Advanced Process Control and Simulation for Chemical Engineers

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Contents

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List of Abbreviations

ANOVA	Analysis of variance
ANN	Artificial neural network
AFD	Average fiber diameter
BM	Bukacek-Maddox
CCD	Central composite design
CA	Contact angle
DOE	Design of experimental
DMF	Dimethylformamide
FTIR	Fourier transforms infrared spectroscopy
GC	Gas chromatographic
GBFS	Granulated blast-furnace slag
HBPs	Hyperbranched polymers
IROST	Iranian Research Organization for Science and Technology
MLP	Multilayer Perception
NRTL	Non-random two-liquid
NMR	Nuclear magnetic resonance
OPC	Ordinary Portland cement
OA	Orthogonal array
PAN	Polyacrylonitrile
PET	Polyethylene terephthalate
PP	Polypropylene
RSM	Response surface methodology
RMSE	Root-mean-square error
SEM	Scanning electron micrographs
SI	Severity index
SSE	Squares due to error
TBA	Tert-butanol
TCD	Thermal conductivity detector
UV–vis	Ultraviolet–visible
UNIQUAC	Universal quasi-chemical
VLE	Vapor-liquid equilibrium
WPLA	Waste PET bottles lightweight aggregate
WPLAC	Waste PET bottles lightweight aggregate concrete
XRD	X-ray diffraction

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List of Symbols

if = Liquid environment near the feed phase
of = Organic environment near the feed phase
os = Organic environment near the stripping phase
is = Liquid environment near the stripping phase
o = Organic phase
i = Liquid phase
δ = Thickness of Mass transfer film
D = Mass transfer diffusion coefficient
N = Mass transfer diffusion
a = optimized interaction parameter
A, B, and C = Antoine equation parameters
B_{ij} = 2^a coefficient of the virial
C = number components
Calc = calculated value
E = excess property
exp = experimental value
G_{ij} = adjustable parameter
2EH = iso octhyl alcohol
NBA = n.butanol
q_i = relative surface area per molecule
r_i = number of segments per molecule
T = absolute teperture (Kelvin)
u_{ij} = interaction energy
x = mole fraction
x_i = equilibrium mole fraction of component i
Z = lattice coordination number, set equal to 10
z_i = number of moles of component i

Greek Symbols
F = segment fraction
q = area fraction
g = activity coefficient
t_{ij} = adjustable parameter in the UNIQUAC equation

Superscript
c = combinatorial part of the activity coefficient
q = UNIQUAC equation
r = residual part of the activity coefficient
i = ith component

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Preface

This book offers a modern view of process control in the context of today's technology. It provides the standard material in a coherent presentation and uses a notation that is more consistent with the research literature in process control. The purpose of this book is to convey to students an understanding of those areas of process control that all chemical engineers need to know. The presentation is concise, readable, and restricted to only essential elements. Topics that are unique include a unified approach to model representations, process model formation and process identification, multivariable control, statistical quality control, and model-based control. The methods presented have been successfully applied in industry to solve real problems. This book is designed to be used as an advanced research guide in process dynamics and control. In addition to chemical engineering courses, the book would also be suitable for mechanical, nuclear, industrial, and metallurgical engineers. The book offers scope for academics, researchers, and engineering professionals to present their research and development works that have potential for applications in several disciplines of engineering and science.

— Hossein Ghanadzadeh Gilani, PhD,
Katia Ghanadzadeh Samper, and Reza Khodaparast Haghi

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1 Artificial Neural Network (ANN) Models and Polymers

CONTENTS

1.1 INTRODUCTION

Hyperbranched polymers (HBPs), due to their unique chemical and physical properties, have attracted increasing attention. These polymers are highly branched, polydisperse, and three-dimensional macromolecules [1]. The HBPs have remarkable properties, such as low melt and solution viscosity, low chain entanglement, and high solubility, as a result of the large amount of functional end groups and globular structure, so they are excellent candidates for use in random applications, particularly for modifying fibers [2, 3].

Recently, the application of HBPs in textile industry has been developed. For instance, in the study on applying HBP to cotton fabric [4-8], it was demonstrated that HBP treatment on cotton fabrics has no undesirable effect on mechanical properties of fabrics. Furthermore, application of HBP to cotton fabrics reduced UV transmission and has good antibacterial activities. The study on dyeability of polypropylene (PP) fibers modified by HBP showed that the incorporation of HBP prior to fiber spinning considerably improved the color strength of PP fiber with C.I. Disperse Blue 56 and has no significant effect on physical properties of the PP fibers [9]. Literature review showed that there has not been a previous report regarding the treatment of amine terminated HBPs on PET fabric and study of its dyeability with acid dyes. In the most recent study in this field, fiber grade PET was compounded with polyesteramide HBP and dyeability of resulted samples with disperse dyes was studied [10]. The results showed that the dyeability of dyed modified samples comprised of fiber grade PET films and a HBP (Hybrane H1500) were better than the neat PET and this was increased by increasing amount of HBP in presence or absence of a carrier. The dyeability of the samples was attributed to decrease in glass transition temperature for blended PET/HBP in comparison with neat PET [10].

In this study, the effect of HBP treatment parameters such as solution concentration, treatment temperature and time on dyeuptake (K/S value) of PET fabric were investigated using ANN models based on a feed forward topology.

1.2 EXPERIMENTAL

1.2.1 Material

A HBP with amine terminal group were synthesized and characterized as described by previous research [4]. Figure 1 represent the structural units of HBPs include terminal,

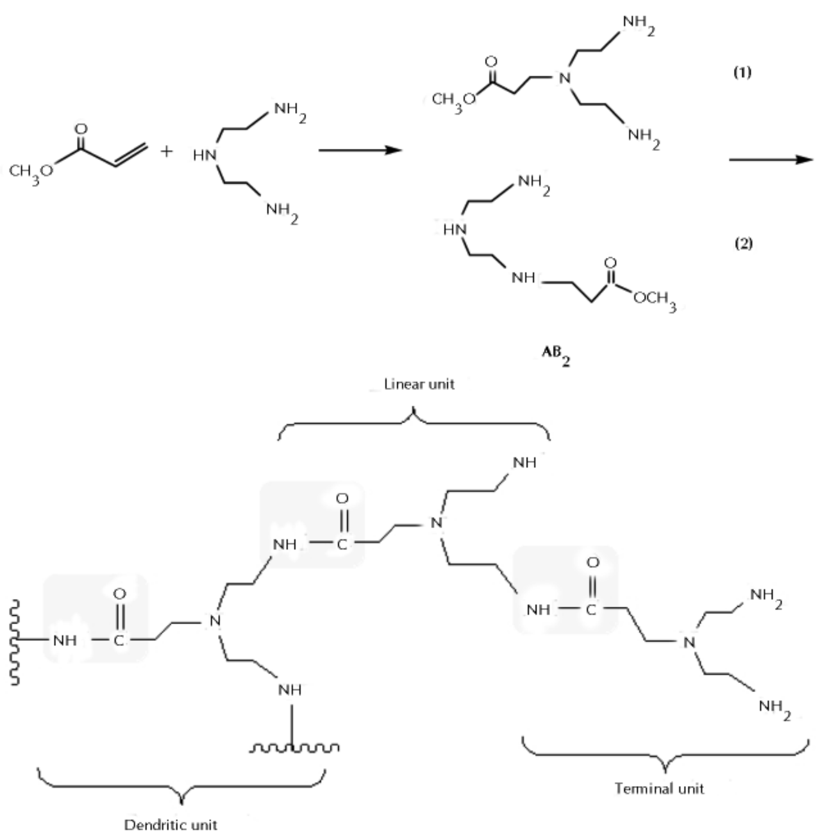

FIGURE 1 Chemical structure of amine terminated hyperbranched polymer.

dendritic and linear units. The PET fabric (28 × 19 count/cm^2) used throughout this work and before use it was treated with a solution containing 5 g/l Na_2CO_3 and 1 g/l of a non-ionic detergent at 60°C for 30 min to remove undesired materials. Distilled water was used for the treatments and washings. Acid dye (C.I. Acid Red 114) was provided by the Ciba Ltd. (Tehran, Iran) and used to evaluate the dye absorption behavior (dyeability) of samples.

1.2.2 PET Fabric Treatment with HBP

The PET fabric samples were immersed in aqueous solution of sodium hydroxide (10% w/v) at the temperature of 94°C for 1 hr with the liquor to goods ratio of 40:1. Then the samples were thoroughly rinsed with distilled water and neutralized with acetic acid, and finally rinsed and dried at room temperature. After the alkaline treatment of fabrics, the HBP was applied to samples using exhaustion process. The alkali-treated PET fabrics were treated with HBP solution and the temperature was raised at a rate of 2.5°C/min. After exhaustion, the samples were thoroughly rinsed with distilled water to remove unfixed HBP and dried at room temperature. Figure 2 show the HBP treatment profile.

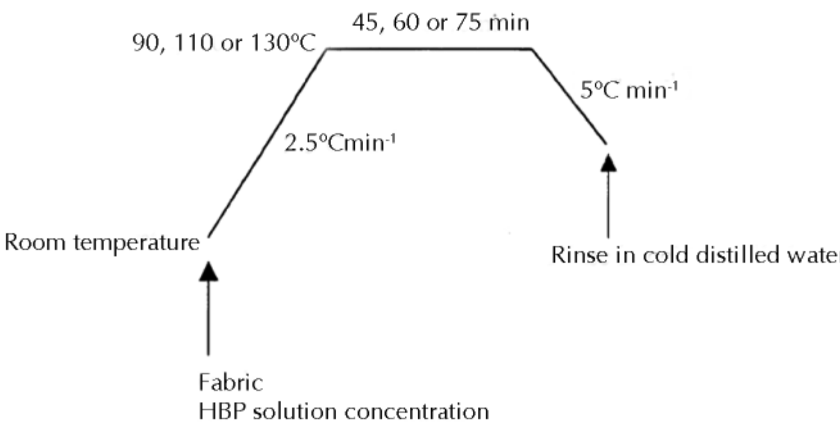

FIGURE 2 Method and graph for HBP treatment of PET fabric.

1.2.3 Dyeing Procedure

The HBP treated fabrics were introduced into the dye baths containing dye (C.I. Acid Red 114) with the liquor to goods ratio of 60:1 at the temperature 40°C, increasing to boil with the constant rate of 3°$Cmin^{-1}$. Dyeing was then continued for 60 min with occasional stirring. At the end of dyeing the dyed samples were rinsed with cold water, then with hot water at about 50°C and finally rinsed with tap water.

1.2.4 Measurement and Characterization

The CIELAB color coordinates of dyed samples were determined under illuminant D_{65} at 10°C standard observers in the visible range using color-eye 7,000A spectrophotometer. As shown by Equation (1), the Kubelka–Munk single-constant theory was employed to calculate K/S values at the wavelength of maximum absorption (λ_{max}) for each fabric [11].

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

where, $R_{M,\lambda}$ and $R_{S,\lambda}$ are the reflectance values at the wavelength of maximum absorbance (λ_{max}) for colored and uncolored substrate respectively, K is the absorption coefficient and S is the scattering coefficient. The HBP treatment conditions and samples K/S value are shown in Table 1.

TABLE 1 The HBP treatment parameters and response.

No.	Inputs			Output
	HBP concentration (wt.%)	**Temperature (°C)**	**Time (min)**	**K/S value**
1	2	90	75	20.38
2	2	130	75	21.57
3	2	110	60	19.86
4	2	130	45	21.09
5	2	90	45	19.78
6	6	110	60	22.68
7	6	110	60	22.18
8	6	110	60	22.67
9	6	110	60	22.97
10	6	110	60	22.64
11	6	110	60	22.26
12	6	110	45	22.59
13	6	110	75	24.47
14	6	90	60	22.58
15	6	130	60	26.07
16	10	90	45	23.35
17	10	90	75	24.97
18	10	130	75	29.92
19	10	130	45	26.01
20	10	110	60	23.23

1.2.5 Artificial Neural Network

The ANN as an information processing technique, are composed of simple unit operating in parallel. A typical ANN represents a network with a several number of layers, consisting of an input layer, one or more hidden layers and an output layer. The ANN can be trained to perform a particular function by adjusting the values of the connections (weights) between elements. The weights between the neurons play an important role during the training process. The interconnection weights are adjusted, based on a comparison of the network output and the actual output, to minimize the error between the network output and the actual values [12, 13].

In this work, the multilayer perceptron ANN was used to process data using the modified backpropagation algorithm. The ANN has three inputs referred to HBP treatment parameter (HBP solution concentrations, treatment temperature and treatment time), and one output referred to K/S value of treated samples. All calculations carried out in Matlab mathematical software (version 7.6) with ANN toolbox. The various topology of neural network are shown in Table 2.

TABLE 2 The topology of neural networks.

No. of model	Number of hidden layer	Number of neuron per hidden layer
1	1	3
2	1	4
3	1	5
4	1	6
5	1	7
6	1	8
7	2	3-2
8	2	4-2
9	2	4-3
10	2	3-3

1.3 RESULTS

In this work, the dyeability of HBP treated PET fabrics is calculated from treatment condition comprising HBP solution concentrations, treatment temperature and treatment time using ANN. The prediction performance is evaluated by calculating R^2 and RMSE through the following equation:

$$RMSE = \sqrt{\frac{\sum_{i=1} (y_{i,\exp} - y_{i,pred})^2}{n}} \quad (2)$$

where, $y_{i,exp}$ and $y_{i,pred}$ are the experimental and predicted values, respectively, and n is the number of the experimental run.

The suitable number of neurons in the hidden layer was determined by changing the number of neurons. As shown in Table 3, the best prediction, based on minimum error, was obtained by ANN with 8 neurons in hidden layer. The R^2 and RMSE were 0.97 and 0.61 respectively. The comparison between the actual and predicted value given by ANN is shown in the Figure 3 and demonstrated that all points are located close to a straight line.

TABLE 3 The results of prediction by artificial neural network.

No. of model	Mean	SD	Max.	Min.	R^2	RMSE
1	0.03	0.04	0.13	0.01	0.85	1.21
2	0.05	0.04	0.16	0.00	0.84	1.42
3	0.05	0.04	0.20	0.00	0.82	1.57
4	0.04	0.03	0.11	0.00	0.89	1.15
5	0.03	0.03	0.10	0.01	0.91	0.96
6	0.02	0.02	0.09	0.00	0.97	0.61
7	0.03	0.03	0.15	0.01	0.93	0.91
8	0.03	0.03	0.12	0.00	0.89	1.11
9	0.03	0.03	0.12	0.00	0.90	1.04
10	0.04	0.04	0.15	0.00	0.87	1.24

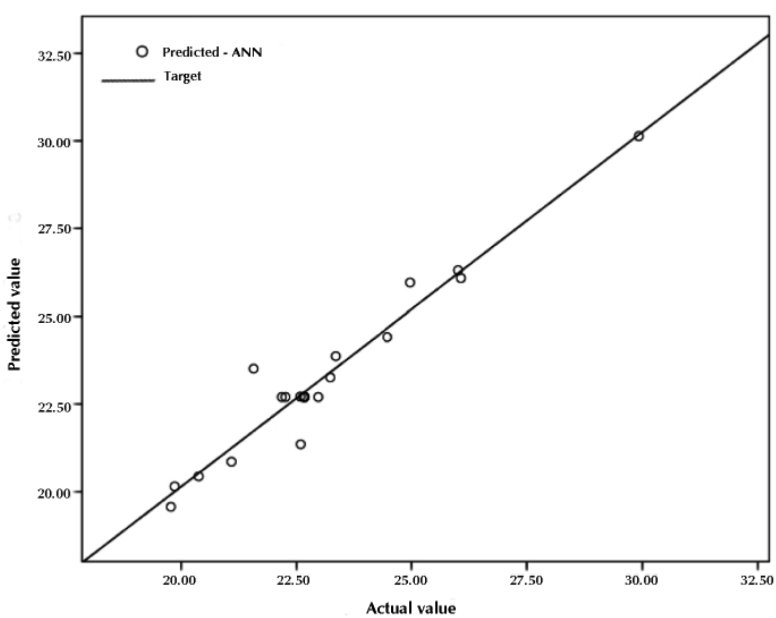

FIGURE 3 Comparison between the actual and predicted K/S value of HBP treated PET fabrics.

1.4 CONCLUSION

In this work, ANN models were developed using a feed forward topology for modeling of HBP treatment on PET fabric. The effects of three HBP treatment parameters namely solution concentrations (wt.%), treatment temperature (°C) and time (min) on dyeability (K/S value) of treated PET fabrics were investigated. The best prediction was obtained by ANN with 8 neurons in hidden layer. In this model the R^2 and RMSE were 0.97 and 0.61 respectively. Furthermore, the mean, standard division, maximum and minimum error are 0.02, 0.02, 0.9, and 0 respectively.

KEYWORDS

- **Artificial neural network**
- **Back-propagation algorithm**
- **Hyperbranched polymers**
- **Kubelka–Munk single-constant theory**
- **Polypropylene**

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