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ORIGINAL ARTICLE

Modeling of dehydration of acetic acid with the help of artificial neural network

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Abstract

In this research, dehydration of acetic acid in the range of 0-100 concentration using Polyimide membrane in the Pervaporation process was studied. The membranes used included Nation membrane and poly (acrylonitrile-co-acrylic acid) [PAC] membranes. Separation of water and acetic acid was performed using these membranes. In this study and in the evaluation of membranes, we used various parameters such as the permeate flux of the product and also the separation factor. In this study, Artificial Neural Network (ANN) was used to evaluate the separation of acetic acid water feed in polymer membranes. The Pervaporation process is able to solve the azeotropic problems in some liquid mixtures such as acetic acid and water. In this study, the experimental data obtained in the separation of acetic acid and water with the help of polymer membranes in the pervaporation process were compared with the data obtained from neural network modeling. Modeling was performed by multi layers perceptron (MLP) neural network feed forward. In this method of Propagation learning algorithm and Levenberg-Marquardt function include of one output and 2 inputs were implemented. The error percentage diagrams for the actual values of the flux output were compared with the values obtained from modeling through polymer membranes to evaluate the efficiency of the pervaporation process in the separation of acetic acid from water. The permeation fluxes of individual components in acetic acid -water mixture through polymeric membranes have been calculated and showed to be in agreement with the experimental values.

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1. Introduction

The Pervaporation (PV) process has the ability to separate different compounds from each other in different liquid mixtures. The separation process in these mixtures can involve the separation of water from a water-organic mixture or the separation of an organic compound from water. This separation can also be done in an organic-organic mixture. This separation takes place after the feed hits a membrane. Across the membrane, the chemical potential gradient works as the driving force for the mass transport of the materials. Also, the use of an ineffective purifier or vacuum pump (typically steam or air) that should be seeped in the side will help maintain proper penetration vapor pressure.

Usually the downstream pressure of the membrane should be less than the feed vapor pressure. After the separation process, the permeated product (permeate) can be taken downstream of the membrane (Fig. 1). This mechanism is not dependent on the relative volatility of components [1- 5].

An efficient membrane requires a suitable membrane material that can enhance performance efficiency in PV performance. Since the minor feed components consume the latent heat,

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therefore PV techniques reduce energy during the process.
The second feature in general is that the best technology for separating liquids is provided by the pervaporation process. In addition, the pervaporation process also provides unparalleled benefits in separating heat-sensitive, azeotropic, and near-boiling compounds [6-8].

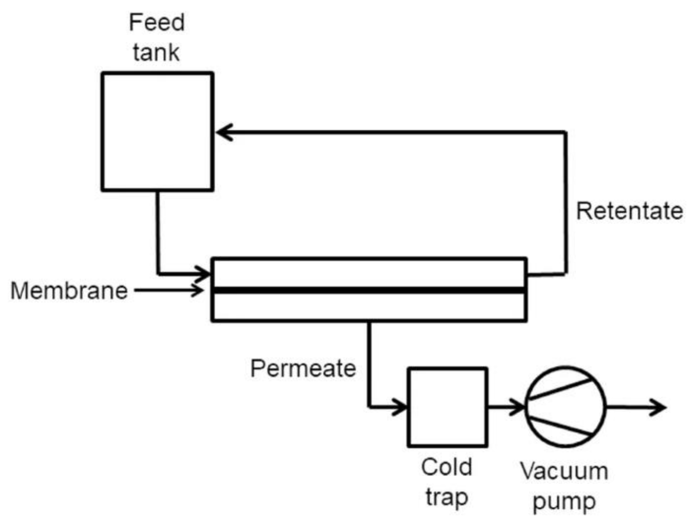

Figure 1: Simplified diagram of pervaporation process

This feature is due to the fact that this process has mild operating conditions, no pollution to the environment and the absence of different species in the feed. Most membrane materials and compounds used in PV processes can be used on a laboratory scale, but if they need to be used on an industrial scale, they must be modified according to application. Thus, there is a need to survey more membrane materials possibilities which is important in order to overcome drawbacks in current membranes.
Most of the membrane materials used in PV techniques is usable in laboratory scale, but not in industrial applications. Thus, there is a need to survey more membrane materials possibilities which is important in order to overcome drawbacks in current membranes.
Dehydration due to the pervaporation of organic acids and bases is important because most of these compounds form azeotropes or create an exertion on the vapor-liquid equilibrium curve. Acetic acid is one of the 20 main organic intermediates used in the chemical industry and in the preparation of several important intermediates such as vinyl acetate, acetic acid itself, phthalic anhydride, acetic anhydride, etc., it is mixed with water. Also, the separation of acetic acid and water using the normal binary distillation process is particularly difficult due to the relative oscillation, especially for acetic acid concentration values. As an alternative candidate, pervaporation dehydration is energy saving and economically more viable [9-16].
There is a need for membrane materials that offer good selectivity and high flux for a wide range of industrially important separations. In general, mechanical separation processes for separating gaseous or liquid streams use membrane technology [20-28]. One of the best technologies for the separation and purification of acetic acid -water is the pervaporation process. Various diagrams in which the amount of leaked products is presented in the experimental data with the data obtained from the ANN simulation for the separation of acetic acid -water feed using by Polyimide membrane, Nation membrane and poly (acrylonitrile-co-acrylic acid) [PAC] membranes by the Pervaporation process.

2. Theory

2.1 Artificial Neural Network (ANN)

The artificial neural networks used are a kind of computational model that is inspired by the human brain. Many advances in artificial intelligence in recent years have been made using artificial neural networks, including voice recognition, image recognition, and robotics. It should be noted that artificial neural networks can be explained as biologically inspired simulations performed to perform specific tasks such as clustering, classification, and pattern recognition. It can be said that artificial neural networks are a biologically inspired network of artificial neurons that have been specially adjusted to be able to use it to do certain things.
It should be noted that the term "nervous" originates from the basic unit of human (animal) neuronal function, the "neuron", or that nerve cells in the brain and other parts of the human (animal) body.
A neural network is a group of algorithms that confirm a fundamental relationship in a similar set of data to the human brain. The neural network can help change the input so that the network can get the best results without redesigning the output method. Here, in Fig. 2, we can see the biological cell as well as the structure of a neuron.

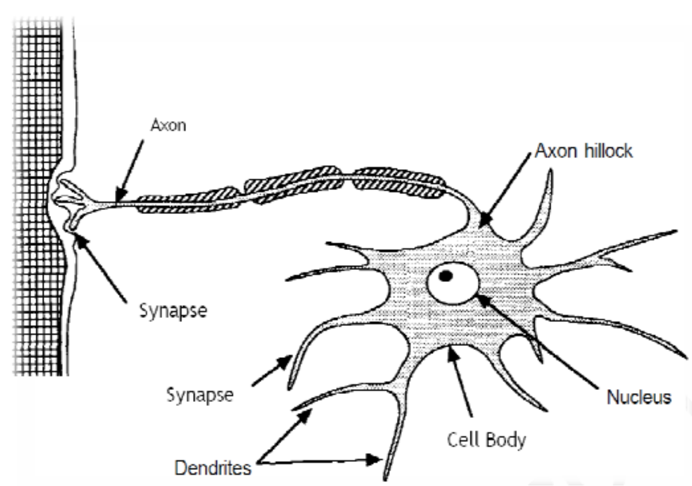

Figure 2. Major parts of a biological cell

We have to consider that an artificial nerve cell is like a mathematical equation in which the symbol p can be defined here as a signal from the input. After amplifying or attenuating as much as the parameter w (mathematically called the weight

parameter), an electrical signal with a value of p_w will enters the neuron. For a simpler mathematical equation, it is assumed that the input signal here is added to another signal with a value of b in the nucluous. Before leaving the cell, the final signal with a value of p_{w+b} undergoes another process that is technically called "Transfer function".
This action is shown as a box in Fig. 3 with f written on it. Here the input of this box is the P_{w+b} signal and the output is represented by a mathematical method. Mathematically, we will have $a = f(pw + b)$

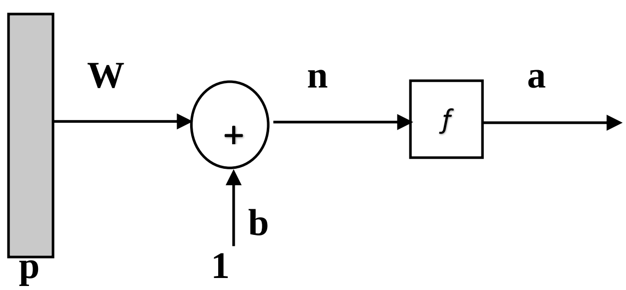

Figure 3. Mathematical model of a neuron

Placing a large number of the above cells creates a large neural network. So it can be said that collecting a large number of the above cells creates a large neural network. It can be concluded that the network developer must assign large values to the parameters w and b. Therefore, this process that was introduced is called the learning process.
In addition, populations of neurons at different layers can be used to increase system efficiency.
It can be said that in the structure of these neural networks, in some cases it is necessary to place a number of neural cells in one layer. In addition, populations of neurons at different layers can be used to increase system efficiency. Therefore, in these conditions, it can be said that the network will be designed with a certain number of inputs and outputs. However, the difference is that there is more than one layer (instead of just one layer).
Therefore, it should be said that (multilayer network), here the input layer is the layer through which the inputs are given to the system, it should also be said that the output layer is the layer in which the desired results are presented and also the other layer Are called hidden layers. Fig. 4 shows a three-layer neural network. Includes input layer, output layer and hidden layer (which in this form is only one layer). We can increase network capabilities by changing the number of hidden layers and the number of nerve cells in each layer.

2.2 Modeling of pervaporation process by use of Neural Network

Here and in this research, it should be noted that the effect of ANN input parameters (operating conditions) on the separation efficiency of acetic acid and water.
Here an ANN is designed for conversion parameter analysis. And Feed-forward multilayer here an ANN is designed for conversion parameter analysis. And Feed-forward multilayer perceptron ANN with Levenberg-Marquardt function include of two inputs and two outputs were used.

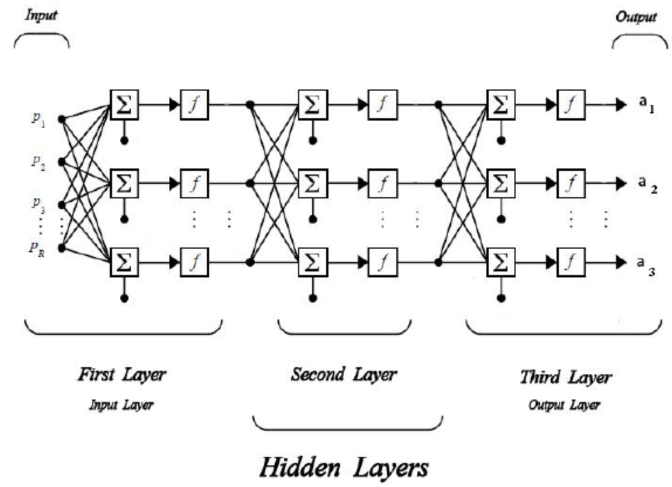

Figure 4. A schematic view of neural network and its constituent layers

In this modeling, the Tansig transfer function was used for the hidden layer and Purelin was used for the output layer Also, five neurons were identified here for the hidden layer after the data processing was done, here 70% of the data was allocated for learning and the remaining 30% for testing. In this research; Matlab version R2014b was used.

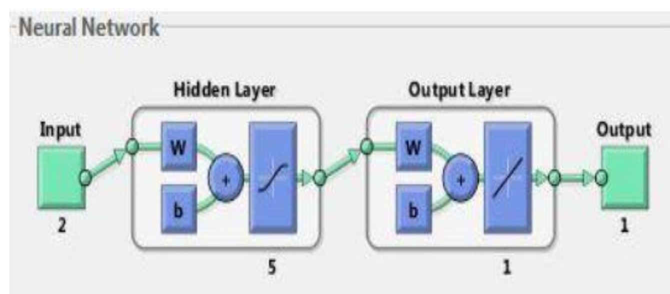

Figure 5. A schematic view of the ANN

Fig. 5 shows a schematic view of a two-layer ANN that, as can be seen, has only one hidden layer and output. Inputs are multiplied by a value of w, and there is a bias factor (b) that is added to the input (bias is a constant value that is added to the input to increase accuracy).
This enclosure randomly defines Train, Validation, and Test data, so that there are instances from anywhere in the environment. The Levenberg-Marquardt function was used in the training phase. Mean square error (MSE) functions are used to measure performance. It is also noted that the default settings for the derivative issue were used here.
It should also be noted that here Epoch is accepted in the range of 0 to 1000 repetitions. This means that continuous weights are changed 1000 times based on Levenberg-Marquardt performance and the training method is performed.

If the number of repetitions reaches 1000, the method stops. There was no time limit (but it could be set for practice to stop after, say, 30 seconds).
Valid check is the maximum number of times it can withstand network failure.

3. Pervaporation experiment

Water- acetic acid separation tests were carried out using evaporative seepage process. These experiments were performed with Nation membrane, Polyimide membrane and poly (acrylonitrile-co-acrylic acid) [PAC] membranes using a laboratory pervaporation system. It should also be noted that different operating conditions such as feed concentration were evaluated in these experiments [29]. The poly (acrylonitrile-co-acrylic acid) [PAC] membranes were three sample PAC-1 (Membrane density was equal 211 (kg/m ^{3})), PAC-2 (Membrane density was equal 415 (kg/m ^{3})) and PAC-3 (Membrane density was equal 658.35 (kg/m ^{3})).
Experimental results as well as predictions of neural network modeling are discussed below.

4. Comparison of neural network modeling results and experimental data

4.1 Effect of feed concentration on flux and selectivity (Polyimide membrane)

Fig. 6, 7 shows the change in water flux and selection with the oral water concentrations for the polyamide membrane at 30° C. Obviously, as the water content in the feed increases, the flux increases and the selectivity decreases.
It can be said that as it is clear from the diagrams, here the neural network model has been able to predict the laboratory results well and accurately

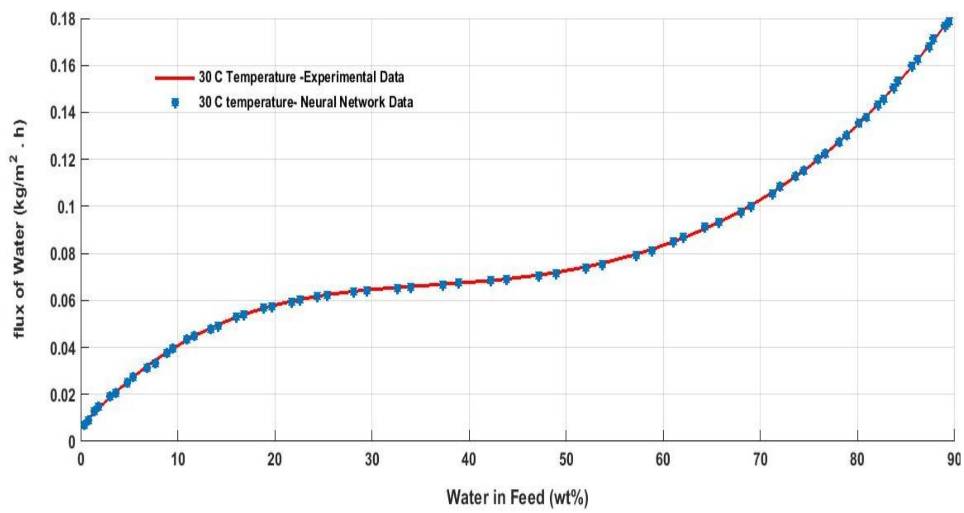

Figure 6: Variation of flux of water with feed concentration of water in polyimide membrane at 30°C (Experimental Data and Network Model Data)

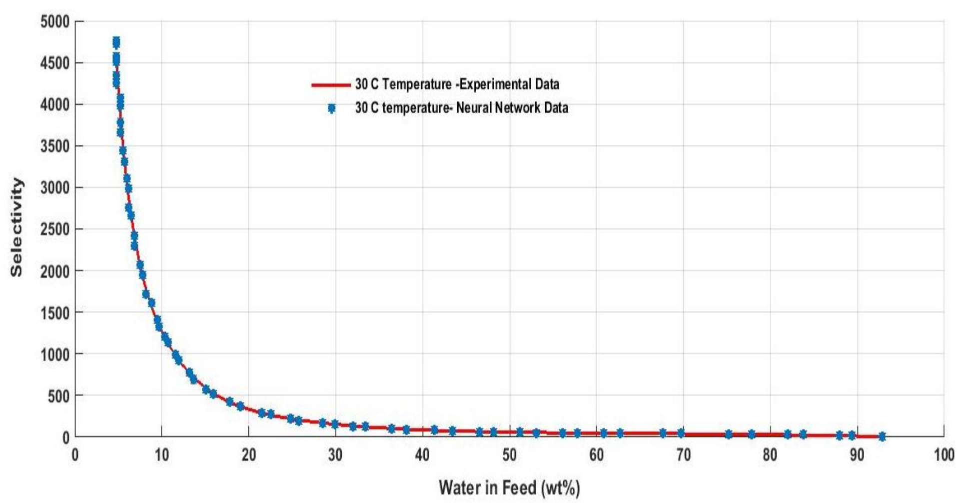

Figure 7: Variation of selectivity of water with feed concentration of water in polyimide membrane at 30°C Polyimide (Experimental Data and Network Model Data)

4.2 Effect of feed concentration on flux and selectivity (Nation membrane)

Figs. 8 and 9 show the variation of water flux and selectivity with feed concentrations of water for Nation membrane at 30°C. It is evident that flux increases and selectivity decreases with increasing water content in the feed. This may be due to plasticization of the membrane by water at low acetic acid content in the feed. As can be seen from the graphs, the neural network model has been able to predict the experimental results well and accurately.

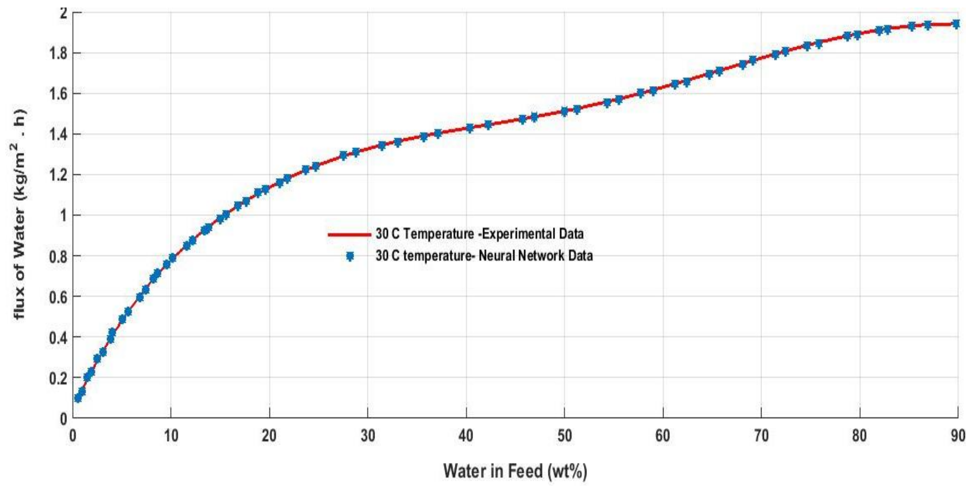

Figure 8: Variation of flux of water with feed concentration of water in Nation membrane at 30°C (Experimental Data and Network Model Data)

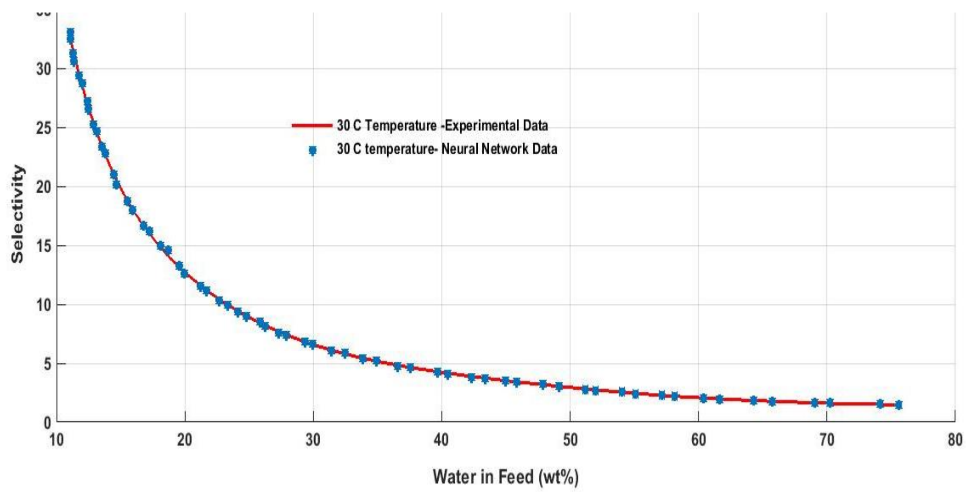

Figure 9: Variation of selectivity of water with feed concentration of water in Nation membrane at 30°C Polyimide (Experimental Data and Network Model Data)

4.3 Effect of feed concentration on flux and selectivity (Acrylonitrile copolymer membranes)

Figs. 10-13 show results of pervaporation through the PAC copolymer membranes. As can be seen, with increasing water concentration in the feed, the water flux increases, while the selectivity decreases. This may again be attributed to plasticization of these membranes at high water content in the feed. From Figs. 10-13, it can be observed that quite predictably in PAC membrane, with increase in density from PAC-1 to PAC-3, water flux increases and selectivity drops. The water fluxes from the above membranes show the following trend:

Nation > PAC > Polyimide

Therefore, as can be seen in Figures 10-13, it can be said that with increasing water concentration in the feed, the amount of water flux in the product initially increases and also the amount of selectivity decreases. These results are similar for different membranes. Also, as can be seen from the figure, the neural network model was able to predict the experimental results well. The three-dimensional figures of the neural network data show the effect of water concentration in the feed on the leached water flux in the product and selectivity were shown in Fig. 11-13.

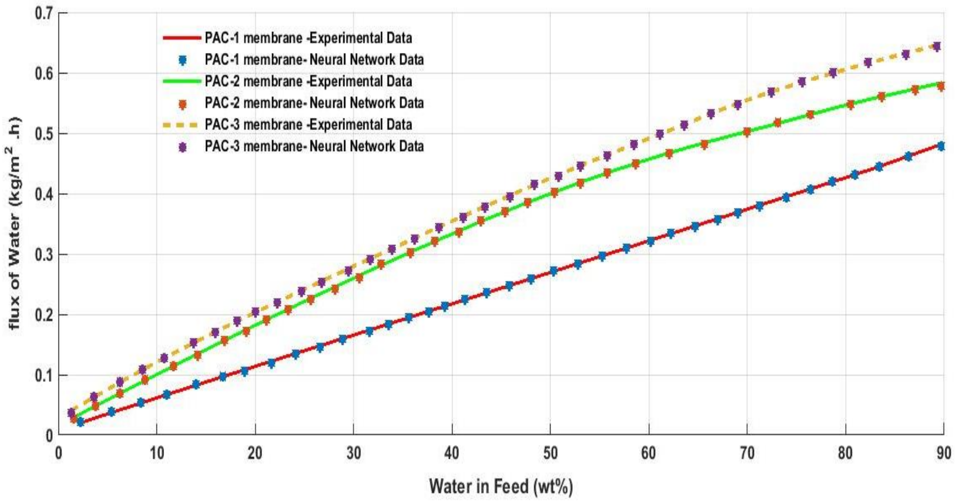

Figure 10: Effect of water in feed concentration on water Flux (Experimental Data and Network Model Data)

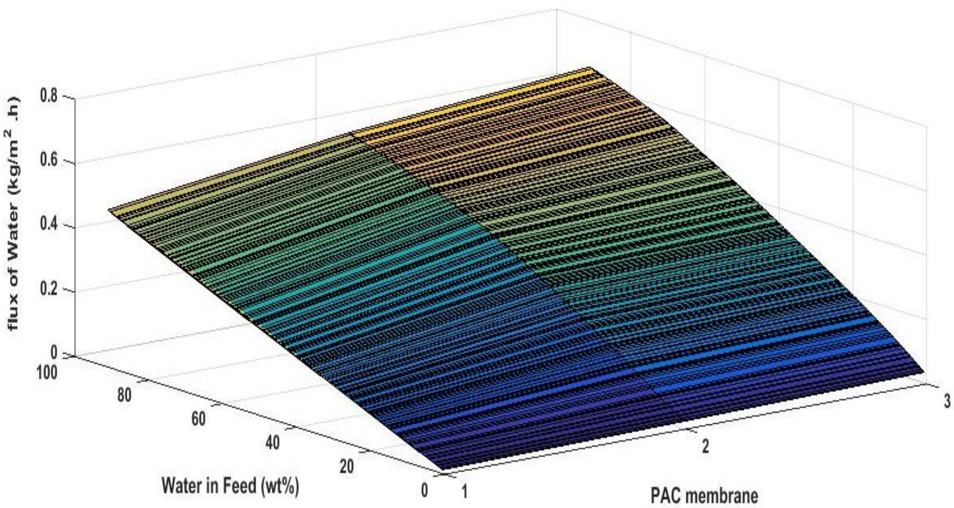

Figure 11: Network Model Prediction for Effect of water concentration in feed on water Flux

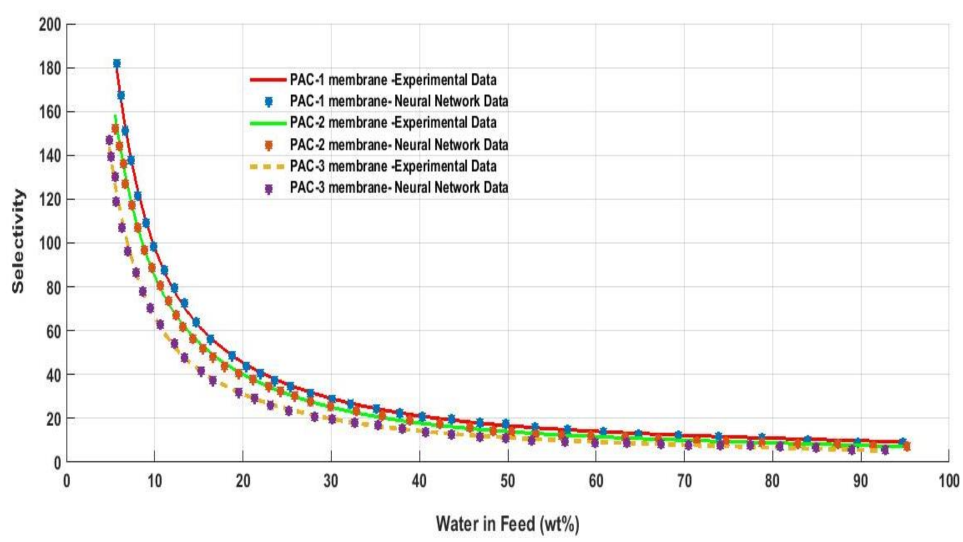

Figure 12: Effect of water in feed concentration on Selectivity (Experimental Data and Network Model Data)

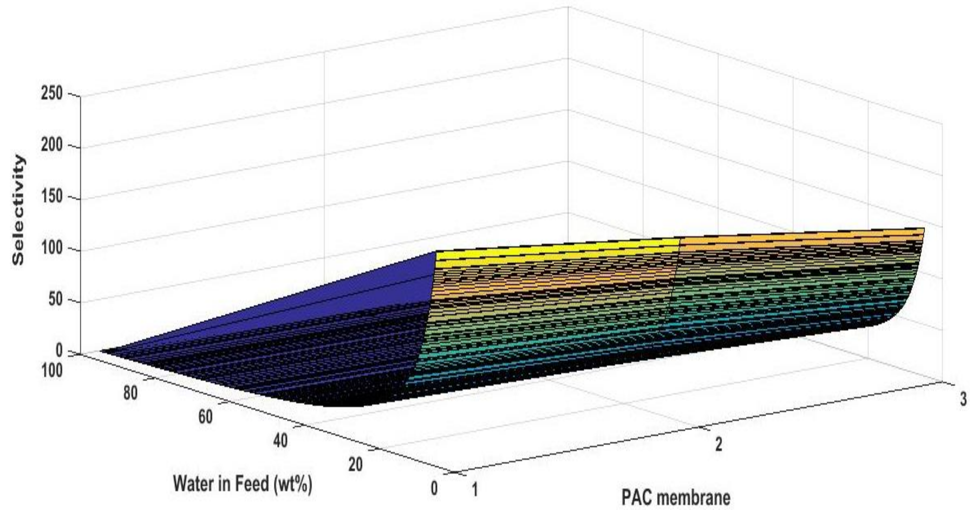

Figure 13: Network Model Prediction for Effect of water concentration in feed on Selectivity

5. Conclusions

In this study, it can be concluded that the results of the neural network model can be used to predict the performance of polymer membranes in the seepage process for the separation of acetic acid water solutions.

It should also be noted that changes in process conditions as well as experimental results are well predictable by the neural network model. On the other hand, the results obtained from neural network modeling showed that this model has the lowest error rate in predicting experimental results.

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