

CHAPTER 5
DISCUSSIONS



5.1 The Mathematical Model based on the Turbid Media Theory.

The mathematical model to be studied in this work was Equation 2.30 ; i.e.,

$$a \frac{K}{S_A} + b \frac{K}{S_B} + \dots + w \frac{K}{S_W} = \frac{K}{S_M} \quad (5.1)$$

Which is essentially the result of the Turbid Media Theory. Assumptions used in deriving Equation 2.30 are :

- 1) the fabrics are opaque
- and 2) refraction in fibers is negligible , i.e., only reflection takes place.

For Equation 2.30 to be true, $\frac{K}{S}$ ratio is a linear function of colorant concentration. Consequently, the value of $\frac{K}{S}$ ratio is additive. This property makes the mathematical model simple and convenient to use.

Unfortunately, experimental data did not confirm the linear relationship between $\frac{K}{S}$ and concentration. Details are discussed in Section 5.2 . Equation was then modified by replacing $\frac{K}{S}$ by $(\frac{K}{S})^n$, where n was a constant. The complete mathematical model is presented in Section 5.3.

5.2 K/S values

Refer to the experimental results, Tables 4.1 to 4.6 and Figures 5.1 to 5.9, it was found that the K/S values which were normalised were not linear with the concentration of dyes. So, it cannot be directly applied to the theory.

Taking account of the surface and internal reflection usually leads to a somewhat better proportionality relation between K/S and concentration c , but some discrepancy of this kind often remains. Whereas for pigment mixtures it is common practice to include in the analysis corrections for surface and internal reflection, for dyestuff mixtures on textiles corrections of this kind are often of little advantage and thus ignored. In the latter case, the colorant concentration is in terms of the concentration of the dyebath and not in terms of the concentration of the dyestuff within or at the surface of the fiber (Gall, 1973). (19) The fiber never absorbs the dye in the dyebath exactly in proportion. Thus there never exists a linear relationship between absorption and concentration and corrections for surface and internal reflection are not going to improve the situation.

Therefore, the equation (5.1) is not feasible. To keep the assumptions and the linearity of the model, the $\frac{K}{S}$ values was replaced by $(\frac{K}{S})^{1.15}$ values and their values are found to give linearity in the range 0 - 3% concentration of dyes, as shown in Figures 5.1 to 5.9 and Tables 4.8 to 4.13. Figures 5.1 to 5.9, shown the diagram of K/S values and $(\frac{K}{S})^{2.15}$ values versus %

(K/S)

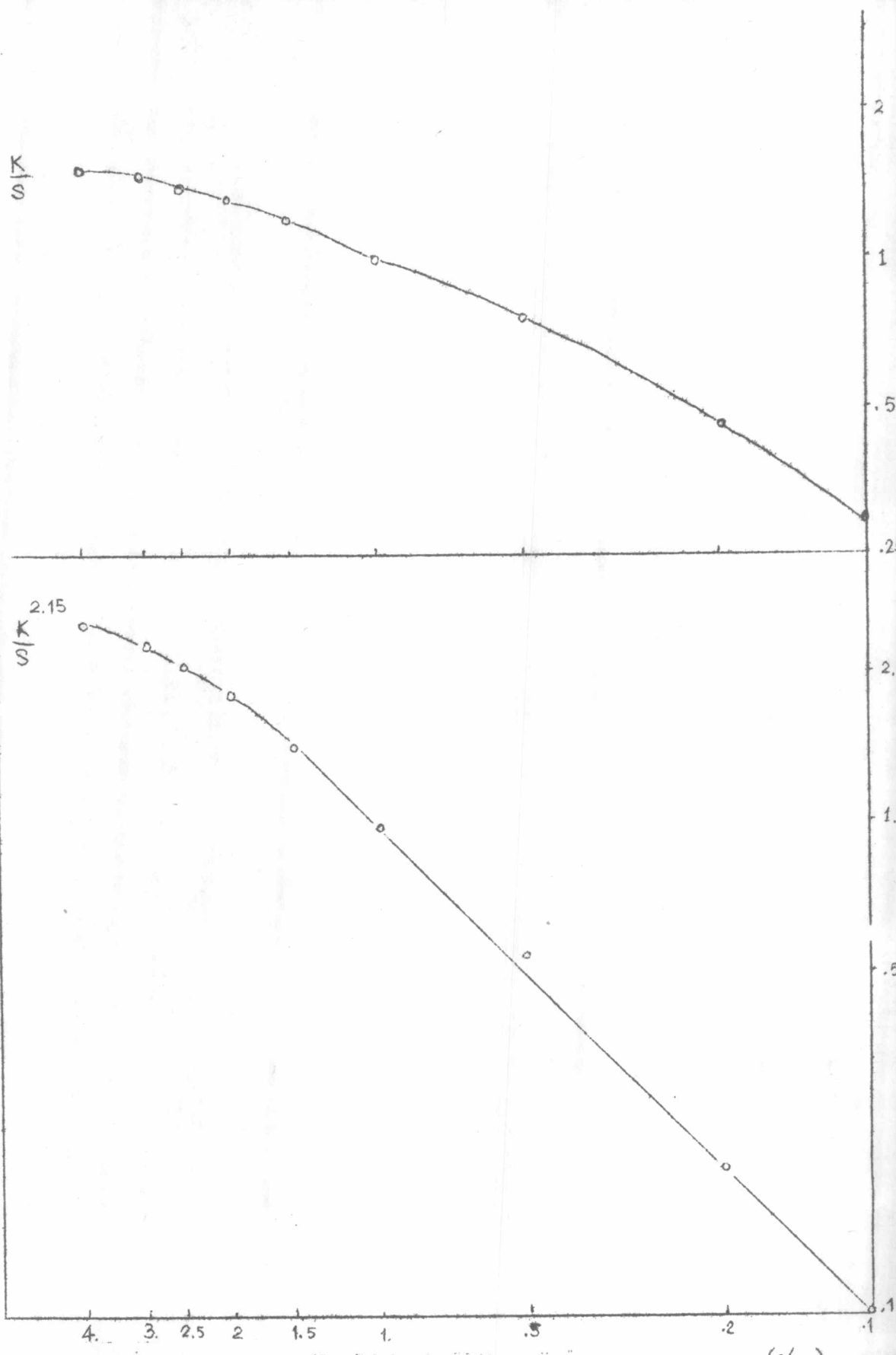
$\frac{K}{S}$

$\frac{K}{S}$

2.15

4. 3. 2.5 2 1.5 1 .5 .2 .1 (%c)

Fig. 5.I K/S vs %c of Procion Blue MX - 4GD (620 nm)



(K/S)

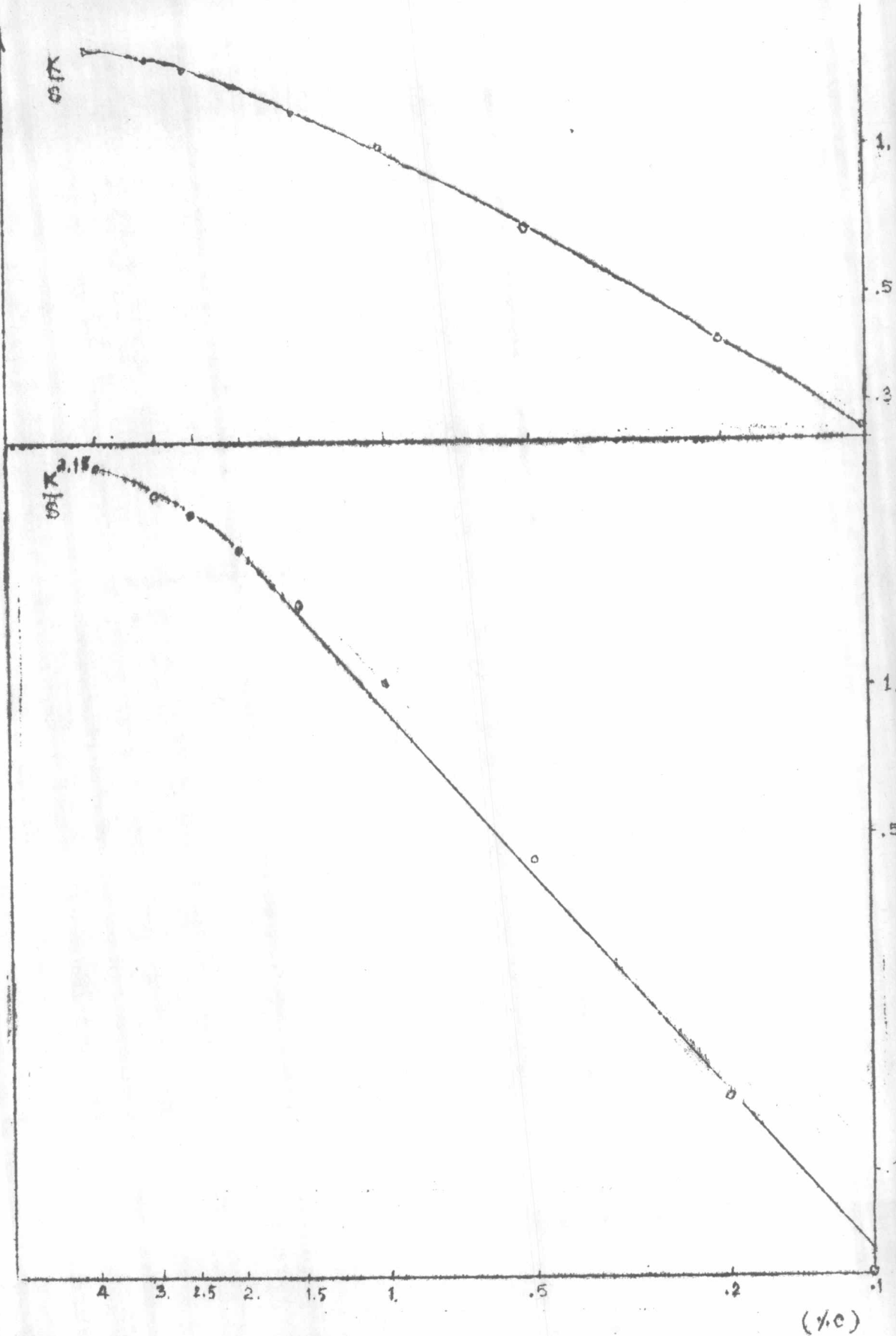


Fig. 5.2 K/S vs %c of Procion Yellow MX-8G (420nm)

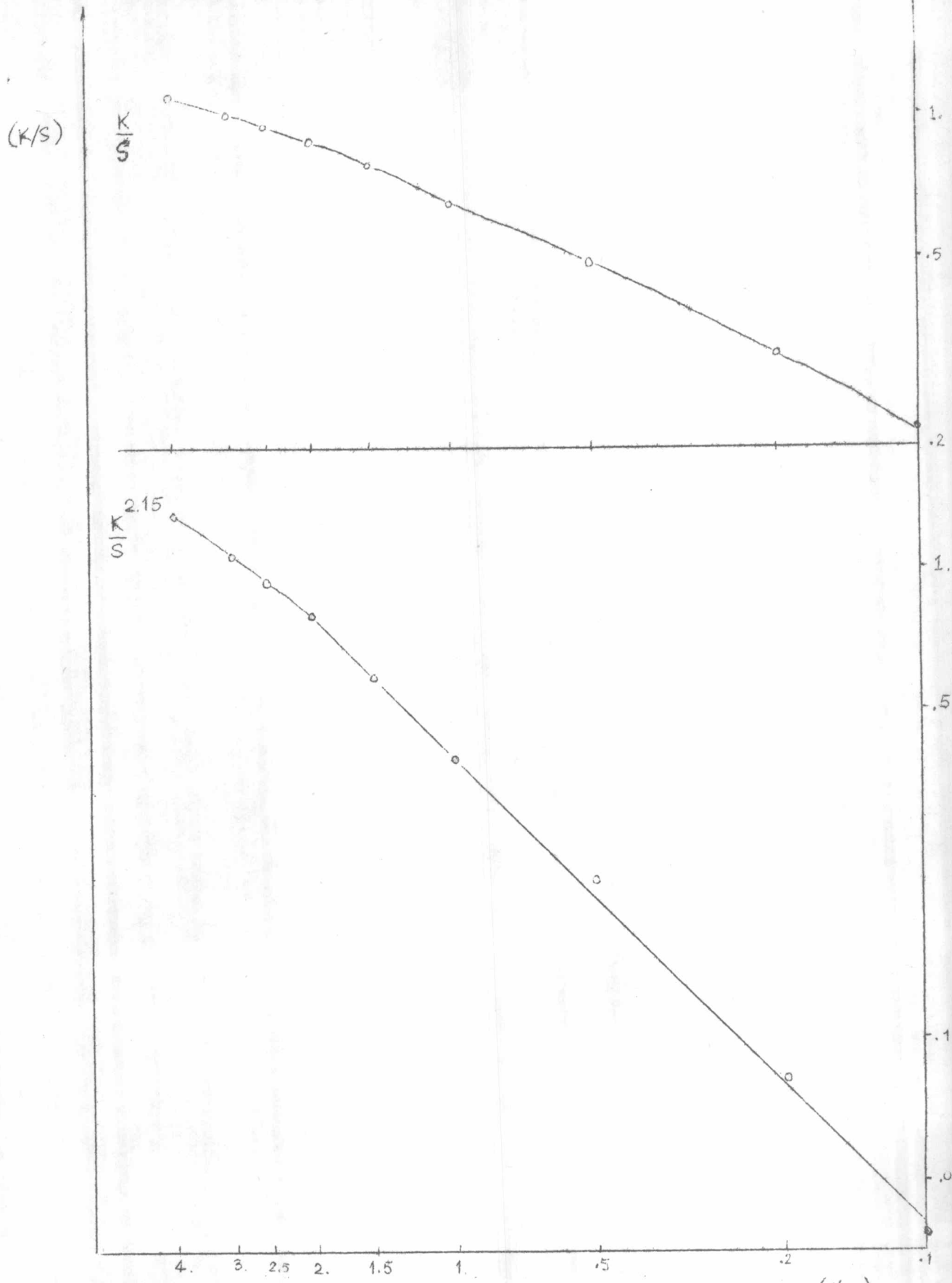


Fig. 5.3 K/S vs %c of Procion Blue MX-G

(%c)
(660 nm)

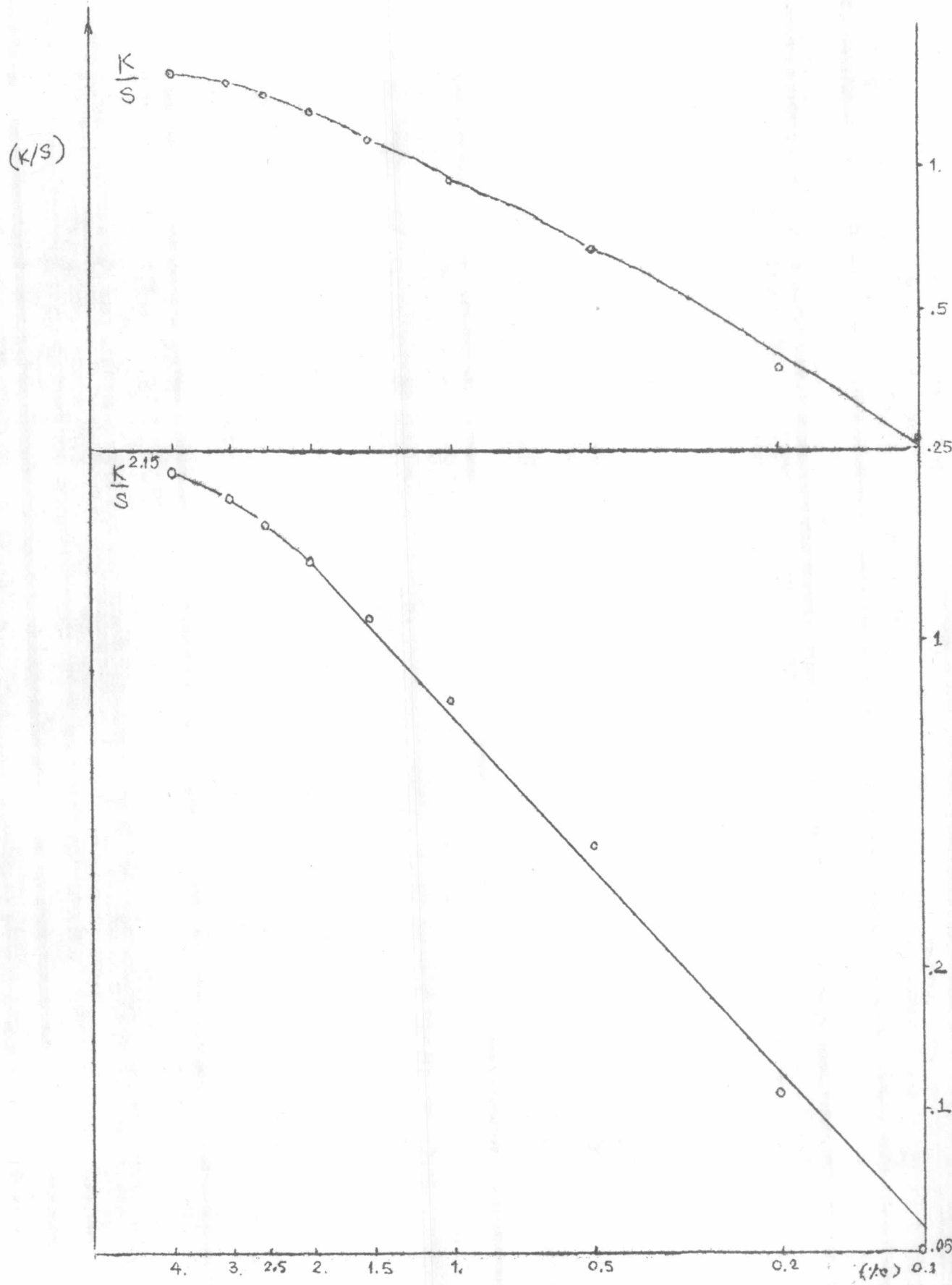


Fig. 5.4 K/S vs %c of Procion Yellow MX - 3R

(420 nm)

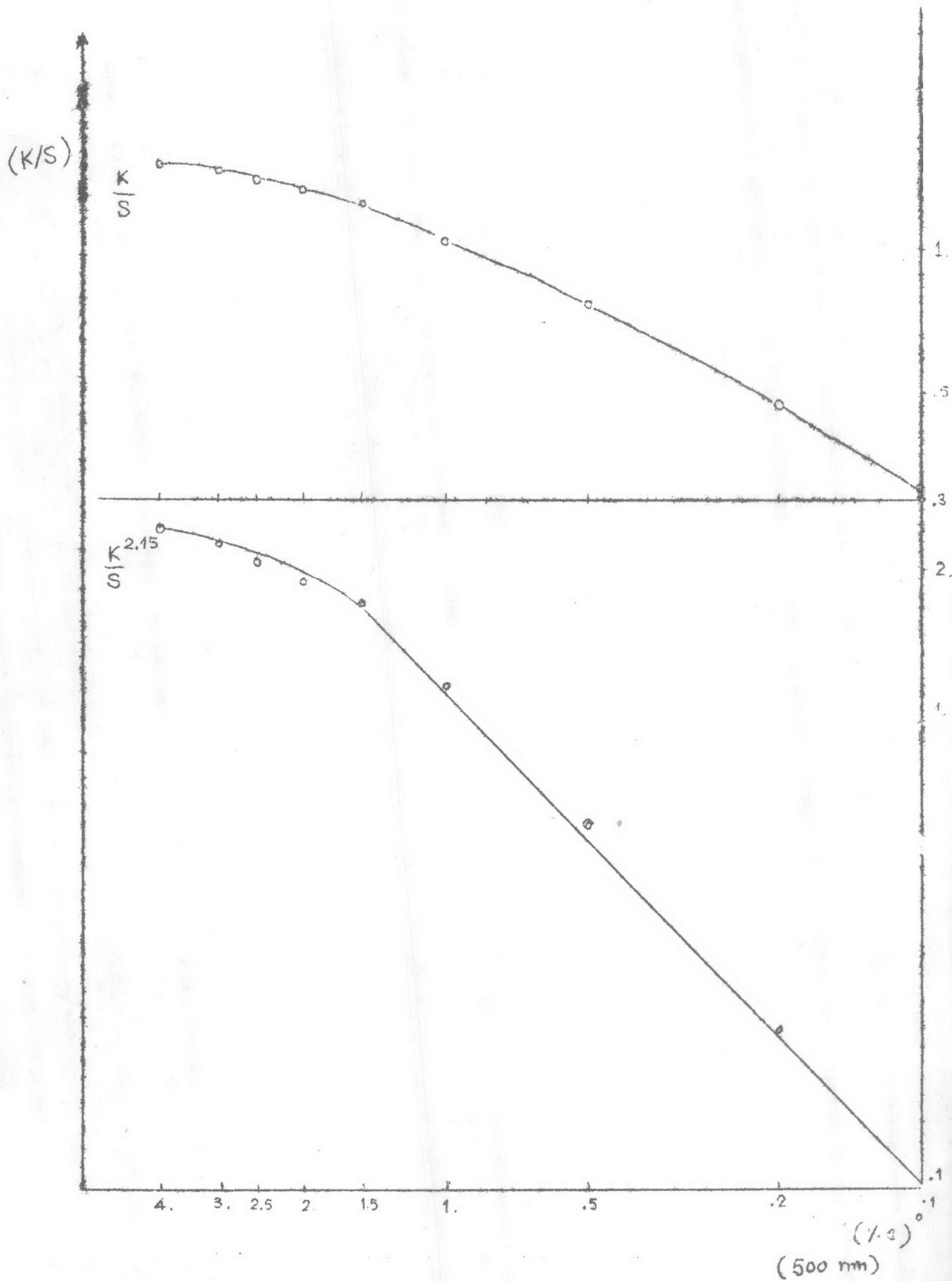


Fig. 5.5 K/S vs %c of Procion Orange MX - 2R

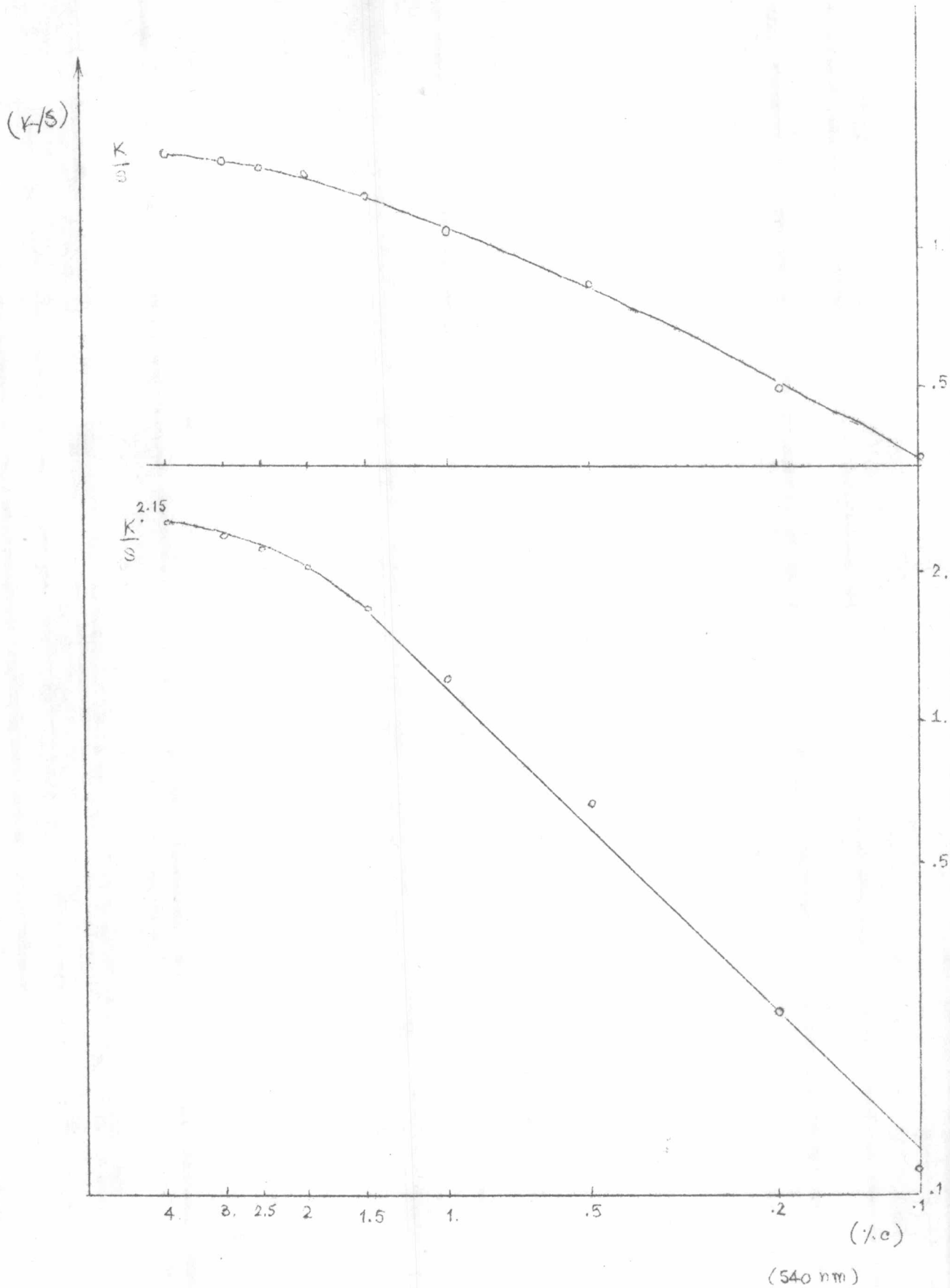


Fig. 5.6 K/S vs %c of Procion Red MX - 5B

(540 nm)

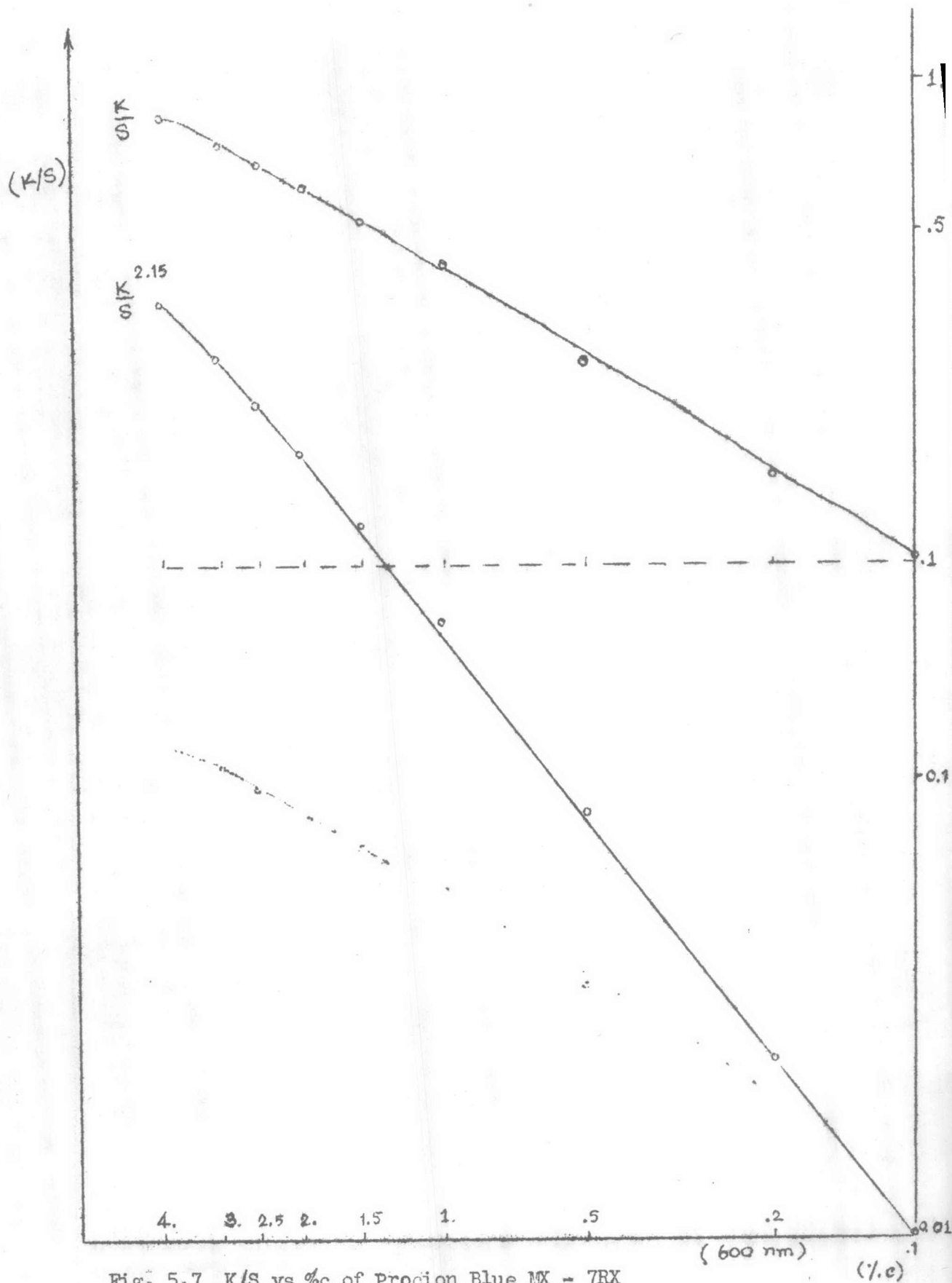


Fig. 5.7 K/S vs %c of Procion Blue MX - 7RX

Fig. 5.7 K/S vs %c of Procion Blue MX - 7RX

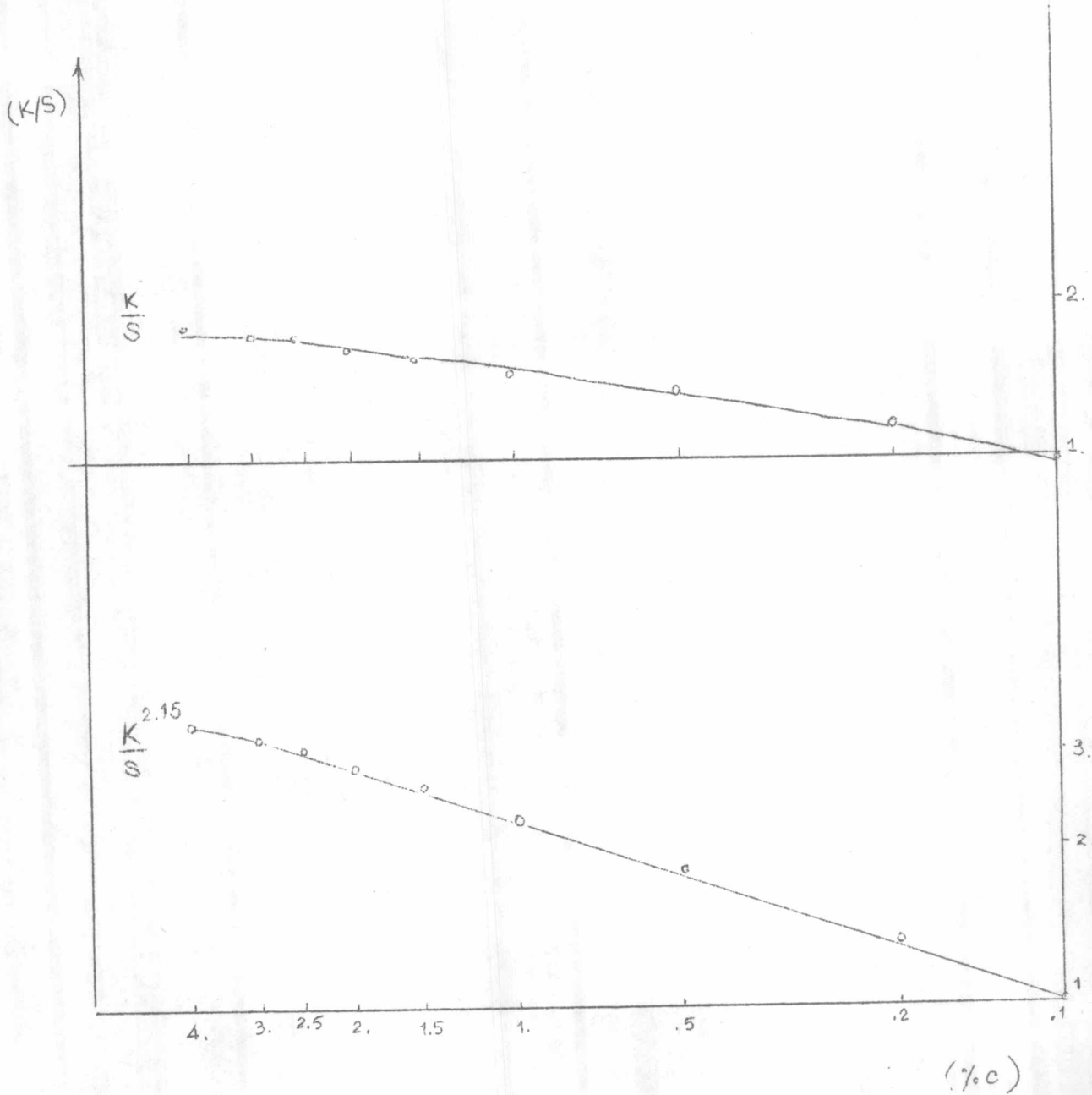


Fig. 5.8 K/S vs %c of Procion Turquoise MX - G (680 nm)

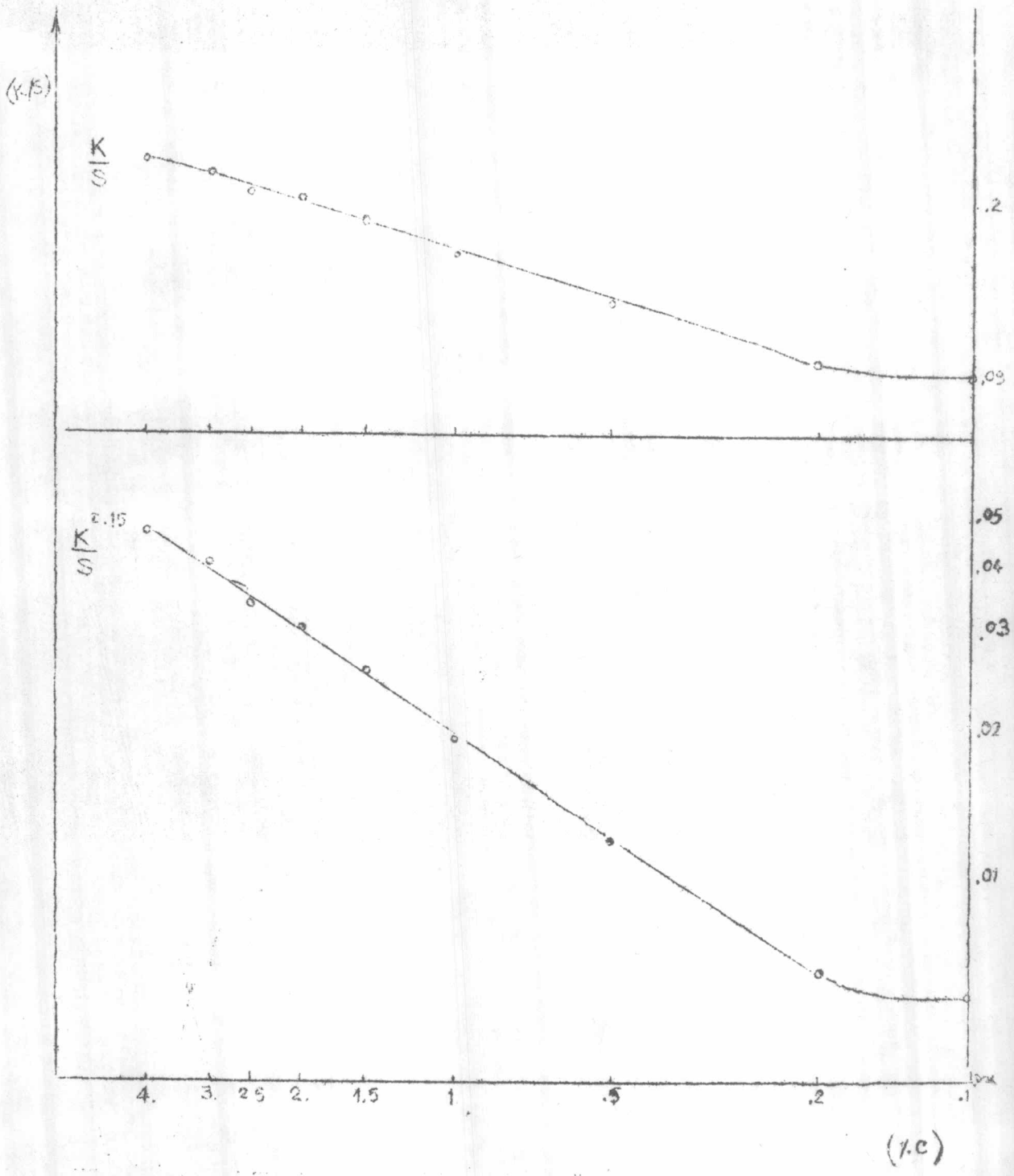


Fig. 5.9 K/S vs %c of Procion Brown MX - 5BR (520 nm)

Fig. 5.10 K/S vs %c of Procion Brown MX - 5BR

concentrations, the lines of $(K/S)^{2.15}$ values are more readily straight than the lines of K/S values, although the end of the lines (at high concentration levels) deviate from straight lines. The causes of its characteristic are :

- (1) the limit of absorption of fiber.
- (2) the affinity and substantivity of its color.

5.3 The Modified Mathematical Model

It is proposed here that the mathematical model based on the turbid media theory be modified by replacing $\frac{K}{S}$ with $(\frac{K}{S})^n$ so as to retain the linearity of the model. Then the modified model consists mainly the following mathematical equations

$$\left(\frac{K}{S} \right)^n = \left[\frac{K}{S} \text{ substrate} + \text{colorant} - \frac{K}{S} \text{ substrate} \right]^n \quad (5.2)$$

$$a \left(\frac{K}{S_A} \right)^n = \left[\frac{K}{S_M} - w \frac{K}{S_W} \right]^n \quad \text{for single color} \quad (5.3)$$

Similarly, for the two color and three color mixture dycings, Equation 5.3 may be rewritten as follows

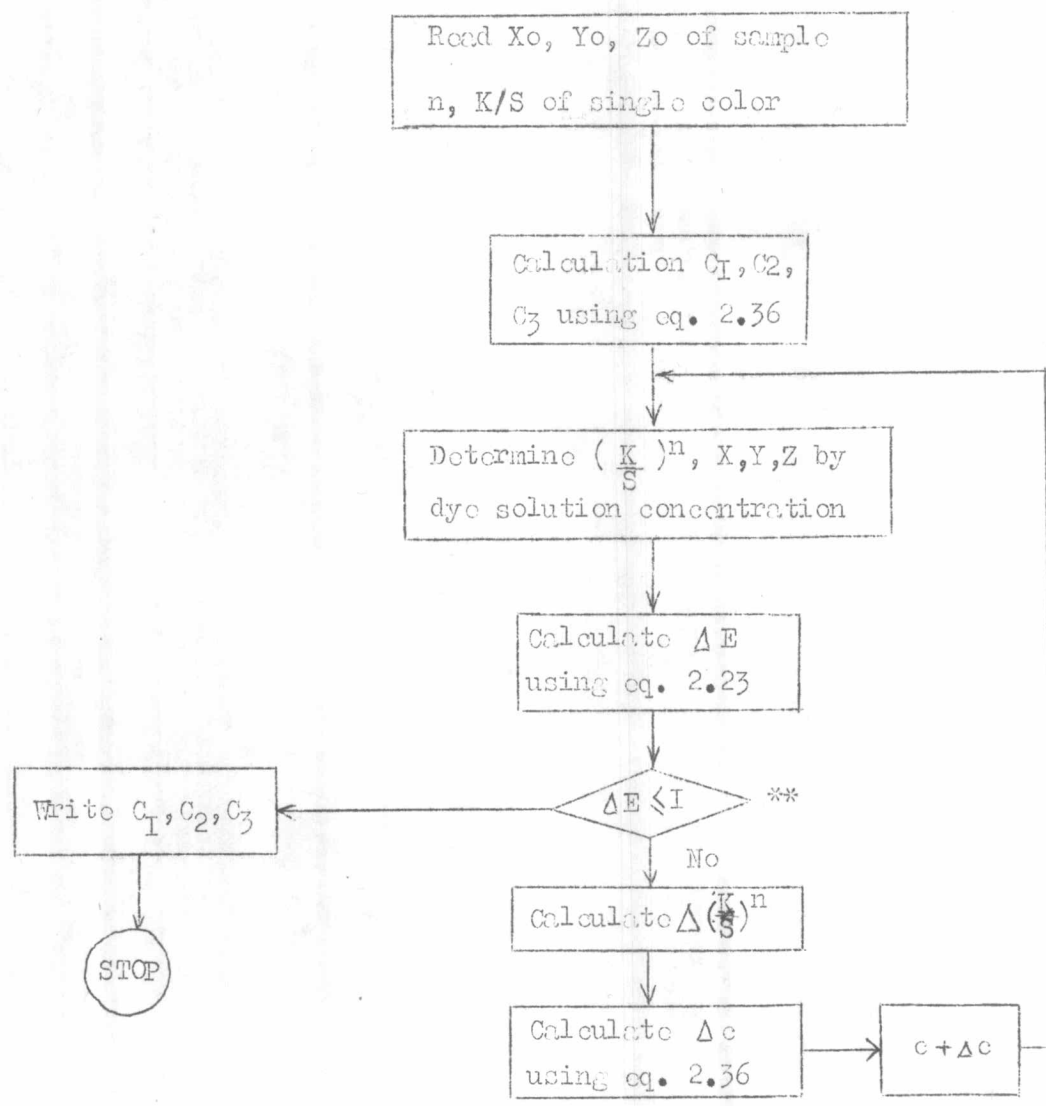
$$a \left(\frac{K}{S_A} \right)^n + b \left(\frac{K}{S_B} \right)^n + c \left(\frac{K}{S_C} \right)^n = \left[\frac{K}{S_M} - w \frac{K}{S_W} \right]^n \quad (5.4)$$

Actually, each dyestuff has its own feasible power n , however, a single value of n is assumed in Equation 5.4. This value is the average values of n 's of dyestuffs. The assumption of single value of n should be feasible, since the experimental result reveals that the values of n 's of different dyestuffs are closed together.

The complete mathematical model consists of Equation 5.4 and Equation 2.36 in which K/S's are replaced by $(K/S)^n$'s.

5.3.I Iterative calculation procedure

The calculation procedure is essentially an iterative one and is shown in Figure 5.I0



** in this work, ΔE was directly obtained from spectrophotometer

Figure 5.I0 Iterative calculation diagram

5.3.2 Alternative calculation procedure

The alternative procedure is shown in Figure 5.II

(7)

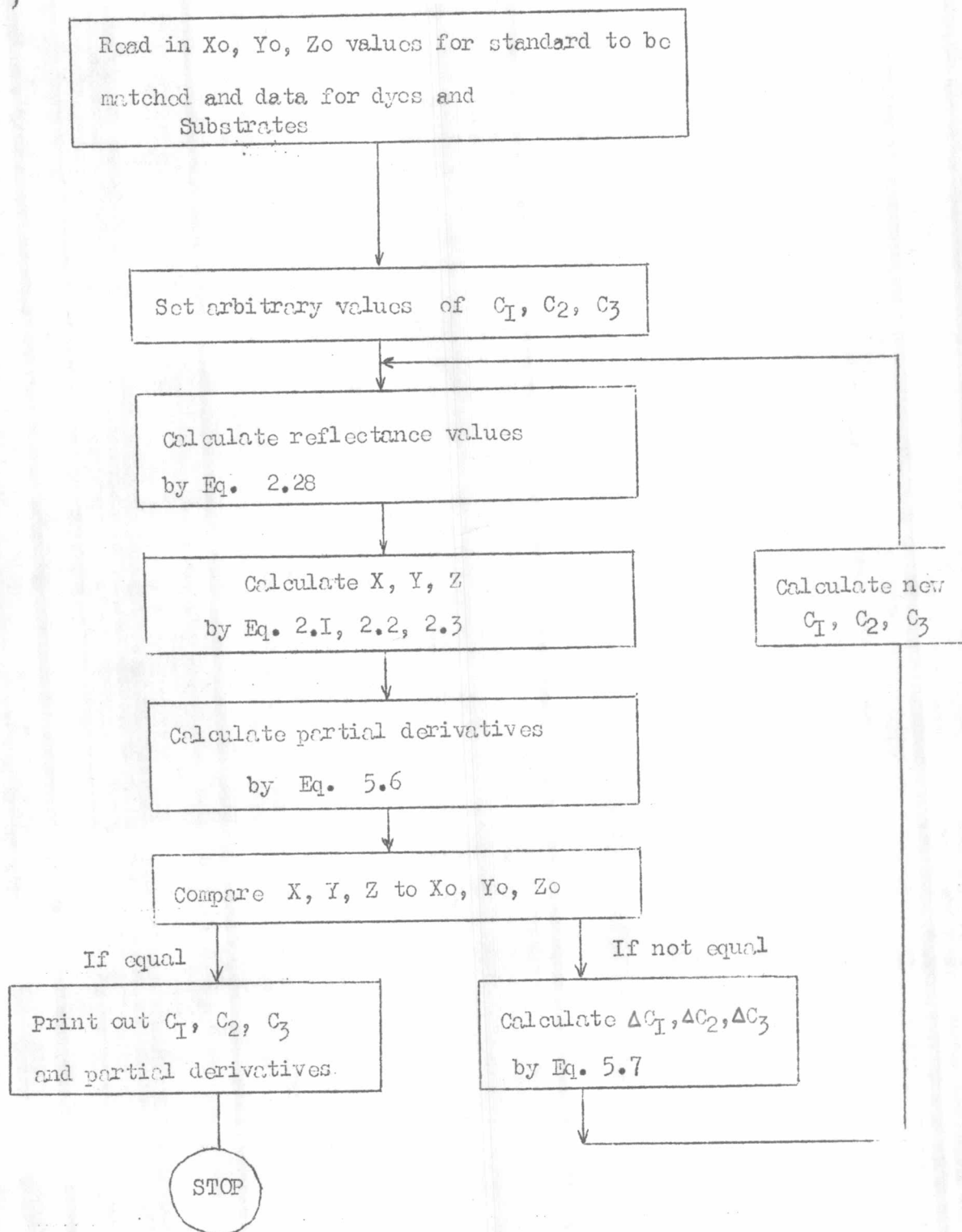


Figure 5.II Flow diagram for colour matching calculation.

The modified mathematical model was used to predict the dyestuff concentration. Iterative calculation procedure outlined in Figure 5.10 was used.

The results of the K/S , $(K/S)^n$ values are shown in Tables 4.15 to 4.16 and Tables 4.19 to 4.20 for standard dyeings and predicted dyeings respectively. The dye concentrations are shown in Tables 4.17 to 4.18 and Tables 4.25 to 4.26 for predicted and corrected concentration respectively.

The $\Delta (K/S)^{2.15}$, Δc , and ΔE values are shown in Tables 4.21 to 4.22 , Tables 4.23 to 4.24 and Tables 4.27 to 4.28 respectively

Only one iteration was required and the final ΔE values were mostly less than 1.00 at which colors are indifferent to the human eyes. Consequently, the modified mathematical model is applicable in cotton fabric dyeing. It can help color matching to be accomplished quickly.

5.4 Applicability of the modified model

Slight experimental error which is discussed in Section 5.5 certainly caused the deviation of predicted values from the theoretical values. Moreover, deviation may also due to the followings :

I) The band of the usable wavelengths are not exact. They are too large to specify the real wavelength of maximum absorption of each dyestuffs. For example, from Table 4.14, The Procion Yellow MX - 8G and Procion Yellow MX - 3R have the

same wavelength of maximum absorption, but in reality they have not. So, the band of wavelength ($\Delta\lambda$) should be decreased.

2) the K/S functions used for calculating the color concentrations are taken from Appendix B which give maximum error up to ± 0.1 . The function $(K/S)^{2.15}$ was changed slightly.

For the $(K/S)^{2.15}$ functions, their additivities also have some errors. See the Figure 2.9, the additivity of the K/S function of Magenta and Yellow is the K/S function of Red., i.e.,

$$K/S_M + K/S_Y = K/S_R - K/S_W$$

but, in calculation, the following equation is used.

$$a \cdot K/S_A^{2.15} + b \cdot K/S_B^{2.15} = (K/S_M - w K/S_W)^{2.15}$$

Certainly, it has error, but **very small**, so it can be neglected.

3) Concentration of Precion Turquoise MX-G, Precion Blue MX - 7RX, and Precion Brown MX-5BR could not be predicted due to low substantivity of the fabric for these dyes. They cannot be dyed together with other high affinity dyes in the same white fabric which has only been bleached. The dyestuffs hardly diffuse into fibers and react less. This situation

can be improved if the white fabric is mercerized to increase the affinity of color to penetrate the fiber thoroughly.

4) Different lots of a color are usually of different color strength. Thus color matching prediction can be effected using different lots when the same set of K/S values are used. In this experiment, different lot of Procion Blue MX - 4GD were used. However, it was found that the total error was very small.

5) The application can be summarized as follows:

5.1) It (colour prediction) will help us in our choice of dyestuffs, in making out our recipes, in speeding up our colour matching.

5.2) It will enable us to work out pass-fail tolerances thereby ensuring less reprocessing and customer rejections

5.3) It will help us to check quickly the levelness of pieces and to grade shades in to acceptable batches.

5.4) It will ease the problem of assessing white shades.

5.5) It will make us more efficient and profitable.

5.5 On the experiment

In this research, the main factors in the actual dyeing process which have to be controlled accurately are :

(I) weight of materials to be dyed, a deviation of $\pm 2\%$ have been found.

(2) weight of dyestuffs, a deviation of 1% is tolerable.

(3) time of dyeing : time lost during the salt addition, the alkali addition and temperature elevation were not accounted for.

(4) temperature of dyeing : there are maximum tolerance of 10°C in fixed temperatures in single dyeing, two color mixture dyeing, and three color mixture dyeing.

(5) pH : The pH of water used for dyeing was not constant and varied from 6.5 to 7.0

(6) liquor ratio, not strictly constant when the predicted and corrected concentrations are used.

(7) electrolyte concentrations, varied slightly due to impurity in the commercial salt.

These 7 factors are not absolutely under control in this research, then the results are slightly effected.

5.6 Recommendations

When color measurement is restricted by the ability of an instrument, the following calculation procedures are recommended:

(I) If the only instrument available is a colorimeter giving either R, G, and B values or X, Y and Z values (I4) it is quite possible to set up a production control system based on such an instrument for 3 colorant mixtures. The system can be operated by using direct readings from the colorimeter. The requirements before calculation starts are a sample of the standard

colour together with three more samples, each one showing the effect of reducing by about 20% each colorant in turn.

All four samples are measured on the colorimeter and the standard X, Y and Z values are subtracted in turn from those of samples 1, 2, and 3 (1 Colorant 1 reduced ΔC_1 , 2 reduced ΔC_2 , and 3 reduced ΔC_3 , respectively) the results being set out as follows:-

in columns corresponding to samples 1, 2 and 3

$\frac{\Delta C_1}{}$	$\frac{\Delta C_2}{}$	$\frac{\Delta C_3}{}$
$X_1 - X_{std.}$	$X_2 - X_{std.}$	$X_3 - X_{std.}$
$Y_1 - Y_{std.}$	$Y_2 - Y_{std.}$	$Y_3 - Y_{std.}$
$Z_1 - Z_{std.}$	$Z_2 - Z_{std.}$	$Z_3 - Z_{std.}$

If the resulting rows are summed across they will give the difference in X, Y, and Z between a sample and the standard but this sample being one in which all the colorants were simultaneously reduced by 20%. The elements of the array are partial derivatives showing the small changes in tristimulus values caused by a small change in colorant concentrations.

$$\begin{aligned} \frac{\delta X}{\delta C_1} + \frac{\delta X}{\delta C_2} + \frac{\delta X}{\delta C_3} &= \Delta X \\ \frac{\delta Y}{\delta C_1} + \frac{\delta Y}{\delta C_2} + \frac{\delta Y}{\delta C_3} &= \Delta Y \\ \frac{\delta Z}{\delta C_1} + \frac{\delta Z}{\delta C_2} + \frac{\delta Z}{\delta C_3} &= \Delta Z \end{aligned} \quad (5.5)$$

This matrix is not exact but becomes more precise the smaller the derivatives and the differences in X, Y and Z become as is normal with differential calculus.

The partial derivatives can be defined in the following manners : $\delta X / \delta C_1 = \sum_{400}^{700} E \cdot \bar{x} \cdot K_1 \cdot \exp(-CK_{11} - CK_{22} - CK_{33})$ (5.6) and etc.,

Any changes in C_1 , C_2 and C_3 may be multiplied into matrix A in the form

$$\begin{array}{ll} \Delta C_1 & \text{to give new approx.} \quad \Delta X \\ \Delta C_2 & \text{values to :-} \quad \Delta Y \\ \Delta C_3 & \quad \quad \quad \Delta Z \end{array}$$

So A is inverted to give :-

$$\begin{pmatrix} \frac{\delta C_1}{\delta X} & \frac{\delta C_1}{\delta Y} & \frac{\delta C_1}{\delta Z} \\ \frac{\delta C_2}{\delta X} & \frac{\delta C_2}{\delta Y} & \frac{\delta C_2}{\delta Z} \\ \frac{\delta C_3}{\delta X} & \frac{\delta C_3}{\delta Y} & \frac{\delta C_3}{\delta Z} \end{pmatrix} * \begin{pmatrix} \Delta X \\ \Delta Y \\ \Delta Z \end{pmatrix} = \begin{pmatrix} \Delta C_1 \\ \Delta C_2 \\ \Delta C_3 \end{pmatrix} \quad (5.7)$$

The System is essentially non - linear so will operate successfully only over small differences in colour space, say about 5 to 7 ANLAB units although this can be extended by various means to about double this limit.

(2) If the only instrument available can not give the total color differences, we can use the Simon & Goodwin charts to estimate them. Simon & Goodwin based their Union Carbide Charts

on recommendations by Davidson & Hanlon. Their method made use of the g_{11} , g_{22} , and $2g_{12}$ constants (14,18). The first equation of this type was derived by Brown and MacAdam, subsequently it was modified on a graphical method by Simon and Goodwin and is :- (15)

$$\Delta E = \left[g_{11} (\Delta x)^2 + 2g_{12} \Delta x \Delta y + g_{22} (\Delta y)^2 + 2g_{23} \Delta y \Delta Y + g_{33} (\Delta Y)^2 + 2g_{13} \Delta x \Delta Y \right]^{\frac{1}{2}}$$

where g_{11} , g_{12} , etc., are metric coefficients whose values depend on the location of the standard x , y , Y space.

The C.I.E. Chromaticity Diagram is partitioned into adjoining rectangles where the g_{11} , g_{22} and g_{12} are essentially constant within each partition. Unit diagonal distances were computed to the nearest 0.100 in terms of x and y , subdivided to the nearest 0.025. The total number of charts to cover the entire diagram was 89. Each chart or partition was numerated by the central calculated point of that region Fig 5-12.

The standard and the batch before adjustment and after adjustment were plotted together on the chart. The distances between the standard and the batches were measured by an inch ruler. Every 1 inch is equivalent to a MacAdam Unit.

These distance give the uncorrected Δc values. These values together with the Y values of the standard and batches are plotted on the Colour Difference Charts. The abscissae give the Y values in decimal fractions, and the ordinates give the Δc uncorrected values, Fig 5.13.

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UNIFORM CHROMATICITY CHART

$x=0.350$

$y=0.300$

CHART 3530

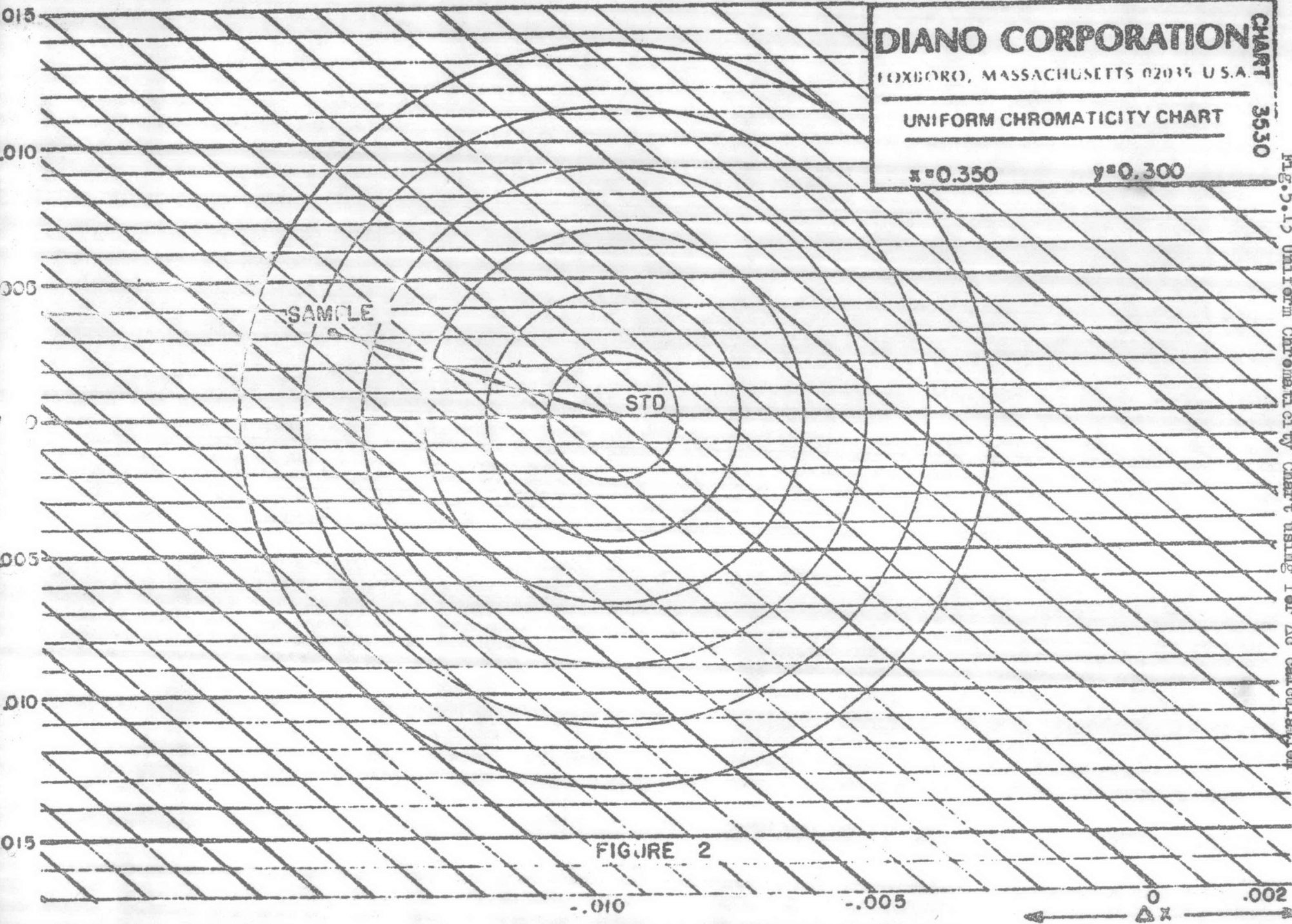


Fig. 5.13 Uniform Chromaticity Chart using for Δd calculation

FIGURE 2

Δx

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COLOR DIFFERENCE CALCULATING CHART
CHART I
Y=0.070 TO 0.115

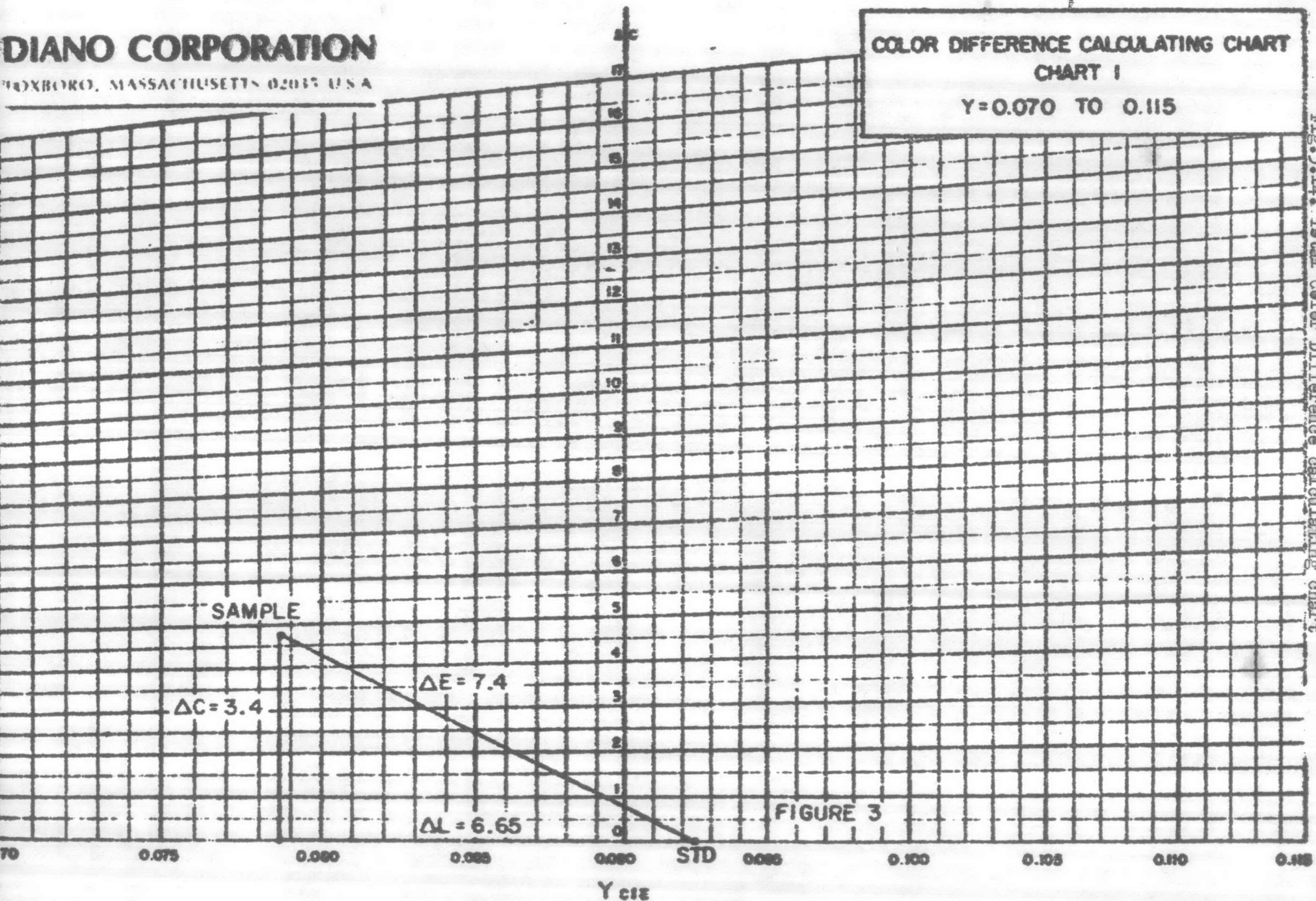


Fig. 5.14. Metal Color Difference calculating chart.

The standard is plotted on the colour difference chart, fig. 5.14, with a zero Δc value. The batches are plotted consecutively with their appropriate Y and C values. A vertical line is drawn from each point, and a line drawn from the batch to the standard. Two right angled triangles are thus formed. The perpendicular give the corrected ΔC the horizontal the ΔL value, and the hypotenuse the total colour difference. Again the distance are measured on the $\frac{1}{2}$ inch scaling.

- ΔC - Chromaticity difference.
- ΔL - Luminosity difference.
- ΔE - Total Color difference.

The recommendations for further work of this study are as follows:-

1. Study the applicability of the mathematical model for other kinds of dyestuffs and fabrics using the commercial plants.
2. Study the metamerism in colour matching to give the best results in prediction (see Appendix C)
3. Study the applicability of the mathematical model for the colour prediction of plastics, paints, papers.

5.7 Conclusions

The results from this study indicate that:

- (I) The K/S values are not linear function of the colorant concentration and the additivity of them are not true.

(2) taking an exponent value n to the K/S value, it can retain the linearity and the additivity of the mathematical model.

(3) the results of using the modified mathematical model for reactive dyeing on cotton fabric are satisfactory and the best results are in the range of 0-3% of dye concentration. However, the model is not applicable for dyes of very low affinity.