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ORIGINAL ARTICLE

Modeling and simulation of membrane separation process using computational fluid dynamics

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Abstract Separation of CO_2 from air was simulated in this work. The considered process for removal of CO_2 was a hollow-fiber membrane contactor and an aqueous solution of 2-amino-2-metyl-1-propanol (AMP) as absorbent. The model was developed based on mass transfer as well as chemical reaction for CO_2 and solvent in the contactor. The equations of model were solved using finite element method. Simulation results were compared with experimental data, and good agreement was observed. The results revealed that increasing solvent velocity enhances removal of CO_2 in the hollow-fiber membrane contactor. Moreover, it was found that counter-current process mode is more favorable to achieve the highest separation efficiency.

1. Introduction

Design and development of novel separation processes for reduction of emissions of carbon dioxide as the major greenhouse gas is of great importance. It has been reported that emission of CO_2 in atmosphere has adverse environmental effects such as global warming. Therefore, there is a definite need for development of efficient and novel separation processes for removal of CO_2 from gas streams. The main criteria for development of efficient separation processes for capture of carbon dioxide include consumption of low energy and high removal rate (Le Moullec et al., 2014; Razavi et al., 2013; Shirazian et al., 2012a). Currently, gas absorption is the most commonly used method for removal of CO_2 from gas streams which is used extensively at industrial scale. The process involves selective absorption of CO_2 into chemical solvents such as aqueous solutions of NaOH or amines.

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Nomenclature

a	inner radius of fiber (m)	D	diffusion coefficient (m^2/s)
b	outer radius of fiber (m)	D_{CO2}	diffusion coefficient of CO_2 (m^2/s)
c	radius of free surface (m)	L	length of fiber (m)
C	concentration (mol/m^3)	m	partition coefficient
C_{gas}	CO_2 concentration in the gas phase (mol/m^3)	p	pressure (Pa)
C_m	CO_2 concentration inside the membrane (mol/m^3)	T	temperature (K)
C_0	inlet concentration of CO_2 in the gas phase (mol/m^3)	r	radial distance (m)
		z	axial distance (m)

Gas absorption is carried out using conventional contactors such as columns and towers in which some usual technical problems are encountered in these contactors. The most common encountered problems in conventional contactors include flooding, foaming, entraining, and channeling (Shirazian and Ashrafizadeh, 2010; Shirazian et al., 2011, 2012b; Sohrabi et al., 2011a,b). These problems detract efficiency of CO_2 capture using conventional separation processes. Therefore, development of alternative separation processes for removal of CO_2 from gas mixtures is of great importance.

Membrane technology can be used for CO_2 capture. CO_2 removal using membrane technology can be accomplished either by porous or by nonporous membranes. Nonporous membranes are usually polymeric which provide low permeation flux. Porous membranes can be used for removal of CO_2 from gas mixtures in which high permeation flux can be obtained that enhances the efficiency of process (Moghadassi et al., 2011; Sohrabi et al., 2011c,d). One of important membrane processes which can be used for CO_2 capture is membrane contactor. Membrane contactors are porous membranes which are used to keep in contact two specific phases such as gas–liquid or liquid–liquid (Gabelman and Hwang, 1999; Mansourizadeh and Ismail, 2009).

Membrane contactors can be used for absorption of CO_2 in which the problems of conventional contactors are not observed in membrane contactors. The most common and useful classes of membrane contactors are hollow-fiber membrane contactors. These novel devices have attracted much attention recently in separation of gas and liquid mixtures (Fadaei et al., 2011a; Fasihi et al., 2012; Ghadiri et al., 2012, 2013a,b,c, 2014; Ghadiri and Shirazian, 2013; Marjani et al., 2012a,b; Marjani and Shirazian, 2010). The main characteristic of hollow-fiber membrane contactors is provision of high surface area per unit volume for separation and reaction. The latter can increase the efficiency of process drastically which in turn makes the process attractive for CO_2 capture. In gas–liquid hollow-fiber membrane contactors, a feed gas is passed through one side while the chemical solvent is passed either co-currently or counter-currently in other side of membrane module.

The main aim of the present work was to develop a mass transfer model for description of CO_2 removal from air in a hollow-fiber membrane contactor. Aqueous solution of 2-amino-2-metyl-1-propanol (AMP) is considered as chemical solvent in the simulations. Computational fluid dynamic technique is used for numerical simulation, and the results of simulations are then compared with the experimental data reported in the literature.

2. Theory

The separation process studied in this work involves a microporous hollow-fiber membrane contactor, a feed gas containing CO_2 and N_2, and an aqueous solution of 2-amino-2-metyl-1-propanol (AMP). The gas mixture flows through the shell side of membrane contactor while the AMP solution is passed through the tube side (see Fig. 1). A gas–liquid interface is formed at the inner side of fiber due to the hydrophobicity of membrane. The latter means that the aqueous solution cannot wet the membrane pores and the membrane pores are filled by the gas phase. The characteristics of the hollow-fiber contactor and operational conditions are the same as those reported in the literature (Kim and Yang, 2000).

A single hollow fiber is considered as model domain in the simulations. The geometry of model is illustrated in Fig. 1. It should be pointed out that the equations of model are derived in cylindrical coordinate while axial symmetry is assumed.

2.1. Equations of gas phase

In the gas phase, feed containing CO_2 and N_2 is contacted with the solvent. Concentration distribution of CO_2 in the gas phase is obtained by numerical solution of mass transfer equation:

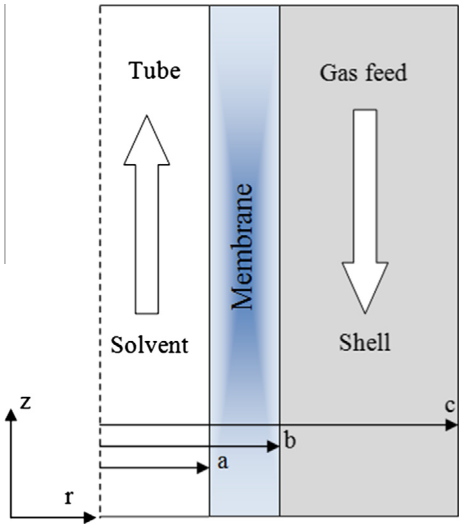

Figure 1 Geometry of hollow-fiber considered in modeling and simulation.

$$D_{gas-Shell}\left[\frac{\partial^2 C_{gas-Shell}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{gas-Shell}}{\partial r}+\frac{\partial^2 C_{gas-Shell}}{\partial z^2}\right] = V_{z-Shell}\frac{\partial C_{gas-Shell}}{\partial z} \quad (1)$$

where D, C, and V are diffusivity (m^2/s), concentration (mol/m^3), and velocity (m/s) respectively. Velocity distribution of gas phase is calculated by the Navier–Stokes equations:

$$-\nabla.\eta\left(\nabla V_{z-Shell}+(\nabla V_{z-Shell})^T\right)+\rho(V_{z-Shell}.\nabla)V_{z-Shell}+\nabla p=0$$
$$\nabla.V_{z-Shell}=0 \quad (2)$$

where η, ρ, and p denote viscosity (Pa s), density (kg/m^3), and pressure (Pa) of gas mixture respectively.

Therefore, simultaneous solution of mass transfer and the Navier–Stokes equations should be carried out to obtain concentration distribution of CO_2 in the shell side of membrane contactor. Boundary conditions for the shell side are listed in Table 1.

2.2. Equations of solvent phase

Concentration distribution of either CO_2 or absorbent (AMP) in the tube side of membrane contactor is obtained by solution of mass transfer equation as follows:

$$D_{i-tube}\left[\frac{\partial^2 C_{i-tube}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{i-tube}}{\partial r}+\frac{\partial^2 C_{i-tube}}{\partial z^2}\right] = V_{z-tube}\frac{\partial C_{i-tube}}{\partial z}-R_i \quad (3)$$

where R refers to chemical reaction rate between CO_2 and AMP (mol/m^3 s), and i refers to either AMP or CO_2. The velocity of solvent phase is estimated using parabolic laminar flow:

$$V_{z-tube}=2u\left[1-\left(\frac{r}{a}\right)^2\right] \quad (4)$$

where u is average velocity of solvent phase (m/s), and a is the inner radius of fiber (m).

Boundary conditions for mass transfer of CO_2 and AMP in the tube side are listed in Table 2. Moreover, the reaction mechanism and kinetics between CO_2 and AMP are taken from the literature (Kim and Yang, 2000).

2.3. Equations of membrane

The mass transfer equation for CO_2 inside the membrane may be written as:

$$D_{gas-membrane}\left[\frac{\partial^2 C_{gas-membrane}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{gas-membrane}}{\partial r}+\frac{\partial^2 C_{gas-membrane}}{\partial z^2}\right]=0 \quad (5)$$

Table 1 Boundary conditions for gas phase.

Position	Navier–Stokes	Mass transfer
$z = L$	$V_{z\text{-}shell} = V_0$	$C_{gas\text{-}shell} = C_{gas,0}$
$z = 0$	$p = p_{atm}$	Convective flux
$r = c$	$V_{z\text{-}shell} = 0$	$\partial C_{gas\text{-}shell}/\partial r = 0$
$r = b$	$V_{z\text{-}shell} = 0$	$C_{gas\text{-}shell} = C_{gas\text{-}membrane}$

Table 2 Boundary conditions for solvent phase.

Position	CO_2	AMP
$z = 0$	$C_{gas} = 0$	$C_{AMP\text{-}tube} = C_{M0}$
$z = L$	Convective flux	Convective flux
$r = 0$	$\frac{\partial C_{gas-Tube}}{\partial r} = 0$	$\frac{\partial C_{AMP-tube}}{\partial r} = 0$
$r = a$	$C_{gas\text{-}tube} = C_{gas\text{-}membrane} \times m$	$\frac{\partial C_{AMP-tube}}{\partial r} = 0$

The transport of CO_2 through the membrane pores is postulated to be due to diffusion. Boundary conditions for membrane are given as:

$$\text{At} \quad r=a, C_{gas-membrane}=C_{gas-tube}/m \quad (6)$$

$$\text{At} \quad r=b, C_{gas-membrane}=C_{gas-shell} \quad (7)$$

where m refers to partition coefficient for CO_2 between gas and liquid which the value is taken from the literature (Kim and Yang, 2000).

The derived equations as well as boundary conditions for all sections of membrane contactor were solved using COMSOL Multiphysics 3.5 package. Finite element is the basic solution procedure which COMSOL utilizes for numerical solution of the model equations. The accuracy of this numerical procedure for simulation of membrane separation processes has been proved in the literature (Razavi et al., 2013; Fadaei et al., 2011a; Fasihi et al., 2012; Ghadiri et al., 2012, 2013a,b,c, 2014; Ghadiri and Shirazian, 2013; Marjani et al., 2012b; Marjani and Shirazian, 2010; Fadaei et al., 2012; Fadaei et al., 2011b; Kohnehshahri et al., 2011; Marjani and Shirazian, 2011a,b,c,d,e, 2012a,b,c,d,e; Marjani et al., 2012c; Moradi et al., 2013; Pishnamazi et al., 2012; Ranjbar et al., 2013; Razavi et al., 2014; Rezakazemi et al., 2013a,b).

3. Results and discussion

3.1. Validation of simulation results

The model findings for removal of CO_2 from N_2 using AMP as solvent in a hollow-fiber membrane contactor were compared with the experimental data reported in the literature to validate the model (Kim and Yang, 2000). The comparisons were conducted between simulated and experimental CO_2 removal at different values of solvent flow rates as indicated in Fig. 2. As it is seen from Fig. 2, enhancement of solvent flow rate (velocity) in membrane contactor results in increasing the removal rate of CO_2. The latter could be due to increasing driving force between gas and liquid phases with increasing solvent velocity. Moreover, Fig. 2 reveals that the model predictions are in good agreement with the experimental data at different values of solvent velocities in the module, and an average deviation of less than 10% was calculated between experimental and simulation results.

3.2. Concentration of CO_2

Concentration distribution of CO_2 in the gas phase is the most important parameter for optimization of process. Decreasing CO_2 concentration in the gas phase determines the removal

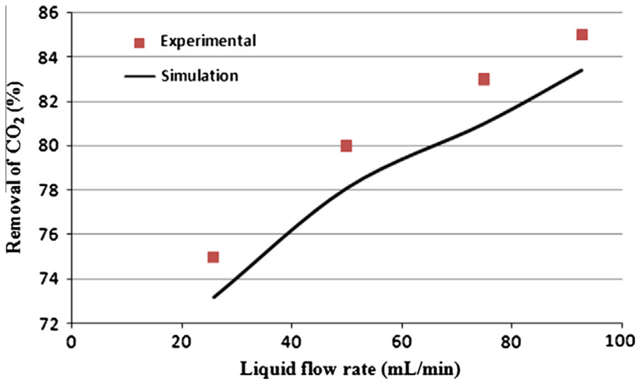

Figure 2 Comparisons between simulation results and experimental data.

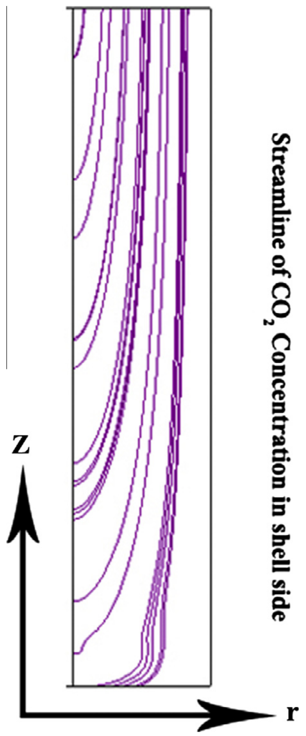

Figure 3 Streamline of CO_2 concentration in the gas phase.

rate of CO_2 using the hollow-fiber membrane contactor. Streamline of CO_2 concentration in the gas phase is shown in Fig. 3. Streamlines show the path of CO_2 transport in the shell side. As it is seen, CO_2 is transferred toward the membrane due to concentration gradient in radial direction. However, a portion of CO_2 is also transferred to the outlet of shell side (axial direction). Fig. 4 also shows total mass transfer flux of CO_2 in all subdomains of membrane contactor. The mass transfer flux in the shell and tube sides is composed of diffusion and convection. The convection mechanism tends to transfer CO_2 to the outlet of contactor due to high contribution of velocity in *z*-direction. CO_2 is transferred toward the membrane by diffusional mass transfer which is responsible for removal of CO_2.

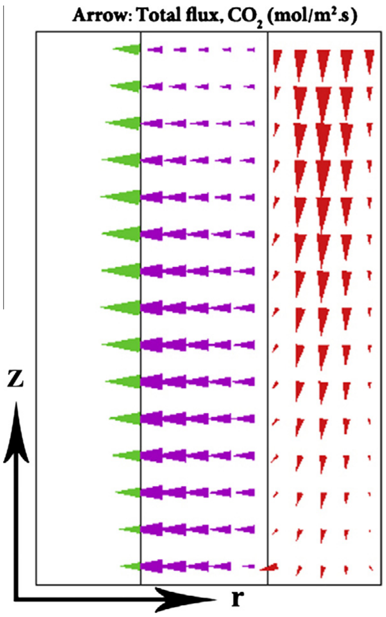

Figure 4 Distribution of total mass transfer flux of CO_2 in the membrane contactor.

3.3. Effect of flow pattern on CO_2 absorption

In the previous section the direction of both streams in simulation was considered to be counter-current, and it was evaluated according to different parameters. In this section the influence of co-current mode on the percent of CO_2 removal rate has been studied (see Table 3) to explore the possibility of co-current operation and compare it with counter-current mode. Comparing these results reveals that the percentage of CO_2 removal from N_2 in membrane module when the direction of streams is counter-current is more than the co-current mode. The latter could be attributed to the higher concentration gradient between two phases in the case of counter-current mode.

3.4. Influence of AMP concentration on CO_2 removal

Fig. 5 illustrates the influence of AMP concentration on CO_2 removal. As it can be seen from Fig. 5, enhancement of absorbent content in the solvent phase increases CO_2 removal in membrane module which is favorable in gas absorption. It should be noted that because the reaction of absorbent and carbon dioxide is assumed to be elementary, it is proportional to concentration of both absorbent and CO_2 in the membrane contactor. Increasing absorbent concentration in the liquid phase enhances reaction rate between CO_2 and absorbent. The latter would result in reduction of CO_2 outlet concentration in the gas phase. The results also reveal that AMP concentration has considerable effect on CO_2 removal from gas mixtures.

3.5. Mass transfer flux of AMP

Absorbent concentration in the tube side of membrane contactor is illustrated as contours in Fig. 6. It is seen that the

Table 3 Comparison of CO_2 removal results between co-current flow and counter-current flow modes.

Removal of CO_2 (%)		Inlet conditions		
With co-current flow	With counter-current flow	CO_2 concentration (vol.%)	Liquid flow rate (ml/min)	Gas flow rate (ml/min)
38	73.2	40	25.8	170
43.3	78.1	40	50	170
46.5	81	40	75	170
49.9	83.4	40	92.8	170

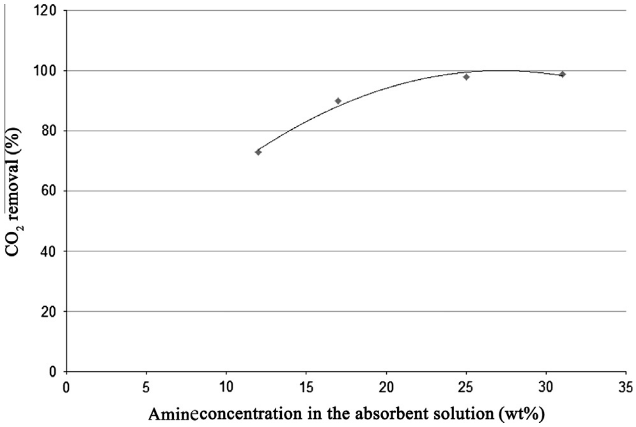

Figure 5 Removal of CO_2 as a function of amine concentration.

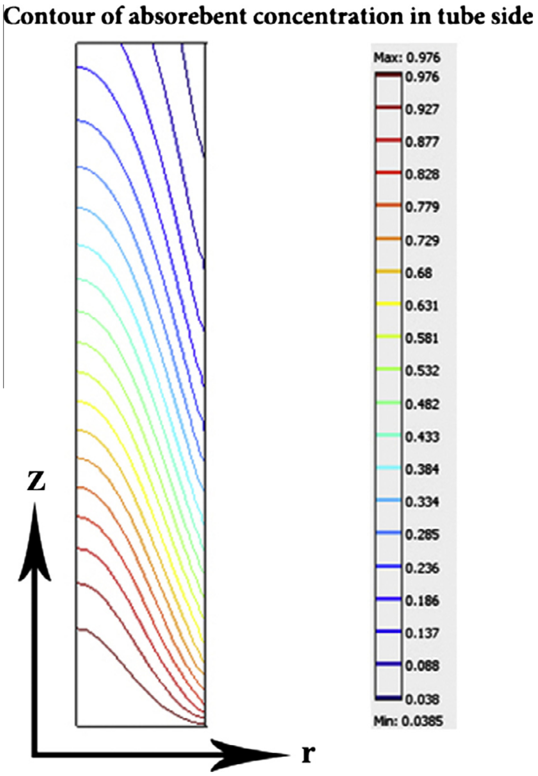

Figure 6 Contours of absorbent concentration.

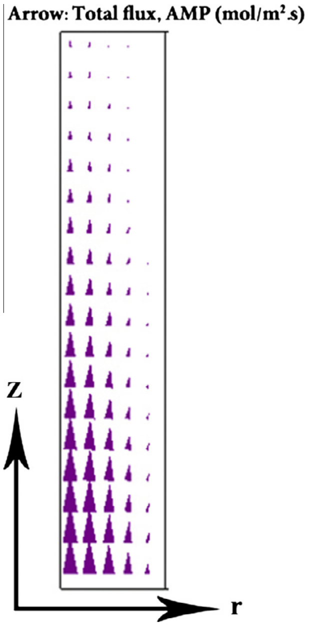

Figure 7 Distribution of total mass transfer flux of absorbent in the liquid phase.

concentration of AMP decreases drastically along the tube side of membrane contactor. The latter could be due to high reaction rate between CO_2 and AMP which results in high consumption of AMP in the process. This can increase the efficiency of process, but increases the cost of separation by consumption of absorbent. Total mass transfer flux of AMP in the tube side is also shown in Fig. 7. The highest mass transfer flux of AMP can be seen at the region near the inlet of tube. As AMP flows in the tube side, its mass transfer flux decreases due to chemical reaction with CO_2.

4. Conclusions

Separation of CO_2 from N_2 as model of air in a hollow-fiber membrane module was studied theoretically in this work. The simulations were based on numerical solution of mass transfer as well as the Navier–Stokes equations for species in the membrane module. FEM analysis was used to solve the governing equations. Amine (AMP) aqueous solution was considered as chemical solvent in the simulations. The simulation results were validated thorough comparing with the experimental data for absorption of CO_2 in AMP aqueous solution. The simulation results were in good agreement with the experimental data for different liquid flow rates. The simulation results for absorption of CO_2 in AMP aqueous solution revealed that CO_2 removal rate increases with enhancement of solvent velocity and AMP concentration in the module. Moreover, the simulation results indicated that the CO_2

absorption in the membrane contactor with counter-current flow mode is higher than co-current mode.

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References

Fadaei, F., Shirazian, S., Ashrafizadeh, S.N., 2011a. Mass transfer simulation of solvent extraction in hollow-fiber membrane contactors. Desalination 275, 126–132.

Fadaei, F., Shirazian, S., Ashrafizadeh, S.N., 2011b. Mass transfer modeling of ion transport through nanoporous media. Desalination 281, 325–333.

Fadaei, F., Hoshyargar, V., Shirazian, S., Ashrafizadeh, S.N., 2012. Mass transfer simulation of ion separation by nanofiltration considering electrical and dielectrical effects. Desalination 284, 316–323.

Fasihi, M., Shirazian, S., Marjani, A., Rezakazemi, M., 2012. Computational fluid dynamics simulation of transport phenomena in ceramic membranes for SO_2 separation. Math. Comput. Model. 56, 278–286.

Gabelman, A., Hwang, S.-T., 1999. Hollow fiber membrane contactors. J. Membr. Sci. 159, 61–106.

Ghadiri, M., Shirazian, S., 2013. Computational simulation of mass transfer in extraction of alkali metals by means of nanoporous membrane extractors. Chem. Eng. Process. 69, 57–62.

Ghadiri, M., Shirazian, S., Ashrafizadeh, S.N., 2012. Mass transfer simulation of gold extraction in membrane extractors. Chem. Eng. Technol. 35, 2177–2182.

Ghadiri, M., Fakhri, S., Shirazian, S., 2013a. Modeling and CFD simulation of water desalination using nanoporous membrane contactors. Ind. Eng. Chem. Res. 52, 3490–3498.

Ghadiri, M., Ghasemi Darehnaei, M., Sabbaghian, S., Shirazian, S., 2013b. Computational simulation for transport of priority organic pollutants through nanoporous membranes. Chem. Eng. Technol. 36, 507–512.

Ghadiri, M., Marjani, A., Shirazian, S., 2013c. Mathematical modeling and simulation of CO_2 stripping from monoethanolamine solution using nano porous membrane contactors. Int. J. Greenhouse Gas Control 13, 1–8.

Ghadiri, M., Fakhri, S., Shirazian, S., 2014. Modeling of water transport through nanopores of membranes in direct–contact membrane distillation process. Polym. Eng. Sci. 54, 660–666.

Kim, Y.-S., Yang, S.-M., 2000. Absorption of carbon dioxide through hollow fiber membranes using various aqueous absorbents. Sep. Purif. Technol. 21, 101–109.

Kohnehshahri, R.K., Salimi, M., Mohaddecy, S.R.S., Shirazian, S., 2011. Modeling and numerical simulation of catalytic reforming reactors. Orient. J. Chem. 27, 1351–1355.

Le Moullec, Y., Neveux, T., Al Azki, A., Chikukwa, A., Hoff, K.A., 2014. Process modifications for solvent-based post-combustion CO2 capture. Int. J. Greenhouse Gas Control 31, 96–112.

Mansourizadeh, A., Ismail, A.F., 2009. Hollow fiber gas–liquid membrane contactors for acid gas capture: a review. J. Hazard. Mater. 171, 38–53.

Marjani, A., Shirazian, S., 2010. CFD simulation of dense gas extraction through polymeric membranes. World Acad. Sci. Eng. Technol. 37, 1043–1047.

Marjani, A., Shirazian, S., 2011a. Simulation of heavy metal extraction in membrane contactors using computational fluid dynamics. Desalination 281, 422–428.

Marjani, A., Shirazian, S., 2011b. Hydrodynamic investigations on heavy metal extraction in membrane extractors. Orient. J. Chem. 27, 1311–1316.

Marjani, A., Shirazian, S., 2011c. Investigation on copper extraction using numerical simulation. Asian J. Chem. 23, 3289–3290.

Marjani, A., Shirazian, S., 2011d. Investigation on numerical simulation of acetone and ethanol separation from water by using membrane. Asian J. Chem. 23, 3293–3294.

Marjani, A., Shirazian, S., 2011e. Computational fluid dynamics simulation of ammonia removal from wastewaters by membrane. Asian J. Chem. 23, 3299–3300.

Marjani, A., Shirazian, S., 2012a. CFD simulation of mass transfer in membrane evaporators for concentration of aqueous solutions. Orient. J. Chem. 28, 83–87.

Marjani, A., Shirazian, S., 2012b. Modeling of organic mixtures separation in dense membranes using finite element method (FEM). Orient. J. Chem. 28, 41–46.

Marjani, A., Shirazian, S., 2012c. Application of CFD techniques for prediction of NH_3 transport through porous membranes. Orient. J. Chem. 28, 67–72.

Marjani, A., Shirazian, S., 2012d. Theoretical studies on copper extraction by means of polymeric membrane contactors. Orient. J. Chem. 28, 23–28.

Marjani, A., Shirazian, S., 2012e. Mathematical modeling and CFD simulation of hydrocarbon purification using membrane technology. Orient. J. Chem. 28, 123–129.

Marjani, A., Mohammadi, P., Shirazian, S., 2012a. Preparation and characterization of poly (vinyl alcohol) membrane for pervaporation separation of water-organic mixtures. Orient. J. Chem. 28, 97–102.

Marjani, A., Rezakazemi, M., Shirazian, S., 2012b. Simulation of methanol production process and determination of optimum conditions. Orient. J. Chem. 28, 145–151.

Marjani, A., Shirazian, S., Ranjbar, M., Ahmadi, M., 2012c. Mathematical modeling of gas separation in flat-sheet membrane contactors. Orient. J. Chem. 28, 13–18.

Moghadassi, A., Marjani, A., Shirazian, S., Moradi, S., 2011. Gas separation properties of hollow-fiber membranes of polypropylene and polycarbonate by melt-spinning method. Asian J. Chem. 23, 1922–1924.

Moradi, S., Rajabi, Z., Mohammadi, M., Salimi, M., Homami, S.S., Seydei, M.K., Shirazian, S., 2013. 3 dimensional hydrodynamic analysis of concentric draft tube airlift reactors with different tube diameters. Math. Comput. Model. 57, 1184–1189.

Pishnamazi, M., Marjani, A., Shirazian, S., Samipurgiri, M., 2012. Mathematical modeling and numerical simulation of wastewater treatment unit using CFD. Orient. J. Chem. 28, 51–58.

Ranjbar, M., Shirazian, S., Ghafarnejad Parto, S., Ahmadi, M., 2013. Computational fluid dynamics simulation of mass transfer in the separation of fermentation products using nanoporous membranes. Chem. Eng. Technol. 36, 728–732.

Razavi, S.M.R., Razavi, S.M.J., Miri, T., Shirazian, S., 2013. CFD simulation of CO_2 capture from gas mixtures in nanoporous membranes by solution of 2-amino-2-methyl-1-propanol and piperazine. Int. J. Greenhouse Gas Control 15, 142–149.

Razavi, S.M.R., Shirazian, S., Najafabadi, M.S., 2014. Investigations on the ability of di-isopropanol amine solution for removal of CO_2 from natural gas in porous polymeric membranes. Polym. Eng. Sci.

Rezakazemi, M., Ghafarinazari, A., Shirazian, S., Khoshsima, A., 2013a. Numerical modeling and optimization of wastewater treatment using porous polymeric membranes. Polym. Eng. Sci. 53, 1272–1278.

Rezakazemi, M., Iravaninia, M., Shirazian, S., Mohammadi, T., 2013b. Transient computational fluid dynamics modeling of pervaporation separation of aromatic/aliphatic hydrocarbon mixtures using polymer composite membrane. Polym. Eng. Sci. 53, 1494–1501.

Shirazian, S., Ashrafizadeh, S.N., 2010. Mass transfer simulation of carbon dioxide absorption in a hollow-fiber membrane contactor. Sep. Sci. Technol. 45, 515–524.

Shirazian, S., Marjanm, A., Azizmohammadi, F., 2011. Prediction of SO_2 transport across ceramic membranes using finite element method (FEM). Orient. J. Chem. 27, 485–490.

Shirazian, S., Marjani, A., Rezakazemi, M., 2012a. Separation of CO_2 by single and mixed aqueous amine solvents in membrane contactors: fluid flow and mass transfer modeling. Eng. Comput. 28, 189–198.

Shirazian, S., Rezakazemi, M., Marjani, A., Rafivahid, M.S., 2012b. Development of a mass transfer model for simulation of sulfur dioxide removal in ceramic membrane contactors. Asia-Pac. J. Chem. Eng. 7, 828–834.

Sohrabi, M.R., Marjani, A., Moradi, S., Davallo, M., Shirazian, S., 2011a. Theoretical studies on membrane-based gas separation using Computational Fluid Dynamics (CFD) of mass transfer. J. Chem. Soc. Pak. 33, 464–473.

Sohrabi, M.R., Marjani, A., Moradi, S., Davallo, M., Shirazian, S., 2011b. Mathematical modeling and numerical simulation of CO_2 transport through hollow-fiber membranes. Appl. Math. Model. 35, 174–188.

Sohrabi, M.R., Marjani, A., Moradi, S., Davallo, M., Shirazian, S., 2011c. Preparation and simulation of polycarbonate hollow-fiber membrane for gas separation. Asian J. Chem. 23, 302–304.

Sohrabi, M.R., Marjani, A., Moradi, S., Davaloo, M., Shirazian, S., 2011d. Simulation studies on H_2S absorption in potassium carbonate aqueous solution using a membrane module. Asian J. Chem. 23, 4227–4228.