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Modelling of Colour Yield in Polyethylene Terephthalate Dyeing with Statistical and Fuzzy Regression

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ABSTRACT

The aim of this study is to investigate and apply two approaches of fuzzy regression as well as statistical regression for modelling the colour yield in polyethylene terephthalate (polyester) high temperature (HT) dyeing as a function of disperse dyes concentration, temperature, and time. The two approaches of fuzzy regression modelling were triangular coefficients and exponential coefficients. The statistical models obtained, did not meet the required conditions to be accepted. However, after applying modification to the original fuzzy regression models with triangular coefficients, acceptable models were obtained. The modification was carried out by means of enabling the centre of coefficients to take positive and negative values as well as dispersing fuzziness in the coefficients. The models obtained with exponential fuzzy coefficients showed weak interaction for the above mentioned variables and hence it seems that for modelling cases such as the one considered in this paper, fuzzy regression with triangular coefficients may be preferred.

Key Words:
polyester;
disperse dye;
statistical regression modelling;
fuzzy regression with triangular coefficients;
fuzzy regression with exponential coefficients.

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INTRODUCTION

Polyethylene terephthalate (PET) commonly known as polyester is the most important man-made fibre. This polymer contains ester groups (-CO-O-) in its main molecular chain and is produced by melt spinning process. Ester groups are a result of the reaction between bi-functional carboxylic acids and bi-functional alcohols [1]. The absence of reactive groups, capable of undergoing reaction with anionic and cationic dyes as well as being a hydrophobe, has limited dyeing and printing of unmodified polyethylene terephthalate fibres to only disperse dyes [2]. Moreover, under normal dyeing conditions, the compact structure of polyethylene terephthalate fibres makes the penetration of disperse dyes inside them very difficult. For this reason, dyeing of polyethylene terephthalate fibres requires special conditions such as high temperature (≈130°C), dry heat (190 - 220°C), or using carrier in the dye bath [3].

The chemical structure of disperse dyes contains polar groups such as -NHR, -OH and $-NH_2$ but there are no ionic groups present which leads to their very low solubility in water [4,5]. Azo, anthraquinone, and nitrodiphenylamine constitute the three main chemical structures of disperse dyes. However, as far as the application is concerned, these dyes are divided into four groups namely: A, B, C, and D [5]. Temperature, time, and disperse dye concentration are the primary factors affecting the colour yield in dyeing polyethylene terephthalate. The overall picture of the relative importance of these factors can be seen in models representing the colour yield as their function. These models may also have applications in processing and cost minimization.

The main objective of this research is to present a model for the colour yield of polyethylene terephthalate dyed with specific disperse dyes by high temperature method. The models will represent colour yield as a function of time, temperature, and dye concentration for each dye. This was attempted by statistical as well as fuzzy regression analysis of K/S and F_k functions. K/S and F_k have a direct relationship with the colour yield.

K/S Shows the ratio of the absorbed light by an opaque substrate relative to the scattered light from it. This ratio is calculated by Kubelka-Munk theory as [6]:

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

where R_λ is the reflectance of sample of infinite thickness to light of a given wavelength, expressed in fractional form. K/S can be used as an estimation of the amount of dye absorbed by the substrate. This function is related to the amount of dye on the substrate by the following relationship [7]:

$$K/S = AC \quad (2)$$

where A is the proportional factor which is constant for each dye.

F_k is in fact an estimation of the area under the absorption curve which considers K/S in different wavelengths of visible light as well as colour matching functions. This function is calculated as follows:

$$F_k = \sum_{400}^{700} (K/S)_\lambda (\bar{x}_{10,\lambda} + \bar{y}_{10,\lambda} + \bar{z}_{10,\lambda}) \quad (3)$$

where $\bar{x}_{10,\lambda}$, $\bar{y}_{10,\lambda}$ and $\bar{z}_{10,\lambda}$ are the colour matching functions (400-700 nm) with observer position at the standard angle of 10 degrees [6].

STATISTICAL AND FUZZY REGRESSION ANALYSIS

Statistical Regression

Regression is a method for analysis and modelling of a dependent variable as a function of one or more independent variable(s). The simplest form of regression is linear. Assuming y and x as the dependent and independent variables, respectively, the function of the straight line relating these two variables is $Y = \beta_0 + \beta_1 x$. Since all the data do not practically lie on the regression line, there exists an error between Y and the straight line $\beta_0 + \beta_1 x$. This error, represented by a random variable η is a sign of shortcoming of the model for the crisp fitting of the data, and is included in the model as follows:

$$Y = \beta_0 + \beta_1 x + \varepsilon \quad (4)$$

Statistical analysis, based on regression model, is carried out by preparing a sample of pair observations (x_i, y_i), i=1,...,n from the population. It is assumed that the following relationship applies to each (x_i, y_i):

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad i=1,...,n \quad (5)$$

The validity of the statistical analysis of the above mentioned regression model depends on the following conditions [8]:

1) The errors must have an expected value equal to zero and a constant variance i.e., $E(\varepsilon_i) = 0$, $var(\varepsilon_i) = \sigma^2$.
2) No correlation should exist between the errors i.e., $Cov(\varepsilon_i, \varepsilon_j) = 0$, $i \neq j$.
3) Errors must have a normal distribution i.e., $\varepsilon_i \sim N(0, \sigma^2)$.

If it happens that the above three conditions are not met, one must either modify the models so that suitable ones emerge [8] or use alternative approaches like spline regression [9] and robust regression [10]. One of the new approaches in this field is fuzzy regression model which do not need the above mentioned conditions [11,12].

Fuzzy Regression

Fuzzy regression was investigated by Tanaka et al. in 1982 for the first time [12]. This work was followed and developed further by others [13-16]. Celmins [17] and Diamond [18] introduced the least squares approach to fuzzy regression analysis. A practical application of fuzzy least squares regression has been reported by Mohammadi and Taheri [19]. It can generally be said that fuzzy regression has found an increasing use in different branches of science. A useful survey about fuzzy regression can be found elsewhere [20]. Generally speaking, fuzzy regression models can be classified into two categories:

- Models with fuzzy coefficients and crisp observations.
- Models with crisp coefficients and fuzzy observations.

In the present work, two main approaches of regression modelling with fuzzy coefficients and crisp observations were employed for the modelling of colour yield. The first approach was the fuzzy regression with triangular fuzzy coefficients. The second one was the regression with a fuzzy coefficient vector defined by an exponential possibility distribution. In the following sections, the definitions and properties of these two approaches are briefly described.

Regression Model with Triangular Fuzzy Coefficients

The regression model with fuzzy coefficients, which is suitable for crisp independent variable(s) and crisp dependent variable, is as follows [12, 21]:

$$y = f(\underline{x}, \underline{A}) = A_0 + A_1x_1 + A_2x_2 + ... + A_nx_n \qquad (6)$$

where,

Y is dependent variable with crisp observation,

$\underline{x} = [x_1, x_2,...,x_n]$ is the vector of independent variabls and $\underline{A} = [A_0, A_1,....,A_n]$ shows the vector of fuzzy numbers.

Assuming that A_i, i= 0,1,2,...,n, are triangular fuzzy numbers, and x_i, i = 0,1,2,...,n, are positive real numbers, then Y (fuzzy output) will be a triangular fuzzy number in the form of $Y = (f^c(\underline{x}), f_s^L(\underline{x}), f_s^R(\underline{x}))_T$, where $f^c(\underline{x})$, $f_s^L(\underline{x})$, and $f_s^R(\underline{x})$ show the mean value, left spread and right spread of Y respectively. These are calculated as follows [21, 22]:

$$f^c(\underline{x}) = a_0^c + a_1^c x_1 + ... + a_n^c x_n \qquad (7)$$

$$f_s^L(\underline{x}) = s_0^L + s_1^L x_1 + ... + s_n^L x_n \qquad (8)$$

$$f_s^R(\underline{x}) = s_0^R + s_1^R x_1 + ... + s_n^R x_n \qquad (9)$$

In other words, the membership function of fuzzy output can be shown in the following way:

$$\mu_Y(y) = \begin{cases} 1 - \dfrac{f^c(\underline{x}) - y}{f_s^L(\underline{x})}, & f^c(\underline{x}) - f_s^L(\underline{x}) \le y \le f^c(\underline{x}) \\ 1 - \dfrac{y - f^c(\underline{x})}{f_s^R(\underline{x})}, & f^c(\underline{x}) < y \le f^c(\underline{x}) + f_s^R(\underline{x}) \end{cases} \qquad (10)$$

The function of right spread can also be represented by the skew coefficients. Using $s_i^R = k_i s_i^L$ the function (9) can be rewritten as:

$$f_s^R(\underline{x}) = k_0 s_0^L + k_1 s_1^L x_1 + ... + k_n s_n^L x_n \qquad (11)$$

If $k_i = 1$, i = 0,1,..., n, then $s_i^L = s_i^R = s_i$

Hence, function (11) reduces to function (8). In this case $f_s^L(\underline{x}) = f_s^R(\underline{x}) = f^s(\underline{x})$.

Determination of the Fuzzy Coefficients

In order to determine the coefficients A_i, i = 0,1,2,...,n, it is assumed that:

1) For all the observations (j = 1,2,...,m), the value of Y_j obtained from the model has a membership degree as big as h i.e.,

$$\mu_Y(y_j) \ge h, \qquad j = 1,2,...,m. \qquad (12)$$

2) The fuzzy coefficients A_i, i = 0,1,2,...,n, should be such that the fuzziness of the model is minimum.

Since the fuzziness of a fuzzy number increases with its spreads, minimizing the sum of the spreads of fuzzy outputs, leads to a minimum value of the fuzziness of the model. So the determination of the fuzzy coefficients leads to a linear programming problem in which the objective function is the sum of the spreads of the fuzzy outputs i.e.,

$$Z = m(s_0^L + s_0^R) + \sum_{i=1}^{n}[(s_i^L + s_i^R)\sum_{j=1}^{m} x_{ji}] \quad (13)$$

where, X_{ji} shows the value of the j^{th} observation for the i^{th} variable.

On the other hand, considering (12) and previous explanations, the constraints of the problem can be written as follows:

$$1 - \frac{f^c(\underline{x}_j) - y_j}{f_s^L(\underline{x}_j)} \geq h \Rightarrow (1-h) f_s^L(\underline{x}_j) - f^c(\underline{x}_j) \geq -y_j \quad j = 1, 2, ..., m$$

$$1 - \frac{y_j - f^c(\underline{x}_j)}{f_s^R(\underline{x}_j)} \geq h \Rightarrow (1-h) f_s^R(\underline{x}_j) + f^c(\underline{x}_j) \geq y_j \quad j = 1, 2, ..., m \quad (14)$$

Substituting (7), (8) and (9) in (14), the constraints can be rewritten as:

$$(1-h)s_0^R + (1-h)\sum_{i=1}^{n} s_i^R x_{ji} + a_0^c + \sum_{i=1}^{n} a_i^c x_{ji} \geq y_j \quad j = 1, 2, ..., m \quad (15)$$

$$(1-h)s_0^L + (1-h)\sum_{i=1}^{n} s_i^L x_{ji} - a_0^c - \sum_{i=1}^{n} a_i^c x_{ji} \geq -y_j \quad j = 1, 2, ..., m \quad (16)$$

Regarding two constraints for each observation, in other words, 2m constraints for observations, one can minimize the objective function (13) using linear programming approaches, such as simplex method [23]. Note that considering $s_i^R = k_i s_i^L$ the objective function (13) and constraint (15) can be rewritten as:

$$Z = m(1+k_0)s_0^L + \sum_{i=1}^{n}\left[(1+k_i)s_i^L \sum_{j=1}^{m} x_{ji}\right] \quad (17)$$

$$(1-h)k_0 s_0^L + (1-h)\sum_{i=1}^{n} k_i s_i^L x_{ji} + a_0^c + \sum_{i=1}^{n} a_i^c x_{ji} \geq y_j, \quad j = 1, 2, ..., m \quad (18)$$

It is reminded that Yen et al. [21] considered objective function Z as follows:

$$Z = (s_0^L + s_0^R) + \sum_{i=1}^{n}[(s_i^L + s_i^R)\sum_{j=1}^{m} x_{ji}]$$

As it can be seen, Z does not represent the total fuzziness of the linear model (6). In other words their objective function is not equal to the sum of spreads of fuzzy outputs for all the data sets. It is probable that this made their models unrealistic. Examples 1 and 2 in the work reported by Yen et al. [21] show that all the vagueness of the model is concentrated in the intercept, and there is no fuzziness in the coefficients of the independent variables i.e., the independent variables have no effect on the fuzziness of the models. Surely, this is a shortcoming for the obtained models. In this research, using the adjusted formula for the objective function Z (17), this difficulty has been overcome. This adjusted approach has been used for obtaining the triangular fuzzy coefficients of the models shown in Tables 6- 8.

It is pointed out that fuzzy regression models are evaluated and compared by means of mean square error (MSE), based on the values of y_i (observed value of the dependent variable) and $def(\tilde{y}_j)$ (defuzzified estimations of the dependent variable) i.e.,

$$MSE = \frac{1}{m}\sum_{j=1}^{m}[y_j - def(\tilde{y}_j)]^2 \quad (19)$$

In this research, mean of maxima method was used for defuzzification [22].

Regression Model with Exponential Fuzzy Coefficients

Regression model with exponential fuzzy coefficients (also called exponential possibility regression) which is suitable for crisp independent variable(s) and crisp dependent variable is presented as follows [16]:

$$Y = A_1 x_1 + A_2 x_2 + \quad + A_n x_n = Ax \quad (20)$$

Where x is a non fuzzy vector of exploratory variables and $A = (A_1, \quad , A_n)$ is a fuzzy coefficient vector. The distribution of the fuzzy coefficient A is an exponential possibility distribution with a centre vector a_c and a symmetrical positive definite matrix D_A as:

$$\Pi_A(a) = \exp\{-(a-a_c)^T D_A^{-1}(a-a_c)\}, \quad (21)$$

$$A=(a_c,D_A)_e. \quad (22)$$

For fitting the above model, the following assumptions are made:

(i) The data are given as (y_j, x_j), j = 1, ,m, where y_j is an output and $x_j = (x_{j1}, \ ,x_{jn})^T$ is an output vector. Assuming m>>n, E = {1, ,n} is the set of subscripts of independent vectors $\{x_1,...,x_n\}$ that are chosen from the given input vectors.

(ii) The data can be represented by the possibility of linear model with the exponential possibility distribution (21)

(iii) Given a threshold h_j, the given output y_j should be included in the h_j level set of estimated fuzzy output y_j, that is:

$$[y_j]_{h_j} = \{y \mid \Pi y_j(y) \geq h_j\} \ni y_j \quad (23)$$

(iv) The index of the spread of the possibility of linear model is defined by:

$$J=\sum_{j=1}^{m} x_j^T D x_j \quad (24)$$

Based on the above assumptions, the problem for finding the possibility distribution Π_A (a) can be written as the following optimization problem:

min J
D_A, a_c

Subject to

$$\Pi_{y_i}(y_j) \geq h_j \quad (25)$$

$D_A>0$.
Where, the constraint (25) which is the same as (23) can be rewritten as

$$x_j^T D_A x_j \geq (y-a_c^T x_j)^2/(-\log h_j). \quad (26)$$

This programme is a non-linear programming problem. In order to transform this problem into a linear programming problem, the following steps are carried out [16]:
(I) Determine the centre vector a_c, using a suitable method, for example the statistical regression.

(II) Substitute the obtained centre vector a_c into (26) and solve the following linear programming problem:

$$\min J = \sum_{j=1}^{m} x_j^T D_A x_j \quad (27)$$
D_A

Subject to:

$$x_j^T D_A x_j \geq (y_j-a_c^{*T} x_j)^2/(-\log h_j) \quad (28)$$

$$x_j^T D_A x_j = 0 \text{ for all } i\#j, \ i, j \in E. \quad (29)$$

Given an input vector x_0, the corresponding fuzzy output Y_0 and its possibility distribution would be $Y_0 = Ax_0$ and Π_{Y0} (y) respectively, where:

$$\Pi_{Y0}(y) = \exp\{-(y-x_0^T a_c)^2 (x_0^T D_A x_0)^{-1}\}. \quad (30)$$

In other words,

$$Y_0=(x_0^T a_c, x_0^T D_A x_0)_e. \quad (31)$$

It is pointed out that the exponential possibility regression models are evaluated and compared by the index

$$J=\sum_{j=1}^{m} x_j^T D_A x_j \quad (32)$$

of the total vagueness of the model i.e.,

LITERATURE REVIEW

The research related to the subject of this work can be summarized as follows:
Hung and Hue [24] used fuzzy inference systems (FIS) to control temperature, pH, and direct dye concentration in continuous dyeing of cellulosic goods. In this model, error constitutes the fuzzy system input, whereas temperature, pH and dye concentration form the fuzzy system output. Marjoniemi and Mantysalo [25, 26] used adaptive neuro fuzzy inference systems (ANFIS) for modelling the relationship between the dye absorption and dye concentration in dyeing leather with two dyes. The result of this work has shown that teaching ANFIS takes less time when compared with artificial neural network (ANN). Um et al. [27] used

fuzzy logic for relating the physical properties of colour, such as hue and intensity to the feelings of the observer. Tavanai et al. [28] used statistical regression for modelling the colour yield as a function of time, temperature and alkali concentration in two phase dyeing (wet fixation) of cotton cloth with reactive dyes.

It is the aim of this research to model the colour yield as a function of time, temperature and disperse dye concentration in high temperature (HT) polyethylene terephthalate dyeing using statistical and fuzzy regression models.

EXPERIMENTAL

Materials

In this research a weft-knitted fabric prepared from a set polyethylene terephthalate yarn (134 dtex) was used for preparing the dyed samples. The disperse dyes employed are listed in Table 1. Acetic acid 98% (Merck) was used to regulate the dye bath pH to 5.5.

Methods

Dyeing of the samples (5 g) was carried out by Polymat laboratory dyeing machine (AHIBA 1000) with the following recipe:

Disperse dye x%
pH 5.5
L:R 50 :1

and according to a set of values for dye concentration, dyeing temperature and dyeing time in the form of a matrix shown in Table 2. After dyeing, reduction clearing for the samples was carried out for 10 min in a bath (65°C) containing sodium hydroxide 38° Be, sodium dithionite and a nonionic detergent.

Table 1. The disperse dyes employed for sample dyeing.

Index name	Commercial name
C.I.Disperse Blue 266	Kayalon Polyester Blue 2R-SF
C.I.Disperse Brown 1	Kayalon Polyester Brown GR-SE
C.I.Disperse Blue 56	Kayalon Polyester Blue EBL-E
C.I.Disperse Red 60	Dispersol Red B-2B
C.I.Disperse Yellow 23	Yohao Disperse Yellow E-R
C.I.Disperse Yellow 7	Yohao Disperse Yellow 4RE
Mixture	Yohao Disperse Red Violet P-R

At the end, the samples were rinsed, dried and prepared for reflection measurements by spectrophotometer (Texflash, Datacolour) with the following conditions:

Diaphragm = 27 mm
Observer = 10°
Light source = D_{65}

The reflection of each sample was measured. Then, K/S and F_k were calculated by considering the dominant wavelength according to the formulae (1 and 3). Table 3 shows the values of K/S and F_K for Kayalon Polyester Blue 2R-SF as an example. Due to space limitation, the data for other dyes [29] are not brought here.

RESULTS AND DISCUSSION

Modelling by Statistical Regression

Assuming zero colour yield, when the independent variables, i.e. time, dye concentration and temperature are zero, enables one to consider a general multiple form for the colour yield model as follows:

$$K/S = k_1 \times \text{Conc.}^{A_1} \times \text{Time}^{A_2} \times \text{Temp.}^{A_3} \tag{33}$$

$$F_K = k_1' \times \text{Conc.}^{A_1'} \times \text{Time}^{A_2'} \times \text{Temp.}^{A_3'} \tag{34}$$

With the help of logarithm, the following linear relationships are obtained:

$$Y_1 = A_0 + A_1X_1 + A_2X_2 + A_3X_3 \tag{35}$$

$$Y_2 = A_0' + A_1'X_1 + A_2'X_2 + A_3'X_3 \tag{36}$$

Coefficients of the above functions are determined by

Table 2. Dyeing conditions.

Dye concentration (%owf)	Temperature (°C)	Time (min)
0.75	100	24
1.5	110	36
3	120	48
4.5	130	

Table 3. The data related to C.I. Disperse Blue 266.

No.	Conc.	Time	Temp.	K/S	F_k	No.	Conc.	Time	Temp.	K/S	F_k
1	0.75	24	100	1.014	9.152	25	0.75	24	120	7.157	61.157
2	1.5	24	100	1.104	10.164	26	1.5	24	120	11.876	100.440
3	3	24	100	1.148	10.760	27	3	24	120	15.878	135.520
4	4.5	24	100	1.178	11.195	28	4.5	24	120	18.878	161.770
5	0.75	36	100	1.421	12.778	29	0.75	36	120	7.223	60.996
6	1.5	36	100	1.518	13.858	30	1.5	36	120	13.697	115.510
7	3	36	100	1.651	15.394	31	3	36	120	20.012	172.650
8	4.5	36	100	1.741	16.378	32	4.5	36	120	17.189	146.920
9	0.75	48	100	1.610	14.502	33	0.75	48	120	7.878	67.660
10	1.5	48	100	1.790	16.413	34	1.5	48	120	12.547	106.000
11	3	48	100	1.928	18.015	35	3	48	120	19.597	167.660
12	4.5	48	100	1.867	17.612	36	4.5	48	120	21.194	183.080
13	0.75	24	110	4.459	39.253	37	0.75	24	130	8.969	74.619
14	1.5	24	110	4.799	42.312	38	1.5	24	130	16.833	141.880
15	3	24	110	5.023	44.646	39	3	24	130	24.352	214.820
16	4.5	24	110	5.422	48.382	40	4.5	24	130	27.678	252.680
17	0.75	36	110	5.797	50.621	41	0.75	36	130	10.198	84.369
18	1.5	36	110	4.974	43.504	42	1.5	36	130	18.605	156.650
19	3	36	110	6.025	53.139	43	3	36	130	27.130	245.090
20	4.5	36	110	6.687	59.236	44	4.5	36	130	29.496	279.500
21	0.75	48	110	5.268	45.948	45	0.75	48	130	10.858	89.721
22	1.5	48	110	6.702	58.253	46	1.5	48	130	18.598	157.130
23	3	48	110	7.325	64.052	47	3	48	130	25.676	229.420
24	4.5	48	110	7.288	64.339	48	4.5	48	130	26.257	257.580

the least squares method. Tables 4 and 5 show the statistical regression models and their related determination coefficients (R^2) as well as MSE values for the dyes employed in this research.

In order to determine the validity of each model, the following conditions must be met [8]:

1- The errors must be independent random variables.
2- The errors must have a constant variance.
3- The errors must have a normal distribution.

The following four conditions can be used as a means of verification of the above mentioned three conditions [8]:

1- Linear form for the normal plot of the residuals.
2- I Chart of residuals should lie between upper and lower control limits without any specific pattern.
3- Histogram of residuals should have approximately normal form.
4- Residuals versus fitted values should show no specific pattern.

As an example, the information related to the statistical regression model obtained for Kayalon Polyester Blue 2R-SF is shown in Figure 1. Regarding the above mentioned four conditions for the validity of the models, it can be said that the statistical model for Kayalon Polyester Blue 2R-SF cannot be accepted. Similar data for the other dyes showed that the necessary conditions for the acceptance of the statistical models were not met.

Table 4. Statistical regression models and their related R^2 and MSE values for K/S.

Chromophore	Name	Regression model	R^2	MSE
Mono azo	Kayalon Polyester Blue 2R-SF	log(K/S)= -20.100+0.335logConc+ 0.354logTime+9.850logTemp	0.918	0.0170
	Kayalon Polyester Brown GR-SE	log(K/S)= -12.900+0.725logConc+ 0.267logTime+6.390logTemp	0.878	0.0171
Diazo	Yohao Disperse Yellow 4R-E	log(K/S)= -1.460+0.559logConc+ 0.042logTime+1.630logTemp	0.947	0.0017
	Yohao Disperse Yellow ER	log(K/S)= -4.090+0.371logConc+ 0.141logTime+2.390logTemp	0.799	0.0058
Anthraquinone	Kayalon Polyester Blue EBL-E	log(K/S)= -7.040+0.680logConc+ 0.170logTime+3.660logTemp	0.917	0.0060
	Dispersol Red B-2B	log(K/S)= -8.100+0.535logConc+ 0.163logTime+4.190logTemp	0.597	0.0379
Not known	Yohao Disperse Red Violet P-R	log(K/S)= -9.610+0.576logConc+ 0.093logTime+4.820logTemp	0.613	0.0441

In such cases one may use the usual statistical modification methods to obtain possibly a suitable model or employ alternative approaches such as fuzzy regression methods.

Modelling by Fuzzy Regression with Triangular Coefficients

As already explained for the statistical regression, a general multiple form can also be considered for the fuzzy models. The models with triangular fuzzy coefficients are:

$$Y_1=(a_0^c,s_0,k_0)_T+(a_1^c,s_1,k_1)_T X_1+ (a_2^c,s_2,k_2)_T X_2+(a_3^c,s_3,k_3)_T X_3 \quad (37)$$

In order to calculate the coefficients of the models, the logarithm of the data related to each dye was made into n×m matrices for independent variables and n 1 matri-

Table 5. Statistical regression models and their related R^2 and MSE values for K/S.

Chromophore	Name	Regression model	R^2	MSE
Monoazo	Kayalon Polyester Blue 2R-SF	Log(F_k) = -18.700+0.363logConc+ 0.356logTime+9.630logTemp	0.921	0.0157
	Kayalon Polyester Brown GR-SE	log(F_k) = -11.800+0.741logConc+ 0.265logTime+6.370logTemp	0.879	0.0171
Diazo	Yohao Disperse Yellow 4R-E	log(F_k) = -7.980+0.571logConc+ 0.092logTime+4.460logTemp	0.614	0.0400
	Yohao Disperse Yellow ER	log(F_k) = -5.190+0.539logConc+ 0.175logTime+3.200logTemp	0.809	0.0105
Anthraquinone	Kayalon Polyester Blue EBL-E	log(F_k) = -5.660+0.713logConc+ 0.163logTime+3.440logTemp	0.925	0.0055
	Dispersol Red B-2B	log(F_k) = -6.530+0.540logConc+ 0.153logTime+3.840logTemp	0.597	0.0347
Not known	Yohao Disperse Red Violet P-R	log(F_k) = -1.090+0.733logConc+ 0.044logTime+1.300logTemp	0.964	0.0019

ces for dependent variables, where:

$$Y_2 = (a_0'^{c}, s_0', k_0')_T + (a_1'^{c}, s_1', k_1')_T X_1 + (a_2'^{c}, s_2', k_2')_T X_2 + (a_3'^{c}, s_3', k_3')_T X_3 \quad (38)$$

m = The number of independent variables
n = The number of samples related to each dye × 2

The chart of operations carried out for fuzzy modelling for each dye could be summarized as follows:

Entering the data related to each model

↓

Determination of h, by taking logarithm and forming the matrix for the coefficients of the constraints

↓

Calculation of the coefficients of the fuzzy model and the minimum value of Z

↓

Defuzzification

↓

Calculation of MSE of the model

To make this approach more clear, an illustration is presented for K/S of Kayalon Polyester Blue 2R-SF. Based on 48 data in Table 3 and using relationship (14), the objective function is:

$$Z = 48(1+k_0)s_0^L + (1+k_1)s_1^L \sum_{j=1}^{48} x_{j1} + (1+k_2)s_2^L \sum_{j=1}^{48} x_{j2} + (1+k_3)s_3^L \sum_{j=1}^{48} x_{j3} \quad (39)$$

For example, if $k_0 = 1.8$, $k_1 = 1.7$, $k_2 = 1.4$, $k_3 = 1.5$, then Z can be written as:

$$Z = 134.4 s_0^L + 38.2806 s_1^L + 177.3197 s_2^L + 247.0350 s_3^L \quad (40)$$

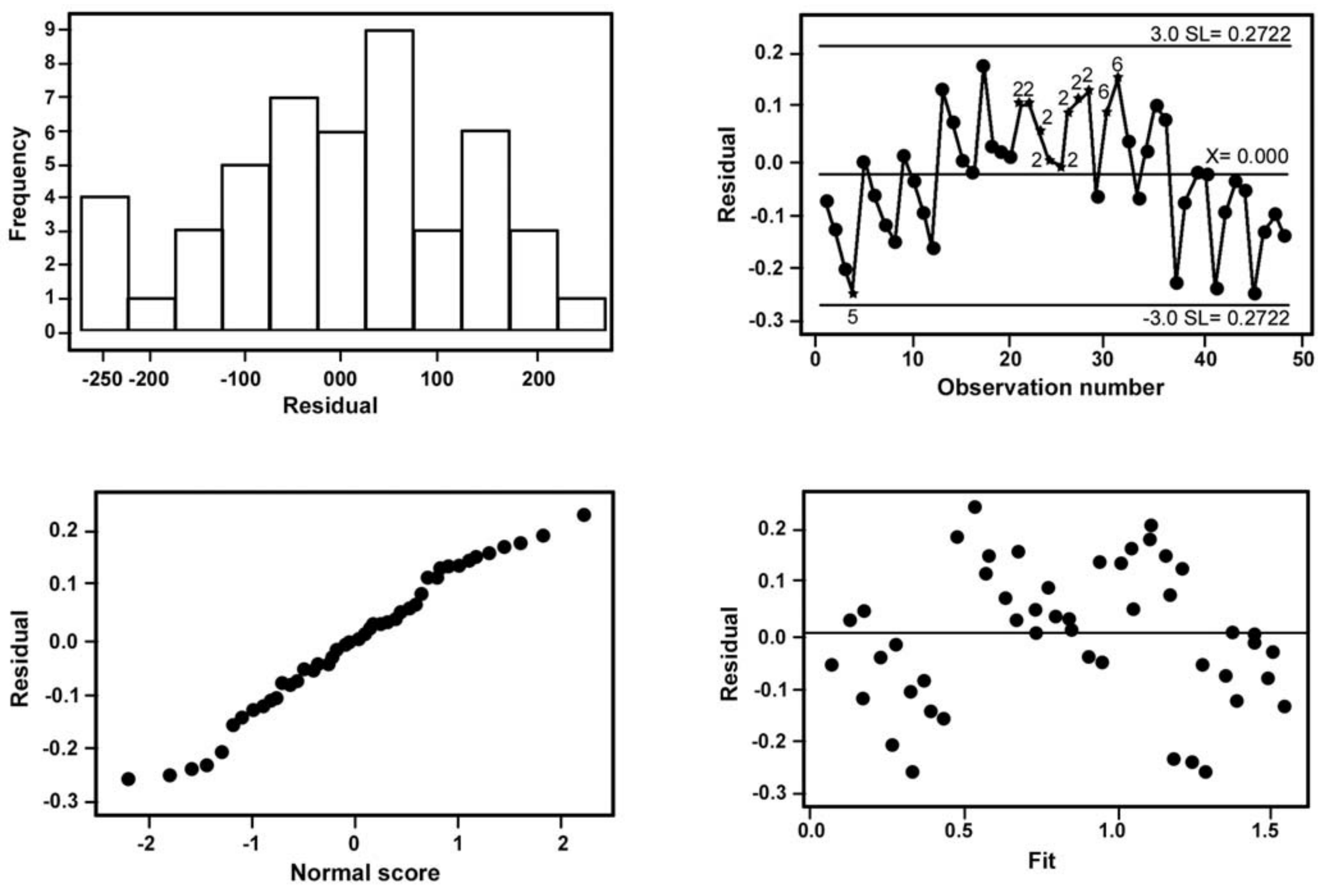

Figure 1. Plots of residuals for K/S of Kayalon Polyester Blue 2R-SF

Table 6. Variation of the MSE for K/S versus different values of $k_0,\ldots k_3$, for Kayalon Polyester Blue 2R-SF.

h	k_0	k_1	k_2	k_3	S_0	S_1	S_2	S_3	a_0	a_1	a_2	a_3	Z	MSE
0.5	1	1	1	1	0	0	0.15	0.11	-19.81	0.28	0.35	9.71	44.29	0.0184
0.5	1	1	1	0.6	0	0	0.15	0.14	-19.81	0.28	0.35	9.70	44.29	0.0203
0.5	1	1	1	0.3	0	0	0.15	0.17	-19.81	0.28	0.35	9.68	44.29	0.0269
0.5	1	1	1	1.5	0	0	0.15	0.09	-19.81	0.28	0.35	9.72	44.29	0.0174
0.5	1	1	1	1.9	0	0	0.15	0.08	-19.81	0.28	0.35	9.73	44.29	0.0174
0.5	1	1	1.4	1.5	0	0	0.12	0.09	-19.81	0.28	0.36	9.72	44.29	0.0173
0.5	1	1.7	1.4	1.5	0	0	0.12	0.09	-19.81	0.28	0.36	9.72	44.29	0.0173
0.5	1.8	1.7	1.4	1.5	0	0	0.12	0.09	-19.81	0.28	0.36	9.72	44.29	0.0173
0.5	1	1	1.5	1.7	0	0	0.12	0.08	-19.81	0.28	0.37	9.73	44.29	0.0190
0.5	1	1	1.6	1.9	0	0	0.11	0.08	-19.81	0.28	0.37	9.73	44.29	0.0190
0.5	1	1	0.6	1.9	0	0	0.19	0.08	-19.81	0.28	0.33	9.73	44.29	0.0178

In addition, based on (16) and (18), 96 constraints related to 48 observations are formulated. As an example, two constraints corresponding to the first observation, with h=0.5, are:

$$0.5s_0^L+0.0624s_1^L+0.6901s_2^L+s_3^L-a_0^c-0.1249a_1^c-1.3802a_2^c-2a_3^c\geq-0.0062 \quad (41)$$

$$0.9s_0^L+0.1062s_1^L+0.9661s_2^L+1.5s_3^L+a_0^c+0.1249a_1^c+1.3802a_2^c+2a_3^c\geq0.0062 \quad (42)$$

The objective function Z (17) is minimized with linear programming methods, subject to 96 constraints. In the following section, it will be illustrated how to find the optimum fuzzy regression model by selecting the optimum k_i s.

Note: In the usual linear programming methods, the variables cannot assume negative values. But when these methods are used for finding the coefficients of the fuzzy regression models, the coefficients can be negative. To eliminate this limitation, the variables a_i^c, i = 1,2,...,n were considered as the subtraction of two positive variables i.e., $a_i^c = a_i^{c_1} - a_i^{c_2}$. Based on $a_i^{c_1}$ and $a_i^{c_2}$ after solving the linear programming problem, the best values for a_i^c which make the objective function (Z) minimum, can be obtained.

In practical situations, one must consider all reasonable values for ki, s and find the best model as the model with minimum MSE. As an example, Table 6 shows the variation of the MSE for K/S versus different values of k_0, ,k_3, for Kayalon Polyester Blue 2R-SF. It can be concluded that, using h=0.5, the model with, k_2 = 1.4, k_2 = 1.4, which lead to a minimum for MSE, is the optimum one for this dye (note that in this case, the intercept and the coefficient of x_1 are obtained as non-fuzzy numbers).

Tables 7 and 8 show the optimum fuzzy regression models with triangular coefficients and their related MSE values for K/S and F_K of all dyes, respectively.

As far as skew coefficients, k_i s are concerned, 1 gives rise to symmetric, while other values lead to non-symmetric models. Both of these conditions were considered in this research. As Table 6 shows, the non-symmetric models obtained for Kayalon Polyester Blue 2R-SF show a lower MSE value. It is pointed out that all the optimum models shown in Tables 7 and 8 are non-symmetric.

Modelling by Fuzzy Regression with Exponential Coefficients

The general exponential possibility regression model (with three exploratory variables) is:

$$Y_j = A_0 + A_1x_{j1} + A_2x_{j2} + A_3x_{j3} = \mathbf{Ax}$$

Where A is a possibility distribution with the centre vector $\mathbf{a_c} = (a_{0c},a_{1c},a_{2c},a_{3c})^T$ and the matrix D_A.

In order to estimate the centre vector a_c*, the statistical regression analysis was employed and resulted in:

Table 7. The optimum fuzzy regression models with triangular coefficients for K/S and their related MSE values.

Construction	Name	Fuzzy regression model	MSE
Monoazo	Kayalon Polyester Blue 2R-SF	log(K/S)= [-19.81,0,0] + [0.25,0,0] logConc + [0.37, 0.12,0.17] logTime + [9.71,0.09,0.14] logTemp	0.0173
	Kayalon Polyester Brown GR-SE	log(K/S)= [-13.34,0.23,0.44] + [0.71,0.25,0.25] logConc + [0.21,0,0] logTime + [6.65,0,0] logTemp	0.0188
Diazo	Yohao Disperse Yellow 4R-E	log(K/S)= [-1.74,0.15,0.12] + [0.57,0.10,0.10] logConc + [0.12,0,0] logTime + [1.24,0,0] logTemp	0.0018
	Yohao Disperse Yellow ER	log(K/S)= [-2.45,0.20,0.20] + [0.25,0.15,0.26] logConc+ [0.12,0,0] logTime + [1.63,0.14,0.28] logTemp	0.0079
Anthraquinone	Kayalon Polyester Blue EBL-E	log(K/S)= [-6.51,0.19,0.36] + [0.62,0,0] logConc + [0.19,0,0] logTime + [3.4,0,0] logTemp	0.0065
	Dispersol Red B-2B	log(K/S)= [-6.6,0,0] + [0.4,0,0] logConc + [0.14,0,0] logTime + [3.49,0.29,0.35] logTemp	0.0407
Not known	Yohao Disperse Red Violet P-R	log(K/S)= [-11.24,0.51,0.76] + [0.73,0,0] logConc + [0.05,0,0] logTime + [4.63,0,0] logTemp	0.0478

Table 8. The optimum fuzzy regression models with triangular coefficients for F_K and their related MSE values.

Construction	Name	Fuzzy regression model	MSE
Monoazo	Kayalon Polyester Blue 2R-SF	log(F_K) = [-18.05,0,0] + [0.30,0,0] logConc + [0.36,0.19,0.19] logTime + [9.32,0.06,0.09] logTemp	0.0173
	Kayalon Polyester Brown GR-SE	log(F_K) = [-13.02,0.30,0.45] + [0.72,0.13,0.13] logConc + [0.19,0,0] logTime + [7.0,0,0] logTemp	0.0188
Diazo	Yohao Disperse Yellow 4R-E	log(F_K) = [-9.83,0.58,0.64] + [0.73,0,0] logConc + [0.03,0,0] logTime + [5.38,0,0] logTemp	0.0018
	Yohao Disperse Yellow ER	log(F_K) = [-2.09,0.17,0.306] + [0.43,0.28,0.48] logConc + [0.11,0,0] logTime + [1.75,0,0] logTemp	0.0079
Anthraquinone	Kayalon Polyester Blue EBL-E	log(F_K) = [-5.64,0.21,0.29] + [0.67,0,0] logConc + [0.18,0,0] logTime + [3.42,0,0] logTemp	0.0065
	Dispersol Red B-2B	log(F_K) = [-5.54,0,0] + [0.43,0,0] logConc + [0.13,0,0] logTime + [3.39,0.29,0.32] logTemp	0.0407
Not known	Yohao Disperse Red Violet P-R	log(F_K)= [-1.67,0.15,0.15] + [0.74,0.10,0.10] logConc + [0.15,0,0] logTime + [1.50,0.25,0.48] logTemp	0.0478

Table 9. The results of fuzzy regression with exponential coefficients for Kayalon Polyester Blue 2R-SF.

Number of observtions	j	D_A
1,6,9,29	19.35	d1= 0.0250, d5=1.5940, d7=0.0800
2,7,9,46	0.48	d2= 0.0003, d7=0.0500, d8=0.0004
5,9,30,42	0.6	d1= 0.0010, d5=0.0640
1,4,27,37	2.99	d1= 0.0120, d5=0.2400, d7=0.0070
21,27,29,46	5.11	d5= 0.4420, d7=0.0004, d8=0.0100
2,16,28,37	1.07	d5= 0.1150, d5=0.0009
1,3,5,44	0.3	d1= 0.0020, d5=0.0250
19,22,33,41	0.47	d2= 0.0001 d5=0.0410, d10=0.0005
5,15,17,31	0.36	d5= 0.0020, d6=0.0320
29,31,32,48	0.57	d1= 0.0120
17,25,33,42	7.77	d2= 0.0700, d4=0.0020, d5=0.6290, d8= 0.0003

$\mathbf{a_c}^* = (-20.10, 0.33, 0.35, 9.85)^T$

Then, the step (II), of the possibility regression approach which has already been explained, was used to solve the linear programming problem (27 - 29). For the case of Kayalon Polyester Blue 2R-SF, n = 4 and m = 48. So, n independent vectors out of m input vectors must be chosen. Attention is drawn to the fact that each input vector x_j, is represented as $(1, x_{ji}, x_{j2}, x_{j3})^T$. There are $C_4^{48} = 5.17 * 10^{59}$ candidates for selecting the 4 independent input vectors. Similar to the procedure used in [16], and with credit level $h_j = 0.5$ for all the given data, linear programming was solved with 12 different randomly choices of input variables. The results are shown in Table 9. Based on these results, first, third, fifth and forty fourth input vectors in Table 3 were selected as the best combination of independent vectors from Table 9. This selection led to the following matrix:

$$D_A = \begin{bmatrix} 0.002 & 0 & 0 & 0 \\ 0 & 0.025 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Now, the fuzzy estimation of K/S for each input x= $(1, x_{01}, x_{02}, x_{03})$ can be calculated using (30). Figure 2 shows the estimated fuzzy outputs for some of the data in Table 3.

As a practical example, assume that in an experiment the values of the obtained input variables are x= (1.0000, 0.6532, 1.6812, 2.0414), corresponding to the values of conc.= 4, time= 48, temp.= 110, then the fuzzy estimation of the output (the value of log K/S) would be an exponential fuzzy set as follows:

$$\Pi_{Y0}(y) = \exp\{-(y - x_0^T a_c)^2 (x_0^T D_A x_0)^{-1}\}$$
$$= \exp\{-(y - 0.8218)^2 / 0.0127\}$$

So, we estimate the value of log K/S as a number approximately 0.8218, with the spread equal to 0.0127. The optimum fuzzy regression models with exponential coefficient, obtained for K/S and F_k for all dyes are given in Tables 10 and 11, respectively.

A Comparison Between Fuzzy Models with Triangular and Exponential Coefficients

It must be pointed out that in regression models with exponential coefficients, the interaction between the variables is represented by the elements of D_A [16]. In fact, near zero value for these elements show ignorable interaction. Hence, from Tables 10 and 11, it is concluded that there is a very weak interaction among the variables considered for the colour yield of the dyes used in this research. Hence, it is concluded that in spite of the ability to represent the interaction between the

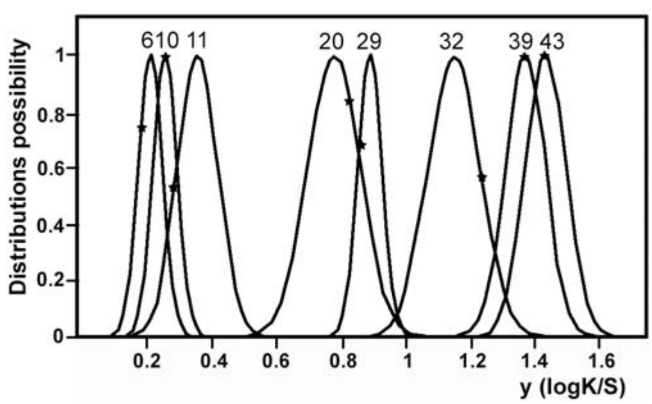

Figure 2. The estimated fuzzy outputs (possibility distributions) for the cases of No. 6, 10, 11, 20, 29, 32, 39 and 43 in Table 3.

Table 10. The optimum fuzzy regression models with exponential coefficients for K/S of dyes and their related J values.

$$Y_0 = (x_0^t a_c, x_0^t D_A^t x_0)_e \qquad D_A = \begin{bmatrix} d_1 & d_2 & d_3 & d_4 \\ d_2 & d_5 & d_6 & d_7 \\ d_3 & d_6 & d_8 & d_9 \\ d_4 & d_7 & d_9 & d_{10} \end{bmatrix}$$

Chromophore	Name	D_A	J
Monoazo	Kayalon Polyester Blue 2R-SF	d_1=0.00200,d_5=0.02500	0.30
	Kayalon Polyester Brown GR-SE	d_5=0.11000, d_8=0.00016, d_{10}=0.00049	1.05
Diazo	Yohao Disperse Yellow 4R-E	d_1=0.00200, d_5=0.01900	0.23
	Yohao Disperse Yellow ER	d_5=0.00300, d_7=0.00004, d_{10}=0.00004	0.03
Anthraquinone	Kayalon Polyester Blue EBL-E	d_5=0.00200, d_7=0.00003, d_{10}=0.00002	0.02
	Dispersol Red B-2B	d_1=0.00040, d_5=0.01000	0.06
Not known	Yohao Disperse Red Violet P-R	d_1=0.00025, d_5=0.00300	0.04

Table 11. The optimum fuzzy regression models with exponential coefficients for FK of dyes and their related J values.

$$Y_0 = (x_0^t a_c, x_0^t D_A^t x_0)_e \qquad D_A = \begin{bmatrix} d_1 & d_2 & d_3 & d_4 \\ d_2 & d_5 & d_6 & d_7 \\ d_3 & d_6 & d_8 & d_9 \\ d_4 & d_7 & d_9 & d_{10} \end{bmatrix}$$

Chromophore	Name	D_A	J
Monoazo	Kayalon Polyester Blue 2R-SF	d_1=0.00200,d_5=0.03000	0.37
	Kayalon Polyester Brown GR-SE	d_5=0.01000, d_8=0.11000	1.36
Diazo	Yohao Disperse Yellow 4R-E	d_1=0.00004, d_5=0.00500	0.06
	Yohao Disperse Yellow ER	d_1=0.00016, d_5=0.00200	0.03
Anthraquinone	Kayalon Polyester Blue EBL-E	d_1=0.00090, d_5=0.01100	0.14
	Dispersol Red B-2B	d_5=0.00200, d_7=0.00003, d_{10}=0.00002	0.02
Not known	Yohao Disperse Red Violet P-R	d_1=0.00067, d_5=0.00800	0.10

variables, in the case of the dyes used in this research, the fuzzy regression with exponential coefficients does not seem to have a major advantage over the fuzzy regression with triangular coefficients.

CONCLUSION

This research showed that statistical regression models obtained for the colour yield in high temperature polyethylene terephthalate dyeing with the dyes specified in Table 1 did not meet the required conditions to be accepted. Models based on triangular coefficient fuzzy regression were obtained and improved by modifying via enabling the centre of coefficients to take positive and negative values as well as dispersing fuzziness in coefficients. Modelling based on exponential coefficient fuzzy regression showed that there was a weak interaction between the three variables namely, time, temperature and dye concentration for the dyes employed and hence, this method of fuzzy regression does not seem to have a major advantage over the fuzzy regression with triangular coefficients.

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