Review Article

Desulfurization Modeling of Mixtures Using Polyether Polyethylene Glycol- Polyether Sulfone Membrane with the Help of Artificial Neural Network and COMSOL Software

Mansoor Kazemimoghadam[1*], Nastatran Sadeghi[2]

[1]Department of Chemical Engineering, Malek-Ashtar University of Technology, Tehran, Iran

[2]Department of Chemical Engineering, South Tehran Branch, Islamic Azad University, Tehran, Iran

*__Corresponding author:__ Mansoor Kazemimoghadam, Department of Chemical Engineering, Malek-Ashtar University of Technology, Tehran, Iran. Tel: +98219676620; Email:mzkazemi@gmail.com

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Abstract

The authors' aim in this study is model in desulfurization of organic compounds by use of Polyethylene glycol- polyether sulfone membrane. The modeling was done based on two completely different methods of Artificial Neural Network (ANN) and implementation of COMSOL software by use of Thiophene alkane (an organic substance), Polyethylene glycol-polyether sulfone membrane. In the modeling process by means of ANN, the error percentage of the actual values for the outputs of separation factor and the flux were calculated, and their graphs were drawn. Moreover, in the modeling process by means of COMSOL, the actual value of flux was calculated by the modeling value by the related membrane. The error percentage was calculated to be 0.013. The authors came to conclusion that the ANN solves the problems in details, but the COMSOL solves the problems in general. For example, ANN considered the temperature part by part; but, COMSOL received temperature ranges. Furthermore, the error percentage in ANN modeling was lowers the error percentage in COMSOL modeling.

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 researches 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 has 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 [1].

As 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 [2]. Moreover, existence of poisoning expensive metal catalysts used in the refineries, and deactivation of these substance while getting in contact with these harmful compounds is another reason of necessity for fuel desulfurization. Regarding the rigid regulations on fuel desulfurization [3], the researchers are trying to find solutions for desulfurization of fuels in the recent years. One of the fuel desulfurization methods that have attracted 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 economic than other common methods of desulfurization regarding the costs, consumed energy, and required equipment [4].

The Evaporation process is a notable progress in the field of solvent dehydration, dehydration of volatile organic compounds, water partial dehydration, and recently, dehydration of organic-organic solutions. Furthermore, it is approved that such method has a good efficiency in 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 pomp provides the required driving force for mass transfer of the compounds [5]. In this study, a membrane procedure will be simulated in Artificial Neural Network (ANN) and COMSOL software. 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 [6,10].

Experimental

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 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 [11]. 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) [12,14].

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, 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.
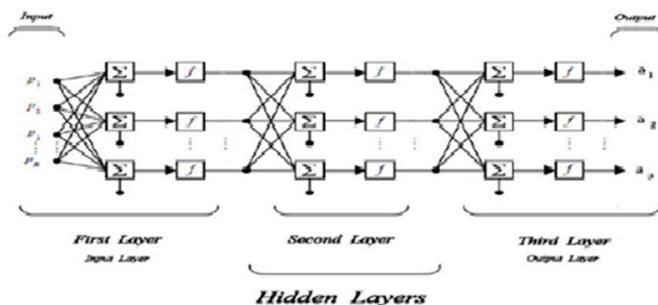

Figure 1: A schematic of ANN and its layers.

The artificial neural cell is in fact a mathematical equation in which denotes an input signal that after strengthening or weakening as much as parameter (in mathematical terminology, it is called weight parameter), it will enter the neuron as an electric signal with a size of. In order to simplify the mathematical model, it is assumed that input signal is added to another signal with the value within the neural cell nucleus. Before getting out of the cell, the result (i.e. a signal with a value of) 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 and 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 [15].

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 were usedthe neurons in the input layer of the network were defined to be 5 neurons. The results can be seen in figures below. The outputs for flux in Thiophene desulfurization by use of Polyethylene Glycol- Polyether Sulfone membrane with 100 number of outputs are as follows [16]. 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 19 that is marked with a circle shows the best validation performance. It means that system had a lower error till the circle, and the excessive training initiated afterward.
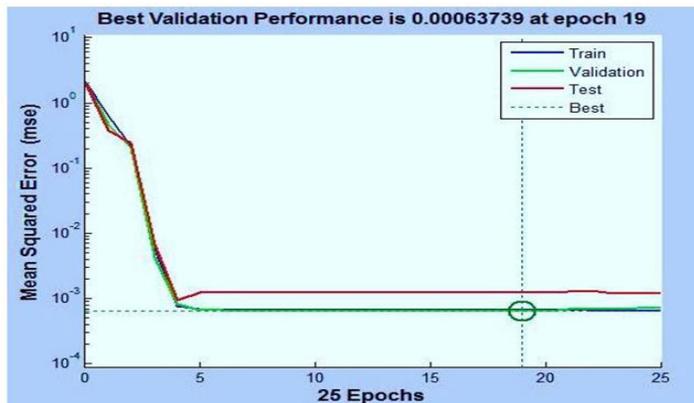
Figure 2: The performance of Alcan- Thiophene dehydration by Polyethylene Glycol- Polyether Sulfone membrane.

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 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.
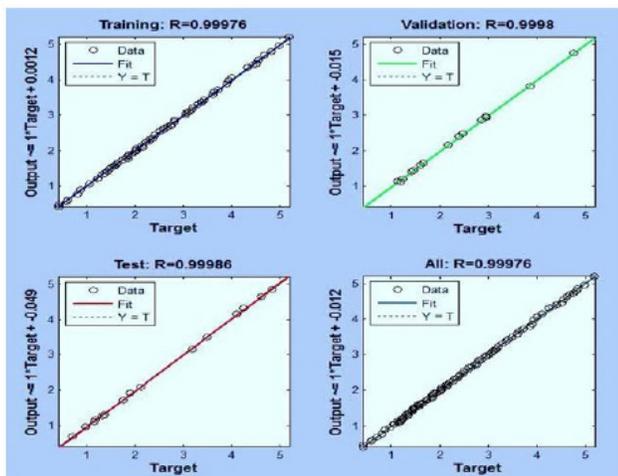

Figure 3: Regression graph for dehydration of Alcan- Thiophene dehydration by Polyethylene Glycol- Polyether Sulfone membrane.

The 3D graph of Thiophene desulfurization can be analyzed as follows:

As the pressure increases, flux decreases too. In other words, with increase of temperature and decrease of pressure, flux increases. The reason of such phenomenon can be decrease of the driving force.
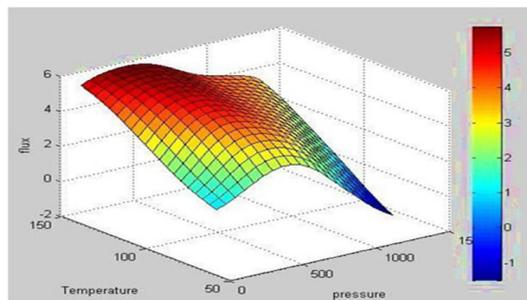

Figure 4: The flux graph for dehydration of Alcan- Thiophene dehydration By Polyethylene Glycol- Polyether Sulfone membrane.

The figure below displays a comparison of the error percentage for real output and the modeled output. As observed in (Figure 5), flux increases with the decrease of pressure. However, flux increases as the temperature increases.
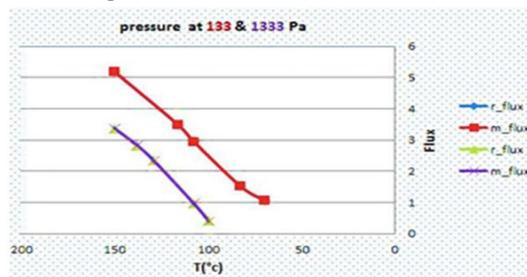

Figure 5: Comparison of the error percentage for real output and the modeled output in dehydration of Alcan-Thiophene by Polyethylene Glycol- Polyether Sulfone membrane.

For desulfurization of Thiophene by use of Polyethylene Glycol- Polyether Sulfone membrane, the output results of separation factor with 100 out   puts are as follows [16]. In the figure below, the best validation performance was achieved in the fourteenth repetition, and excessive training initiated afterward.
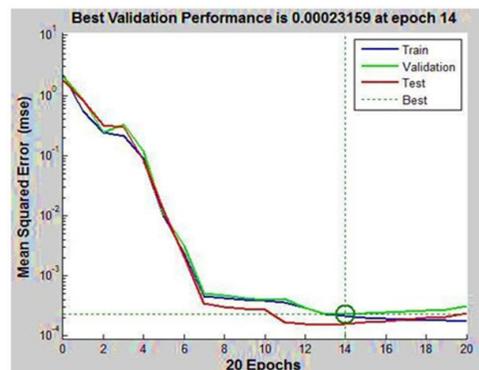

Figure 6: The performance graph for dehydration of Alcan- Thiophene by Polyethylene Glycol- Polyether Sulfone membrane.

The regression graph is depicted in figure below. As observed in the total graph, the best line with the lowest error is achieved by the equation 1.Output=1*Target+0.0084
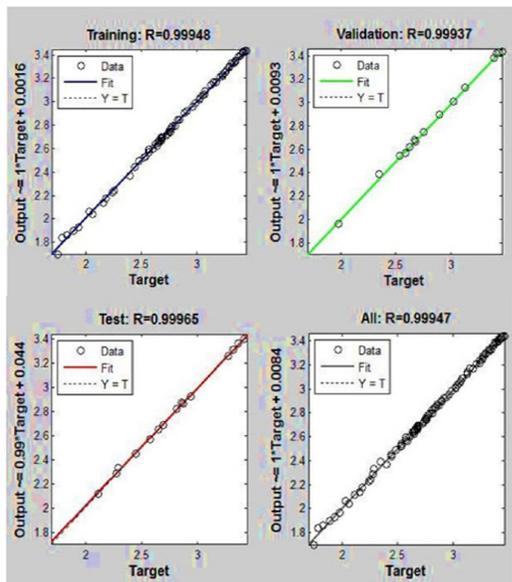
Figure 7: Regression graph for separation factor in dehydration of Alcan-Thiophene by Polyethylene Glycol- Polyether Sulfone membrane.

As analysis of the 3D graph below, it can be mentioned about the separation factor that at beginning, separation factor increases with increase of temperature, and decreases afterward. About alteration of pressure, it can be said that by increase of pressure, separation factor decreases; however, the separation factor increases at beginning, and decreased slightly afterward.
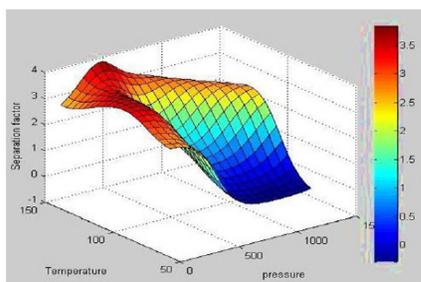

Figure 8: Separation factor 3D graph for dehydration of Alcan- Thiophene by Polyethylene Glycol- Polyether Sulfone membrane.

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 figure, in dehydration of Thiophene, flux and separation factor increase with the increase of temperature. However, increase of separation factor is little, and afterward, separation factor increases as the temperature decreases.

Multiphysics COMSOL software

Multiphysics COMSOL software is modeling software that runs all the phases in the modeling process. Different modeling phases that COMSOL is capable of phase by phase modeling are drawing geometric structure of the model, meshing model, draw-ing the major physics of model, resolving the model, and graphical presentation of the modeling results. Due to usage of default physical structures in this software, modeling in this software is done very fast. It is possible to electromagnetically analyze a vast range of mechanical structures by this software. It is also possible to define the material characteristics, source parts, and the approximate border of objects as arbitrary functions of the independent variables. Modeling dehydration of organic compounds by use of COMSOL Multiphysics software Such organic compounds as acetone, butanol, ethanol, isopropanol, and methanol were selected for this study, and the COMSOL Multiphysics version 4.2.0.150 was used for modeling. The procedure description is as follows [17]. After opening the software, select the 2D mode to enter the phase definition phase. In the phase definition section, select "Transport of Concentrated Species" (that is applicable for thick solutions) for the mass transfer mode. Forthe fluid mechanics issue, select the "laminar Flow" mode, and for the heattransfer mode, select "Heat Transfer Solids". Select the study type to be "Type Dependent". This type is applicable for solving equations that depend on time. On the setting page, for length unit select mm, and for size unit select degrees. Now, it is time for definition of geometry, draw the first rectangle as vertical, and the second rectangle as horizontal. The next step will be selection of materials. As the name suggests, water and alcohols are needed for this study. Water enters the system from the top, and alcohol enters from the bottom, Then, the materials will be mixed, and exit from the right. So, the system will have two inputs and one output. Mesh is the starting point for Finite Element Method, and its mission is partitioning geometry into smaller units with simpler shapes.
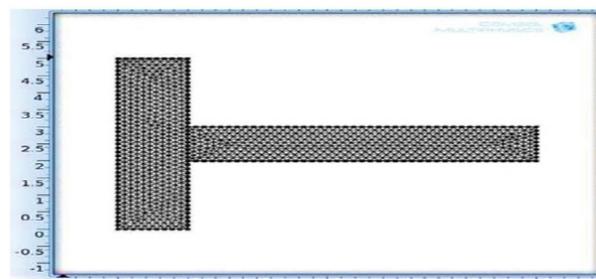

Figure 9: Meshing the membrane module in the dehydration process of Alcan- Thiophene by different membranes.

Now, it is time to draw geometry. Right click on the "Study", and click "Compute" option. On the "Results" part, you see counters that display temperature, flux, velocity, and pressure. The results for the Polyethylene Glycol and Polyether Sulfone membrane are as follows [18]. In the temperature graph, the input equals with the atmosphere temperature, and temperature gradually decreases along the membrane. The reason is that due to existence of vacuum in membrane output, condensation occurs, andaccordingly, temperature in the membrane output decreases from thermodynamic point of view, and becomes cool.
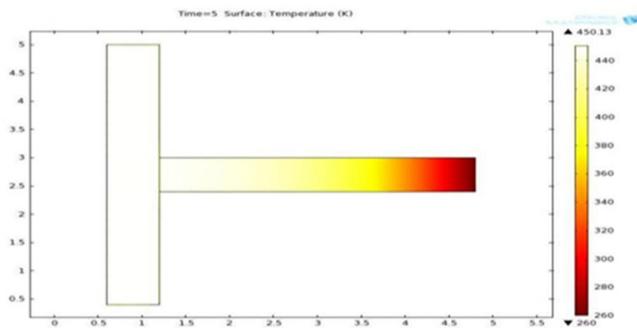
Figure 10: The temperature graph in dehydration process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane.

As there is feed in the input of the flux graph, the flux decrease is not so notable. The flux did not change in the membrane walls. However, due to increase of pressure within the membrane, flux increased. The error percentage for flux is 0.013.
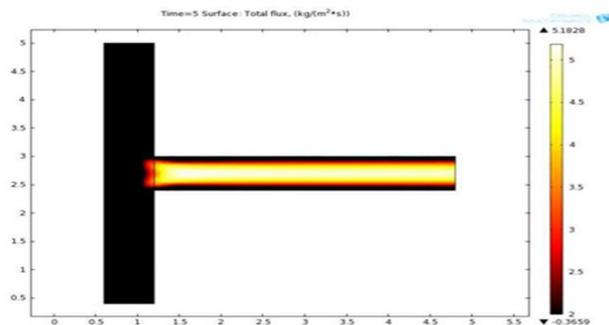

Figure 11: The flux graph in dehydration process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane it is witnessed that in velocity graph, the current velocity in the input is low, and it decreased along the wall too. However, the velocity increased within the membrane as the temperature decreased along the membrane, and sulfur concentration increased.
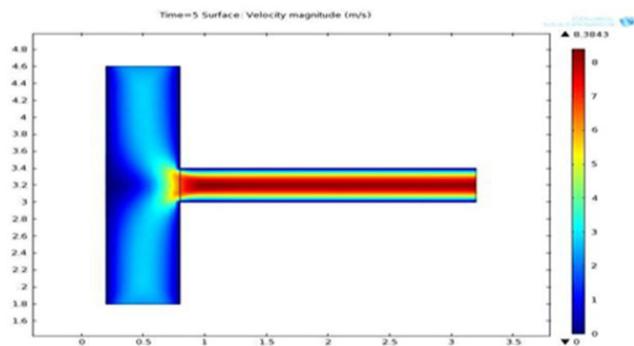

Figure 12: The velocity graph for dehydration process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane.

In the pressure graph, the pressure is equal to atmosphere pressure at the input, and it decreased along the membrane. The reason can be increase of the driving force along the membrane.
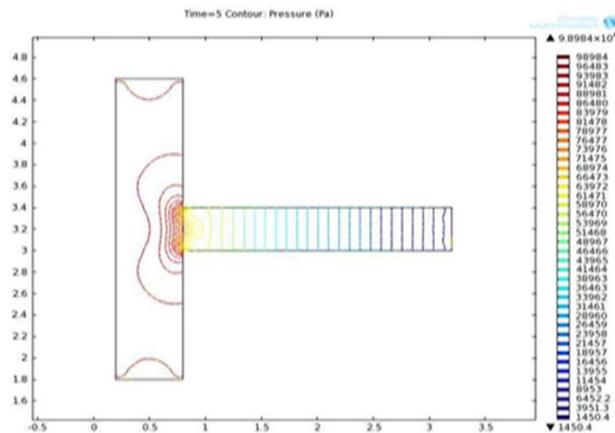

Figure 13: The pressure graph for dehydration process of Alcan- Thiophene by Polyethylene Glycol and Polyether Sulfone membrane.

Comparison of the ANN and COMSOL in desulfurization of organic compounds by polyethylene glycol- polyether sulfone glycol membrane

With regard to the error percentage, it can be concluded that both modeling results were acceptable, and the ANN had a lower error percentage than the COMSOL. As a result, ANN is more accurate, because it considers problems in more detail, but COMSOL solves the problems in general.

Achieved flux in membranes (kgm-2h-1) Modeling type	PEG-PES membrane (Ligang Lin, et al.)
ANN	5.2
COMSOL	5.1828
Real amount	5.18212
Error percentage in ANN (%)	0.34
Error percentage in COMSOL	0.013

Conclusion

The maximum amount of flux modeled by ANN, the maximum amount modeled by COMSOL, and the real amount of flux were compared in this study. The amount of error percentage in ANN was 0.34, and in COMSOL was achieved to be 0.013 that both were acceptable. Consequently, it can be concluded that the results of both modeling methods were acceptable.

Desulfurization of organic compounds by means of evaporation was modeled in ANN. It was concluded that Polyethylene Glycol- Polyether Sulfone Glycol membrane is suitable for desulfurization of organic compounds. Moreover, the ANN could reflect the error very well.Desulfurization of organic compounds by means of evaporation was modeled in COMSOL too. It was

concluded that polymer membrane used for so doing is suitable for desulfurization of organic compounds. Moreover, the COMSOL could reflect the flux error very well in this study.

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