Statistical method of experimentation for the analysis and optimization of berberine finishing of cellulose fiber

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1. Introduction

A recent trend in cellulose chemistry is the search for high tech materials with special properties such as antibacterial, UV protecting, insect repellent, fire retarding and even medical properties[1]. Berberine chloride, a natural cationic colorant was successfully employed as antimicrobial finisher for cellulose fiber. In this context, Statistical method of experimentation[2] has been successfully applied for determining the optimal values of three important designing parameters for berberine finishing of reactive anionic agent modified cellulose fibers.

2. Experimental and model development

Experiments were designed using Statistical Experimental Design[2] by MINITAB 14 (PA, USA). Experiments were carried out in a laboratory-scale infra red dyeing machine (ACE-6000T) by varying pH, temperature, concentration on level of dye exhaustion and fixation. The results of experimental design were studied and interpreted by MINITAB 14 (PA, USA) statistical software to estimate the response of the dependent variable (% exhaustion and % fixation). Using the date, empirical model was developed. The behaviour of the system was explained by the following empirical model[3]:

$$Y = \beta_0 + \sum \beta_i x_i + \sum \beta_{ii} x_i^2 + \sum \beta_{ij} x_i x_j \quad (1)$$

Where, Y is the dependent variable, β are the regression coefficients, x are independent data. RMSE (Root Mean Square Error) is the important tool to validate the model equation for its prediction capacity and was calculated using the following formula[3],

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{0}^{N} (\mathrm{Exp.} - \mathrm{Pred.})^2}{N}} \quad (2)$$

Where, Exp. is the experimental value, Pred. is the predicted value from model equations and N is the total number of experiments. Statistical analysis of the experimental data was performed. The quality of the fit of the polynomial model equation was expressed by the coefficient of determination R^2.

3. Results and Discussion

Cellulose was first treated with anionic agent to impart anionic sites and then treated with berberine at various process conditions. The main effect plot shows (Fig. 1.) that higher pH conditions, a lower range of temperatures and liquid ratio leads to higher % exhaustion of berberine.

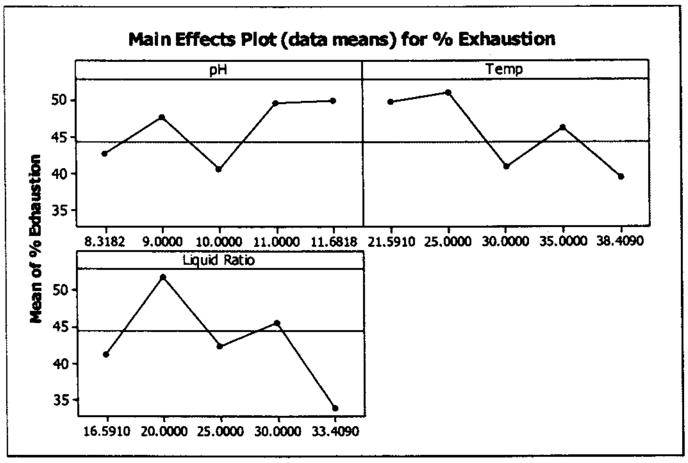

Fig. 1. Main effect plots of berberine exhaustion with cellulose fiber.

Using the experimental results, regression model equation (second order polynomial) relating the % exhaustion and process variables were developed and is given in equation (3)

Polynomial regression equation for % exhaustion of berberine into cellulose fiber (3)

$$Y= 0.9717 + 0.7467 X_1+ 0.6643 X_2 + 0.4675 X_3 - 0.01932 (X_1X_2) - 0.00483 (X_1X_3) - 0.00427 (X_2X_3) - 0.00072 (X_1X_1) - 0.00512 (X_2X_2) - 0.00648 (X_3X_3) \quad (R^2 = 0.9985)$$

The empirical model developed for the experimental data have high coefficient of determination values (R^2=0.9985). This implies that 99.85% of sample variation for berberine is explained by independent variables and also means that the model did not explain only about 0.0015% of sample variation for berberine. The predicted values (using model equations) were compared with experimental results and are shown in Fig. 2. The surface plots given in Fig. 3 show relative effects of any two variables when the remaining one variable is kept constant for all combinations. The optimum values drawn from these figures are in close agreement with those obtained by optimizing the regression model equation (3) using Monte-Carlo techniques. Experiments were carried out at optimum conditions obtained by the theoretical analysis and highly feasible results were obtained.

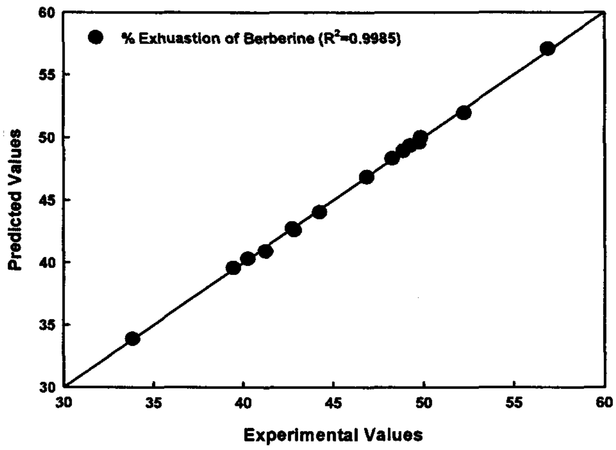

Fig. 2. Experimental and predicted values of berberine exhaustion with cellulose fiber.

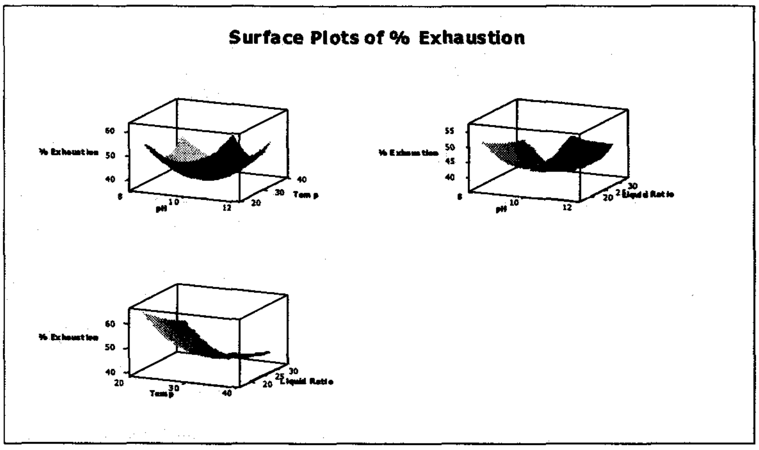

Fig. 3. Surface plots for optimization of process condition of berberine treatment.

4. Conclusions

Statistical experimental design was successfully applied to study the main effects of process parameters for the berberine treatment of anionic agent modified cellulose. Empirical model was developed using experimental data and process conditions were optimized using surface plots.

Acknowledgement

This research was supported by the Program for the Training of Graduate Students in Regional Innovation which was conducted by the Ministry of Commerce Industry and Energy of the Korean Government.

References

1. T.Rosenau, A.H.M. Renfew, C.Adelwohrer, A.Potthast, P.Kosma, Cellulosics modified with slow-release reagents. Part I. Synthesis of triazine-anchored reagents for slow release of active substances from cellulosic material s Polymer, 2005,46,1453 - 1458.
2. D.C.Montgomery, Design and Analysis of Experiments, 3rd ed.; John Wiley & Sons Inc: New York,1991.
3. E.Mordecai, Methods of correlation analysis, 3rd ed.; John Wiley & Sons Inc: New York, 1951.

제 3 발표장

좌 장 : 전 근 박사(한국화학연구원)

14:40-15:00 고압기류 Relaxer의 노즐 유동에 관한 수치해석적 연구
박시우, 조경철, 이호준, 나혜중*, 노석홍 ,전두환*
(재)한국섬유기계연구소, *영남대학교 섬유패션학부

15:00-15:20 Nylon/Spandex 염색의 Spandex 오염 방지에 관한 연구
한태성, 박준호, 전병대
한국생산기술연구원

15:20-15:40 PET섬유용 Phthalimide 염료의 합성 및 염색특성
전정민, 최재홍, 박준수, 김미현
경북대학교 섬유시스템공학과

15:40-16:00 Coffee break

좌 장 : 전병대 박사(한국생산기술연구원)

16:00-16:20 카제인 교직물의 염색특성
김미현, 최재홍
경북대학교 섬유시스템공학과

16:20-16:40 Synthesis and properties of novel azo dyes derived from phthalimide
박준수, 전정민, 최재홍
경북대학교 섬유시스템공학과

16:40-17:00 Coffee break

좌 장 : 최재홍 교수(경북대학교)

17:00-17:20 고기능성 직물의 보온성 향상에 관한 연구
최종덕, 조영원, 박영미*, 최종석**, 구 강
영남대학교 섬유패션학부, *연세대학교 의류환경학과, **미광다이텍(주)

17:20-17:40 Dyeing Properties of 4-Amino-4'-fluorosulfonylazobenzene Disperse Dyes and their 4'-nitro Analogues on PET
Joonseok Koh, Kwang Soo Kim, Sung Dong Kim
Department of Textile Engineering, Konkuk University

17:40-18:40 간친회