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Use of Polymer Membranes for Modeling Desulfurization in the Process of Pervaporation through Artificial Neural Network

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ABSTRACTS

The present study considered the amount of thiophene_alkane separation within the process of pervaporation by use of-of membrane polyethylene glycol and polydimethylsiloxane-polyacrylonitrile with the help of Artificial Neural Network Modeling. In this research, the effects of such parameters as Volumetric flow rate and temperature, as well as feedstuff properties (separation factor and flux) on the Desulfurization process efficiency were evaluated, and the Multi Layers Perceptron (MLP) neural network feed forward along with Propagation learning algorithm and Levenberg-Marquardt function with inputs and outputs were implemented. Tansig activation algorithm was used for the hidden layer, and Purelin algorithm was utilized for the output layer. Furthermore, 5 neurons were defined for the hidden layer. After processing the data, 70 percent were allocated for learning, 15% were allocated for validity, and the remaining 15% was allocated for the experience. The achieved results with the aforementioned method had a suitable accuracy. The graphs of the error percentage for the actual values of the separation factor and flux outputs were compared to the achieved values from modeling through related membranes for evaluating the efficiency of pervaporation process in a separation of ethanol, Acetone, and butanol from the water. Finally, the graphs were drawn.

Keywords: Modeling, desulfurization, artificial neural networks, polyethylene glycol
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1. Introduction

Sulfur-containing compounds are one of the most important pollutants in petroleum products, and removing them is considered as a goal in the refinement process. The desulfurization process emerged in 1933, and so far, a great number of researchers have been conducted on this subject. Environmental regulations for sulfur content in fossil fuels are getting more and more rigid, and international regulation-making organizations have defined the permissible amount of sulfur content in petroleum products to be 15 ppm in order to limit and lower the amount of this dangerous substance. However, the amount of sulfur content in the petroleum products produced in Iranian refineries is about 500-1000 ppm, and this amount of sulfur content can seriously pollute the air and environment (Abdullah et al., 2014).

As the reduction of sulfur content in the fuel is influential over the Diesel engine performance, automobile-makers are obliged to design and manufacture automobiles that are compatible with low-sulfur fuels (Al-Shahrani et al., 2007). Moreover, the existence of poisoning expensive metal catalysts used in the refineries, and deactivation of this substance while getting in contact with these harmful compounds is another reason of necessity for fuel desulfurization. Regarding the rigid regulations on fuel desulfurization (Li et al., 2014), the researchers are trying to find solutions for desulfurization of fuels in the recent years. One of the fuel desulfurization methods that have attracted the attention of the researchers in the recent years is desulfurization by use of membrane processes. In this technology, a semi-permeable membrane is used for separation of different compounds. This method is much more economical than other common methods of desulfurization regarding the costs, consumed energy, and required equipment (Bösmann et al., 2001). The pervaporation process is a notable progress in the field of solvent desulfurization, desulfurization of volatile organic compounds, water partial desulfurization, and recently, desulfurization of organic- organic solutions. Furthermore, it is approved that such method has a good efficiency in a separation of sulfur impurities. Due to high overall efficiency and high energy efficiency, this method is getting more popularity in the industries right now. Selection of the proper membrane is one of the most important phases in the evaporation process. In most of the evaporation processes, the driving force is the pressure difference between the feed current and the permeated current, and, the vacuum pump provides the required driving force for mass transfer of the compounds (Mulder, 1996).

In this study, a membrane procedure will be simulated in Artificial Neural Network (ANN). The produced feed from Sulfur and hydrocarbon compounds undergo the procedure and will be analyzed under different conditions regarding temperature and pressure in separation efficiency. Moreover, other influential parameters on the evaporation process will be defined (Huang et al., 2004; Yazu et al., 2004; Dooley et al., 2013; Wang et al., 2014; Fattahi et al., 2014).

2. Materials and Methods

2.1. Artificial Neural Network (ANN)

The ANN system is inspired by the brain and neural system of human beings and is composed of a great number of neurons. Like the human brain, the ANN networks are capable of training. One of the advantages of ANN networks is that in problems where an algorithm (in the form of a formula) is not found, or there are a number of examples of the inputs and outputs of the desired system available, usage of ANN for proposition of a model or giving structure to the information will be useful (Mohaghegh, 2000).

High calculation speed of the computers and faster training algorithms can make the ANN more popular in future. This issue can make usage of ANN possible in industrial problems that have a great volume of calculations. Regarding the fact that ANN is not comparable with the natural neural networks, they (ANN) have some characteristics that make them unique where training a linear or nonlinear mapping is required (for example in the field of image resolution, robotics, and control) (Maier and Dandy, 2001; Goda et al., 2005; Shoikir et al., 2006).

2.2. The structure of ANN

Regarding the fact in many cases, a neuron with a great number of inputs is not enough for resolving a technical-engineering problem, gathering a number of neurons in a layer are required in some cases. Moreover, a compilation of neurons in different layers is possible for increasing the system efficiency. In this case, the network will be designed with a particular number of inputs and outputs, with a difference that the network will have more than one layer. Under this condition, the layer to which the data enters is called input layer, the layer from which the processed data gets out is called the output layer, and other layers are called hidden layers. Figure 1 displays an ANN with three layers. In this network, the input, hidden, and output layers are composed of only one layer. The network capabilities can be modified by altering the number of hidden layers, and the number of neurons in each layer. The artificial neural cell is, in fact, a mathematical equation in which p denotes an input signal that after strengthening or weakening as much as w parameter (in mathematical terminology, it is called weight parameter), it will enter the neuron as an electric signal with a size of pw. In order to simplify the mathematical model, it is assumed that input signal is added to another signal with the b value within the neural cell nucleus. Before getting out of the cell, the result (i.e. a signal with a value of $+b$) undergoes another process that is called transfer function in the technical terminology.

When a huge ANN is formed due to gathering a great number of neural cells, too many of the b and w parameters must be initialized by the network designer. This process is called training process. Sometimes, compiling a number of neurons in a layer is required. Moreover, compiling neurons in different layers is also possible for improving the system efficiency. In this case, the network will be designed with a particular number of inputs and outputs, with a difference that the network will have more than one layer. The network capabilities can be modified by altering the number of hidden layers, and the number of neurons in each layer (Rautenbach and Albrecht, 1985).

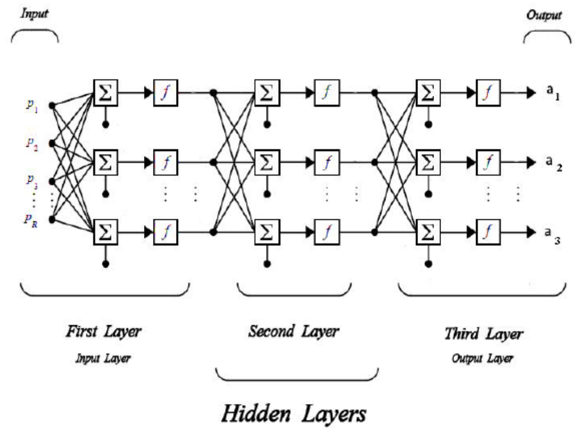

Fig. 1. A schematic of ANN and its layers

3. Results and Discussion

The network inputs include volumetric flow rate and temperature. The network outputs include separation factor and flux. A separate ANN was designed for the separation factor and flux parameters. The MATLAB software version R2012a (7.14.0.739), propagation training algorithm for neural network modeling, and Levenberg-Marquardt function for neural network modeling was used. The neurons in the input layer of the network were defined to be 5 neurons. The results can be seen in figures (Fig. 2 to Fig. 11) below.

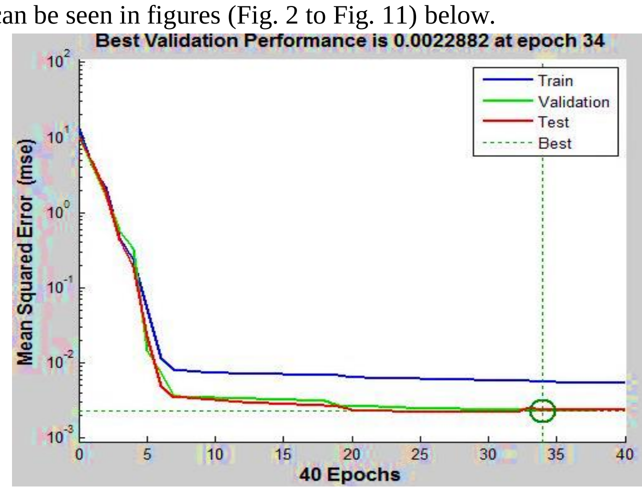

Fig. 2. The performance of Alcan-Thiophene desulfurization by polydimethylsiloxane-polyacrylonitrile membrane

The outputs for flux in Thiophene desulfurization by use of a polydimethylsiloxane-polyacrylonitrile membrane with 141 numbers of outputs are as follows (Lin et al., 2006).

There is a system performance graph in the ANN that shows the number of steps in terms of error. As shown in Figure 2, the error performance of the network for train, test, and validation is descending. Phase 34 that is marked with a circle shows the best validation performance. It means that system had a lower error around the circle, and the excessive training initiated afterward.

After the required data were defined and trained to the ANN, other results were achieved in the regression section. In the figure below, the target axis depicts the goal parameter outputs (in fact, the thing to be achieved at the end). The vertical axis depicts the output achieved by the ANN. These two graphs are usually drawn according to each other, and if the ANN would be able to conduct an exact modeling, the graph will be drawn on a line with $Y = T$ coordination (a line with the slope 1 that passes the origin of the coordinates). In order to statistically calculate the best line with the lowest error, the linear equation in the total graph should be used.

$$Output = 1 * Target + 0.0019 \qquad (1)$$

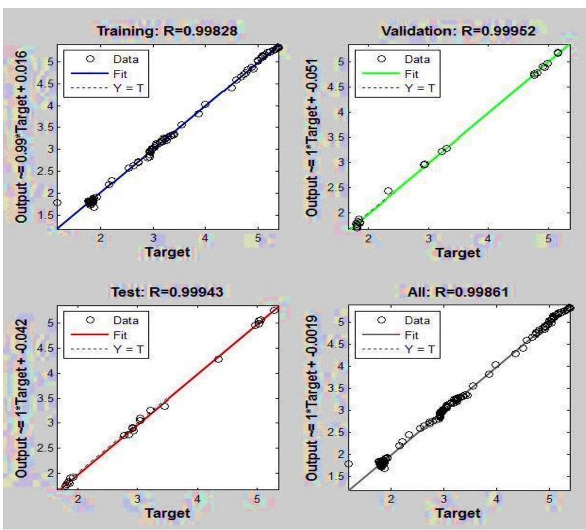

Fig.3. Regression graph for desulfurization of Alcan-Thiophene desulfurization by polydimethylsiloxane-polyacrylonitrile membrane

The 3D graph of Thiophene desulfurization can be analyzed as follows (Fig. 4). As the temperature increases, the flux increases along the membrane and the temperature has a direct effect on the transfer of the components into the feed and membrane.

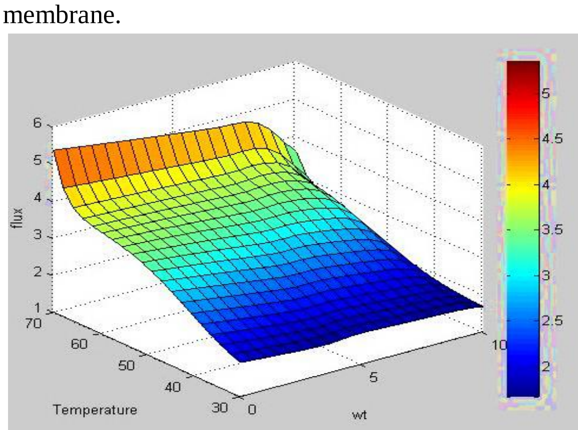

Fig.4.The flux graph for desulfurization of Alcan-Thiophene desulfurization by polydimethylsiloxane-polyacrylonitrile membrane

The figure below displays a comparison of the error percentage for real output and the modeled output. As observed in Fig. 5. The temperature affects the transfer of compounds in the liquid feed and in the membrane, and increasing the concentration decreases the slope of the flux.

Fig. 5. Comparison of the error percentage for real output and the modeled output in desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

For desulfurization of Thiophene by use of a poly-dimethylsiloxane-polyacrylonitrile membrane, the output results of separation factor with 141 outputs are as follows (Lin et al., 2006). In the figure below, the best validation performance was achieved in the Sixty one repetitions, and excessive training initiated afterward.

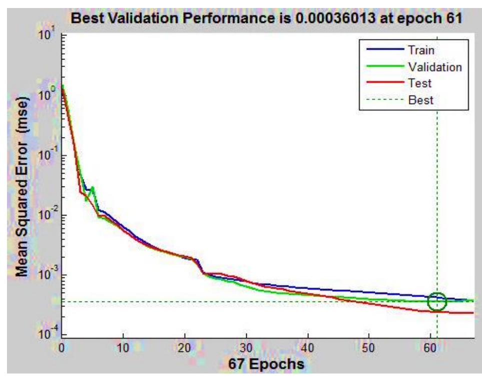

Fig. 6. The performance graph for desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

The regression graph is depicted in the figure below. As observed in the total graph, the best line with the lowest error is achieved by the equation 2.

$$Output = 1 * Target + 0.003 \qquad (2)$$

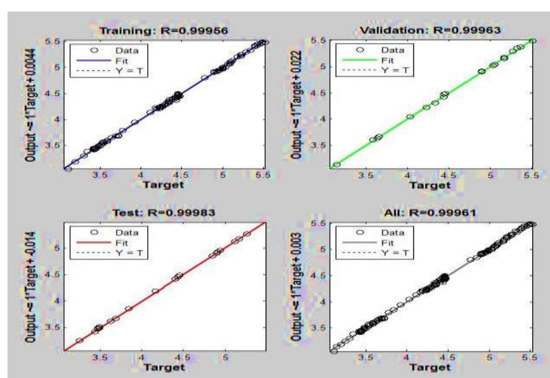

Fig. 7. Regression graph for separation factor in desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

As analysis of the 3D graph below, it can be mentioned about the separation factor that at the beginning, separation factor decreases with the increase of temperature.

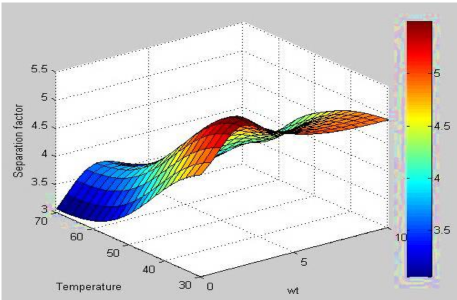

Fig. 8. Separation factor 3D graph for desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

The graph for calculation of error percentage of the real output and the modeled output is depicted in the figure below. As observed in the Fig. 9, in desulfurization of Thiophene, flux with increasing temperature and concentration the separation factor first increases and then decreases.

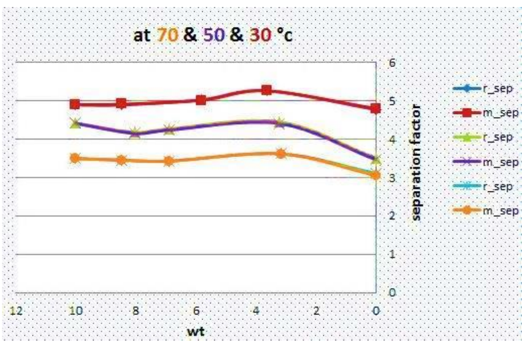

Fig. 9. Comparison of error percentage for overall flux in reality and modeling for desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

106 data were used for desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane was utilized. The results for separation factor are as below (Qi et al., 2007; Lin et al., 2007; Srikanth, 2008). The best validation performance in performance graph was in the Sixteenth repetition. The regression coefficient for all the data in regression graph was equal to 0.99919 that was a very good result. The graph for calculating the error percentage of the real output value and the modeling output value is displayed below. As reflected in this graph, as time went down and the volumetric flow decreased, sulfur decreased to a constant value.

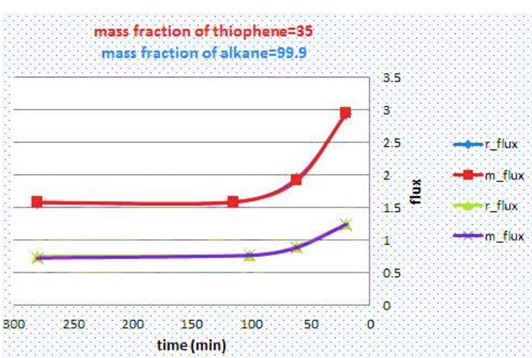

Fig. 10. Comparison of the error percentage for real separation factor and modeling in desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

The results of overall flux output in desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane are as follows: The best validation performance in the performance graph was in the Sixteenth repetition. The regression coefficient for all data in the regression graph was calculated to be 0.99986 that is a very good result. The graph for calculation of the error percentage for real flux and modeling is as follows. It can be seen that with an increase of volumetric flow rate in desulfurization of Alcan-Thiophene, the overall flux increases.

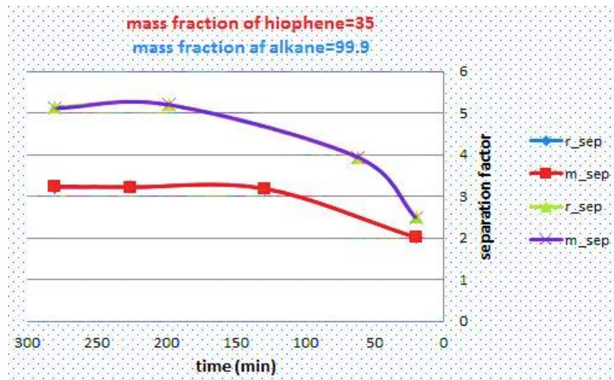

Fig. 11. Comparison of error percentage for overall flux in reality and in modeling of desulfurization of Alcan-Thiophene by polydimethylsiloxane-polyacrylonitrile membrane

4. Conclusion

The maximum amount of flux modeled by ANN and the real amount of flux were compared in this study. The amount of error percentage in ANN was 0.34, which was acceptable. Consequently, it can be concluded that the results of modeling method were acceptable. Desulfurization of organic compounds by means of evaporation was modeled in ANN. It was concluded that Polyether polydimethylsiloxane-polyacrylonitrile membrane is suitable for desulfurization of organic compounds. Moreover, the ANN could reflect the error very well.

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Conflict of interest: Non declare