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Prediction of impacts of fabrication conditions on the filtration performance of homemade VC-co-VAc-OH microfiltration membrane by Support Vector Machine (SVM)

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ABSTRACT

In this study, the support vector machine (SVM) model which was based on restricted data sets (the size of the training set is small or small training sample) was applied to predict the permeate flux and rejection of Bovine serum albumin (BSA) of homemade VC-co-VAc-OH microfiltration membrane as the function of fabrication conditions. The membrane preparation conditions (the solid content, the additive content, environmental temperature, the relative humidity, evaporation time of a volatile solvent, precipitation temperature, and precipitation time) were input variables; pure water flux and rejection of BSA were output variables. The results showed that the detailed relationships between fabrication conditions and filtration performance of the membranes could be established. Excellent agreements between the prediction of SVM model and the experiments validate that SVM model has sufficient accuracy. Furthermore, the results predicted by SVM model were compared with those predicted by artificial neural network (ANN) model which was widely used in the optimization of nonlinear relationships. It is found that the deviations of both the training and the predicting data obtained by SVM model are much smaller than those by ANN models. Hence, SVM model can be used as an efficient approach to optimize fabrication conditions of homemade VC-co-VAc-OH microfiltration membrane.

Keywords: Support vector machine; Artificial neural network; Flux; Rejection; Comparison

1. Introduction

Membrane separation technology has become more and more important in modern industry due to its advantage of energy-saving and environmental friendly nature [1,2]. However, membrane fouling is an inevitable phenomenon during industrial operation process, which will greatly shorten membrane longevity and increase its operating costs [3]. Therefore, the membrane fouling is a hot point in the membrane research field [4–6]. Though there are many kinds of

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methods, such as pretreatment of feed solutions [7–10], membrane washing and cleaning [11,12], operation optimization [13,14], and so on, were used to overcome this problem, the anti-fouling membrane fabrication still remains as the most efficient way to improve membrane fouling [15,16].

The quality of the membrane depends on many fabrication conditions, for example, the composition of membrane casting solution, surrounding environmental condition, and the type of coagulation bath, etc. This implies that in order to select the best membrane fabrication condition, a large amount of experiments have to do. Though experimental workload can be reduced by orthogonal method [17], it is unable to predict filtration performance of the membrane. So, how to predict the membrane filtration performance based upon experimental data has practical significance. Many forecasting methods, such as Multiple Linear Regressions [18], artificial neural network (ANN) [19] and support vector machine (SVM) [20] were explored and used as an efficient prediction method.

Compared with multiple linear regression and other traditional prediction methods, ANN model shows high accuracy despite some shortcomings such as design in advance of the network structure or construction of the network structure in training process using heuristic algorithm; absence theoretical guidance for the network adjustment and weight initialization; overfitting problem; etc. All these problems are arising from the theoretical statistical basis of ANN, which needs a large size of training sets. So, ANN is often unable to solve specific practical issues, where data sets were restricted. To overcome this limitation, Vapnik et al. proposed SVM approach based on the statistical learning theory [20]. SVM is known as the excellent tool for the classification and regression problems of good generalization ability and provides a unified framework for restricted data sets' learning [21].

Recently, SVM as a highly effective approach of system modeling with restricted data sets has been widely applied in many fields for predicting [20,21], such as pattern recognition problem [21–25], classification [26,27], regression [28,29], image analysis [30], drug design [31–33], time series analysis [34–36], quality control of food [37,38], protein structure function prediction [39–42], genomics [43], and usually outperformed the traditional statistical learning methods [44,45]. Thus, SVM have been receiving increasing attention and quickly become quite a hot spot. For example, in order to make this approach easy for junior learners to comprehensively understand the basic ideas of SVM, C. Burges reviewed the support vector classification machines [46] and A. J. Smola also gave a review on the Support Vector Regression Machines [47]. Specifically, as SVM is gaining popularity in a wide variety of biological applications, W.S. Noble described in detail what exactly SVM is and how they work mainly for biologists [48]. In addition, Xu et al. have also developed SVM for classification in chemometrics [49]. Jia et al. showed that SVM was applicable to forecast the synthesis characteristics of hydraulic valve and with high accuracy [21]. A predictor is constructed to predict the true and false splice sites for higher eukaryotes based on SVM [50]. Liang et al. proposed an effective approach for content-based sketch retrieval [51]. All these contribute to the development and application of SVM and make it become a very active area. Ergun Gumus present an evaluation of using various methods for face recognition [52]. All these results show that SVM can provide better or comparable results than that by ANN or other statistical models. However, up to now, the application of SVM in membrane fabrication process was not reported.

In this study, the SVM was used to validate its application for the simulation of the permeate flux and rejection of Bovine serum albumin (BSA) of homemade VC-co-VAc-OH microfiltration membrane as function of membrane fabrication conditions with restricted data sets.

2. SVM

In SVM regression approach, the nonlinear regression problem in low-dimensional feature space can be transformed to the linear regression problem in high-dimensional feature space by a nonlinear mapping ϕ. In order to endow the SVM predicted models, good function approximation and generalization capabilities, a linear estimation function f, which makes the empirical risk minimum [55], as follows:

$$f(x) = (\omega, \varphi(X)) + b \tag{1}$$

where $\omega(\omega \in F)$ is the weight vector, (,) is the inner product, $\varphi(X)$ denotes a mapping function in the feature space, i.e. it represent the non-linear mapping from low-dimensional feature spaces $R^m(X \in R^m)$ to high-dimensional feature space F; b is a constant.

The values of ω and b in formula (1) can be derived substituting the set (sample) data (Xi, Yi) into the following function:

$$R_{\mathrm{reg}}[f] = R_{\mathrm{emp}}[f] + \lambda\|\omega\|^2 = \sum_{i=1}^{s} C(e_i) + \lambda\|\omega\|^2 \tag{2}$$

where $R_{reg}[f]$ is the sum of empirical risk and experience risk; $R_{emp}[f]$ is the experience risk; λ is the regularization parameter for controlling the loss of training set (sample) and the compromise of model complexity; $\|\omega\|^2$ is the confidence risk and reflects the model complexity in high-dimensional feature space, and the smaller $\|\omega\|^2$ means smaller confidence risk; s is the size of the set (sample); and $C(.)$ is the Loss function, $e_i = f(X_i) - Y_i = \hat{Y}_i - Y_i$ represents the difference between the predicted values and the experimental data, and $C(e_i)$ represents the experience loss of the model. Based on the structured risk minimization principle, SVMs seek to minimize the sum of empirical risk and confidence risk.

For a given loss function, the problem of finding function f can be solved as a quadratic programming problem as following:

$$\max J = -\frac{1}{2}\sum_{i,j=1}^{s}(\alpha_i - \alpha_i^*)(\alpha_j^* - \alpha_j)(\varphi(X_i), \varphi(X_j)) + \sum_{i=1}^{s}\alpha_i^*(Y_i - \varepsilon) - \sum_{i=1}^{s}\alpha_i^*(Y_i + \varepsilon) \tag{3}$$

$$\text{s.t.}\left\{\begin{array}{l} \sum_{i=1}^{s}\alpha_i = \sum_{i=1}^{s}\alpha_i^* \\ 0 \leqslant \alpha_i \leqslant C \\ 0 \leqslant \alpha_i^* \leqslant C \end{array}\right\} \tag{4}$$

By solving the functions (3) and (4), $\omega = \sum_{i=1}^{s}(\alpha_i - \alpha_i^*)\varphi(X_i)$ can be gotten; b can be obtained by substituting any supported vector into the functions (3) and (4). In this way, the function is transformed into the following form:

$$f(x) = \sum_{i=1}^{s}(\alpha_i - \alpha_i^*)(\varphi(X_i), \varphi(X)) + b \tag{5}$$

Definite the inner product of high-dimensional feature transformation space as the kernel function of SVM:

$$K(X_i, X_j) = (\varphi(X_i), \varphi(X_j)) \tag{6}$$

The inner product in high-dimensional space can be obtained only by computing the kernel function in the low-dimensional space. Finally, by introducing Lagrange multipliers and exploiting the optimality constraints, the decision function has the following explicit form [53]:

$$f(x) = \sum_{i=1}^{s}(\alpha_i - \alpha_i^*)K(X_i, X) + b \tag{7}$$

Based on the theory above, the structure of SVM used to model the prediction of the effects of membrane fabrication conditions on pure water flux and rejection of BSA were shown in Fig. 1, respectively.

In present paper, the SVM system used in this work is LIBSVM tool loaded into MATLAB (R2010b) and the membrane fabrication conditions (the solid content, the additive content, environmental temperature, the relative humidity, evaporation time of a volatile solvent, precipitation temperature, and precipitation time) were input variables, and the filtration performance of the

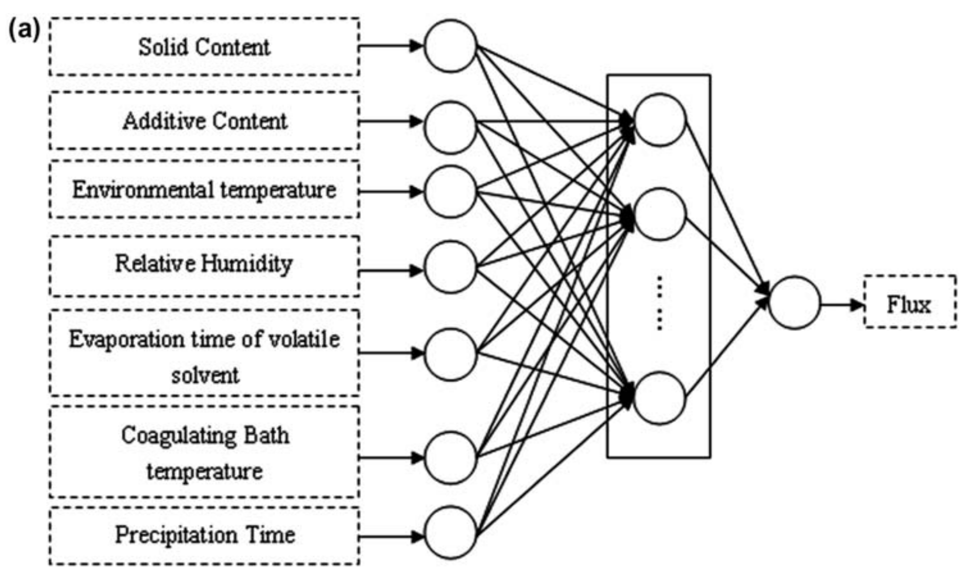

Fig. 1. (a) Structure of the SVM used for modeling the flux prediction process and (b) structure of the SVM used for modeling the rejection prediction process.

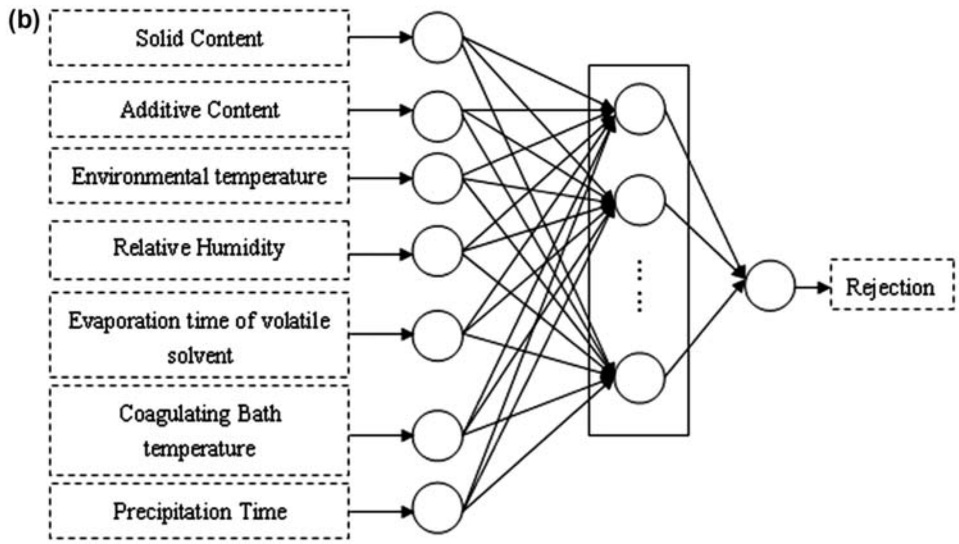

Fig. 1. (b) (*Continued*)

membrane (pure water flux and rejection of BSA) were output variables. The network structure was optimized by adjusting the program.

3. Experimental

3.1. Materials

Dimethylformamide (DMF), Dimethylacetamide (DMAc), and *N*-methyl-2-pyrrolidone (NMP), all of analytical grade, were purchased from Tianjin Fuchen Chemical Reagent Factory. Poly (ethylene glycol) of molecular weight of 2000 g/mol, i.e. PEG 2000, which was chosen as the additive in casting solution, N-butanol used as santomerse was purchased from Beijing Chemical Engineering Factory. BSA used as reagent for determining the rejection of BSA of the membrane was purchased from Beijing Microorganism Culture Medium Manufacturing Corporation, and its isoelectric point of pH is 4.8. Homemade VC-co-VAc-OH was used as the membrane material [54].

3.2. Membrane fabrication procedure

Firstly, VC-co-VAc-OH polymer was dissolved in a solution of DMF and uniformly stirred. PEG was added after the polymers have been completely dissolved. The casting solution was placed in the vacuum oven at 60℃ for 3 days. Meantime, Non-Woven Fabrics (NWFs) were put into deionized water to remove the impurities and dried at the environmental temperature of 25℃, then immersed in different solvents for certain time. Secondly, the immersed NWFs were evaporated for certain time under different environmental temperatures and relative humidities. Thirdly, the casting solution was cast onto NWFs with solvent by a casting blade under certain environmental temperature and relative humidity, and then the cast film along with the glass plate was gently immersed into coagulation bath with a temperature of 20℃ for 30 min. Finally, the formed membrane was immersed into the deionized water bath for 24 h to remove residual solvent at room temperature.

3.3. Membrane characterization

Pure water flux and rejection of BSA (average molecular weight is 67,000 g/mol) of the membrane were conducted via a dead-end membrane cell with an effective filtration area of 24 cm^2. The experiments were measured at transmembrane pressure of 0.2 MPa, and the experimental results were calculated as follows:

$$J = \frac{V}{A \times t} \tag{8}$$

where J is the pure water flux of the membrane ($mL\,cm^{-2}\,h^{-1}$), V is the total permeate volume during the experiment (mL), and A is the effective area of membrane (cm^2), t is operation time (h), respectively.

$$R(\%) = \left(1 - \frac{C_p}{C_f}\right) \times 100\% \tag{9}$$

where R is the rejection of the membrane, C_p and C_f is the concentration of permeate and the feed solution ($g{\cdot}L^{-1}$), respectively. The analysis of BSA was performed by the UV spectrophotometer (HP 8451-A) at $\lambda = 280$nm. In addition, the experimental setup can be found elsewhere [55].

3.4. Data scaling

Because raw data of various factors (polymer concentration, the additive content, environmental temperature, the relative humidity, evaporation time of a volatile solvent, precipitation temperature, precipitation time, pure water flux, and rejection of BSA) are not in the same order of magnitude. In order to prevent such raw data causing increased training time or causing that the network not to converge, raw data needs to undergo preprocessing. One approach for scaling of the data is performed with following formula Eq. (10), which normalizes the data to values between − 1 and 1 [56]:

$$x_i' = 2\left[\frac{x_i - x_{min}}{x_{max} - x_{min}}\right] - 1 \qquad (10)$$

where x_i is the initial value of parameter, x_i' is the normalized value of x_i, x_{max} and x_{min} are the maximum and minimum of x_i, respectively.

After the training and testing of SVM, the output data were scaled to the real-world values through the following equation:

$$x_i = 0.5(x_i' + 1)(x_{max} - x_{min}) + x_{min} \qquad (11)$$

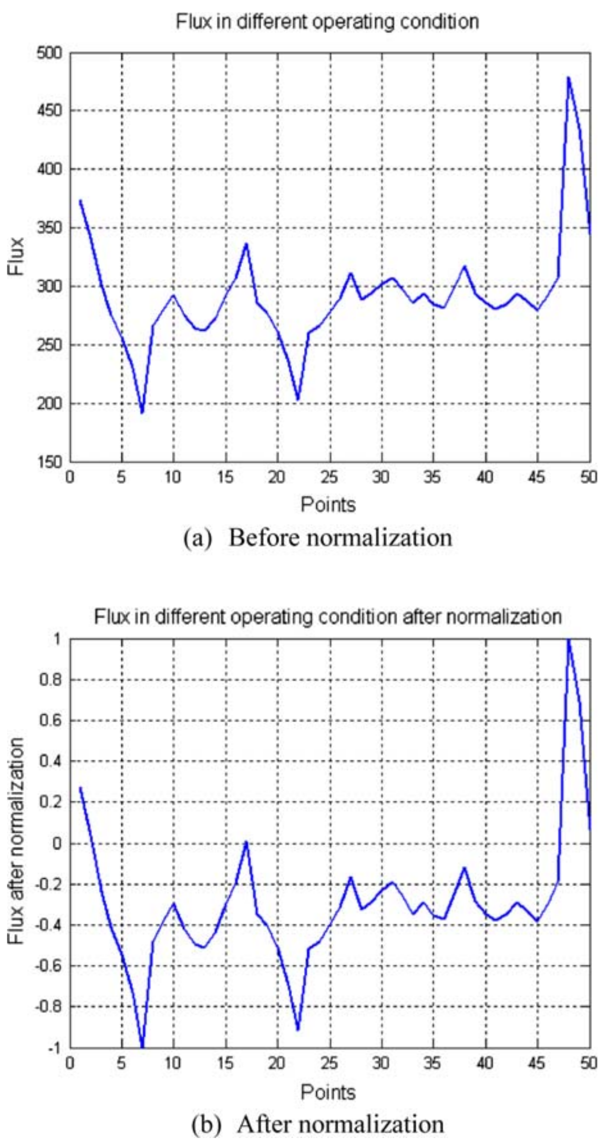

Fig. 2. Normalization of membrane flux.

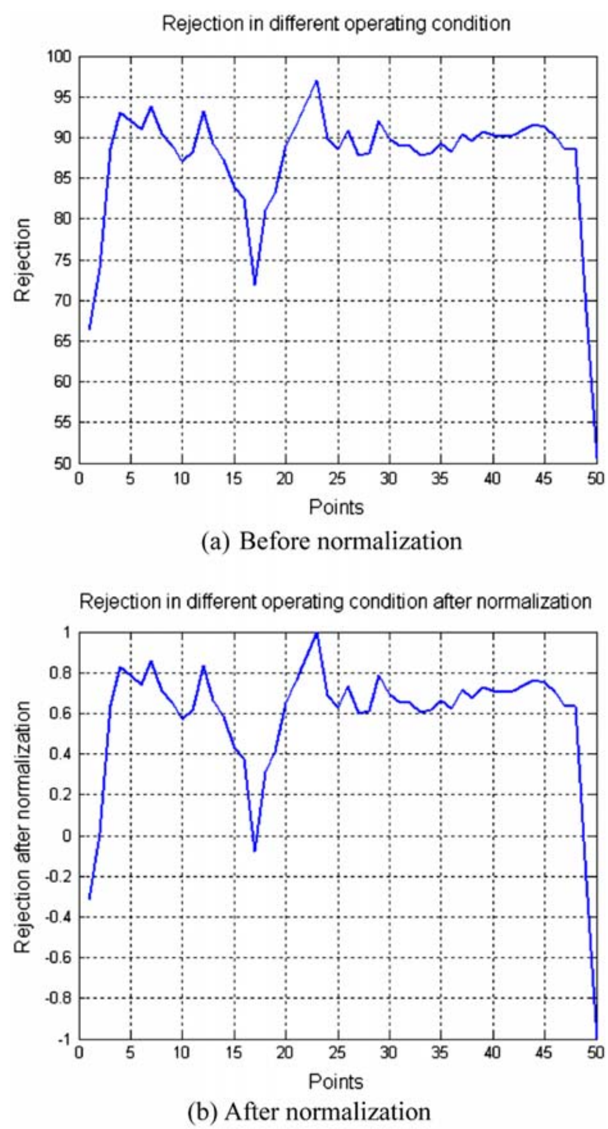

Fig. 3. Normalization of rejection.

4. Results and discussion

4.1. Data scaling

Raw data were normalize and scaled, respectively. As shown in Figs. 2 and 3, pure water flux and rejection of BSA of the membrane with different orders of magnitude were normalized between −1 and +1 by Eq. (10), respectively.

4.2. Comparison of experimental data and predicted values by SVM

4.2.1. Fit of SVM to pure water flux

The network structure of SVM was trained with 100 training points and 50 test points. The inputs are the membrane fabrication conditions, such as the composition of the casting solution (polymer concentration and the additive content), surrounding environmental condition (environmental temperature, the relative humidity, evaporation time of a volatile solvent), and precipitation condition (temperature and precipitation time); and the outputs are pure water fluxes. If comparing the experimental data and the predicted values by SVM under the different conditions, it can be seen from Fig. 4 that the predicted values by SVM and experimental data agreed quite well. According to Fig. 5, the relative error of pure water fluxes between predicted values by SVM and experimental data relative errors lie in the range −6 to 5%, and the average absolute error is 2.84%. This means that the agreement between the experimental data and the predicted values by SVM is excellent.

From what has been discussed above, we may safely draw the conclusion that the SVM can be used to predict the effects of membrane fabrication conditions on the pure water flux of homemade VC-co-VAc-OH microfiltration membrane.

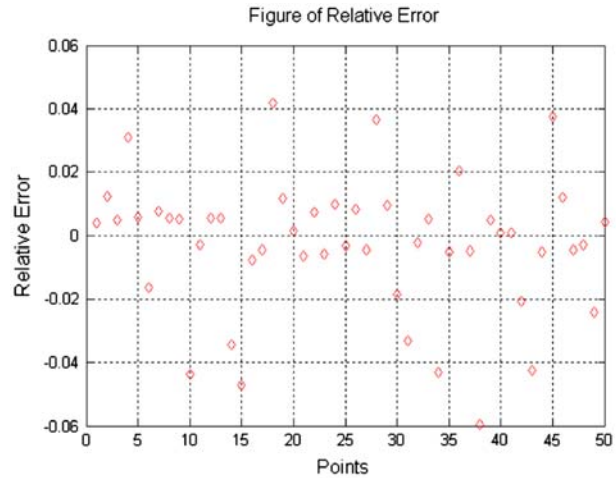

Fig. 5. Relative error of flux by SVM.

4.2.2. Fit of SVM to the rejection of BSA

The inputs are the membrane fabrication conditions, such as the composition of the casting solution (polymer concentration and the additive content), surrounding environmental condition (environmental temperature, the relative humidity, evaporation time of a volatile solvent) and precipitation condition (temperature and precipitation time), and the output are the rejections of BSA of the membrane. If comparing the experimental data and the predicted values by SVM under the different conditions, it can

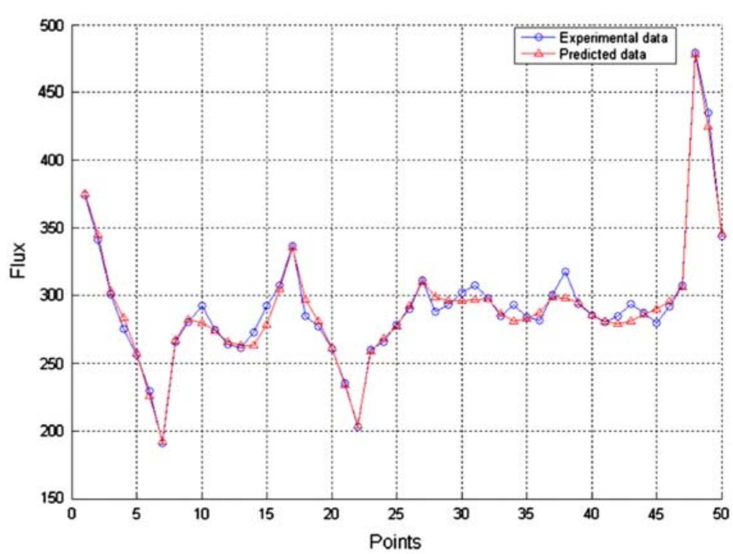

Fig. 4. Comparison between experimental data and predicted data of flux under different operation by SVM.

be seen from Fig. 6 that the predicted values by SVM and experimental data agreed very well. According to Fig. 7, the relative error of rejection of BSA of the membrane between predicted values by SVM and experimental data lie in the range −5 to 6%, and the average absolute error is 2.37%. This means that the agreement between the experimental data and the predicted values by SVM is excellent.

Taking into account all these factors, we may come to the conclusion that the SVM can be used to predict the effects of fabrication conditions of the membrane on rejection of BSA of homemade VC-co-VAc-OH microfiltration membrane.

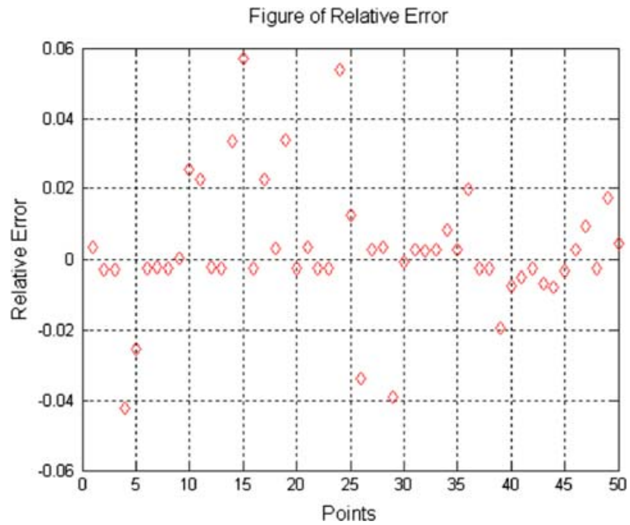

Fig. 7. Relative error of rejection by SVM.

4.3. Comparison of prediction accuracy by SVM and ANN

In order to comparing the prediction accuracy by SVM and ANN, the ANN was used to fit the same experimental data used in 4.2. In this study, the network was trained by the neural network toolbox of MATLAB functions in training network. The transfer function and the number of hidden layer nodes in the training process of BP neural network were chosen as in our previous study [19], i.e. the transfer function is Traindx function, the hidden layer node is seven and the learning rate is 0.1. In such circumstances, the results were showed in Figs. 8 and 9, respectively.

Figs. 8 and 9 revealed the good prediction accuracy of pure water flux and rejection of BSA of the membrane by ANN, respectively. Moreover, the results in Table 1 shown that predicted data by SVM model were more accurate than that of ANN model. This can be explained by the following reasons: (i) SVM is based on statistical theory-based, and it has a rigorous theoretical and mathematical foundation, while ANN needs to rely on the designer's experience and knowledge; (ii) Large size of experimental set needed for ANN methods to achieve desired prediction accuracy, while the SVM method can get the high accuracy only with a small size of experimental set; (iii) SVM has good generalization ability, which can get the global optimal solution.

Therefore, SVM can reach an optimal balance between sensitivity and specificity in the small size of the training set (small training sample or restricted data sets) and give predictive values with high accuracy.

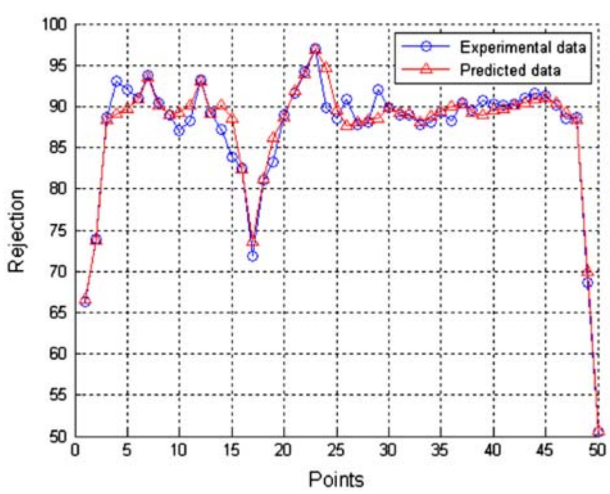

Fig. 6. Comparison between experimental data and predicted data of rejection under different operation by SVM.

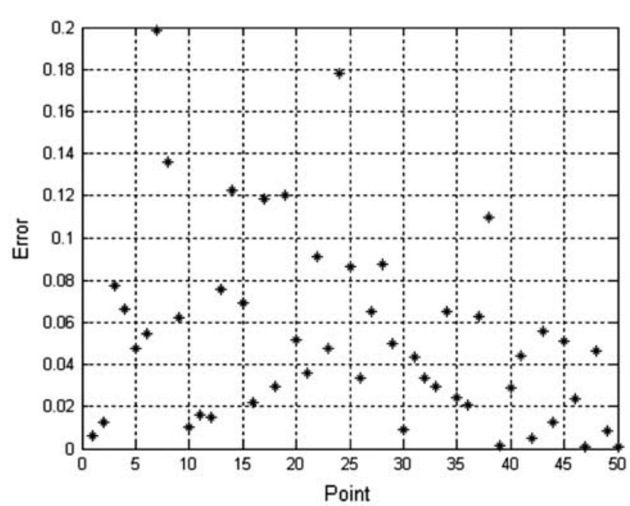

Fig. 8. Relative error of flux by ANN.

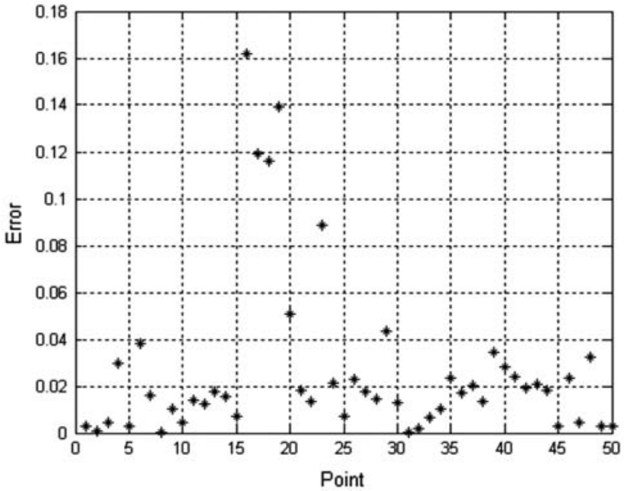

Fig. 9. Relative error of rejection by ANN.

Table 1
Comparison between the different prediction methods

Methods of prediction	Average error of flux (%)	Average error of rejection (%)
SVM	2.84	2.37
ANN	13.72	3.55

5. Conclusion

SVM model was constructed to predict the effects of fabrication conditions on filtration performance of homemade VC-co-VAc-OH microfiltration membranes. The detailed relationships between fabrication conditions and filtration performance of membrane were established by the SVM model. SVM possesses good ability in the prediction of pure water flux and rejection of BSA of homemade VC-co-VAc-OH microfiltration membrane, whose relative error varies from −6 to 6%. In addition, the prediction accuracy by SVM and ANN were compared. The average errors of prediction of pure water flux and rejection of BSA of the membrane by SVM are 2.84 and 2.37%, respectively, while the value by ANN is 13.72 and 3.55%. That is to say, SVM shows better learning and generalization ability in the small size of the training set. The ANN model can be applied to predict the filtration performance of homemade VC-co-VAc-OH microfiltration membranes and thereby design the membrane fabrication conditions to obtain the desired filtration performance of the membrane in the fabrication process of homemade VC-co-VAc-OH microfiltration membranes.

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Nomenclature

F	—	a high dimensional feature space
ϕ	—	a nonlinear mapping
ω	—	weight vector
(,)	—	inner product
$\varphi(x)$	—	a mapping function in the feature space
b	—	a constant (the bias)
$R_{emp}[f]$	—	experience risk
λ	—	regularization parameter
$\|\omega\|^2$	—	confidence risk
S	—	size of the sample
$C(.)$	—	Loss function
e_i	—	difference between the predicted values and the experimental data
$C(e_i)$	—	experience loss of the model
J	—	flux of the membrane
V	—	total permeate volume
A	—	effective membrane area
t	—	operation time
R	—	rejection of the membrane
C_p	—	concentration of the permeation
C_f	—	feed solution

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