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Part II: Prediction of the dialysis process performance using Artificial Neural Network (ANN)

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ABSTRACT

In the present research, an experimental based Artificial Neural Network (ANN) model is developed to describe the dialysis process performance under different operating conditions in the charged and neutral states of dialysis. The transfer behavior of charged micelles through the charged and neutral conductive membranes was investigated using this model. The parameters are highly interconnected in this system. Moreover, using the available deterministic models for tracking the process performance and the switch of the diffusion mechanisms is not completely realizable. Therefore, using neural networks is highlighted as a recommended model for this type of situations. The concentration gradient, absolute feed concentration and membrane electrical charge are the main parameters which affect the process performance.

The experimental system consists of aqueous sodium dodecyl sulphate (SDS) solution above critical micelle concentration (CMC) and commercial micro-filtration membrane (GVHP) coated by conductive poly-pyrrol (PP) or silver. The amounts and the mechanisms of mass transfer were analyzed for the two types of membranes in a variety of operating conditions. Moreover, the study over the competitive state of the process was performed where the parameters are manipulated simultaneously. The developed ANN is able to predict the process performance under individual manipulation and simultaneous manipulation of the parameters. Therefore it is able to track the governing mechanisms any time.

The experimental data and the developed model show that in low concentration and concentration gradients, the diffusion mechanism and value, are different in comparison to the state with high values of concentration and concentration gradient. The neural network approach was found to be capable of modeling this complex process accurately.

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1. Introduction

Dialysis process has a wide range of technological applications for metal ions separation in waste water treatment, food processing, protein separation and etc. Although all those technologies are governed by the same basic phenomenon (diffusion), a suitable modeling approach should consider the special characters of each process as well. For example, a recent study [1] shows that the transfer of charged particles is affected not only by the concentration gradient of the particles across the membrane, but also by the parameters like feed phase concentration and induced electrical charge over the membrane surface. A new approach of modeling is required to describe this observed behavior. The nonlinear interactions of parameters in this dialysis process make it difficult to track the source of the observed effects using a conventional mathematical model. In this process, the expected effect of concentration gradient on the diffusion rate is influenced by the charge available on the membrane surface. The same is true about the effect of absolute concentration. These strong nonlinearities, pose a complex problem in predicting the dynamic process performance where the parameters are changed continually. As a result, the development of general equation-based model for this system has proved extremely challenging [1]. Therefore beside any effort to develop a deterministic model, the data-based models should be also tried, among which Artificial Neural Network (ANN) models are more flexible and appropriate.

In 2005, Bandini [2] developed a simple "adsorption-amphoteric" model to describe the mechanism of membrane charge formation in nanofiltration membranes. Samuel de Lint and Benes [3] used a predictive charge-regulation transport model in which no adjustable parameter was used. Moreover, in a fundamental research [4], the charge-regulation concept was combined with the theory of irreversible processes to predict the multi-component electrolyte transport across the nanofiltration membranes. In all of these mentioned studies, the model considers the electrostatic repulsions as a straightforward factor which is obviously an over-simplification for this system. In another related study, Szymczyk et al. [5] focused on modeling the



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Fig. 1. Schematic of a three-layer feed forward neural network model.

rejection rate via a dielectric model. This model includes an adjustable parameter in order to track the system's behavior. This adjustable parameter in this model is the effective dielectric constant of the solution inside the pores. In two other studies [6–8], theory of electrostatic repulsion and Brownian diffusion mechanism has been used to describe the observed patterns in the experimental data. The fact that the generalized mass transfer equations like the Stephan– Maxwell equation lead to the same result for the charged and neutral state of the dialysis, is another motivation to develop a new model for the general state of the dialysis process. Detailed information in this regard is available in Part I where the modeling is performed based on the physical model.

To mention another potential for this research, it should be noted that, feed phase concentration has an individual effect on the performance of the charged dialysis process which has not been modeled as an individual parameter yet. However, the affected partition of ions due to the membrane charge has been modeled under the well-known framework of the rejection theory [9]. Takagi in this reference [9] developed an equation which generally shows that the rejection varies linearly with the inverse of the volume flow which implicitly represents the effect of feed phase concentration. In this study like several other researches [6,10], effects of parameters have been modeled based on the mobility concept. In this manner effects of electrical charge and concentration on the process behavior are modeled by considering the mobility of solutes while they are passing through the membrane.

Moreover, in another related study [11], the concentration profile was modeled for the charged solute in the concentration polarization layer based on the Maxwell–Stephan (MS) equation and Gouy– Chapman model. They provided an analytical equation in terms of three dimensionless numbers, although, even this generalized equation and fundamental model does not directly reflect the effect of feed phase concentration.

As a novel approach, the individual and interactive effects of concentration and electric charging the membrane surface on the charged dialysis performance are modeled here for the first time.

The main motivations for developing the dialysis process ANN model in this research are summarized as below:

Presenting a flexible model based on the experimental data for the dialysis process might avoid the biasing risk.

 Developing a model as a new and unique tool for modeling both neutral and charged states of the dialysis process.



Fig. 2. SDS concentration versus conductivity of solution.

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