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Optimization of ultrafiltration membrane fabrication using backpropagation neural network and genetic algorithm

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ABSTRACT

Hybrid models based on backpropagation neural network (BPNN) and genetic algorithm (GA) were constructed to optimize the fabrication of polyetherimide (PEI) ultrafiltration (UF) membrane via dry/wet phase inversion. BPNN was employed to capture the detailed relationships between the preparation conditions and the UF membrane performances, and GA was used to choose the initial connection weights and biases of BPNN to avoid convergence at suboptimal solutions. The excellent agreements between the model predictions and the testing data indicate that the hybrid models have sufficient accuracy. The effects of preparation conditions on membrane performances were predicted by the hybrid models successfully, which indicate that PEI/N,N-dimethylacetamide (DMAc)/1,4-butyrolactone (GBL) is the best membrane casting system investigated in this study. Furthermore, the optimal preparation conditions were forecasted, and membranes with desired performances, for instance, higher pure water flux (PWF) and bovine serum albumin (BSA) rejection ratio (RR) 80–90% were fabricated with the standard deviation between the predicted performances and validation experimental values less than 10%. The hybrid models can contribute to collaborative optimization of multiple parameters and designing the preparation conditions to obtain desired UF membrane performances and avoiding large experimental data scattering in the fabrication of phase inversion membranes.

1. Introduction

Ultrafiltration (UF) membrane is extensively applied to the product recovery and pollution control in chemical, electronic, food, pharmaceutical, water treatment and biotechnological industries [1,2]. Pure water flux (PWF) and rejection ratio (RR) are the most important performances to characterize UF membranes [3,4]. To optimize the fabrication of UF membrane via dry/wet phase inversion, traditional orthogonal method is the most widely used owing to its sufficient accuracy [5,6]. However, the method cannot get a function expression between preparation conditions and membrane performances and hence it is difficult to find out the optimal factor combination [7,8].

Backpropagation neural network (BPNN) due to its good robustness and fault tolerance is widely used in optimization and function approximation [9–13]. The biggest problem involved in the application of BPNN is easily convergent to a local solution [14,15]. To overcome this problem, several global search techniques including genetic algorithm (GA) have been developed. Up until now, GA has mainly been used to search the optimal solution of BPNN function [16–20].

In the field of membranes, BPNN models have been used frequently in membrane filtration process, to predict the evolution of membrane fouling [21–25] or membrane performances under different separation parameters, for instance, concentration of solute, solution viscosity, transmembrane pressure difference, temperature and filtration time [10,11,26–30]. The application of BPNN to the membrane fabrication has rarely been reported yet. In our previous work [31], we successfully constructed hybrid models which employed GA to choose the initial connection weights of BPNN to predict the effects of preparation conditions on pervaporation performances of polydimethylsiloxane (PDMS)/ceramic composite membranes. However, the UF membrane which is porous is totally different from the pervaporation membrane that is nonporous. Therefore, it is necessary to construct hybrid models for optimization of UF membrane fabrication.

Abbreviations: BPNN, backpropagation neural network; BSA, bovine serum albumin; BuOH, n-butanol; Da, Dalton; DE, diethyl ether; DMAc, N,N-dimethylacetamide; GA, genetic algorithm; GBL, 1,4-butyrolactone; PEG400, polyethylene glycol with average molecular weight of 400 Da; PEI, polyetherimide; PDMS, polydimethylsiloxane; PVP, polyvinylpyrrolidone; PWF, pure water flux; RR, rejection ratio; SSE, sum square error; UF, ultrafiltration.

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Nomenclature

Symbols

b_1	biases of input/hidden layer
b_2	biases of hidden/output layer
C_{add}	the concentration of additive
C_f	BSA concentration of the feed
C_p	BSA concentration of the permeate
C_{PEI}	the concentration of PEI casting solution
F_n	output of the PWF prediction model
F_p	predicted PWF (de-normalized of F_n)
IW	connection weights of input/hidden layer
logsig	log-sigmoid transfer function
LW	connection weights of hidden/output layer
$\max(n_i)$	maximum value of n_i
$\min(n_i)$	minimum value of n_i
n_i	numerical value of each preparation condition
$\hat{n}_i$	normalized value of n_i
P	model input vector composed of the normalized value of n_i
Q	volume of the permeate pure water (m^3)
R_p	predicted RR (output of the RR prediction model)
S	effective area of the membrane (m^2)
t	evaporation time
T	temperature of the water coagulation bath
tansig	tan-sigmoid transfer function
t_{add}	the type of additive
t_p	permeation time (h)

Subscripts

F	PWF
R	RR

In this study, the fabrication of polyetherimide (PEI) UF membrane via dry/wet phase inversion was optimized by the hybrid models. Effects of PEI concentration, temperature of water coagulation bath, additive type and concentration on membrane performances were predicted by the hybrid models and verified by experimental data. According to the hybrid models, the best membrane casting system of the six was determined. Furthermore, the optimal preparation conditions were forecasted, and membranes with desired performances were fabricated.

2. Experimental

2.1. Materials

PEI purchased from General Electric Plastics (USA) in pellet form and polyvinylpyrrolidone (PVP) supplied by Shanghai Chemical Reagent Station (China), were dried in a vacuum oven at 105 °C to constant weight. 1,4-Butyrolactone (GBL) purchased from Tianjin Guangfu Fine Chemical Research Institute (China) and N,N-dimethylacetamide (DMAc) supplied by Beijing Chemical Plant (China) were dried over molecular sieve beads (50 nm, Dalian Liaodong Chemical Reagent Co., China) before used. Bovine serum albumin (BSA) with average molecular weight of 67,000 Dalton (Da) bought from Beijing Aoboxing Biological Product Company (China), n-Butanol (BuOH) purchased from Shenyang Reagent Plant 3 (China), Diethyl Ether (DE) supplied by Tianjin Tanggu Industrial and Commercial Industry Co. (China), and polyethylene glycol with average molecular weight of 400 Da (PEG400) bought from Guangdong Province Xilong Chemical Factory (China) were used without further purification. All the chemicals were of analytical grade.

2.2. Membrane preparation

The PEI UF membranes were prepared by dry/wet phase inversion method. Polymer PEI without or with a kind of additive (BuOH, DE, PEG400, PVP and GBL) was dissolved in solvent DMAc by mechanical stirring for 8 h at 90 °C to form a homogenous membrane casting solution. Air bubbles in the casting solution were removed by vacuum degassing for 30 min. The casting solution was cast on a non-woven fabric (Ahlstrom, Finland). After exposed to air with the relative humidity of around 55% for a few seconds, the cast films were immersed in a water coagulation bath for 24 h, where the polymer precipitation occurred due to the exchange of solvent in the cast film and non-solvent (water) in the coagulation bath, and then the membrane was formed.

2.3. Membrane characterization

A home made UF cell was used to measure pure water flux (PWF) and rejection ratio (RR), with the effective membrane area of $33.18 \times 10^{-4}\ m^2$ and transmembrane pressure difference of 0.1 MPa. Prior to the experiments, the as-prepared membrane was compacted in the cell by deionized water for 30 min under the transmembrane pressure difference of 0.15 MPa.

The PWF ($m^3/(m^2\ h)$) is defined by Eq. (1).

$$\mathrm{PWF} = \frac{Q}{S \cdot t_p} \tag{1}$$

where Q is the volume of the permeate pure water (m^3), S is the effective area of the membrane (m^2), and t_p is the permeation time (h).

The RR, tested with 0.5 kg/m^3 BSA solution, is calculated by Eq. (2).

$$\mathrm{RR} = 1 - \frac{C_p}{C_f} \tag{2}$$

where C_p and C_f is the BSA concentration of permeate and feed, respectively, which is determined by ultraviolet–vis spectrophotometer (Shanghai xinmao instrument Co., Ltd., China) at 280 nm.

3. Modeling schemes of the hybrid models

A commercially available software program (MATLAB Version 7.0.0.19920, genetic algorithm and direct search toolbox v. 1.0.1, neural network toolbox v. 4.0.3, the Math Works Inc.) was used to implement GA and BPNN on a personal computer.

3.1. Training/testing data

In the dry/wet phase inversion process, membrane performances are mainly determined by the concentration of PEI casting solution (C_{PEI}), the type of additive (t_{add}), the concentration of additive (C_{add}), evaporation time (t), temperature of the water coagulation bath (T) and relative humidity of air [32]. In our preparation processes, relative humidity of air remained constant at about 55%. Therefore, the variables that influenced the membrane performances were C_{PEI}, t_{add}, C_{add}, t and T, which were considered as the model inputs.

Model inputs must be normalized to avoid numerical overflows due to very large or very small weights [33,34]. The normalization