Modeling Dehydration of Acetone by Use of Polyacrylonitrile Membrane and Polyethylene Glycol with the Help of Artificial Neural Network

Mansoor Kazemimoghdam1* and Zahra Amiri2

1Department of Chemical Engineering, Malek-Ashtar University of Technology, Tehran, IRAN; 2Department of Chemical Engineering, South Tehran Branch, Islamic Azad University, Tehran, IRAN

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ABSTRACT

The authors of this research analyzed the amount of water-acetone separation in the pervaporation process by means of polyacrylonitrile membranes and polyethylene glycol with the help of artificial neural network. The pervaporation process can be applied for separation of many liquids (separation of acetone from water in this research). Due to azeotropic with water, acetone has purity problems. The amounts achieved from the experimental data were compared to the modeling data, and the results were analyzed. 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 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 purely 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 polyacrylonitrile membranes and polyethylene glycol for evaluating the efficiency of pervaporation process in the separation of acetone from the water. Finally, the graphs were drawn.

Keywords: Modeling, dehydration, acetone, polymer membrane, Artificial Neural Network

* Corresponding author: mzkazemi@gmail.com

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” (Seader and Henely, 1998). 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 repairment (Baker, 2004; Srikanth, 2008). The six major processes in membrane separation include micro-filtration, ultrafiltration, reverse osmosis, electrodialysis, gas separation, and pervaporation (in such fields as water purification, chemical and food processing, medical application, and biological separations) (Kujawski, 2000).

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 takes place in three phases of absorption, penetration, and evaporation (or disposal) (Huang, 1991). As a result, selectivity and permeation are generally based on the interaction between membrane and penetrating molecules, the size of leaking molecules, and
the empty volume of the 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 by low-pressure steam from the other side of the membrane. The product will be collected after changing into a 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 (Feng and Huang, 2004). Due to such advantages as excellent performance and high energy efficiency, this process has recently gained the 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 (Mulder, 1996).

The results of this study by use of Artificial Neural Network (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 acetone using by polyacrylonitrile polymer and polyethylene glycol polymer membrane.

2. Materials and Procedures

2.1. Artificial Neural Network

Recently, there have been a number of researches 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. Fig. 1 displays the structure of a neuron.

Dendrites, as an electric signal receiving areas, are composed of cell fibers with unsmooth surface and many split extensions. That is why they are called tree-like receiving networks. The dendrites transfer the electrical signals into the cell nucleus. The cell body provides the required energy for neuron activity that can be easily modeled through an addition and comparison with a 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 influence 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.

2.2. Mathematical equation of artificial neural cells

The artificial neural cell is a mathematical equation in which \( p \) represents an input signal (Fig. 2). 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 Fig. 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:

\[
a = f(pw + b)
\]

Fig. 2. Mathematical model of a neuron

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

Fig. 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 (Rautenbach and Albrecht, 1985).

![Fig. 3. A schematic view of neural network and its constituent layers (Rautenbach and Albrecht, 1985).](image)

3. Results and Discussion

3.1. Modeling dehydration of acetone 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 the 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 compound as acetone was selected in this research; and, Matlab version R2012a (7.14.0.739) was used. The results of the study are displayed (Fig. 4). Fig. 4 displays a schematic view of a two-layer ANN with only one hidden and an 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.

![Fig. 4. A schematic view of the ANN](image)

The following points about the algorithms (Fig. 5) 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.
- The Levenberg-Marquardt function was used in the training phase.
- The Mean Squared Error (MSE) functions for performance measurement.
- The default settings were used for derivative issue.

![Fig. 5. Algorithms compartment in ANN](image)

The number of data for modeling acetone dehydration was 91. By use of polyacrylonitrile and polyethylene glycol membrane for the output of separation factor (Zhao et al., 2008; Fouad and Feng, 2009; Zhan et al., 2009; Olukman and Sanli, 2015), the following results were achieved. 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. There was no limit for time (but it could be set for training to stop after 30 seconds for example).

The performance graph shows the number of phases based on the errors. As shown in Fig. 6, the network performance for Train, Validation, and Test has decreased to an acceptable level. Phase 27 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.

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 27 times, and failed 6 times afterward; consequently, excessive training happened to it.

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 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:

\[
\text{Output} = 0.99 \times \text{Target} + 0.13
\]

This shows the fitting desirability, i.e. there is a low difference between the target outputs and the ANN outputs in the modeling.

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. As shown in Fig. 9, with an increase in temperature and increase of volumetric flow rate, the separation factor decrease 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-ethanol solubility and diffusion rate decreases and the separation factor declines accordingly.

The output of overall flux in water-acetone dehydration through polyacrylonitrile and polyethylene glycol polymer membranes, with 91 data is as follows (Fig. 10). In the performance graph, the best validation performance was in the seventeenth repetition, and the excessive learning started afterward. Fig. 11 displays the regression graph.
As depicted in all graphs, the best line with the lowest error would be as follows.

As shown in the Fig. 12 below, with the increase of temperature and volumetric flow rate in dehydration of acetone, the total fluxes increases. With the increase in 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.

The numbers of data used for dehydration of acetone were 91 data, and polyacrylonitrile and polyethylene glycol membranes were utilized (Takegami et al., 1992; Sridhar et al., 2006; Zhao et al., 2009; Villegas et al., 2015). The results for separation factor are as below. 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 in Fig. 14 below. As reflected in this graph, with an 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.

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 0.999009 that was a very good result. The graph for calculation of the error percentage for real flux and modeling is shown in Fig. 15. It can be seen that with an increase in temperature and volumetric flow rate in dehydration of acetone, the overall flux increases. This phenomenon can be justified in this manner: with an 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.

![Fig. 15. Comparison of error percentage for overall flux in reality and in modeling of acetone dehydration by polyacrylonitrile and polyethylene glycol membranes](image)

4. Conclusion

In this study, dehydration of water-acetone by use of pervaporation process was modeled in ANN. The polymer membranes polyacrylonitrile and polyethylene glycol, hydrophilic membranes, are appropriate for separation of low amounts of water in acetone. Moreover, the ANN in this study reflected the error suitably.

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Conflict of interest: Non declare