Mechanistic Modeling of Organic Compounds Separation from Water *via* Polymeric Membranes

Marjani, Azam*[+]

Department of Chemistry, Arak Branch, Islamic Azad University, Arak, I.R. IRAN

ABSTRACT: *A mathematical model considering mass and momentum transfer was developed for simulation of ethanol dewatering via pervaporation process. The process involves removal of water from a water/ethanol liquid mixture using a dense polymeric membrane. The model domain was divided into two compartments including feed and membrane. For a description of water transport in the feed solution, Maxwell-Stefan approach was used, while for mass transfer inside the membrane the molecular diffusion mechanism was assumed. The governing equations were solved numerically using finite element method. The concentration profile inside the membrane showed a linear decrease and a parabolic fully developed velocity profile was obtained on the feed side. The results also confirmed that formation of concentration layer can be easily predicted using Maxwell-Stefan approach in dewatering of organic compounds using pervaporation process.*

KEYWORDS: *Mass transfer; Membranes; Modeling; Pervaporation; Maxwell-Stefan model.*

INTRODUCTION

Dehydration of organic solvents is an important unit operation in the production of solvents at industrial scale. The operation can be conducted using typical separation units such as distillation, adsorption, etc. These processes involve removal of water from the solvent by application of energy as heat or by application of another phase like in adsorption. The major problem with conventional dehydration processes is the consumption of much energy in these processes especially for those processes that use heat for the creation of vapor phase [1]. Moreover, the conventional separation processes suffer from other difficulties such as difficult scale up, design, high capital and maintenance costs, and huge equipment.

Researchers are trying to find alternative separation processes for dehydration of chemical solvents. The main criteria for alternative separation processes are efficiency, consumption of low energy, low cost, and easy design and operation. Recently membrane separation technology has attracted much attention in separation processes due to its superior properties compared to other processes [2-33]. Membrane processes can provide a great medium for separation of close-boiling point materials such as water-alcohol. Moreover, membrane technology is also capable of separation of liquid mixtures that form an azeotrope at specific concentration [34-37]. Additionally, design and scale-up of membrane processes is easy and linear which can make the process fascinating for industrial applications. Research on membrane separation processes mostly focuses on synthesis and fabrication of novel and composite material for the purpose of separation [15]. However, development of mathematical models for simulation of membrane processes is of great importance.

* *To whom correspondence should be addressed.*
+ E-mail: a-marjani@iau-arak.ac.ir
1021-9986/2017/5/139-149 11/$/6.10

Development of a mechanistic model which can relate process parameters to product properties is of great interests for design and optimization of separation processes [38-46].

Some researchers have developed mechanistic models for simulation of polymeric and inorganic membranes to predict the performance of process [47-58]. Recently, data-driven models have shown great capability if process modeling and simulation [59-64]. However, these models are a black box and cannot capture the process.

Various models have been developed for prediction and description of membrane processes. *Shirazian et al.* [38-44, 49, 65] developed a mathematical model for prediction of transport phenomena in porous membranes. They developed a 2D comprehensive model for prediction of CO_2 & SO_2 concentration in hollow-fiber membrane contactors. The model considers both diffusional and convective mass transfer in the membrane module. Their results revealed that 2D mathematical model based on Computational Fluid Dynamics (CFD) can provide a powerful tool for design and optimization of membrane processes. *Rezakazemi et al.* [66] developed a mathematical model for prediction of water transport through dense membranes in a pervaporation process. The model considers mass transfer flux in the membrane and the feed solution. The mass transfer equations were coupled with the momentum equation to completely model the process. CFD technique was used for simulation of the process. The results showed satisfactory agreement with the experimental data. Shirazian and *Ashrafizadeh* [67] developed a 3D mass transfer model for simulation of water transport in membrane evaporation process. The authors considered Fick's law of diffusion for prediction of mass transfer in feed solution and membrane pores. In the developed models for modeling and simulations of membrane processes, the authors used Fick's law of diffusion for estimation of diffusional mass transfer. The latter could produce satisfactory results at low concentration and also for binary systems. For concentrated systems, the model would deviate from experimental data.

Therefore, there is a definite need for a comprehensive mathematical model for simulation of separation in membrane systems. The model should be capable of predicting mass transfer flux as well as hydrodynamics of process at various feed concentrations. Application of multicomponent mass transfer theory, i.e. Maxwell-Stefan model for simulation of membrane processes can provide a better understanding of the separation mechanism in membrane processes. The main objective of the present work is to develop a 2D mathematical model based on Maxwell-Stefan theory for simulation of membrane separation processes. The model is developed for dehydration of ethanol using pervaporation.

THEORETICAL SECTION

In this work, a 2D comprehensive model is developed for simulation of membrane process. The considered process here is a pervaporation process for removal of water from ethanol (ethanol dehydration). For modeling of the process, a model domain is considered and model equations are then derived. Fig. 1 shows model domain used for modeling. The feed solution involving a mixture of 10 % wt. water and 90% wt. ethanol flows through the feed side of the membrane module (at $y = 0$). The feed solution exits from the upper side and recirculates inside the module. The membrane module at $x = 0$ is assumed to be insulated. Therefore, the model domain consists of two subdomains called membrane and feed sides. The governing equations are derived and solved for these two regions separately.

Model development

In order to develop the mechanistic model for prediction of the process, the following assumptions are made:

(1) Steady state and isothermal conditions for both feed and membrane sides

(2) The feed flow is in the laminar regime

(3) Thermodynamic equilibrium is established the feed - membrane interface

(4) Water is the only penetrant.

The next step is to derive the governing equations for description of water transport in the feed and membrane side. It should be pointed out that the permeate side is neglected in the simulation because the considered process here is pervaporation and the permeate pressure is very low. Therefore the concentration at the permeate side is assumed to be zero.

The main equation that describes the transfer of water from the feed phase to permeate side is continuity equation. The continuity equation is used to obtain

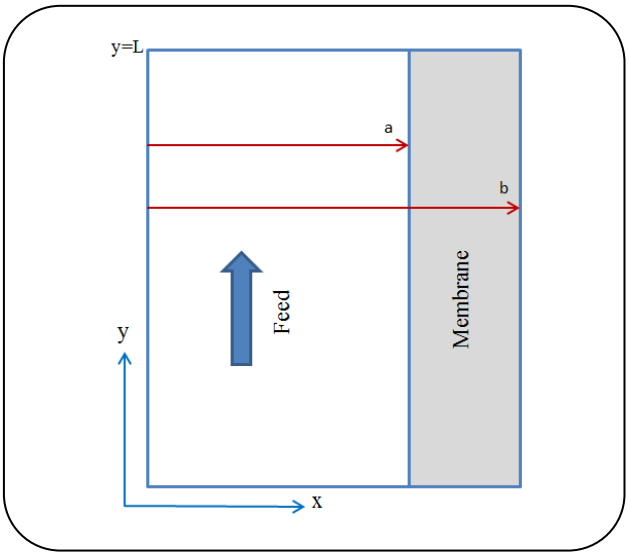

Fig. 1: Model domain.

concentration and mass transfer flux of water in the membrane module. The basic form of continuity equation is as follows [68]:

$$\frac{\partial C_w}{\partial t} + \nabla \cdot (J_w + C_w V) = R_w \qquad (1)$$

Where C_w denotes the concentration of water (mol/m^3), J_w refers to diffusive mass transfer flux of water (mol/m^2.s), V stands for the velocity vector (m/s), t the time (s), and R_w refers to the chemical reaction (mol/m^3.s) which is zero in this case. Now the equations are derived for each subdomain, i.e. feed and membrane.

Feed phase equations

Equation (1) is the main equation of mass transfer which should be solved numerically to obtain the concentration and mass flux distribution of water in the membrane module. In order to solve this equation, velocity distribution is required to be coupled to the continuity equation. Velocity distribution can be calculated by solving the Navier-Stokes equations. Therefore, the Navier-Stokes, as well as continuity equation, should be solved simultaneously to specify the concentration distribution of water on the feed side. It is worth mentioning that the Navier-Stokes equations describe flow in viscous fluids through momentum balances for each of the components of the momentum vector in all spatial dimensions. In laminar flow regime, Navier-Stokes equations are given as [68]:

$$-\nabla \cdot \eta(\nabla V_y + (\nabla V_y)^T) + \rho(V_y.\nabla)V_y + \nabla p = F \qquad (2)$$

$$\nabla . V_y = 0$$

where η denotes the dynamic viscosity (kg/m.s) of feed solution, V_y refers to the velocity of feed in y-direction (m/s), ρ is the density of the feed solution (kg/m^3), p is the pressure (Pa) and F refers to a body force term (N) which is zero in this case.

Another important issue in deriving feed equation is estimation of diffusive mass transfer flux, i.e. J_w in equation (1). J_w stands for the amount of mass (water) transferred to the tube side of membrane module by a diffusion mechanism. The latter can be estimated by either Fick approach or Maxwell-Stefan approach. Fick approach is useful for dilute and binary systems, whereas Maxwell-Stefan (MS) approach is capable of prediction of diffusion in multicomponent systems. MS approach is used for estimation of diffusional mass transfer. In the steady state condition, Maxwell-Stefan can be expressed as [68]:

$$d_i = -\sum_{j \neq i}^{n} \frac{x_j J_i - x_i J_j}{c D_{ij}} \qquad (3)$$

Where d is diffusion driving force, x is mole fraction, c is a total concentration of the solution (mol/m^3), n is a number of components and D is MS coefficient (m^2/s). The assumptions for Equation (3) are constant pressure and ideal mixture. Therefore, Equations 1-3 should solve to obtain the concentration and velocity distribution in the feed side of the membrane module. It should be noted that the convective mass transfer in the x-direction is neglected due to its negligible contribution to the total mass transfer flux.

The boundary conditions for the continuity equation are:

y = 0, $C_{w\text{-}feed} = C_0$ (Inlet concentration) (4)

y = L, convective flux (5)

x = 0, $\frac{\partial C_{w-feed}}{\partial y} = 0$ (Insulation boundary) (6)

The convective flux boundary condition imposed on the boundary at y=L (Equation (5)) assumes that all mass transfer through this boundary is convection.

x = a, $C_{w\text{-}feed} = C_{w\text{-}feed}/m$ (7)
(thermodynamic equilibrium)

where m refers to partition coefficient for water between the feed and the membrane wall.

The boundary conditions for Navier-stokes equations are as follow:

$y = 0,\ V_y = V_0$ (Inlet velocity) (8)

$y = L,\ p = p_{atm}$ (9)

$x = 0,\ V = 0$ (no slip condition) (10)

$x = a,\ V = 0$ (no slip condition) (11)

Membrane equation

Inside the membrane, diffusion is the predominant phenomenon; therefore a diffusion mass transfer equation is derived and solved. For prediction of diffusion inside the membrane, Fick's law of diffusion is applied which has shown great results in the literature [22, 41, 44, 67, 69]. The steady-state continuity equation for transport of water through the membrane is as following [66]:

$$D_{w-membrane}\left[\frac{\partial^2 C_{w-membrane}}{\partial x^2}+\frac{\partial^2 C_{w-membrane}}{\partial y^2}\right]=0 \quad (12)$$

The boundary conditions for the continuity equation in the membrane are:

$$x = a,\ C_{w-membrane} = C_{w-feed} \times m \quad (13)$$

$$x = b,\ C_{w-membrane} = 0 \quad (14)$$

$$y = 0\ \&\ y = L,\ \frac{\partial C_{w-membrane}}{\partial y} = 0 \quad (15)$$

The boundary condition (14) states that the concentration of water is zero at membrane/permeate interface. Since the membrane is kept at vacuum condition at permeate side (at x=b), the water concentration at this boundary is assumed to be negligible. The latter means that when the water reaches this boundary, it evaporates instantaneously.

Numerical simulation of the process

The model equations including continuity, Maxwell-Stefan, and Navier-Stokes equations for the feed and the membrane with the boundary conditions were solved numerically using COMSOL Multiphysics software version 3.5. The continuity equation is used to obtain a concentration In order to simulate the process, the software utilizes finite element technique for discretization of equations and numerical solution. The latter method has shown great capability in the simulation of transport phenomena in membrane separation processes [7-11, 22-26, 30, 32, 70-78]. The numerical solver of UMFPACK was set entire the simulation for the numerical solution of the governing equations. An IBM-PC-Pentium 5 (CPU speed was 2600 MHz and 4 GB of RAM) was used to solve the set of equations within a short time. It should be pointed out that the COMSOL mesh generator creates triangular meshes that are isotropic in size. Adaptive mesh refinement in COMSOL, which generates the best and minimal meshes, was used to mesh the domain of process. Fig. 2 indicates the nodes generated by software for the process simulation [66]. The membrane and process parameters used in the simulations are listed in Table 1.

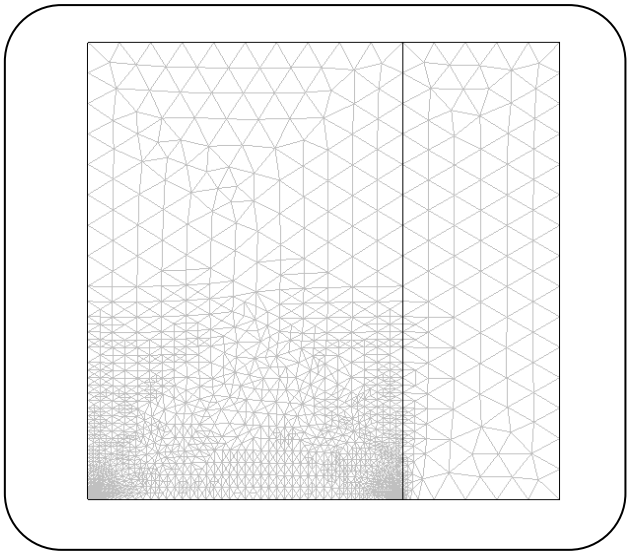

Fig. 2: Magnified segments of the mesh used in the numerical simulation.

RESULTS AND DISCUSSION

Concentration distribution in the feed

The concentration distribution of water on the feed side is illustrated in Fig. 3. The water concentration is shown in terms of mass fraction. Moreover, concentration profiles of water in x and y directions are shown in Figs. 4 and 5 respectively. As it is clearly seen, concentration change is very sharp near the membrane wall whereas at the zones far from the membrane, the concentration does not change considerably. This is also clearly seen in Fig. 4

Tab. 1: Parameters used in numerical simulations [12, 68].

Parameter	value	unit
Feed side width	2e-5	m
Feed side length	3e-5	m
Membrane thickness	1e-5	m
Feed temperature	300	K
MS diffusivity	1e-10	m^2/s
Membrane diffusivity	1e-12	m^2/s
Inlet water mass fraction	0.1	-
Inlet feed velocity	0.001	m/s

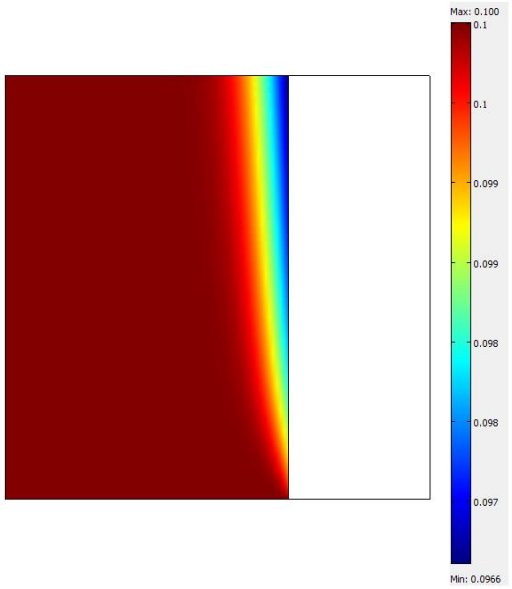

Fig. 3: Concentration distribution of water on the feed side.

where the concentration of water is almost constant at the bulk of feed while a sharp decrease in water concentration is observed in the vicinity of membrane wall. The latter could be an evidence for the formation of mass transfer boundary layer. Therefore, the developed model is capable of predicting concentration boundary layer in the feed side.

Concentration distribution inside the membrane

The concentration distribution of water inside the membrane is shown in Fig. 6. Moreover, the concentration profile of water inside the membrane in the x-direction is depicted in Fig. 7. Since the only diffusional mass transfer is assumed for transport of water through the membrane, a uniform and linear concentration profile in the x-direction is observed. Moreover, two upper and bottom sides of membranes (at y=0 & y=L) are assumed Insulation boundary. However, a sharp decrease in water concentration is observed whereas the concentration reaches zero at the feed/permeate interface. The latter is due to the implementation of zero concentration for water in the boundary.

Velocity profile

Velocity distribution of feed solution in 2 dimensions is represented in Fig. 8. As mentioned before, velocity field of the feed solution is obtained by numerical solution of the Navier-Stokes equations. Analysis of velocity field reveals that the maximum of velocity occurs at the middle of feed side, whereas the velocity decreases sharply in the vicinity of membrane wall and also feed wall. The latter is also an evidence for the formation of velocity boundary layer which is well predicted by the developed model. The reduction in the velocity near the membrane wall could be attributed to the effect of viscous forces exerted on the layer of fluid.

Distribution of mass transfer flux

Fig. 9 shows the distribution of mass transfer flux along with arrows of flux in the feed side of the membrane module. The only diffusional mass transfer is depicted in Fig. 9, because it has a major effect on the transport of water from feed phase to the membrane phase. As it is clearly seen, the diffusion in the bulk of feed solution is almost zero,

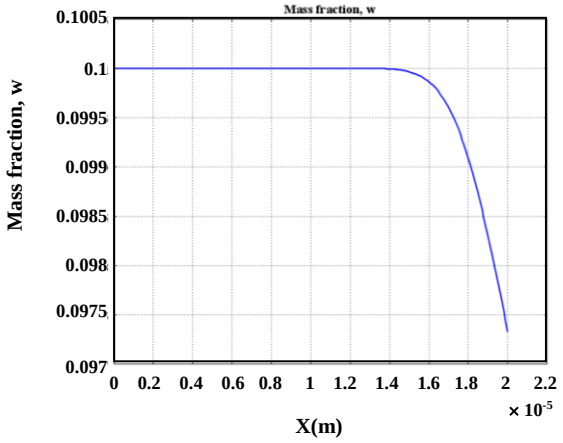

Fig. 4: Concentration profile of water in the feed side (x-direction).

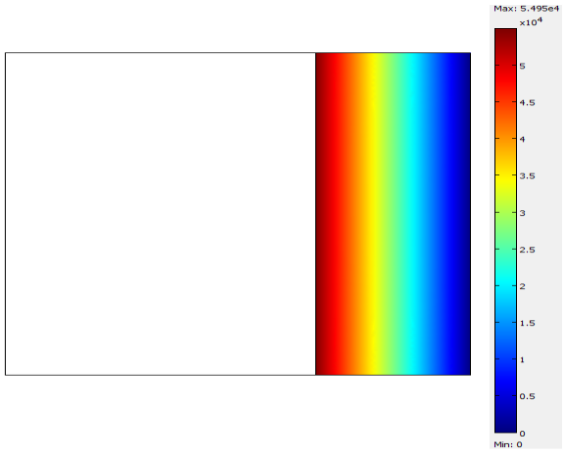

Fig.6: Concentration distribution of water inside the membrane.

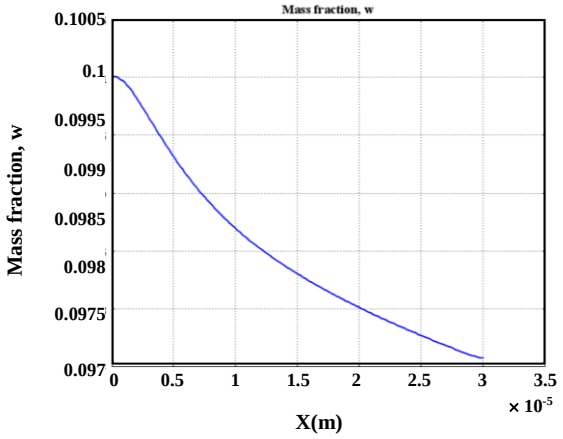

Fig. 5: Concentration profile of water on the feed side (y-direction).

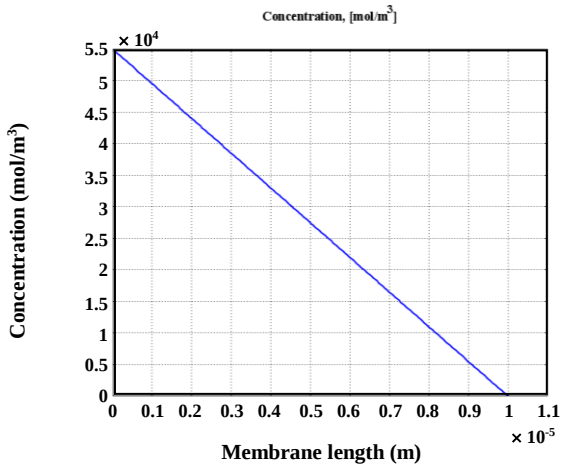

Fig. 7: Concentration profile of water inside the membrane.

whereas in the area near the membrane wall, a significant increase in diffusion is observed. Basically, mechanism of mass transfer for water in the feed side is diffusion and convection. Convection is controlled by the velocity of the fluid, whereas diffusion is mainly controlled by the concentration gradient of species. Since the velocity in the bulk of feed solution is high (see Fig. 8), convection contribution in the bulk is high and diffusion is negligible. On the other hand, diffusion is significant near the membrane wall due to the reduction of velocity in this zone. This can also be from the arrows of mass transfer flux in Fig. 9 which is high near the membrane wall.

CONCLUSIONS

A two-dimensional mathematical model was developed in this work considering mass transfer as well as momentum transfer. The process studied in this work involved removal of water from alcohol/water solution by means of a dense polymeric membrane. Evaporation is considered to be the separation method in which the separation is achieved by applying a vacuum pressure at the permeate side. Therefore, vapor pressure gradient is the main driving force of the process. Maxwell-Stefan approach was used for estimation of diffusional mass transfer in the model, and the velocity of fluid was modeled using the Navier-Stokes equation. Finite element

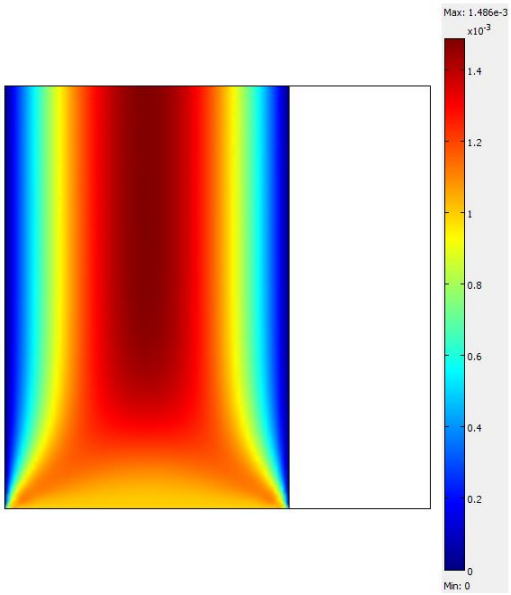

Fig. 8: Velocity profile of feed.

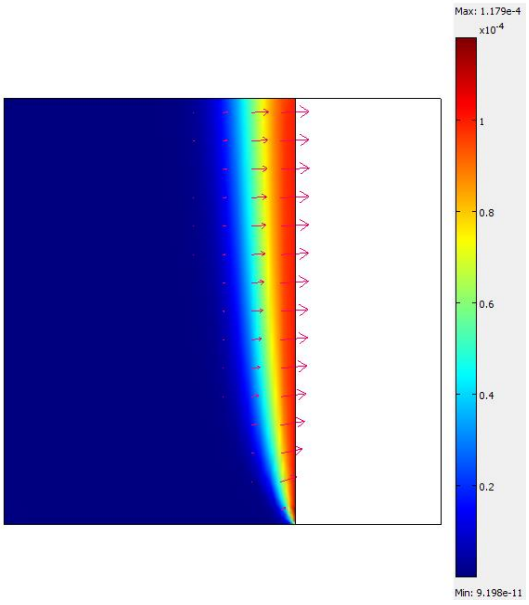

Fig. 9: Diffusive mass transfer flux of water in the feed.

the method was used for numerical solution of the model equation and the results indicated that increasing feed velocity decreases the removal of water due to a reduction in residence time of feed solution in the membrane module.

Received: Sep. 15, 2016 ; Accepted May 8, 2017

REFERENCES

[1] Chien I.L., Opportunities for Energy Savings in Azeotropic Separation Processes, in: A.K. Iftekhar, S. Rajagopalan (Eds.) "Computer Aided Chemical Engineering", Elsevier, pp. 75-82 (2012).

[2] Koorepazan Moftakhar M., Habibi L., Yaftian M.R., Selective and Efficient Ligandless Water-in-Oil Emulsion Liquid Membrane Transport of Thorium(IV) Ions, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, **35**: 125-134 (2016).

[3] Kohnehshahri R.K., Salimi M., Mohaddecy S.R.S., Shirazian S., Modeling and Numerical Simulation of Catalytic Reforming Reactors, *Oriental Journal of Chemistry*, **27**: 1351-1355 (2011).

[4] Marjani A., Mohammadi P., Shirazian S., Preparation and Characterization of Poly (Vinyl Alcohol) Membrane for Pervaporation Separation of Water-Organic Mixtures, *Oriental Journal of Chemistry*, **28**: 97-102 (2012).

[5] Marjani A., Rezakazemi M., Shirazian S., Vapor Pressure Prediction Using Group Contribution Method, *Oriental Journal of Chemistry*, **27**: 1331-1335 (2011).

[6] Marjani A., Rezakazemi M., Shirazian S., Simulation of Methanol Production Process and Determination of Optimum Conditions, *Oriental Journal of Chemistry*, **28**: 145-151 (2012).

[7] Marjani A., Shirazian S., Hydrodynamic Investigations on Heavy Metal Extraction in Membrane Extractors, *Oriental Journal of Chemistry*, **27**: 1311-1316 (2011).

[8] Marjani A., Shirazian S., Investigation on Copper Extraction Using Numerical Simulation, *Asian Journal of Chemistry*, **23**: 3289-3290 (2011).

[9] Marjani A., Shirazian S., Investigation on Numerical Simulation of Acetone and Ethanol Separation From Water by Using Membrane, *Asian Journal of Chemistry*, **23**: 3293-3294 (2011).

[10] Marjani A., Shirazian S., Computational Fluid Dynamics Simulation of Ammonia Removal From Wastewaters by Membrane, *Asian Journal of Chemistry*,**23**: 3299-3300 (2011).

[11] Marjani A., Shirazian S., CFD Simulation of Mass Transfer in Membrane Evaporators for Concentration of Aqueous Solutions, *Oriental Journal of Chemistry*, **28**: 83-87 (2012).

[12] Marjani A., Shirazian S., Modeling of Organic Mixtures Sparation in Dense Membranes Using Finite Element Method (FEM), *Oriental Journal of Chemistry*, **28**: 41-46 (2012).

[13] Marjani A., Shirazian S., Application of CFD Techniques for Prediction of NH_3 Transport Through Porous Membranes, *Oriental Journal of Chemistry*, **28**: 67-72 (2012).

[14] Marjani A., Shirazian S., Theoretical Studies on Copper Extraction by Means of Polymeric Membrane Contactors, *Oriental Journal of Chemistry*, **28**: 23-28 (2012).

[15] Marjani A., Shirazian S., Mathematical Modeling and CFD Simulation of Hydrocarbon Purification Using Membrane Technology, *Oriental Journal of Chemistry*, **28**: 123-129 (2012).

[16] Marjani A., Shirazian S., Ranjbar M., Ahmadi M., Mathematical Modeling of Gas Separation in Flat-Sheet Membrane Contactors, *Oriental Journal of Chemistry*, **28**: 13-18 (2012).

[17] Moghadassi A., Marjani A., Shirazian S., Moradi S., Gas Separation Properties of Hollow-Fiber Membranes of Polypropylene and Polycarbonate by Melt-Spinning Method, *Asian Journal of Chemistry*, **23**: 1922-1924 (2011).

[18] Pishnamazi M., Marjani A., Shirazian S., Samipurgiri M., Mathematical Modeling and Numerical Simulation of Wastewater Treatment Unit Using CFD, *Oriental Journal of Chemistry*, **28**: 51-58 (2012).

[19] Ranjbar M., Shirazian S., Ghafarnejad Parto S., Ahmadi M., Computational Fluid Dynamics Simulation of Mass Transfer in the Separation of Fermentation Products Using Nanoporous Membranes, *Chemical Engineering and Technology*, **36**: 728-732 (2013).

[20] Razavi S.M.R., Razavi S.M.J., Miri T., Shirazian S., CFD Simulation of CO_2 Capture From Gas Mixtures in Nanoporous Membranes by Solution of 2-Amino-2-Methyl-1-Propanol and Piperazine, *International Journal of Greenhouse Gas Control*, **15**: 142-149 (2013).

[21] Shirazian S., Marjani A., Fadaei F., Supercritical Extraction of Organic Solutes From Aqueous Solutions by Means of Membrane Contactors: CFD Simulation, *Desalination*, **277**: 135-140 (2011).

[22] Shirazian S., Marjani A., Rezakazemi M., Separation of CO_2 by Single and Mixed Aqueous Amine Solvents in Membrane Contactors: Fluid Flow and Mass Transfer Modeling, *Engineering with Computers*, **28**: 189-198 (2012).

[23] Shirazian S., Marjanm A., Azizmohammadi F., Prediction of SO_2 Transport Across Ceramic Membranes Using Finite Element Method (FEM), *Oriental Journal of Chemistry*, **27**: 485-490 (2011).

[24] Shirazian S., Moghadassi A., Moradi S., Numerical Simulation of Mass Transfer in Gas-Liquid Hollow Fiber Membrane Contactors for Laminar Flow Conditions, S*imulation Modelling Practice and Theory*, **17**: 708-718 (2009).

[25] Shirazian S., Pishnamazi M., Rezakazemi M., Nouri A., Jafari M., Noroozi S., Marjani A., Implementation of the Finite Element Method for Simulation of Mass Transfer in Membrane Contactors, *Chemical Engineering and Technology*, **35**: 1077-1084 (2012).

[26] Shirazian S., Rezakazemi M., Marjani A., Moradi S., Hydrodynamics and Mass Transfer Simulation of Wastewater Treatment in Membrane Reactors, *Desalination*, **286**: 290-295 (2012).

[27] Shirazian S., Rezakazemi M., Marjani A., Rafivahid M.S., Development of a Mass Transfer Model for Simulation of Sulfur Dioxide Removal in Ceramic Membrane Contactors, *Asia-Pacific Journal of Chemical Engineering*, **7**: 828-834 (2012).

[28] Sohrabi M.R., Marjani A., Moradi S., Davallo M., Shirazian S., Theoretical Studies on Membrane-Based Gas Separation Using Computational Fluid Dynamics (CFD) of Mass Transfer, *Journal of the Chemical Society of Pakistan*, **33**: 464-473 (2011).

[29] Sohrabi M.R., Marjani A., Moradi S., Davallo M., Shirazian S., Preparation and Simulation of Polycarbonate Hollow-Fiber Membrane for Gas Sparation, *Asian Journal of Chemistry*, **23**: 302-304 (2011).

[30] Sohrabi M.R., Marjani A., Moradi S., Davallo M., Shirazian S., Mathematical Modeling and Numerical Simulation of CO_2 Transport Through Hollow-Fiber Membranes, *Applied Mathematical Modelling*, **35**: (2011) 174-188.

[31] Sohrabi M.R., Marjani A., Moradi S., Davaloo M., Shirazian S., Simulation Studies on H_2S Absorption in Potassium Carbonate Aqueous Solution Using a Membrane Module, A*sian Journal of Chemistry*, **23**: 4227-4228 (2011).

[32] Sohrabi M.R., Marjani A., Shirazian S., Moradi S., Simulation of Ethanol and Acetone Extraction from Aqueous Solutions in Membrane Contactors, *Asian Journal of Chemistry*, **23**: 4229-4230 (2011).

[33] Valavi M., Shirazian S., Pour A.F., Ziary M., Calculation of the Density and Activity of Water in ATPS Systems for Separation of Biomolecules, *Journal of Solution Chemistry*, **42** 1423-1437 (2013).

[34] Nagy E., Pervaporation, in: E. Nagy (Ed.) Basic Equations of the Mass Transport through a Membrane Layer, Elsevier, Oxford, pp. 267-291 (2012).

[35] Shirazi Y., Ghadimi A., Mohammadi T., Recovery of Alcohols From Water Using Polydimethylsiloxane–Silica Nanocomposite Membranes: Characterization and Pervaporation Performance, *Journal of Applied Polymer Science*, **124**: 2871-2882 (2012).

[36] Shirazi Y., Mohammadi T., Effects of CNTs Content on Physicochemical and Pervaporation Separation Properties of PVA Membranes, *Separation Science and Technology*, **48**: 716-727 (2013).

[37] Shirazi Y., Tofighy M.A., Mohammadi T., Synthesis and Characterization of Carbon Nanotubes/Poly Vinyl Alcohol Nanocomposite Membranes for Dehydration of Isopropanol, *Journal of Membrane Science*, **378**: 551-561 (2011).

[38] Fadaei F., Hoshyargar V., Shirazian S., Ashrafizadeh S.N., Mass Transfer Simulation of Ion Separation by Nanofiltration Considering Electrical and Dielectrical Effects, *Desalination*, **284**: 316-323 (2012).

[39] Fadaei F., Shirazian S., Ashrafizadeh S.N., Mass Transfer Modeling of Ion Transport Through Nanoporous Media, *Desalination*, **281**: 325-333 (2011).

[40] Fadaei F., Shirazian S., Ashrafizadeh S.N., Mass Transfer Simulation of Solvent Extraction in Hollow-Fiber Membrane Contactors, *Desalination*, **275**: 126-132 (2011).

[41] Fasihi M., Shirazian S., Marjani A., Rezakazemi M., Computational Fluid Dynamics Simulation of Transport Phenomena in Ceramic Membranes for SO_2 Separation, *Mathematical and Computer Modelling*, **56**: 278-286 (2012).

[42] Ghadiri M., Fakhri S., Shirazian S., Modeling and CFD Simulation of Water Desalination Using Nanoporous Membrane Contactors, *Industrial and Engineering Chemistry Research*, **52**: 3490-3498 (2013).

[43] Ghadiri M., Fakhri S., Shirazian S., Modeling of Water Transport Through Nanopores of Membranes in Direct-Contact Membrane Distillation Process, *Polymer Engineering and Science*, **54**: 660-666 (2014).

[44] Ghadiri M., Ghasemi Darehnaei M., Sabbaghian S., Shirazian S., Computational Simulation for Transport of Priority Organic Pollutants Through Nanoporous Membranes, *Chemical Engineering and Technology*, **36**: 507-512 (2013).

[45] H. Du-shu, Zhong-zhou, Yi, H. Zhao-long, Ping, Yi, L. Zi-jin, Mass Transfer Mechanism and Mathematical Model for Extraction Process of L-Theanine across Bulk Liquid Membrane, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, **31**: 53-58 (2012).

[46] Kambarani M., Bahmanyar H., Mousavian M.A., Mousavi S.M., Crossflow Filtration of Sodium Chloride Solution by A Polymeric Nanofilter: Minimization of Concentration Polarization by a Novel Backpulsing Method, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, **35**: 135-141 (2016).

[47] Asgarpour Khansary M., Kazemi Nezhad Estahbanati A., Shams B., Marjani A., S. Shirazian, Correlation of Sorption-Induced Swelling in Polymeric Films with Reference to Attenuated Total Reflectance Fourier-Transform Infrared Spectroscopy Data, *European Polymer Journal*, **91**: 429-435 (2017).

[48] Asgarpour Khansary M., Marjani A., Shirazian S., Prediction of Carbon Dioxide Sorption in Polymers for Capture and Storage Feasibility Analysis, *Chemical Engineering Research and Design*, **120**: 254-258 (2017).

[49] Ghadiri M., Shirazian S., Computational Simulation of Mass Transfer in Extraction of Alkali Metals by Means of Nanoporous Membrane Extractors, *Chemical Engineering and Processing: Process Intensification*, **69**: 57-62 (2013).

[50] Ghasemi A., Asgarpour Khansary M., Marjani A., Shirazian S., Using Quantum Chemical Modeling and Calculations for Evaluation of Cellulose Potential for Estrogen Micropollutants Removal From Water Effluents, *Chemosphere*, **178**: 411-423 (2017).

[51] Hemmati M., Nazari N., Hemmati A., Shirazian S., Phenol Removal from Wastewater by Means of Nanoporous Membrane Contactors, *Journal of Industrial and Engineering Chemistry*, **21**: 1410-1416 (2015).

[52] Khansary M.A., Marjani A., Shirazian S., On the Search of Rigorous Thermo-Kinetic Model for Wet Phase Inversion Technique, *Journal of Membrane Science*, **538**: 18-33 (2017).

[53] Khansary M.A., Sani A.H., Shirazian S., Mathematical-Thermodynamic Solubility Model Developed by the Application of Discrete Volterra Functional Series Theory, *Fluid Phase Equilibria*, **385**: 205-211 (2015).

[54] Razavi S.M.R., Rezakazemi M., Albadarin A.B., Shirazian S., Simulation of CO_2 Absorption by Solution of Ammonium Ionic Liquid in Hollow-Fiber Contactors, *Chemical Engineering and Processing: Process Intensification*, **108**: 27-34 (2016).

[55] Razavi S.M.R., Shirazian S., Nazemian M., Numerical Simulation of CO_2 Separation From Gas Mixtures in Membrane Modules: Effect of Chemical Absorbent, *Arabian Journal of Chemistry*, **9**: 62-71 (2016).

[56] Rezakazemi M., Dashti A., Asghari M., Shirazian S., H_2-Selective Mixed Matrix Membranes Modeling Using ANFIS, PSO-ANFIS, GA-ANFIS, *International Journal of Hydrogen Energy*, **42**(22): 15211-15225 (2017).

[57] Shirazian S., Ashrafizadeh S.N., Synthesis of Substrate-Modified LTA Zeolite Membranes for Dehydration of Natural Gas, *Fuel*, **148**: 112-119 (2015).

[58] Shirazian S., Ashrafizadeh S.N., LTA and Ion-Exchanged LTA Zeolite Membranes for Dehydration of Natural Gas, *Journal of Industrial and Engineering Chemistry*, **22**: 132-137 (2015).

[59] Sajjia M., Shirazian S., Egan D., Iqbal J., Albadarin A.B., Southern M., Walker G., Mechanistic Modelling of Industrial-Scale Roller Compactor 'Freund TF-MINI Model, *Computers & Chemical Engineering*, **104**: 141-150 (2017).

[60] Shirazian S., Kuhs M., Darwish S., Croker D., Walker G.M., Artificial Neural Network Modelling of Continuous Wet Granulation Using a Twin-Screw Extruder, *International Journal of Pharmaceutics*, **521**: 102-109 (2017).

[61] Marjani A., Khansary M.A., Shirazian S., Development and Validation of a Graphical Sorption Model: Application to Sorption of Organic Liquids Into Low Density Polyethylene Polymeric Membrane, *Asia-Pacific Journal of Chemical Engineering*, In Press.

[62] Rezakazemi M., Marjani A., Shirazian S., Development of a Group Contribution Method Based on UNIFAC Groups for the Estimation of Vapor Pressures of Pure Hydrocarbon Compounds, *Chemical Engineering & Technology*, **36**: 483-491 (2013).

[63] Sajjia M., Shirazian S., Kelly C.B., Albadarin A.B., Walker G., ANN Analysis of a Roller Compaction Process in the Pharmaceutical Industry, *Chemical Engineering & Technology*, **40**: 487-492 (2017).

[64] Shirazian S., Ashrafizadeh S.N., 3D Modeling and Simulation of Mass Transfer in Vapor Transport through Porous Membranes, *Chemical Engineering & Technology*, **36**: 177-185 (2013).

[65] Ghadiri M., Marjani A., Shirazian S., Mathematical Modeling and Simulation of CO_2 Stripping From Monoethanolamine Solution Using Nano Porous Membrane Contactors, *International Journal of Greenhouse Gas Control*, **13**: 1-8 (2013).

[66] Rezakazemi M., Shahverdi M., Shirazian S., Mohammadi T., Pak A., CFD Simulation of Water Removal From Water/Ethylene Glycol Mixtures by Pervaporation, *Chemical Engineering Journal*, **168**: 60-67 (2011).

[67] Shirazian S., Ashrafizadeh S.N., 3D Modeling and Simulation of Mass Transfer in Vapor Transport through Porous Membranes, *Chemical Engineering and Technology*, **36**: 177-185 (2013).

[68] Bird R.B., Stewart W.E., Lightfoot E.N., "Transport Phenomena", Revised 2nd Edition, Wiley (2007).

[69] Rezakazemi M., Ghafarinazari A., Shirazian S., Khoshsima A., Numerical Modeling and Optimization of Wastewater Treatment Using Porous Polymeric Membranes, *Polymer Engineering and Science*, **53**: 1272-1278 (2013).

[70] Al-Marzouqi M.H., El-Naas M.H., Marzouk S.A.M., Al-Zarooni M.A., Abdullatif N., Faiz R., Modeling of CO_2 Absorption in Membrane Contactors, *Separation and Purification Technology*, **59**: 286-293 (2008).

[71] Shavit U., Bar-Yosef G., Rosenzweig R., Assouline S., Modified Brinkman Equation for a Free Flow Problem at the Interface of Porous Surfaces: The Cantor-Taylor Brush Configuration Case, *Water Resources Research*, **38**: 1320-1334 (2002).

[72] Shavit U., Rosenzweig R., Assouline S., Free Flow at the Interface of Porous Surfaces: A Generalization of the Taylor Brush Configuration, *Transport in Porous Media*, **54**: 345-360 (2004).

[73] Abdullah N.S., Das D.B., Ye H., Cui Z.F., 3D bone Tissue Growth in Hollow Fibre Membrane Bioreactor: Implications of Various Process Parameters on Tissue Nutrition, *The International Journal of Artificial Organs*, **29**: 841-851 (2006).

[74] Shirazian S., Ashrafizadeh S.N., Mass Transfer Simulation of Carbon Dioxide Absorption in a Hollow-Fiber Membrane Contactor, *Separation Science and Technology*, **45**: 515-524 (2010).

[75] Ye H., Das D.B., Triffitt J.T., Cui Z., Modelling Nutrient Transport in Hollow Fibre Membrane Bioreactors for Growing Three-Dimensional Bone Tissue, *Journal of Membrane Science*, **272**: 169-178 (2006).

[76] Abdullah N.S., Das D.B., Modelling Nutrient Transport in Hollow Fibre Membrane Bioreactor for Growing Bone Tissue with Consideration of Multi-Component Interactions, *Chemical Engineering Science*, **62**: 5821-5839 (2007).

[77] Shirazian S., Ashrafizadeh S.N., Mass Transfer Simulation of Caffeine Extraction by Subcritical CO2 in a Hollow-Fiber Membrane Contactor, *Solvent Extraction and Ion Exchange*, **28**: 267-286 (2010).

[78] Shirazian S., Ashrafizadeh S.N., Near-Critical Extraction of the Fermentation Products by Membrane Contactors: A Mass Transfer Simulation, *Industrial and Engineering Chemistry Research*, **50**: 2245-2253 (2011).