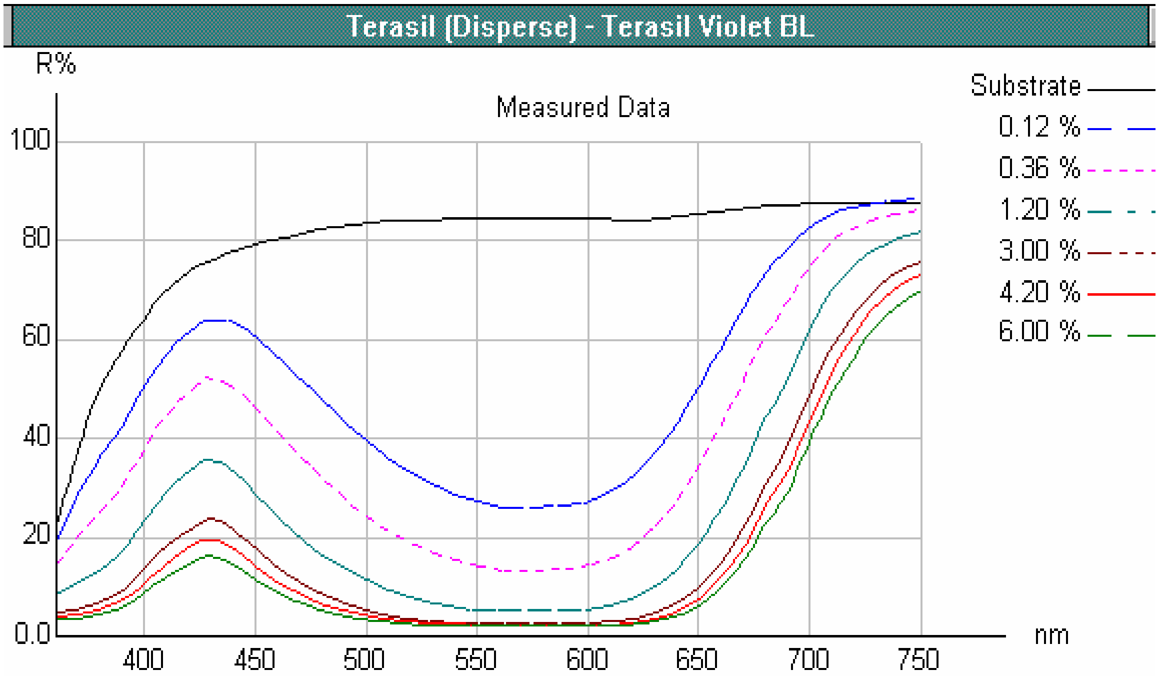

Figure 7: %R vs. Wavelength

The reflectance curves for the set of primary dyeings should all have the same basic shape with no lines that cross. There will be occasions, however, when some line crossing occurs at higher reflectance values, especially above 600nm for yellow to red dyes. As long as the crossing is not significant, there is no need to remove or redye the sample. If the reflectance curve exhibits significant crossing as in Figure 8 for the 0.15% level of the red dye, then the sample has become contaminated during the dyeing process or by some other means. This point should definitely be redyed or, if the remaining points have a linear K/S versus concentration build, simply deleted.

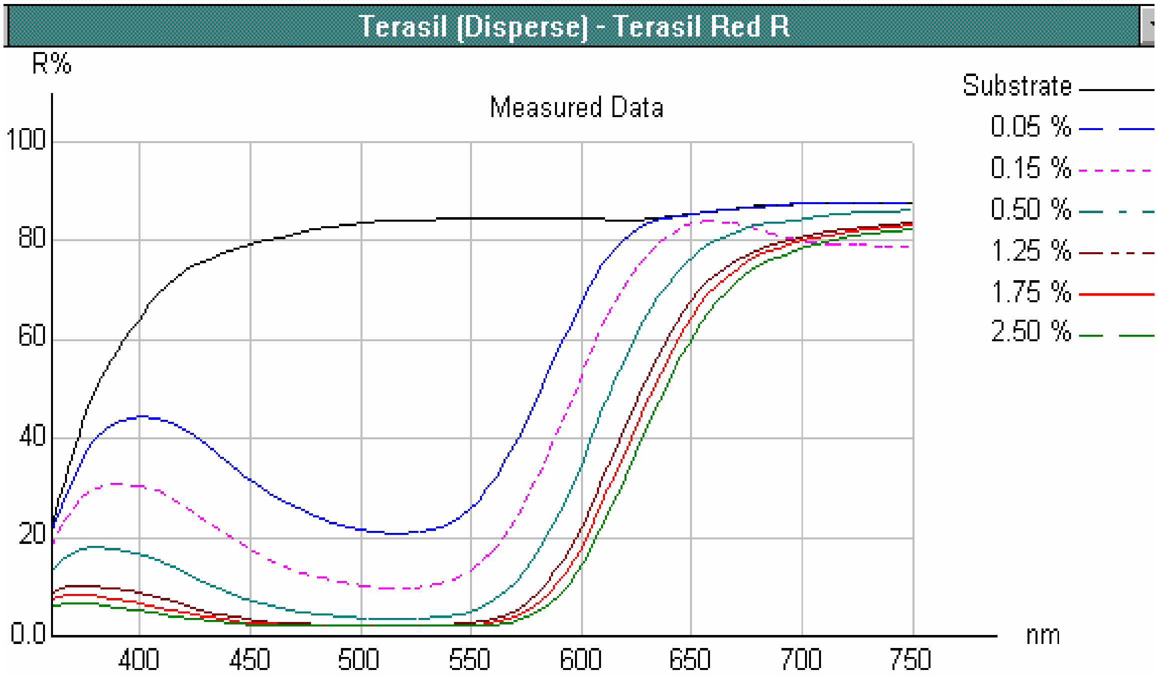

Figure 8: %R vs. Wavelength with Contamination

For most dyes, the percent reflectances for the darker concentrations are so low relative to that of the light concentrations that it is difficult to determine from the %R graph if there are any problems with the darker dyeings. To make evaluation easier, a plot of K/S versus wavelength is used. In Figure 9, K/S versus wavelength is plotted for the violet dye seen previously in Figure 7.

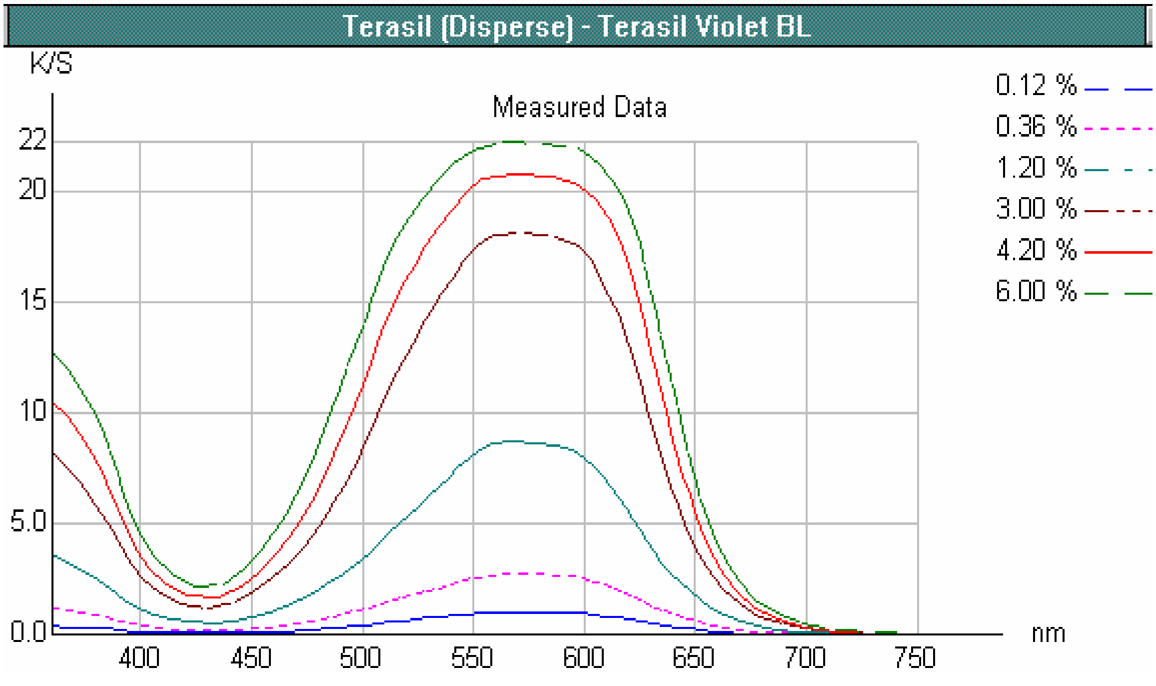

Figure 9: K/S vs. Wavelength

Reexamining Figure 7 does indicate that for the darker primaries, the reflectance curves seem to merge between 525nm and 600nm. It can be seen in the K/S versus wavelength graph that the reflectance curves have been reversed, with the darker concentrations at the top of the graph while the lighter concentrations are at the bottom. It can be concluded from the graph that the darker primaries are also consistent.

A point to remember when evaluating reflectance versus wavelength graphs is that some dyes do exhibit a change in hue as the concentration increases. For these dyes, the reflectance curves of all concentrations will not be identical in shape, but this does not mean that a particular sample is necessarily contaminated. For these dyes, absence of crossing is the critical characteristic.

Confirmation of Primary Accuracy

K/S and reflectance graphs are essential tools in determining the quality of the primary data. After any questionable points have been deleted or replaced, the accuracy of the database should be confirmed by generating match predictions for a series of dyed “knowns”.

A “known” is simply a piece of material that has been dyed using the same techniques and substrate that were used to dye the primaries. When asked to predict a formula for a known sample, the computer formulation software should produce a formula reasonably close to the actual concentrations that were used to produce the sample. Small variations are common and are typically due to dye interaction that cannot be accounted for when the primaries are dyed separately.

If the computer prediction is significantly different from the actual formula, then there may be a problem with one or more sets of primary data. A secondary technique for confirmation of primary quality is to dye a known that contains only one dye. This will eliminate dye interaction as a possible source of the error. If the software cannot accurately predict the concentration of the single dye, then a problem does exist with the set of primary data and the set should be redyed. This test is also useful when changing to a new lot of dyestuff to determine the degree of error that will be introduced when the new lot is used in the lab or in production.

In most cases, variations between predicted and actual formulas are consistent within shade families and among particular dye combinations. To take advantage of this fact, some computer formulation systems have the ability to “learn” about dye interaction and to compensate for it by modifying the initial formula prediction. This means that the first lab dyeing based on a modified prediction will be much closer to the target color than a formula based only on primary data. This process works well if the materials being dyed are consistent for an extended period of time. Application of this technology can significantly reduce the number of lab dyeings required to match new shades.

Primaries Provided by Dye Manufacturers

Many companies choose to use primaries provided by dye manufacturers. This data is usually very consistent and offers a way for a lab to immediately begin shade matching or to evaluate a new dye or family of dyes. The dye manufacturer's primaries are usually available on a computer diskette in a form suitable for a large number of color-matching programs.

Although these primaries are usually very consistent when evaluated using the techniques discussed earlier, this does not guarantee that the formulas predicted will be accurate. This is caused by the use of different materials, different chemicals, different equipment and dyeing procedures, and even by different water supply. This does not mean that the supplier primaries cannot be useful, it simply means that the initial computer predictions will not be as accurate as ones based on primaries dyed in the lab's own environment. One solution to this problem, especially if the primaries are not required immediately, is to provide the supplier with fabric, chemicals, dyeing procedures, and water to use to produce the dyeings. The only remaining variable will be the equipment.

Conclusions

A computer color matching system is not a "black box" that magically produces the exact formula for a sample on demand. The accurate preparation of dye primaries and the careful evaluation of the stored data are essential if a color matching system is to be able to predict formulas with any consistency. As this is accomplished, significant reductions in the number of dyeings required to match new shades are made possible.

References

1 - Billmeyer, Jr., F.W. and M. Saltzman, *Principles of Color Technology, 2nd Edition,* Wiley, New York, 1981, p140.

2 - Billmeyer, p140.