



Scan to know paper details and
author's profile

Research of Two Different Types of Modeling on Polymer Membranes

*Mansoor Kazemimoghadam & Zahra Amiri
Malek - Ashtar University of Technology*

ABSTRACT

In this research, two different types of modeling for the decontamination process of organic compounds using polymer membranes are investigated. In this research, experimental results are analyzed using the neural network algorithm as well as the Comsol software. The researcher in this study used a Feed Forward multilayer Perceptron neural network with a back propagation algorithm and Levenberg-Marquardt function with two inputs and two outputs. The output values of Artificial Neural Network modelling were compared with the real values of pervaporation for separation of water from Ethanol and Acetone. The results revealed that the proposed model had a good performance. Moreover, the output of COMSOL software for pervaporation of five different alcohols were compared with the real values, and the error percentage of the actual amount of flux was calculated with the modeling value by means of related membranes. The results of COMSOL modeling showed that the error percentage of 3.049 achieved for dehydration process of Acetone.

Keywords: Modeling, Dehydration, Polymer membrane, COMSOL Multiphysics, Artificial Neural Network.

Classification: FOR Code: 280213

Language: English



LJP Copyright ID: 661864
ISBN 10: 153763156
ISBN 13: 978-1537631561

London Journal of Engineering Research

Volume 18 | Issue 1 | Compilation 1.0



Research of Two Different Types of Modeling on Polymer Membranes

Mansoor Kazemimoghadam^α & Zahra Amiri^σ

I. ABSTRACT

In this research, two different types of modeling for the decontamination process of organic compounds using polymer membranes are investigated. In this research, experimental results are analyzed using the neural network algorithm as well as the Comsol software. The researcher in this study used a Feed Forward multilayer Perceptron neural network with a back propagation algorithm and Levenberg-Marquardt function with two inputs and two outputs. The output values of Artificial Neural Network modelling were compared with the real values of pervaporation for separation of water from Ethanol and Acetone. The results revealed that the proposed model had a good performance. Moreover, the output of COMSOL software for pervaporation of five different alcohols were compared with the real values, and the error percentage of the actual amount of flux was calculated with the modeling value by means of related membranes. The results of COMSOL modeling showed that the error percentage of 3.049 achieved for dehydration process of Acetone.

Keywords: Modeling, Dehydration, Polymer membrane, COMSOL Multiphysics, Artificial Neural Network.

Corresponding author α: Associate Professor, Department of Chemical Engineering, Malek-Ashtar University of Technology, Tehran, Iran.

σ : Department of Chemical Engineering, South Tehran Branch, Islamic Azad University, Tehran, Iran.

II. INTRODUCTION

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) [1-5]. 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 and acetone. Moreover, the error percentage for the real flux and modeled flux by the related membranes for each of the five alcohols were modeled by the COMSOL Multiphysics.

III. EXPERIMENTAL

3.1 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 and Acetone were selected in this research; and, Matlab version R2012a (7.14.0.739) was used. Figure 1 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.

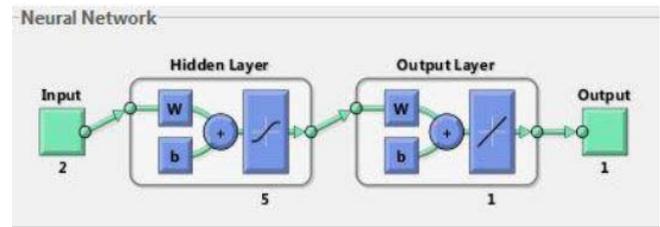


Figure 1: A schematic view of the ANN

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.

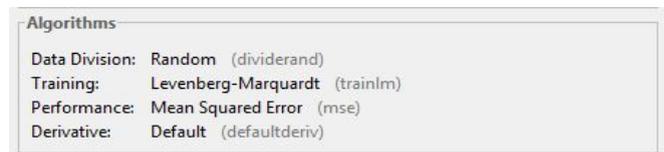


Figure 2: Algorithms compartment in ANN

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 [8]:

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.

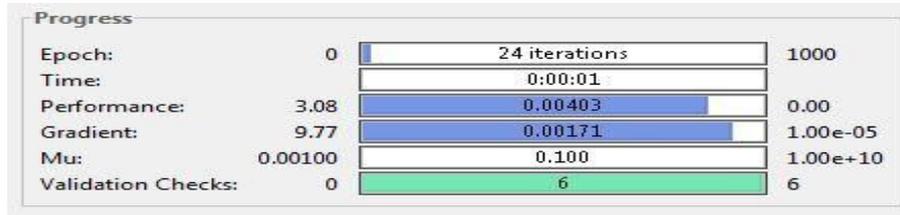


Figure 3: Graph of Water and ethanol dehydration progress by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

The performance graph shows the number of phases based on the errors. As shown in Figure 4, 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.

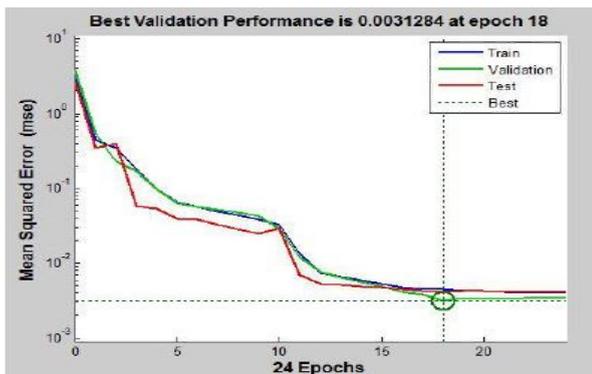


Figure 4: The water- ethanol dehydration performance by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

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.

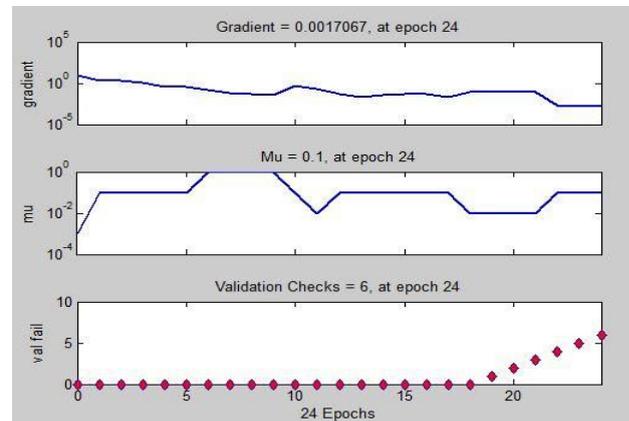


Figure 5: State training graph for water- ethanol dehydration by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

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.

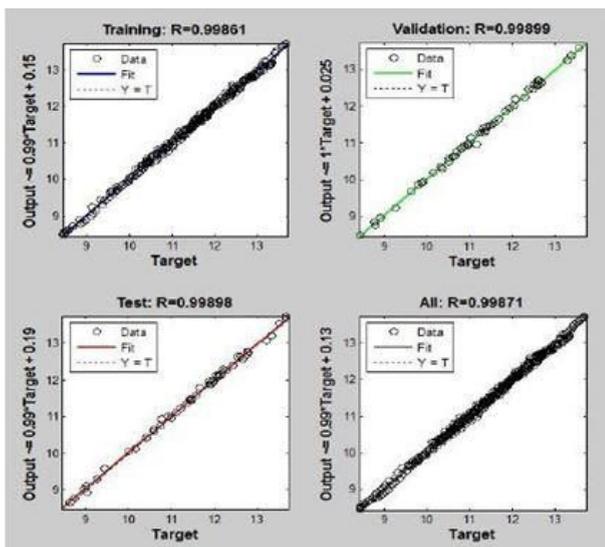


Figure 6: Regression graph for water-ethanol dehydration by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

Figure 7 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.

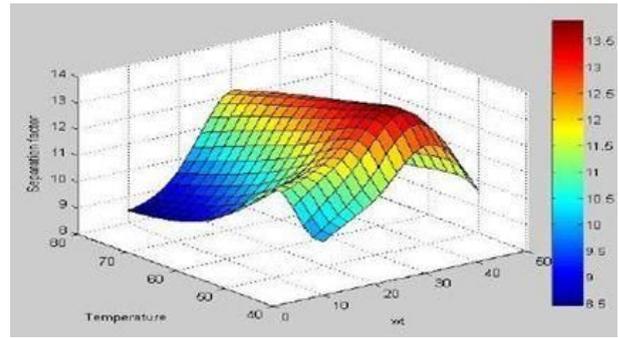


Figure 7: Figure graph for Water- ethanol dehydration by Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

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 8, 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- ethanol solubility and diffusion rate decreases, and the separation factor declines accordingly.

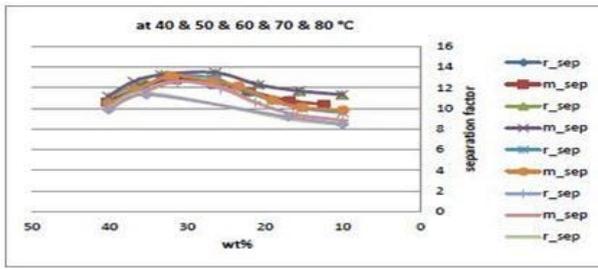


Figure 8: A comparison between the error percentage of real separation factor and the modeling separation factor for water and ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

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.

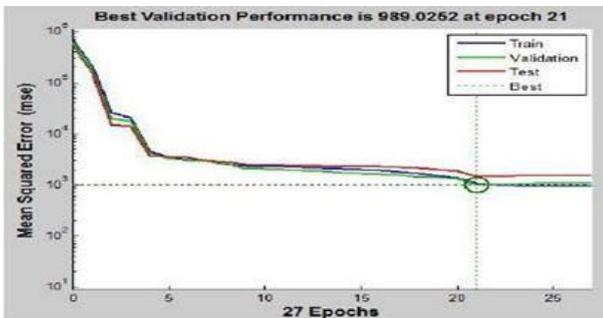


Figure 9: Performance graph for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

Figure 9 displays the regression graph. As depicted in ALL graph, the best line with the lowest error would be as follows:

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

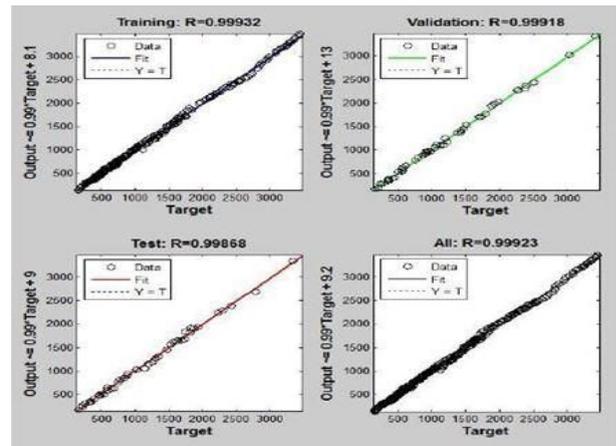


Figure 10: Regression graph for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

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.

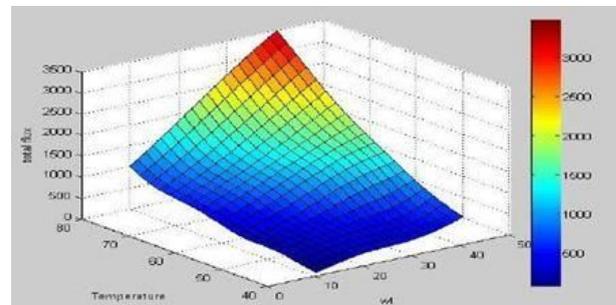


Figure 11: Figure graph for water- ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

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.

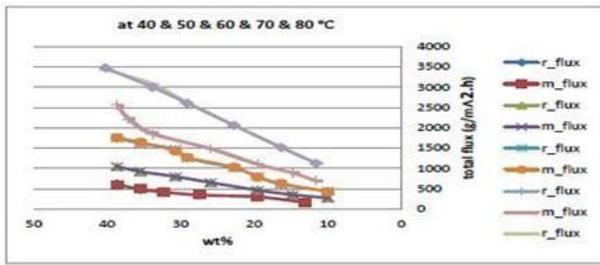


Figure 12: Comparison of error percentage for overall flux in reality and modeling for water-ethanol dehydration by ethanol Polydimethylsiloxane polymer membrane and Polyvinylidene fluoride

91 data were used for dehydration of acetone, and Polyacrylonitrile and polyethylene glycol membranes were utilized. The results for separation factor are as below [8-10]:

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.

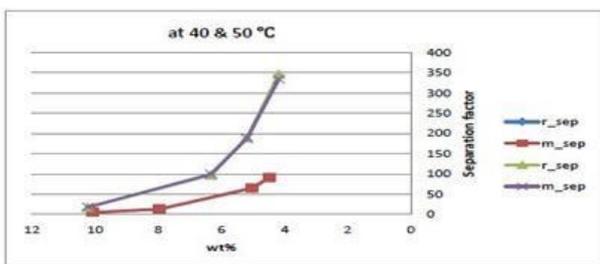


Figure 13: Comparison of the error percentage for real separation factor and modeling in water-acetone dehydration by Polyacrylonitrile and polyethylene glycol membranes

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 regressio 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.

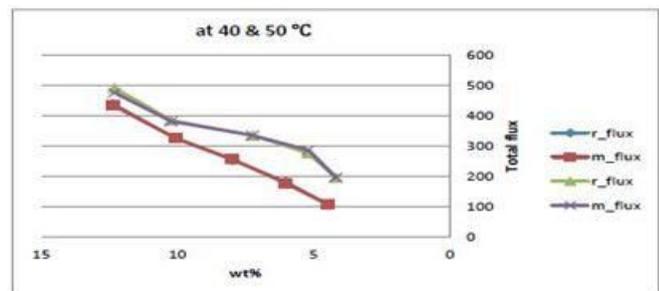


Figure 14: Comparison of error percentage for overall flux in reality and in modeling of acetone dehydration by Polyacrylonitrile and polyethylene glycol membranes

3.2 Modeling dehydration of organic compounds by use of COMSOL Multiphysics Software

The organic compound including acetone was utilized in this study, and the COMSOL Multiphysics version 4.2.0.150 was implemented to data analysis. The procedure description is as follows:

Mesh is the starting point for the Finite Element method that partitions geometry into simpler and smaller units.

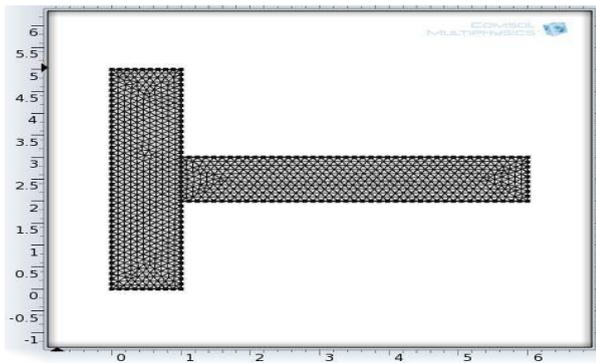


Figure 15: Meshing the membrane module in the water- alcohol processing by different membranes

In this method, you can see counters in the results section that includes temperature (ht), mass fraction, flux (chcs), velocity (spf), and pressure (spf).

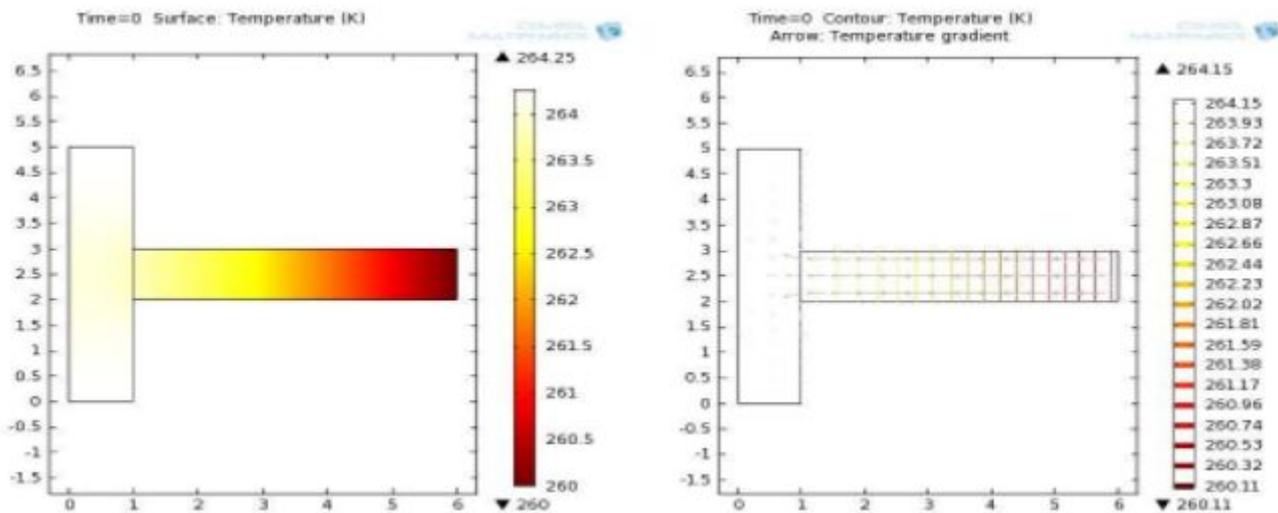


Figure 16: Temperature in water-acetone processing by Acrylonitrile and 2- Hydroxyethyl methacrylate grafted polyvinyl alcohol

As can be seen in the mass fraction graph below, the amount of mass fraction is fixed across the module. The reason is that after balancing the membrane swelling and saturation concentration of water on the membrane surface, flux and water separation factor change slightly with the increase of the feed's water amount.

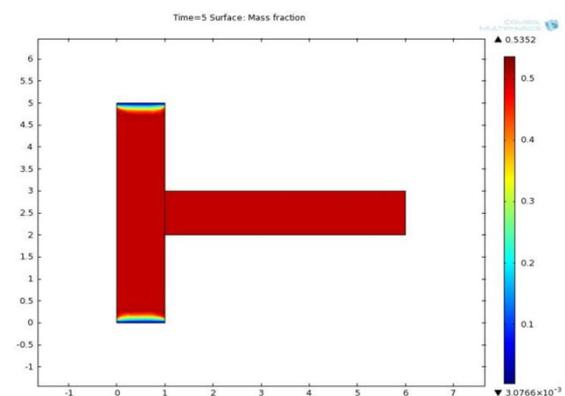


Figure 17: Mass fraction in water- acetone processing by Acrylonitrile and 2- Hydroxyethyl methacrylate grafted polyvinyl alcohol

As shown in the figure, flux is stable and low in the membrane entries and walls due to the low driving force. However, the flux increased within the membrane, as the pressure increased. The error percentage in flux was 3.049.

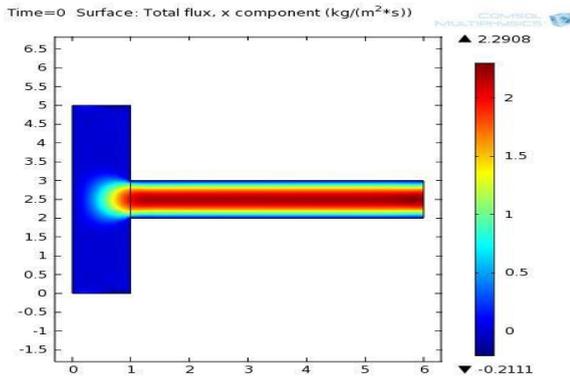


Figure 18: Flux graph for water- acetone processing by Acrylonitrile and 2- Hydroxyethyl methacrylate grafted polyvinyl alcohol

The current velocity in the entry is low, and it decreased across the walls too in the velocity graph; however, the velocity increased in the membrane. The reason of this phenomenon can be reduction of temperature across the membrane and increase of water concentration in membrane. Afterward, the separation factor for water increases due to increase of the driving force for the mass transfer.

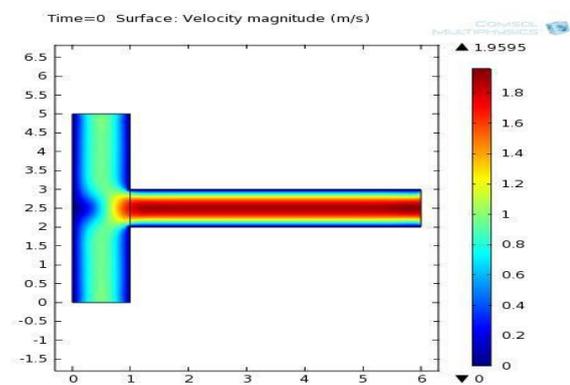


Figure 19: Velocity graph for water- acetone processing by Acrylonitrile and 2- Hydroxyethyl methacrylate grafted polyvinyl alcohol

As observed in the figure, the input is under the atmosphere pressure, and the pressure decreased

across the membrane module. The reason can be said to be reduction of the driving force across the membrane.

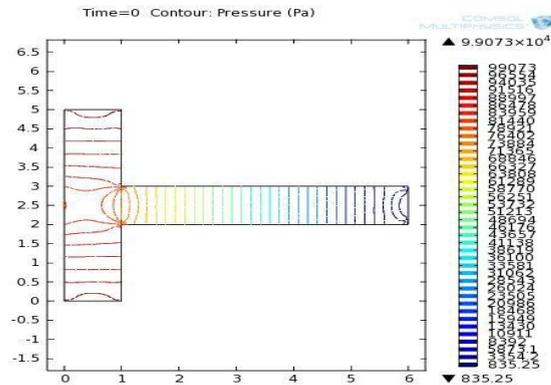


Figure 20: Pressure graph for water- acetone processing by Acrylonitrile and 2- Hydroxyethyl methacrylate grafted polyvinyl alcohol

IV. COMPARISON OF ANN AND COMSOL IN DEHYDRATION OF ACETONE BY POLYACRYLONITRILE AND POLYETHYLENE GLYCOL

The error value in the ANN was 1.86, and the error value in COMSOL was 2.11. Regarding the error value, it can be concluded that both modeling methods were appropriate, and the error percentage in ANN is lower than the COMSOL. As a result, ANN is more accurate, and the reason is that ANN considers the problems in detail, while COMSOL considers the problems in general.

V. CONCLUSION

In this study, dehydration of water-ethanol and water- acetone 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.

The dehydration of water- acetone by pervaporation process were also modeled in the COMSOL. The hydrophilic membranes were used

that are good for separation of low amounts of water in alcohols. Moreover, the COMSOL in this study reflected the error suitably.

REFERENCES

1. Seader and Henely, Separation process principles, *John Wiley and Sons*, (1998).
2. Srikanth, G., Membrane separation processes technology and business, *Opportunities. Water conditioning & purification*, (2008).
3. Baker, R.w., Membrane technology and application, *John Wiley & Sons, Ltd*, (2004).
4. Kujawski. W, Application of pervaporation and vapor permeation in environmental protection, *Polish journal of environmental studies*, 9 (1), 13-26, (2000).
5. Huang, R. Pervaporation membrane separation process, *ELSEVIER*, 11(120), 181-191, (1991).
6. Feng, X. and R.Y.M. Huang, Liquid separation by membrane pervaporation A review, Industrial Baker, R.w., *Membrane technology and application*, (2004).
7. Mulder, M., Basic principles of membrane technology, ed. S. Edition, *Kluwer*, (1996).
8. Rautenbach R. and Albrecht, R., The separation potential of pervaporation: part 1. Discussion of transport equations and comparison with reverse osmosis, *Journal of membrane science*, 1 (23), (1985).
9. Xia Zhan, Ji-ding Li, Jian Chen and Jun-qi Huang, Pervaporation of ethanol/water mixtures with high flux by zeolite-filled PDMS/PVDF composite membranes, *Chinese Journal of polymer science*, 771-780 (2009).
10. Qiang Zhao, Jinwen Qian, Quanfu An, Zhihui Zhu, Peng Zhang, Yunxiang Bai, Studies on pervaporation characteristics of polyacrylonitrile-b-poly (ethylene glycol)-b-polyacrylonitrile block copolymer membrane for dehydration of aqueous acetone solutions, *Journal of membrane science* 311, 284-293, (2008).
11. Elsayed A. Fouad, Xianshe Feng, Pervaporation separation of n-butanol from dilute aqueous solutions using silicalite-filled poly (dimethyl siloxane) membranes, *Journal of Membrane Science* 339, 120-125, (2009).
12. Merve Olukman Oya Sanli, A novel in situ synthesized magnetite containing acrylonitrile and 2-hydroxyethylmethacrylate grafted poly (vinyl alcohol) nanocomposite membranes for pervaporation separation of acetone/water mixtures, *Journal of Membrane Science*, 1-10, (2015).
13. Sridhar, S., Smitha, B., Amarnath Reddy, A., Separation of 2-butanol-water mixtures by pervaporation through PVA-NYL 66 blend membranes, Membrane Separations Group, Chemical Engineering Division, *Indian Institute of chemical technology*, (2006).
14. Takegami, Shinsuke., Yamada, Hideki., Tsujii, Shoji., Dehydration of water/ethanol mixtures by pervaporation using modified poly(vinyl alcohol) membrane, *Toyobo Research Institute*, (1992).
15. Zhao, Qiang., Qian, Jinwen., An, Quanfu., Meihua, zhu., Poly(vinyl alcohol)/ polyelectrolyte complex blend membrane for pervaporation dehydration of isopropanol, *Department of polymer science and engineering*, (2009).
16. Mercedes Villegas Elza F. Castro Vidaurre Juan C. Gottifredi, Sorption and pervaporation of methanol/water mixtures with poly (3-hydroxybutyrate) membranes, (2014).