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Modeling dehydration of organic compounds by use of polymer membranes with the help of artificial neural network

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Abstract

The present study considered the amount of water-alcohol separation within the process of pervaporation by use of polymer membranes with the help of Artificial Neural Network modeling. Pervaporation can be utilized for separation of many liquids (in this study, it was used for separation of ethanol, Acetone, and butanol from water). All the mentioned alcohols have purity problems due to azeotropics with water. The experimental data were compared and analyzed with the model data. 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 dehydration process efficiency were evaluated, and the Multi Layers Perceptron (MLP) neural network feed forward along with Propagation learning algorithm and Levenberg-Marquardt function with 2 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% were 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 separation of ethanol, Acetone, and butanol from water. Finally, the graphs were drawn.

Keywords: Modeling, dehydration, Organic compounds, polymer membrane, Artificial Neural Network

1. Introduction

The traditional purification methods like distillation and extraction require much energy consumption. Moreover, due to heating the product or mixing it with a solvent, it is possible that the final product would be decomposed or impure. Furthermore, the traditional systems usually bring about environmental pollutions due to their purification systems. As a result, searching for an alternative more economic method that would be able to solve the environmental pollution problems (while dismissing the previous restrictions) seems absolutely reasonable.

Membrane separation is the most privileged method among the whole other separation methods. In a membrane separation process, the feed includes a mixture of two or more parts. While passing through a semi-permeable environment (membrane), these parts partially get purified. The feed gets divided into two parts in a membrane process. The part of the feed which does not pass through the membrane is called "Retentate". Another part that passes through the membrane is called "Permeate" [1]. The common membrane separation technology has such advantages as lower energy consumption for separation, enabling conduction of separation process in situ, easy access to the separated phases, conduction of separation process by means of light and compact equipment, easy installation and operation, and the minimum requirements for control, maintenance and repairmen [2, 3]. The six major processes in membrane separation include microfiltration, ultrafiltration, reverse osmosis, electro dialysis, gas separation, and pervaporation (in such fields as water purification, chemical and food processing, medical application, and biological separations) [4].

Use of pervaporation for separation of organic compounds has attracted the attention of many researchers in recent years. Pervaporation is one of the complicated membrane separation processes in which transfer through non-porous (non)polymer

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takes place in three phases of absorption, penetration, and evaporation (or disposal) [5]. As a result, selectivity and permeation is generally based on the interaction between membrane and penetrating molecules, the size of leaking molecules, and the empty volume of membrane. This process is generally very good for excluding little impurity from a liquid mixture. In general, pervaporation is accompanied with penetrating material phase change from liquid to gas. The passed product through the membrane will be separated as low-pressure steam from the other side of the membrane. The product will be collected after changing into liquid. In fact, this process is the known evaporation process, while a membrane is used between the two phases of liquid and gas. The presence of membrane adds selectivity to the process and increases the advantages of the process. With the help of such process, it is possible to separate two liquids from each other [6]. Due to such advantages as excellent performance and high energy efficiency, this process has recently gained attention of many industries. In most pervaporation processes, the driving force is the pressure difference between the feed stream and the permeate stream. The vacuum pump provides the driving force for mass transfer of components [7].

The results of this study by use of ANN reflected a suitable accuracy. The graph of error percentage for the real outputs of separation factor and flux and the modeled separation factor and flux by the related membranes for pervaporation performance were drawn in dehydration of ethanol, acetone, and butanol.

2. Experimental

2.1 Artificial Neural Network (ANN)

Recently, there has been a number of research conducted on data processing for problems for which there is no solution, or problems that are not easily solvable. The ANN pattern is inspired by the neural system of living organisms that includes some constituent units called 'Neuron'. Most of the neurons are composed of the three main parts including cell body (that includes nucleus and other protective parts), dendrites, and axon. The last two parts are the communicative parts of the neuron. Figure 1 displays the structure of a neuron.

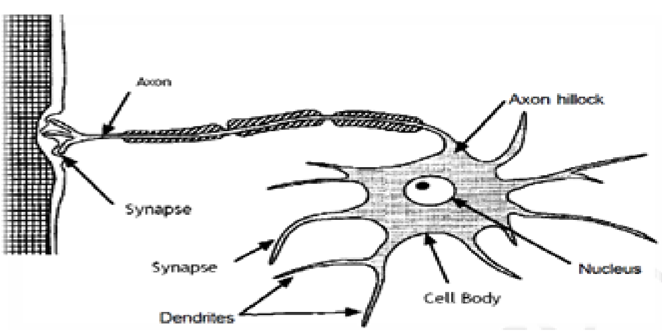

Figure 1. Major parts of a biological cell [7]

Dendrites, as electric signal receiving areas, are composed of cell fibers with unsmooth surface and many splitted extensions. That is why they are called tree-like receiving networks. The dendrites transfer the electrical signals into cell nucleus. The cell body provides the required energy for neuron activity that can be easily modelled through an addition and comparison with threshold level. Unlike Dendrites, axon has a smoother surface and fewer extensions. Axon is longer and transfers the received electro-chemical signal from the cell nucleus to other neurons. The confluence of a cell's axon and dendrites is called synapse. Synapses are small functional structural units that enable the communication among neurons. Synapses have different types, from which one of the most important ones is the chemical synapse.

Artificial neural cell is a mathematical equation in which p represents an input signal. After strengthening or weakening as much as a parameter w (in mathematical terms, it is called weight parameter), an electric signal with a value of pw will enter the neuron. In order to simplify the mathematical equation, it is assumed that the input signal is added to another signal with b value in the nucleus. Before getting out of the cell, the final signal with a value of $pw + b$ will undergo another process that is called "Transfer function" in technical terms. This operation is displayed as a box in Figure 2 on which f is written. The input of this box is the $pw + b$ signal and the output is displayed by a. mathematically, we will have:

$a = f(pw + b)$

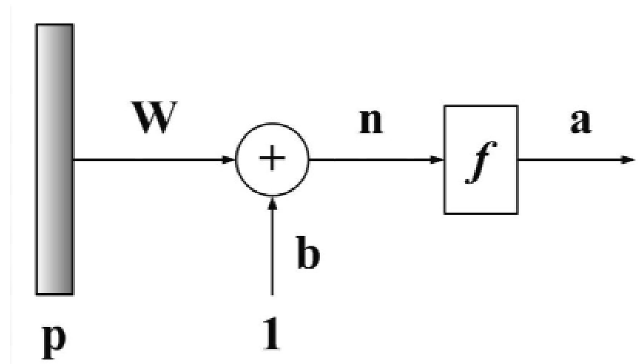

Figure 2. Mathematical model of a neuron [8]

Putting together a great number of the above-mentioned cells brings about a big nueral network. As a result, the network developer must assign values for a huge number of w and b prameters; this process is called learning process.

Within the structure of neural networks, sometimes it is needed to stack up a number of neurons in a layer. Moreover, it is possible to take advantage of neuron crowds in different layers to increase the system efficiency. In this situation, the network will be designed with a certain number of inputs and outputs too; while the difference is that there would be more than one layer (instead of having only one layer). In this manner (multi-layer network), the input layer is the layer through which the inputs are given to the system, the output layer is the layer in which the desired the results are delivered, and the other layers are called hidden layer. Figure 3 displays a neural network with three layers. Input layer, output layer, and hidden layer (that is only one layer in this figure). Through changing the number of hidden layers, and changing the number of present neurons in each layer, it is possible to enhance the network capabilities [8].

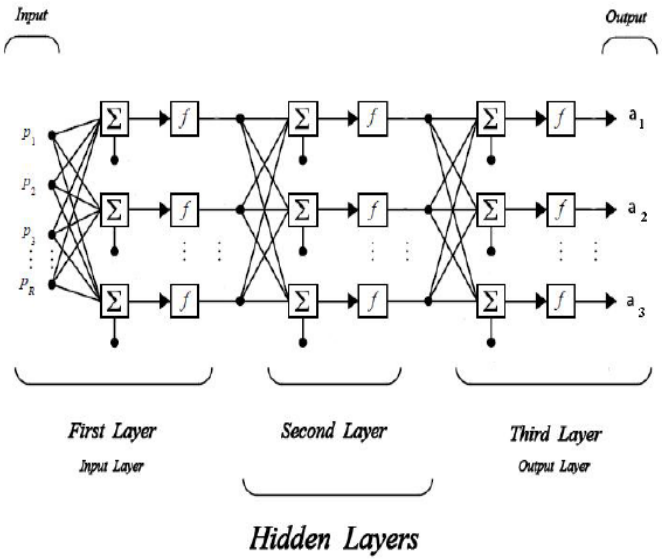

Figure 3. A schematic view of Neural Network and its constituent layers [8]

2.2 Modeling dehydration of organic compounds by use of Neural Network

In this research, the influence of ANN input parameters (volumetric flow and temperature) as well as the feed characteristics (the feeds are the network output) (separation factor and flux) on the efficiency of dehydration process. Two ANNs were designed for analysis of the separation factor and flux parameters. Feed-forward multilayer perceptron ANN and Levenberg-Marquardt function with two inputs and two outputs were used. The Tansig transfer function was used for the hidden layer, and Purelin was utilized for the output layer. Five neurons were determined for the hidden layer. After data processing, 70 percent was dedicated for learning, 15 percent was dedicated for validation, and the remaining 15 percent was dedicated for testing. Such organic compounds as ethanol, acetone, and butanol were selected in this research; and, Matlab version R2012a (7.14.0.739) was used. The results of the study are displayed in figures below. Figure 4 displays a schematic view of a two-layer ANN with only one hidden and output layer. The inputs are multiplied by a *w* value, and there is a bias factor (b) that is added to the input (bias is a fixed value that is added to the input in order to increase the accuracy). Afterward, the result will undergo a function and the resulted value will be multiplied by a weight and added with a bias. The final result will pass another function (with different form and functionality) and output is made. There are five neurons and two inputs on the first layer; however, the number of neurons in the output layer is the same as the number of outputs.

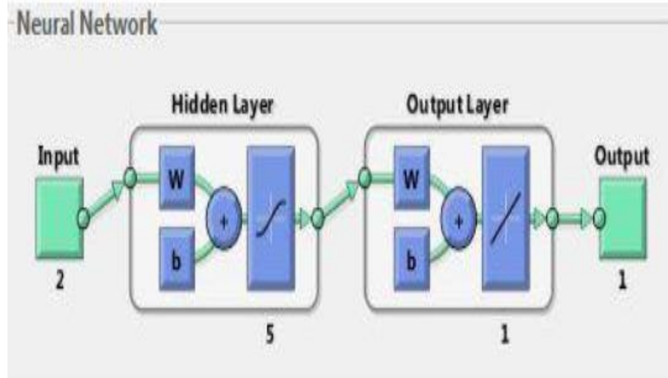

Figure 4. A schematic view of the ANN

The following points about the algorithms must be considered:

- The Data Division compartment totally scrambles the defined data for the system. This compartment randomly defines the Train, Validation, and Test data, so that there will be samples from everywhere of the environment.
- Levenberg-Marquardt function was used in Training phase.
- The Mean Squared Error (MSE) functions for performance measurement.
- The default settings were used for derivative issue.

Figure 5. Algorithms compartment in ANN

The number of data for modeling ethanol dehydration was 326. By use of polydimethylsiloxane and Polyvinylidene fluoride membrane for the output of separation factor, the following results were achieved [9]:

The whole procedure is displayed through some status bars in the progress compartment. The initial values are displayed on the left side of the status bar, and the present value is displayed on the right side.

Epoch is accepted from iteration 0 to 1000. It means the weights consecutively changed for 1000 times based on the Levenberg-Marquardt function, and the training procedure was done. If the iteration number reaches 1000, the procedure stops (here it stopped at 24). There was no limit for time (but it could be set for training to stop after 30 seconds for example).

The performance rate was 3.08 at the beginning. If this rate reaches 0, the error would be acceptable. Finally, the error rate reached 0.00403.

Gradient is the error function and it means the value of derivatives. The range for this variable starts from 9.77, and would be acceptable if it reaches 1.00e-05. Finally, it reached

0.00171. Mu is one of the Levenberg-Marquardt algorithm parameters. Validation check is the maximum number of times that network failure can be tolerated.

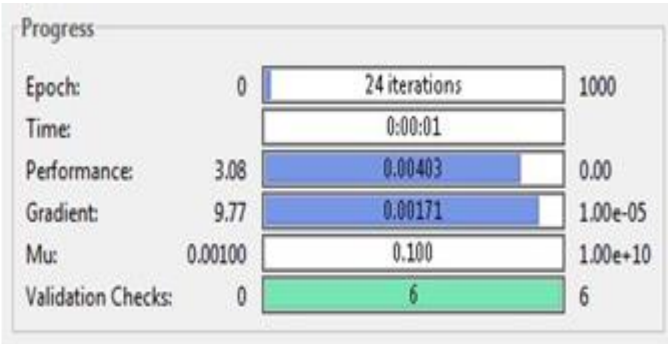

Figure 6. Graph of Water and ethanol dehydration progress by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The performance graph shows the number of phases based on the errors. As shown in Figure 7, the network performance for Train, Validation, and Test has decreased to an acceptable level. Phase 18 that is marked with a circle was the best validation performance; i.e. there were fewer errors before the circle, and excessive training phase started after the circle.

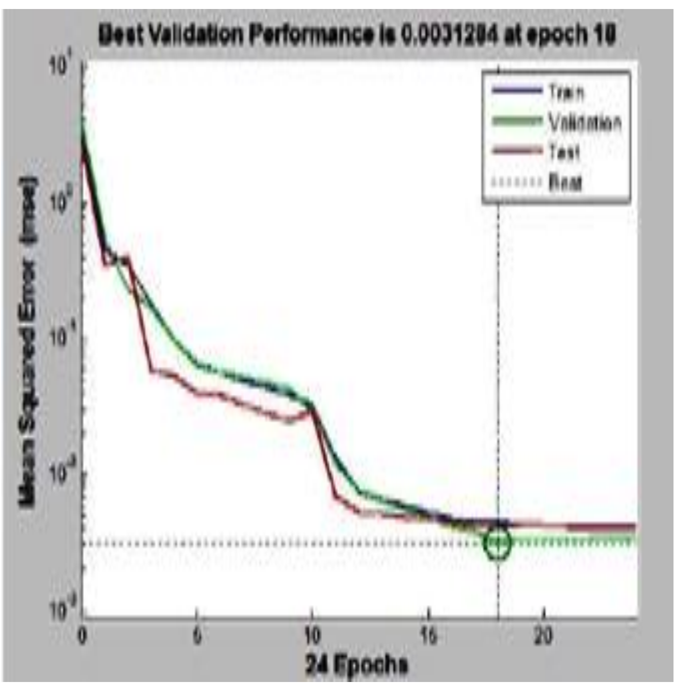

Figure 7. The water- ethanol dehydration performance by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The training state graph shows different status in training phase. The first graph is for gradient error function. The second is for Mu, and the third is for validation fail. Regarding the fact that the third graph reached 6 in the vertical axis and stopped, it shows failure. Moreover, the validation fail graph shows that the system has been stable for 18 times, and failed 6 times afterward; consequently, excessive training happened for it.

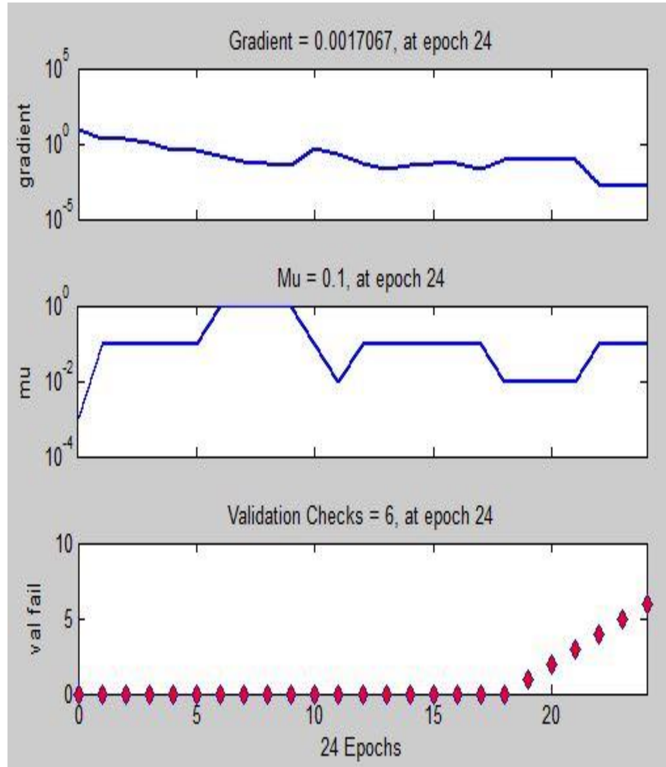

Figure 8. State training graph for water- ethanol dehydration by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The regression graph demonstrates regression separately. The horizontal axis displays the outputs of the target parameters (in fact, what to be achieved). The vertical axis displays the ANN output. As a result, the graph is drawn based on these two parameters. If the ANN would be able to model exactly, the graph should be placed the $Y = T$ line (a line with a slope of 1 that passes the origin of coordinates). In order to statistically calculate the best line with the lowest error, the linear equation achieved in all graph must be used:

$$Output = 0.99 \times Target + 0.13$$

The result would be better if the value of F will be closer to 1. This shows the fitting desirability, i.e. there is a low difference between the target outputs and the ANN outputs in the modeling. In general, the regression coefficient for all the data was calculated to be 0.99871 that is considered a very good result.

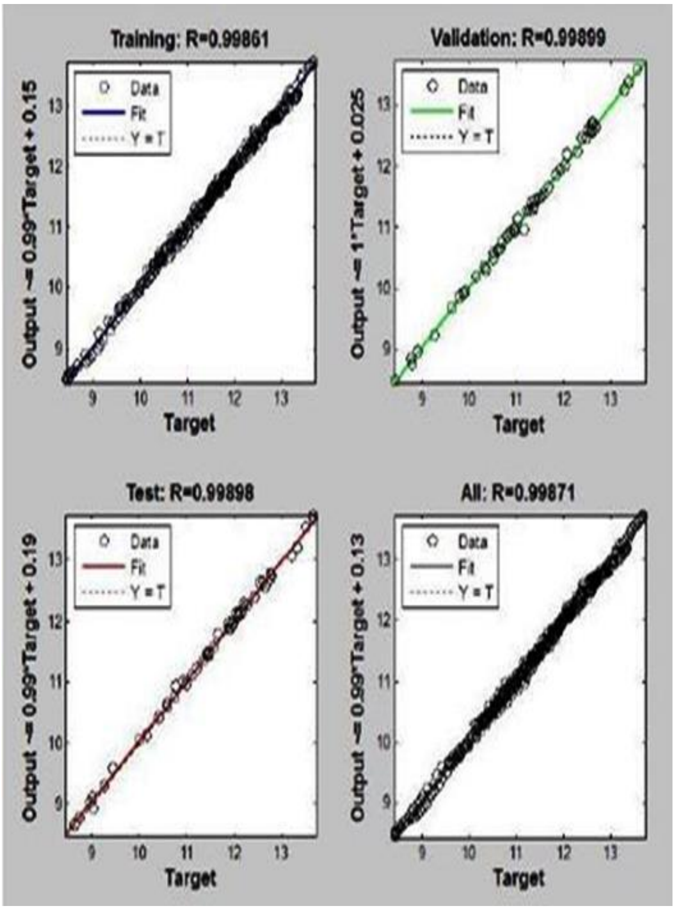

Figure 9. Regression graph for water-ethanol dehydration by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

Figure 10 displays the water- ethanol figure graph for Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride. According to this figure, with increase of temperature and decrease of volumetric flow rate in ethanol dehydration, the separation factor increases in the beginning, and decreases afterward.

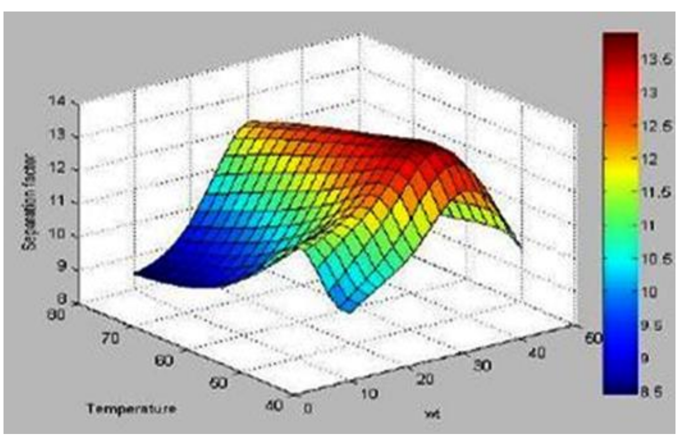

Figure 10. Figure graph for Water- ethanol dehydration by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The graph for calculation of error percentage of real output and modeling output is as below. Using the related formula, the error percentage of the real data and modeling data can be achieved. The lower percentage of error would be more desirable. As an example, a number of accidental cases of data were selected, and their error percentage were calculated. A comparison between the separation factor of the real values and the modeling values was conducted then. The results of the comparison revealed that there was a little difference between the real data and the modeling data. As a result, the modeling has been successful.

As shown in Figure 11, with increase of temperature and decrease of volumetric flow rate, the separation factor increases first, and decreases afterward. The cause of this phenomenon is that the propulsion increases with the increase of temperature at first. However, as the temperature continuously raises, the difference between the water- athanol solubility and diffusion rate decreases, and the separation factor declines accordingly.

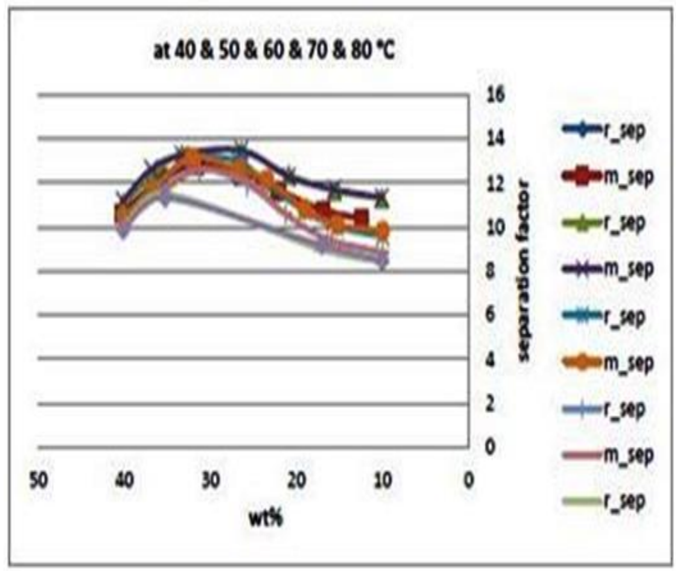

Figure 11. A comparison between the error percentage of real separation factor and the modeling separation factor for water and ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The output of overall flux in water- ethanol dehydration through ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride, with 326 data is as follows.

In the performance graph, the best validation performance was in the twenty-first repetition, and the excessive learning started afterward.

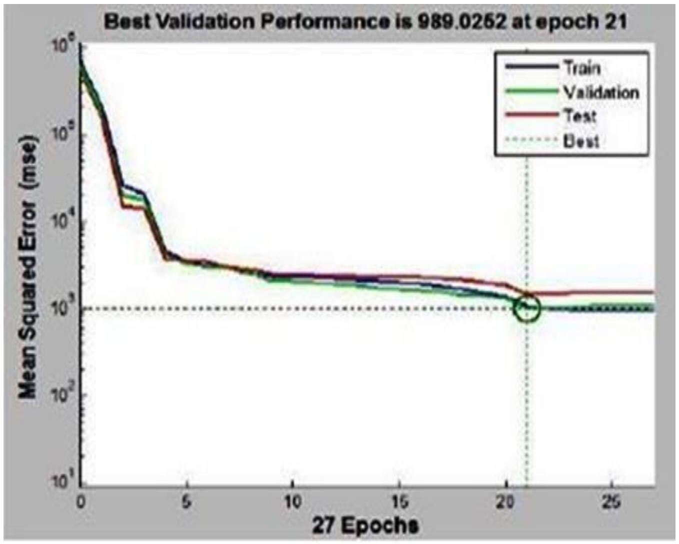

Figure 12. Performance graph for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

Figure 13 displays the regression graph. As depicted in ALL graph, the best line with the lowest error would be as follows

$$Output = 0.99 \times Target + 92$$

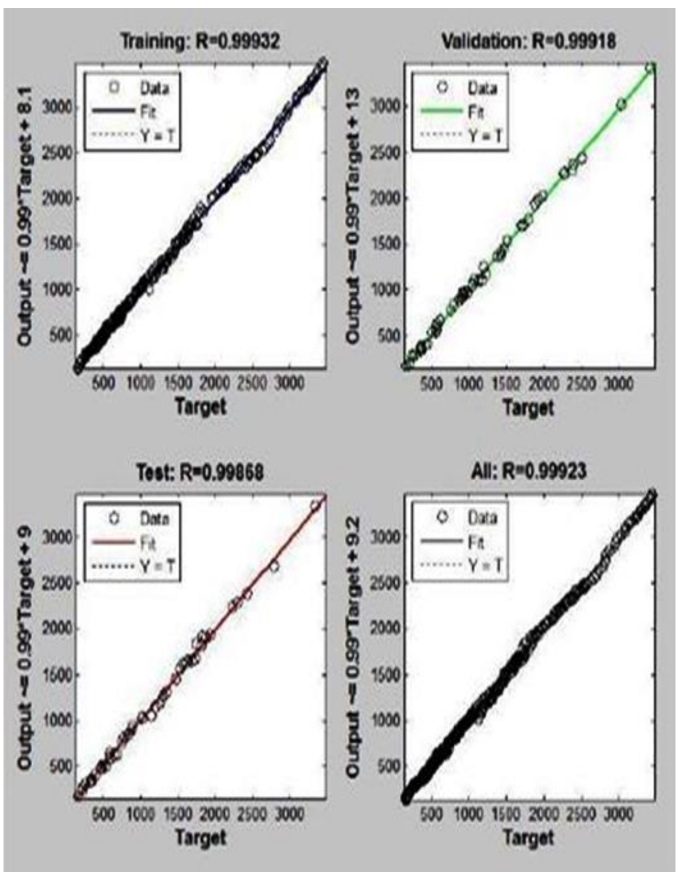

Figure 13. Regression graph for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

As shown in the figure below, with the increase of temperature and volumetric flow rate in dehydration of ethanol, the total flux increases. With the increase of temperature, the driving force of mass transfer and the saturated vapor pressure of useful compounds while penetration in membrane increases, and the flux increases accordingly.

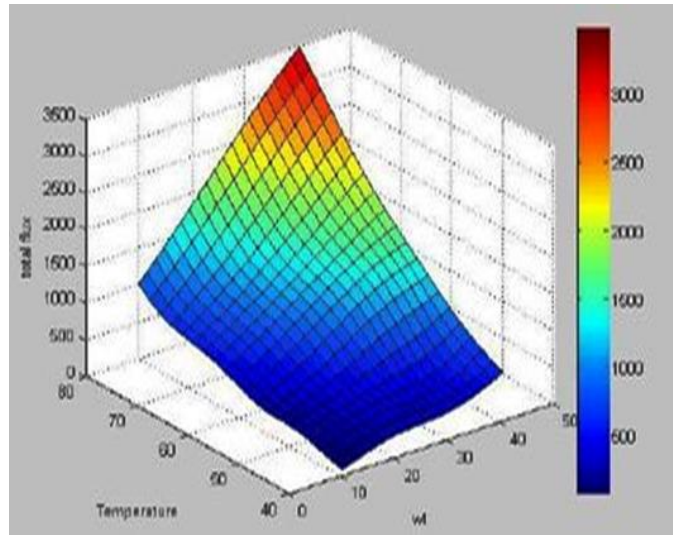

Figure 14. Figure graph for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The figure below displays a comparison between the error percentage of the real outputs and the modeling outputs. According to this figure, with increase of temperature and volumetric flow rate in water- ethanol dehydration, the overall flux increases.

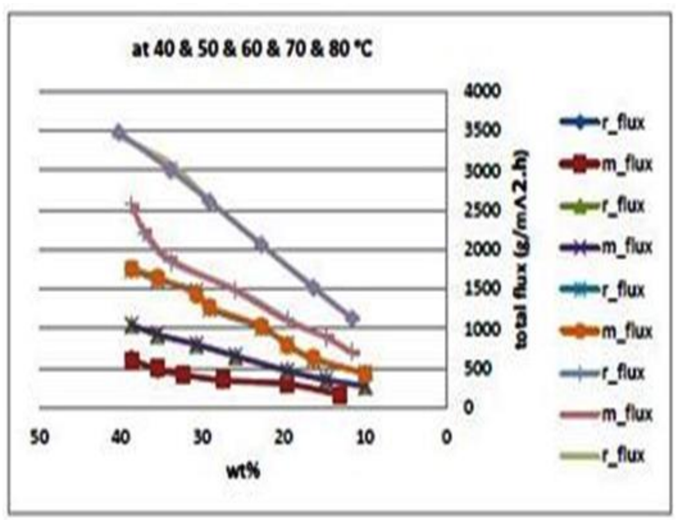

Figure 15. Comparison of error percentage for overall flux in reality and modeling for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

91 data were used for dehydration of acetone, and

Polyacrylonitrile and polyethylene glycol membranes were utilized. The results for separation factor are as below [10-13]:
The best validation performance in performance graph was in the twenty-seventh repetition.
The regression coefficient for all the data in regression graph was equal to 0.99946 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, with increase of temperature and volumetric flow rate in dehydration of acetone, the separation factor decreases. This phenomenon can be justified in this manner: continuous increase of the feed temperature decreases the water-acetone penetration and solubility difference, and decreases the separation factors of acetone accordingly.

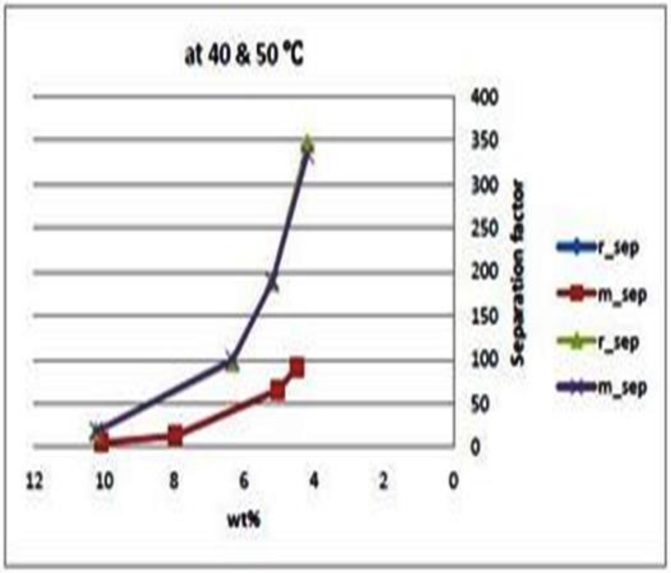

Figure 16. Comparison of the error percentage for real separation factor and modeling in water-acetone dehydration by Polyacrylonitrile and polyethylene glycol membranes

The results of overall flux output in dehydration of acetone by Polyacrylonitrile and polyethylene glycol membranes are as follows:
The best validation performance in the performance graph was in the seventeenth repetition.
The regression coefficient for all data in the regression graph was calculated to be 0.99909 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 increase of temperature and volumetric flow rate in dehydration of acetone, the overall flux increases. This phenomenon can be justified in this manner: with increase of temperature, the driving force of mass transfer and the saturated vapor pressure of useful compounds while penetration in membrane increases, and the flux increases accordingly.

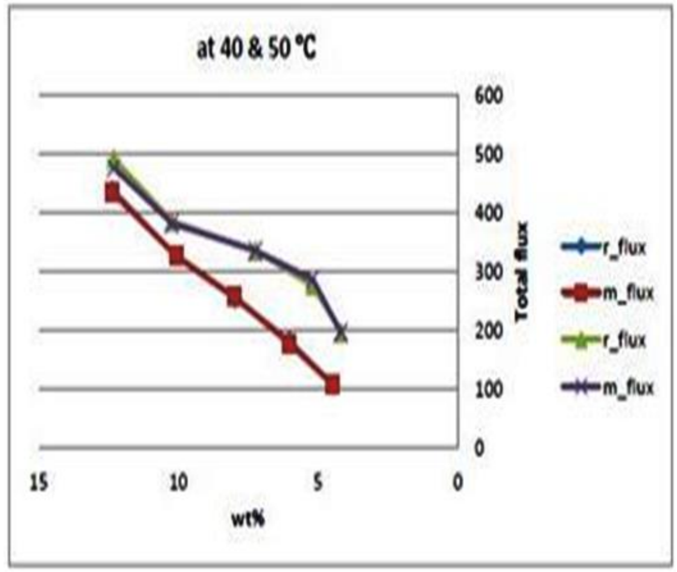

Figure 17. Comparison of error percentage for overall flux in reality and in modeling of acetone dehydration by Polyacrylonitrile and polyethylene glycol membranes

302 data objects were used for modeling butanol dehydration, and polydimethylsiloxane membrane was used. The results of the modeled separation factor are as follows [11-16]:
In the performance graph, the best validation performance was in the 151 repetition. The regression coefficient for all the data was 0.9922 that was a good result. In the error percentage graph for the real outputs and modeling outputs of the butanol dehydration, it was observed that with increase of temperature and decrease of volumetric flow rate, the separation factor increased at the beginning and decreased afterward.

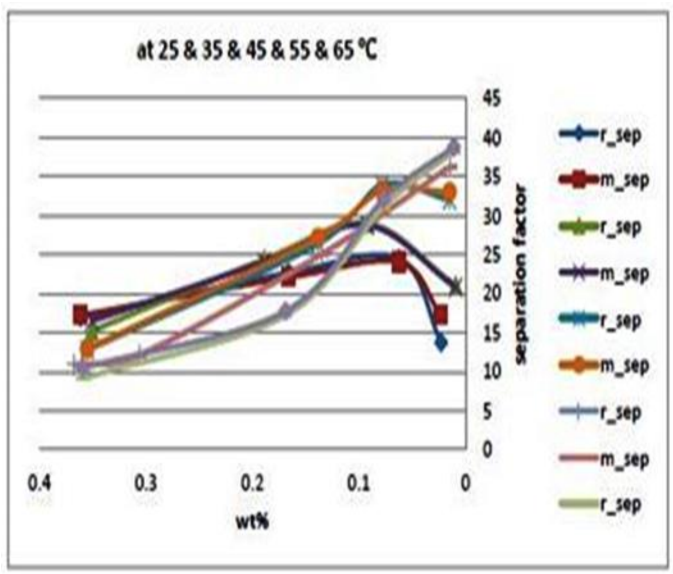

Figure 18. Comparison of the error percentage of real separation factor and modeled separation factor for buthanol dehydration by polydimethylsiloxane membrane

The results for the dehydration of butanol by means of polydimethylsiloxane membrane with 302 data objects, the results for flux output are as follows:
The best validation performance in the performance graph was in the 202 repetition.
The regression coefficient for all the data in regression graph was 0.9998 that was a very good result. In the error percentage graph for the real outputs and modeling outputs of the butanol dehydration, it was observed that with increase of temperature and increase of volumetric flow rate, the overall flux increased.

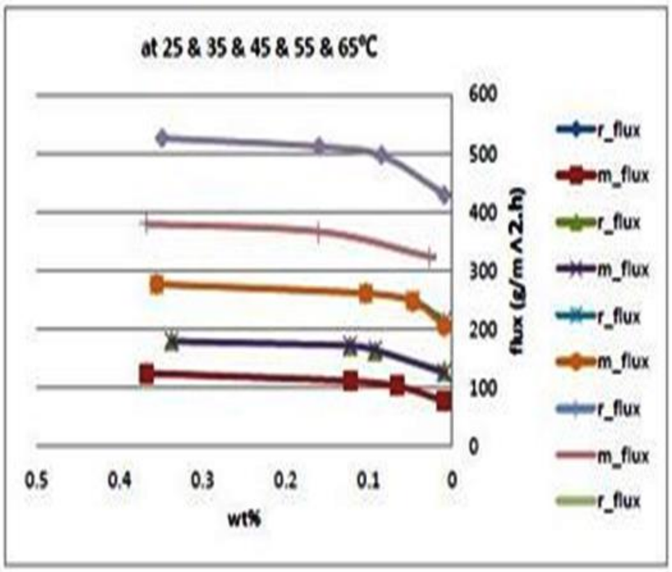

Figure 19. Comparison of the overall flux error percentage for real and modeled dehydration of butanol by polydimethylsiloxane membrane

3. Conclusion

In this study, dehydration of water-ethanol, water- acetone, and water butanol by use of pervaporation process was modeled in ANN. The polymer membranes Polydimethylsiloxane, Polyvinylidene fluoride, Polyacrylonitrile, and Polyethylene glycol are hydrophilic membranes, and are appropriate for separation of low amounts of water in alcohols. Moreover, the ANN in this study reflected the error suitably.

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