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Ultrafiltration of BSA in pulsating conditions: an artificial neural networks approach

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Abstract

The aim of the present paper is to analyze membrane systems behavior, operating in pulsating conditions, by means of artificial neural networks (ANNs). Different ANNs have been developed, by means of Matlab® Neural Network Toolbox, to model the ultrafiltration process of aqueous BSA solutions through poly-ethersulfone membranes. A specific neural network architecture, constituted by one input layer, two hidden layers and one output layer, has been finally identified by a trial-and-error procedure. The network has been trained through a selected set of experimental data obtained for a lab-scale flat sheet membrane module, equipped with a device capable of producing periodic pulses of the applied trans-membrane pressure (TMP) and feed flow rate. It has been found that the developed neural network is capable of offering very accurate predictions of actual system behavior either when it is tested within the range used for training or when the inputs combination has been never exploited during learning phase. The observed reliability of neural networks predictions of membrane performances has suggested to use them for searching an optimal pulsation frequency profile able to maximize permeate flux. The utilization of such a pulse frequency profile allows obtaining, on the basis of theoretical evaluations only, significant improvements of membrane performances with respect to UF experiments performed at fixed and constant pulsation frequencies.
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1. Introduction

Membrane ultrafiltration (UF) is a pressure driven process used for separation, concentration and purification of macromolecules from solutions [1,2]. UF offers plenty of advantages; nevertheless, one of the main drawbacks of this process is the rapid permeate flux decay, due to the membrane fouling. In order to improve membrane performances, several different methods, based either on the chemical modifications of the surface or on the variation of system fluid dynamics, have been proposed [3–5]. One of the most successful fluid dynamics techniques consists in periodically changing both the velocity profiles in the membrane module and the applied trans-membrane pressure (TMP), thus promoting a periodic relaxation of the deposited cake and the disruption of concentration polarization layer. The application of pulsating conditions has shown that the permeate flux decay is not so steep as it is found in traditional membrane processes [6], thus promising very interesting perspectives for the improvement of membrane module productivity by changing feed flow rate and TMP during the experiment.

The individuation of operating parameters values that maximize membrane performances can be accomplished if a dynamic model is available. This has to be able to predict the permeate flux decay as a function of all the phenomena involved in the process. The formulation of such a model is complicated, however, by several aspects that, in some cases, have not yet been fully understood. At present, the available models are based either on some restrictive hypothesis that limit their applications to a few of simple cases, or on

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the utilization of adjustable parameters that are difficult to determine experimentally, or are expressed in terms of complex mathematical equations for which an analytical solution cannot be provided [7–9].

Therefore, different modeling techniques that, by means of appropriate algorithms, directly analyze the systems responses to various forcing inputs (black-box models) represent an alternative option that may be chosen to develop predictive models. The artificial neural networks (ANNs) demonstrated to be an effective predictive instrument for modeling non-linear dynamic systems, as those typical of several engineering applications. ANNs have been successfully employed to model the dynamic evolutions of membrane processes, like ultrafiltration and microfiltration, thus allowing predicting the permeate flux decay as a function of process operating parameters. In fact, a neural network approach was used to model membrane fouling in raw cane sugar microfiltration, accounting for the effects that hydrodynamic conditions have on the variation of total hydraulic resistance of the membrane with respect to time [10]. Permeate flux and membrane rejection were estimated by means of a neural model as functions of process variables, i.e. solute concentration, flow velocity, pressure and temperature [11]. According to the authors, neural network models have several advantages; in fact they are easy to use and are characterized by shorter computing time as compared to traditional approach based on the solution of mass transfer equations. A neural network approach was also used to predict the total hydraulic resistance of ultrafiltration membranes employed for the production of drinking water [12]. By means of some characteristic parameters regarding water quality, i.e. turbidity and temperature, and accounting for the effects of the main operating variables, it was possible to obtain a very accurate prediction of membrane resistance. The rate of BSA ultrafiltration as a function of pH and ionic strength was predicted by a single hidden layer neural network [13]. The authors proved that network training is affected much more by the quality of experimental training points than by their amount; in the specific application, the agreement with experimental results was excellent, with average errors lower than 2.7%. Two different neural network models were developed to predict the permeate flux at any time instant, within a process in which ultrafiltration was followed by backwashing with demineralized water [14]. Both the trained networks were capable of accurately analyzing the non-linear process characteristics up to experiment durations of 2500 s. The ANNs were used also to dynamically model cross-flow ultrafiltration of milk, thus allowing a prediction of time-dependent rate of flux/total resistance and membrane rejection [15,16]. The authors demonstrated the ANN ability of foreseeing new data that were not used during the training, showing a good agreement between the validation points and the model predictions. Moreover, the same authors developed feed-forward perceptron networks with a single hidden layer, used to simulate the time-dependent rate of ultrafiltration from a few experimental data [17]. They analyzed the effect of the number of training points, hidden neurons and training data arrangements on the simulation correctness.

In the present paper, a neural black-box model has been developed and trained to predict the ultrafiltration performances under pulsating conditions. This, in order to answer two different questions that were not fully analyzed in the literature:

- Is neural technology suitable to model the membrane processes behavior even if the operating conditions are periodically changed during the experiments?
- May artificial neural network be used to design an advanced control system that indicates the best trend of pulse frequency that has to be chosen to maximize the permeate flux?

2. Theory

The artificial neural networks (ANNs) are computational models that simulate a few functions and capacity of human brain whose structure and operation they somehow reproduce [18]. An ANN is constituted by a certain number of single elaborating elements, operating in parallel that are called neurons or units or knots. The units are combined so as to form a layer within the ANN. If several layers are present, a multilayer network is obtained; in a multilayer network each neuron receives several inputs from other related units and, by means of an activation function, produces an output, i.e. a signal that is fed to the other neurons connected to it. The supervised back-propagation learning technique is based on the knowledge of a reference output (target), represented—in most cases—by the experimental results obtained after a specific experimental protocol. The inputs and the corresponding outputs are used to train the network until it can associate input vectors to specific system responses. Trained back-propagation networks are able to give reasonable responses when presented with inputs never exploited during learning phase. This generalization property permits to train a network on a representative set of input/target pairs and get good results without training the network on all possible input/output couples [19]. Learning process is called back-propagation because the error signal propagates backward within the network. In multilayer feed-forward architecture (MLP), the back-propagation learning technique is applied so that the output of each single unit is transmitted only to the neurons belonging to the following layer and never to units of the same level or to those of the previous ones. MLP networks make use of the so-called generalized delta rule (GDR) that, in standard version, utilizes the method of descending gradient so that the connections weights change proportionally to the derivative of the deviation between the network output and the target (error) [20,21]. A certain input is fed to the neurons of first layer, is processed and, then, transmitted through each of the following layers until an output is produced. The obtained output is compared with the corresponding target and an error signal is calculated for every output unit. The

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