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Comparison between artificial neural networks and Hermia's models to assess ultrafiltration performance

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ABSTRACT

In this work, flux decline during crossflow ultrafiltration of macromolecules with ceramic membranes has been modeled using artificial neural networks. The artificial neural network tested was the multilayer perceptron. Operating parameters (transmembrane pressure, crossflow velocity and time) and dynamic fouling were used as inputs to predict the permeate flux. Several pretreatments of the experimental data and the optimal selection of the parameters of the neural networks were studied to improve the fitting accuracy.

The fitting accuracy obtained with artificial neural networks was compared with Hermia pore blocking models adapted to crossflow ultrafiltration. The artificial neural networks generate simulations whose performance was comparable to that of Hermia's models adapted to crossflow ultrafiltration. Considering the computational speed, high accuracy and the ease of the artificial neural networks methodology, they are a competitive, powerful and fast alternative for dynamic crossflow ultrafiltration modeling.

1. Introduction

In the last decades, the interest in the use of ultrafiltration (UF) technology has focused on wastewater treatment, recovery of high value compounds from wastewater currents, and the production of drinking water and process water [1]. However, membrane fouling is the main obstacle to a wider application of UF processes as it implies great energy consumption and high operation and maintenance costs [2]. Therefore, a better understanding of membrane fouling is the key to solve the problems arising in the application of this technology [1]. The characterization of membrane fouling makes possible to estimate the capacity and efficiency of the membrane under certain conditions.

Artificial neural networks (ANNs) have been used in the last years in a wide range of scientific and business fields [3–6]. One of the main advantages of ANNs is their capability to learn and recognize trends in a series of input and output data without having into consideration prior assumptions or hypothesis about the relationships governing the process parameters [7]. Compared to the conventional mathematical models used to predict the evolution of permeate flux decline with time during membrane filtration processes, it is noteworthy that these models have certain shortcomings: they involve complex mathematical equations, experimental data is sometimes necessary to infer the input parameters, their empirical equations are only valid in the range of experimental conditions tested and should be fitted for each experimental condition at a time [7]. On the contrary, ANNs are able to accurately predict the complex non-linear relationships between input and output variables of a system and to simulate all the experimental conditions tested at once. For these reasons, some authors concluded that ANNs are a competitive, powerful and fast alternative for dynamic crossflow UF modeling [7–17]. One of the latest applications of ANNs corresponds to the dynamic and steady-state modeling [7] for process control purposes [8], especially in the membrane technology field. Some previous works available in the literature have successfully developed and employed ANNs for different applications from microfiltration and UF to nanofiltration and reverse osmosis and different feed solutions [9–17]. For instance, Chakraborty et al. [11] studied the UF of aqueous solutions containing chromium (VI) and correlated the permeate flux and the membrane performance index to different operating conditions (feed flow rate, transmembrane pressure, polymer to metal ratio and pH) using an ANN model. They developed a feed-forward ANN consisting of two hidden layers and based on a Bayesian algorithm. These authors found more accurate

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Nomenclature

A	membrane area (m^2)
A_0	membrane porous surface (m^2)
a	specific resistance of the gel layer (m/kg)
a_p	radius of the solute molecule (m)
CFV	crossflow velocity (m/s)
E_m	average deviation (dimensionless)
E_{max}	maximum deviation (dimensionless)
E_{min}	minimum deviation (dimensionless)
J_0	initial permeate flux ($L/m^2 \cdot h$)
J_p	permeate flux ($L/m^2 \cdot h$)
J_{pss}	steady-state permeate flux ($L/m^2 \cdot h$)
K_c	constant for complete blocking model for crossflow filtration (m^{-1})
K_{CF}	phenomenological coefficient—constant
K_{gl}	constant for gel layer formation model for crossflow filtration (s/m^2)
K_S	constant for standard blocking model ($m^{-1/2} \cdot s^{-1/2}$)
K_i	constant for intermediate blocking model for crossflow filtration (m^{-1})
n	constant for fouling mechanism (dimensionless)
Neur	number of neurons in the intermediate layer of the ANNs
Norm	normalization of the permeate flux
Weights	initialization of the weights in the ANNs
Pret	data pretreatment
R^2	square regression coefficient (dimensionless)
$R(t)$	fouling indicator (m^{-1})
R_m	membrane resistance (m^{-1})
RE	relative error (dimensionless)
T	time (s)
TMP	transmembrane pressure (MPa)

Greek letters

μ	viscosity (kg/m·s)
ρ	density (kg/m^3)
χ_m	solute concentration over the membrane surface (dimensionless)
ψ	solute form factor (dimensionless)
Δ^L and Δ^U	margins used to give the network limited extrapolation capability in Eq. (10) (dimensionless)

Abbreviations

ANN	artificial neural network
FF ANN	Feed Forward Artificial Neural Network
LSD	Least Significant Difference
MF	microfiltration
MP ANN	Multilayer Perceptron Artificial Neural Network
MSE	mean square error
MWCO	molecular weight cut-off (g/mol)
NF	nanofiltration
NMSE	normalized mean square error
PEG	polyethylene glycol
RMSE	root mean square error
UF	ultrafiltration

predictions by means of the ANN model in comparison with those obtained using a conventional multiple regression analysis. Soleimani et al. [12] predicted the permeate flux and fouling resistance after the UF of oily wastewaters by applying ANN models. They created the feed-forward ANN with the Levenberg-Marquadt back-propagation algorithm and they used the transmembrane pressure, the crossflow velocity, the feed temperature and the pH as input variables. They obtained an excellent agreement (values of coefficient of determination greater than 0.99) between the predicted values and the experimental data. Purkait et al. [13] investigated the prediction of permeate flux obtained in nanofiltration and reverse osmosis treatments of leather plant effluents. They applied a multi-layered feed-forward ANN with back-propagation algorithm for both batch and crossflow experiments. The optimal ANN consisted of two hidden layers and provided mean absolute error values lower than 1%. Finally, Rahmanian et al. [17] designed an ANN to predict the experimental data obtained from a wastewater micellar-enhanced UF process. These authors tested a three-layer feed-forward ANN using the Levenberg-Marquadt algorithm for training and seven variables as input (transmembrane pressure, pH, electrolyte concentration, feed SDS concentration, etc.). They observed that there was a good agreement between the ANN model results and the experimental data, being the ANN developed an effective tool to predict complex non-linear relationships.

In this paper, feed-forward ANNs with one intermediate layer and based on a Levenberg-Marquadt training algorithm were created to predict the permeate flux decline with time during the crossflow UF of polyethylene glycol (PEG). In addition, the influence of two pretreatment methods (the normalization of the output variable and the introduction of a fouling indicator as an additional input) of the experimental data on the fitting accuracy of the ANNs models was evaluated. Since only few papers available in the literature deal with the comparison between the goodness of fit provided by the ANN models and the classical ones [18,19], in this paper ANN predictions were compared with those of Hermia's classical fouling models, once the optimum ANN parameters were determined and the training of the network with a set of UF experimental data was performed.

2. Theory

2.1. Hermia's models adapted to crossflow ultrafiltration

Hermia's models adapted to crossflow UF are four semi-empirical models based on constant pressure filtration laws [20], whose general equation is as follows (Eq. (1)):

$$\frac{d^2t}{dV^2} = K_{DF} \cdot \left(\frac{dt}{dV}\right)^n \quad (1)$$

where t is the filtration time, V is the permeate volume, K_{DF} is a phenomenological coefficient for dead-end filtration and n is the characteristic model constant.

The classical dead-end filtration models were modified by Field et al. [21] to account for the back-transport mass transfer occurring in crossflow filtration by including the permeate flux obtained at the steady-state [22–24]. This modification results in the following general differential equation Eq. (2).

$$-\frac{dJ_P}{dt} = K_{CF} \cdot (J_P - J_{PSS}) \cdot J_P^{2-n} \quad (2)$$

where J_P is the permeate flux at a given time, J_{PSS} is the permeate flux when steady-state was achieved and K_{CF} is a phenomenological coefficient for crossflow filtration. The value of the characteristic model constant (n) depends on the type of fouling mechanism and thus, Hermia distinguished four different types of fouling named as complete blocking ($n = 2$), intermediate blocking ($n = 1$), standard blocking ($n = 3/2$) and gel layer formation ($n = 0$).