Modeling and Cost Minimization of Weight Reduction Process of a Polyethylene Terephthalate Fabric by Sodium Hydroxide

Mehdi Seifollazade Ledari, Hossein Tavanai and Ali Zeinal Hamadani

***Abstract*—Weight reduction is a chemical surface modification process with the aim of improving mainly the handle and touch of polyethylene terephthalate fabrics through hydrolysis, with the help of usually sodium hydroxide solution. The amount of weight reduction depends on processing parameters such as concentration of sodium hydroxide, treatment time and temperature. This paper describes the modeling of weight reduction of a polyethylene terephthalate fabric as a function of the three aforementioned parameters, using full factorial experimental design. Three levels were assigned to each parameter. After acquiring the model, the conditions leading to minimum cost for a given weight reduction percentage were found.**

Key words: Weight reduction, polyethylene terephthalate fabric, modeling, full factorial experimental design, cost minimization

I. INTRODUCTION

Weight reduction or de-weighing of polyethylene terephthalate (PET) fibers by, usually, an alkaline solution is in fact a surface modification process patented in 1958[1]. In weight reduction process which is based on hydrolysis, hydroxyl ions of the alkali solution employed e.g. aqueous sodium hydroxide attack the electron-deficient carbonyl carbons of PET and lead to chain scission, formation of carboxylate and hydroxyl end groups, weight loss and considerable surface modifications. Because of surface modification, a better hand (silk like feel) and drape results. Moreover, hydrophilicity and resistance against soil and pilling improves [2]. It has been found that adding ethylene diamine to sodium hydroxide solution or dissolving sodium hydroxide in ethanol or methanol give rise to an accelerated hydrolysis process [3,4].

Although, it was believed that the action of alkali on PET was limited to the fiber surface (topochemical) [2], in a recent work, with the help of WAXS and SAXS, Tavanai [5] showed that the micro-structure of PET fiber is affected by weight reduction process. The atomic force microscopy (AFM) images also showed that weight reduction of PET fibers cannot be looked upon as a simple slimming down process and in fact a special roughness forms on the surface of PET fibers. Moreover, it was also shown that higher degrees of weight reduction lead to an increase in the coefficient of friction of the surface and a decrease in the tenacity and flexural rigidity of PET fabrics. The following literatures are also examples of similar works already carried out in the field of alkaline polyester weight reduction. Haghighat Kish and Nouri [6] have reviewed the alkalin hydrolysis of polyester fibers. Haghighat Kish and Nouri [7] also compared the effect of sodium hydroxide and calcium hydroxide in the weight reduction of polyester fabrics and found that calcium hydroxide needs higher temperatures when compared with sodium hydroxide. Mousazadegan *et al.* [8] investigated the effect of weight reduction on the physical and mechanical properties of microfilament polyester fabrics. Davis and Amirbayat [9] studied the effect of weight reduction on the performance of a polyester fiber satin pending shear, drape and drop. The main factors affecting the weight reduction process are alkaline concentration, temperature and treatment time. This research aimed to model the amount of weight reduction of a PET fabric as a function of the three aforementioned parameters with the help of full factorial experimental design. Moreover, this research aimed also at finding the conditions leading to minimum cost for a given amount of weight reduction.

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II. EXPERIMENTAL DESIGN

Experimental design is an action or a series of actions in which input variables of the process or systems are changed on purpose so that the reasons for changes in the output response can be identified and observed. Recognition of the statement of problem, determination of effective factors with their levels, and finally specifying response variable constitute the basis of any experimental design system. Choice of experimental design depends on the objectives as well as the conditions such as the number of input factors, their levels, cost of experiments etc. Experimental design provides the order of carrying out experiments from which data is obtained. The data is then analyzed using analysis of variance; leading to the determination of significant factors affecting the response variable. Finally a model representing the response variable as a function of the significant factors is worked out [10–12].

Factorial designs constitute one of the experimental designs and are subdivided into:

- Full factorial designs
- Fractional factorial designs
- Taguchi designs

Considering the conditions of present research, three levels full factorial design was found to suit best and hence employed. Using three levels for each factor enables us to fit a quadratic response surface to the experimental results and use optimization method to find the best combination of factor levels.

III. MATERIALS AND METHODS

A scoured ready to dye 100% PET plain woven fabric with a warp and weft density of 29 and 24 per centimeter respectively and 95.2 g/m2 was employed. Both warp and weft were set textured PET yarns (denier per filament ≈ 3). Three levels were chosen for each of the independent factors i.e. weight reduction bath temperature (A), treatment time (B) and sodium hydroxide concentration (C). Table I shows the three levels coded as +1, 0 and -1. A replica of 2 was chosen. So, considering three factors, each at three levels and a replica of 2 led to a total of 54 experiments. It is worth mentioning that as the degree of freedom for residual in this work is greater than 6, a replica of 2 is sufficient. Fabric samples (left in conditioning room for 24 hours) of 5g (W1) were weight reduced according to the experimental design shown in Table II. Table II was provided by minitab 15 software. It is reminded that the order of carrying out experiments was observed as per Table II. All the experiments were carried out with a liquor ratio (L:R) of 15. After weight reduction, the samples were rinsed, neutralized in water containing 1ml of acetic acid (98%) and rinsed again. The samples were left to dry for 24 hours in conditioning room and finally weighed (W2). The weight reduction percentage was calculated by Weight reduction (%) = [(W1 – W2) / W1] × 100 relation.

TABLE I
CODING OF THREE LEVELS OF THE INPUT FACTORS A, B AND C

	Levels		
Factors	-1	0	1
Temperature (°C) (A)	40	60	80
Treatment time (min) (B)	10	20	30
Sodium hydroxide concentration(g/L) (C)	100	200	300

IV. RESULTS AND DISCUSSION

Weight reduction (%) for each of the 54 samples is shown in Table II accordingly. In order to find the significant main effects i.e. A (bath temperature), B (treatment time) and C (sodium hydroxide concentration) as well as the interaction effects i.e. AB (interaction between A and B), AC, and BC, analysis of variance (ANOVA) was used. It is worth mentioning that in this work, second order polynomial modeling was considered. Table III shows the result of model fitting for all the main and interaction effects (α = 0.05). It is reminded that the insignificance of block shows the fact that there is essentially no difference between the two replicas. Having found the significant effects, a preliminary model is obtained by regression response surface using minitab 15 software as shown by Eq. (1).

$$W=5.3530+11.096A+4.6778B+8.3239C+5.7294A\times A+2.8794C\times C+5.1417A\times B+9.4192A\times C+4.000B\times C \quad (1)$$

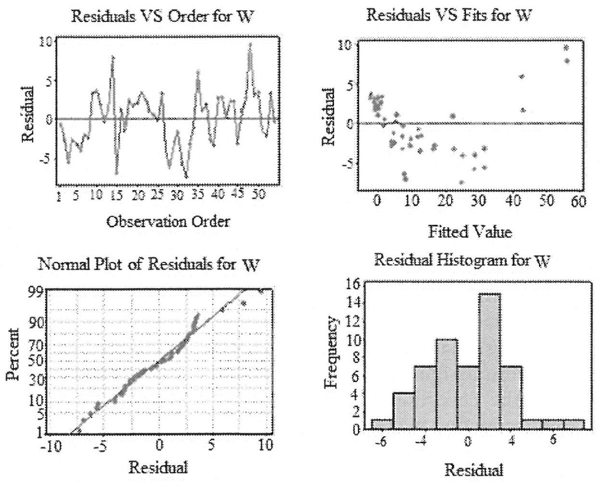

Fig. 1. The normal plot, I chart and histogram of residuals and residuals VS fits for the preliminary model.

To examine the adequacy of this model, residual versus order of experiment, residual versus fitted values, residual histogram and normal plot of residual for W were obtained by Minitab 15 software. As shown in Figure 1.These plots show that the model does not enjoy a good adequacy, since the plot of the residuals versus fitted values shows a pattern. This means that the variance of the residuals is not constant. Moreover, lack of normality is also present. Therefore the preliminary model cannot be accepted and should be modified. To carry out the modification, Box – Cox transformation [11] is employed. Figure 2 shows the box – Cox plot which is obtained also by Minitab 15 software. This plot proposes a transformation of natural logarithm type because λ = 0 (rounded). After the transformation, analysis of model fitting is applied again to find the significant factors (Table IV) and then the new model is obtained as shown in Eq. (2).

$$Ln(w)=1.71664+1.23373A+0.37718B+0.67723C-0.13371B\times B+0.14159A\times B+0.38163A\times C+0.14136B\times C \quad (2)$$

The adequacy of the new model is verified by considering the corresponding residual plots as shown in Figure 3. As can be seen, in this case, the plots are adequate. Table V shows the values of RMSE, R^2 adj and R^2_{adj} for the preliminary and final models. It is obvious that all the three indices of the final model are improved. In the final model, the level of factors is given by coded values to make the model usable. In other words, prediction of weight reduction (%) with known amounts of concentration, time and temperature is possible. It is

reminded that by considering a linear relationship between the code and real values with a gradient of 1, real values are changed to coded ones. For example the code of temperatures 45, 50, 65 and 75°C are -0.75, -0.5, +0.25 and +0.75 respectively. So, considering temperature, time and concentration of, 70°C (code = 0.75), 20 min. (code = 0) and 275 g/l (code = 0.75) respectively gives:
Ln(W) = 3.3645 and
W = 28.92%

TABLE II
DESIGN OF EXPERIMENTS

	Coded factor levels			
Run Order	A	B	C	W(%)
1	1	-1	0	11.2
2	0	0	1	14.0
3	1	1	0	26.0
4	-1	0	-1	1.4
5	1	0	0	19.2
6	0	1	1	20.8
7	0	1	0	7.6
8	-1	1	1	2.4
9	0	1	-1	3.4
10	-1	-1	1	1.4
11	-1	1	-1	0.8
12	1	0	-1	7.2
13	0	0	0	6.6
14	1	1	1	62.0
15	-1	-1	-1	1.0
16	-1	-1	0	1.2
17	1	1	-1	11.2
18	0	-1	0	2.6
19	1	0	1	44.7
20	0	0	-1	2.0
21	1	-1	-1	4.4
22	-1	1	0	1.6
23	-1	0	0	1.2
24	-1	0	1	2.4
25	0	-1	1	7.2
26	0	-1	-1	2.0
27	1	-1	1	24.6
28	-1	-1	-1	1.4
29	1	1	0	28.2
30	1	-1	0	10
31	1	-1	1	22.6
32	0	1	1	17.2
33	0	0	1	13.2
34	-1	1	1	3.4
35	1	0	1	48.6
36	1	0	0	23.0
37	-1	0	0	1.8
38	0	1	0	6.6
39	1	1	-1	9.0
40	0	-1	-1	1.2
41	-1	1	0	1.6
42	0	0	0	5.4
43	0	0	-1	2.0
44	-1	1	-1	1.0
45	1	0	-1	4.0
46	-1	-1	0	0.8
47	1	-1	-1	3.4
48	1	1	1	63.4
49	0	1	-1	3.0
50	0	-1	0	3.4
51	0	-1	1	5.6
52	-1	0	-1	1.6
53	-1	-1	1	0.8
54	-1	0	1	1.4

Figures 4 to 7 show the contour plot of Ln(W) for two factors with the third one kept constant as shown on the graphs. As can be seen, 5 zones has been considered for Ln(W). Each zone of the contour plot is in fact a locus of a known weight reduction range. In other words, it is possible to get the weight reduction (%) in this known zone with all the conditions specified for the factors.

TABLE III
RESPONSE SURFACE ANALYSIS FOR THE PRELIMINARY MODEL

Term	Coef.	SE of Coef.	T	P - Value
Constant	5.3530	1.4125	3.790	0.000
Block	0.1196	0.5339	0.224	0.824
A	11.0961	0.6539	16.970	0.000
B	4.6778	0.6539	7.154	0.000
C	8.3239	0.6539	12.730	0.000
A*A	5.7294	1.1325	5.059	0.000
B*B	-0.5922	1.1325	-0.523	0.604
C*C	2.8794	1.1325	2.542	0.015
A*B	5.1417	0.8008	6.421	0.000
A*C	9.4192	0.8008	11.762	0.000
B*C	4.0000	0.8008	4.995	0.000

TABLE IV
RESPONSE SURFACE ANALYSIS FOR THE FINAL MODEL

Term	Coef.	SE of Coef.	T	P - Value
Constant	1.71664	0.08718	19.691	0.000
Block	0.04002	0.03295	1.215	0.231
A	1.23373	0.04036	30.571	0.000
B	0.37718	0.04036	9.346	0.000
C	0.67723	0.04036	16.781	0.000
A*A	-0.04596	0.06990	-0.658	0.514
B*B	-0.13371	0.06990	-1.913	0.062
C*C	-0.02058	0.06990	-0.294	0.770
A*B	0.14159	0.04943	2.865	0.006
A*C	0.38163	0.04943	7.721	0.000
B*C	0.14136	0.04943	2.860	0.007

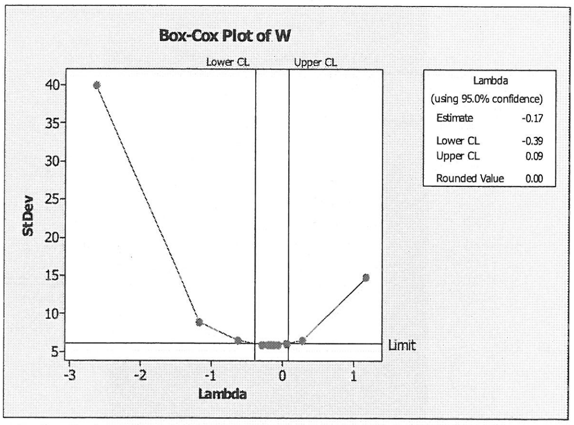

Fig. 2. The Box – Cox plot for the data employed for the preliminary data.

In order to carry out a weight reduction process with minimum cost, a cost function for a known weight of fabric e.g. 1Kg must be set up. A simple cost function can be defined as follows:

$$Cost=a(X-20)(L:R)+bY+cZ(L:R) \quad (3)$$

Where:

a = cost of heating one liter of water for 1°C (room temp. = 20°C), X= Temp. (°C)

b = cost of running a workshop per min (fixed cost, labor, etc.), Y = Time (min)

c = cost of 1g of sodium hydroxide, Z = sodium hydroxide concentration (g/L)

Assumptions:

The time needed for rising the bath temperature from 20°C to the required temperature is negligible.

After reaching the required level, the temperature remains unchanged.

The cost function for the coded values of factors is given as:

$$\text{Cost} = a\,(A-2)\,(L{:}R) + b\,B + c\,C\,(L{:}R) \qquad (4)$$

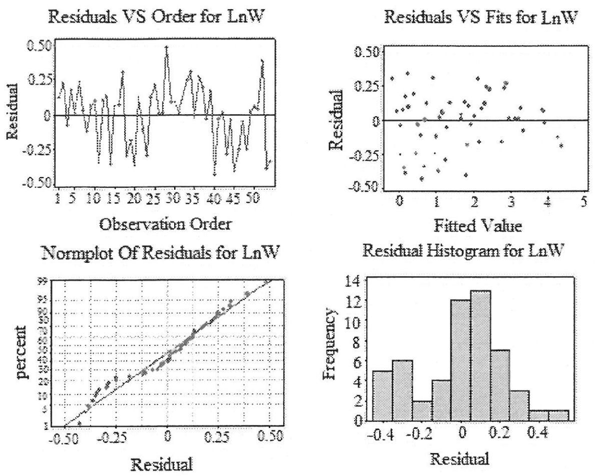

Fig. 3. The normal plot, I chart and histogram of residuals and residuals VS fits for the final model.

TABLE V
DESCRIPTIVE INDICES OF THE PRELIMINARY AND FINAL MODEL

Indicator	First model	Modified model
R^2	94.50%	96.99%
R^2_{adj}	93.21%	96.29%
RSME	3.5008	0.2160

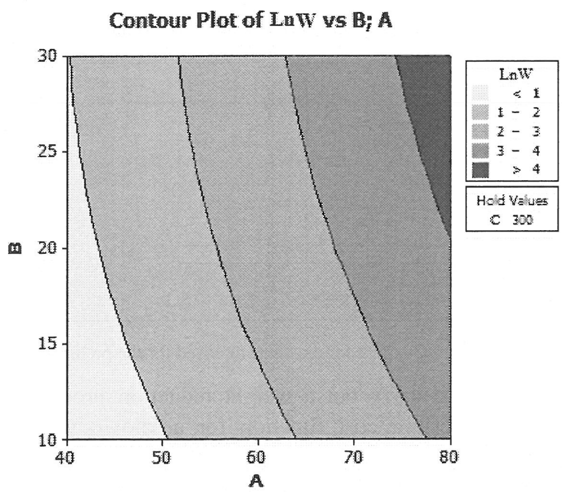

Fig. 4. The contour plot of Ln (W) for A and B (C= constant).

Considering values of a, b and c as 0.4, 1.5, and 0.6 unit currency, respectively and L:R = 15, to minimize the weight reduction cost for a given weight reduction (%), the cost function for the coded values must be minimized. Substituting the values of a, b, c, and L:R in the cost function for the coded values of factors gives:

$$\text{Cost} = 6\,(A-2) + 1.5B + 9\,C \qquad (5)$$

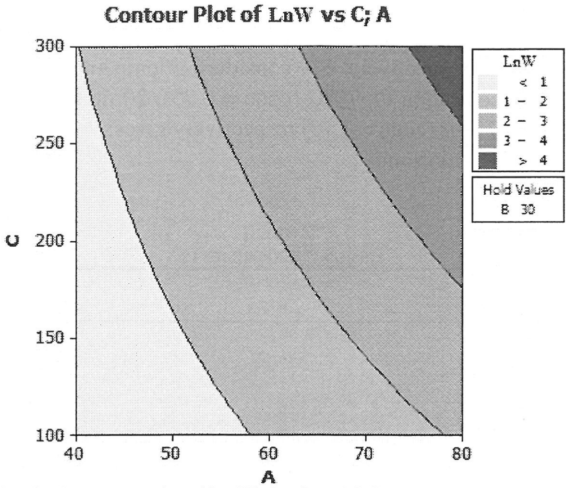

Fig. 5. The contour plot of Ln(W) for A and C (B= constant).

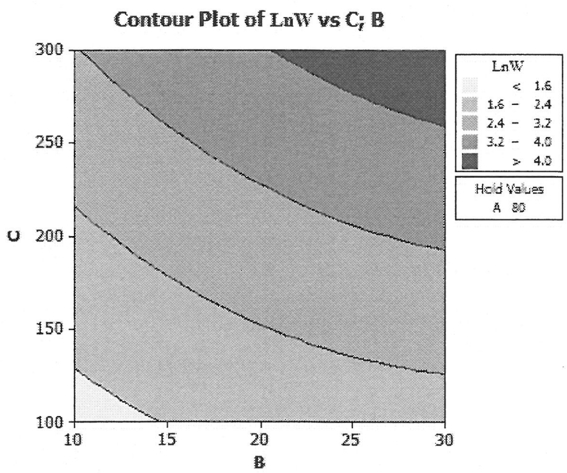

Fig. 6. The contour plot of Ln(W) for B and C (A= constant).

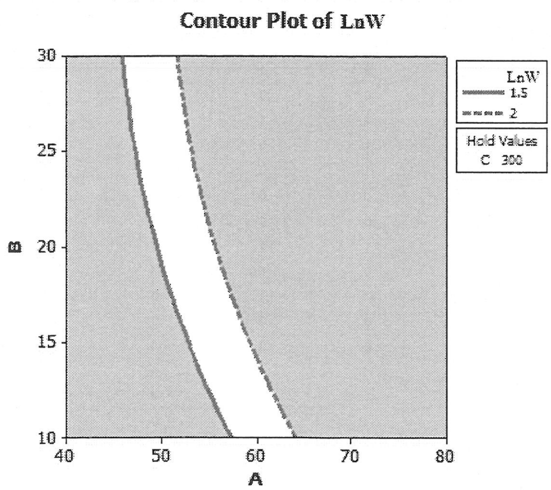

Fig. 7. Overlaid contour plots for A and B variable.

Using the Excell solver program, one can find the optimum values of temperature, time and sodium hydroxide concentration for a known value of weight reduction (W) in percent with minimum cost. For example for W = 15%, the conditions leading to minimum cost are as follows:

Temp. 93.4°C

Time = 28.5 min.

Sodium hydroxide concentration = 95.8 g/L

The conditions leading to minimum cost for weight reductions (%) of 20, 10 and 5% are as follows:

Weight reductions = 20 %

Temp. 96°C

Time = 29 min.

Sodium hydroxide concentration = 104 g/L

Weight reductions = 10 %

Temp. 89°C

Time = 27 min.

Sodium hydroxide concentration = 83 g/L

Weight reductions = 5 %

Temp. 80°C

Time = 25 min.

Sodium hydroxide concentration = 58 g/L

It must be pointed out that apart from the parameters considered in this research, a good number of other factors such as warp and weft density, yarn denier, polymer characteristics and fabric weight per square meter could affect the weight reduction percentage. So, the fitted model cannot be considered as a general model, but a model representing the fabric employed in this research.

V. CONCLUSION

A model representing the weight reduction of a polyethylene terephthalate fabric as a function of treatment time, temperature and sodium hydroxide concentration has been put forward using full factorial experimental design. Three levels were assigned for each factor. The preliminary model did not satisfy the conditions to be approved. However, after applying Box-Cox transformation, the final model acquired the required qualifications and was accepted. Finally, by defining a cost function, the optimum values of the factors leading to minimum cost for a given weight reduction was found.

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