International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:5, No:10, 2011

CFD Simulation of SO_2 Removal from gas Mixtures using Ceramic Membranes

Azam Marjani*, Saeed Shirazian

***Abstract*—**This work deals with modeling and simulation of SO_2 removal in a ceramic membrane by means of FEM. A mass transfer model was developed to predict the performance of SO_2 absorption in a chemical solvent. The model was based on solving conservation equations for gas component in the membrane. Computational fluid dynamics (CFD) of mass and momentum were used to solve the model equations. The simulations aimed to obtain the distribution of gas concentration in the absorption process. The effect of the operating parameters on the efficiency of the ceramic membrane was evaluated. The modeling findings showed that the gas phase velocity has significant effect on the removal of gas whereas the liquid phase does not affect the SO_2 removal significantly. It is also indicated that the main mass transfer resistance is placed in the membrane and gas phase because of high tortuosity of the ceramic membrane.

***Keywords*—**Gas separation; Finite element; Ceramic; Sulfur dioxide; Simulation

I. Introduction

NOWADAYS, capture of greenhouse gases is a subject of great interest in research community. Greenhouse gases have adverse effects on human life and health. Among adverse gases, sulfur dioxide (SO2) has been known as a highly reactive gas. This gas is emitted mostly from fossil fuel combustion at power plants (73%) and other industrial facilities (20%). Other sources of SO_2 emissions are industrial processes such as extracting metal from ore, and the burning of high sulfur containing fuels. SO_2 has a number of adverse effects on human health [1].

Capture of SO_2 by selective absorption into a solvent is a common method to reduce the amount of SO2. The current sulfur dioxide (SO_2) separation processes are based on physical and chemical processes. The separation of SO_2 through ordinary processes experiences a number of shortcomings such as channeling, flooding, entraining, foaming, and also high capital and operating costs [2-5]. Some studies have been conducted to evaluate the possibilities of enhancing the efficiency of the latter processes to overcome the problems. New recently, the gas-liquid membrane contactors as gas absorption devices have become a subject of interest. In these devices, the membrane contactor acts as a physical barrier between the two phases, i.e. gas and liquid.

Extensive researches about the gas-liquid membrane contactors have been conducted since Qi and Cussler first studied these contactors [6]. They used a hollow-fiber membrane contactor for absorption of CO2. After that, Kreulen et al. [7] investigated the chemical absorption of CO_2 into water/glycerol liquid mixtures as absorbent. All studies have been conducted on CO_2 absorption in polymeric membrane contactors. A few studies have been done on ceramic membrane contactors. In industrial applications, harsh feed conditions or high temperature operations precludes the use of polymeric membranes. The main advantage of ceramic membranes compared with polymeric membranes is the thermal and chemical resistance of the ceramic membranes which makes these membranes favorable for industrial applications. Recently a few experimental studies have been carried out for SO_2 absorption [8-9]. Luis et al. [8-9] studied absorption of SO_2 in N,N-dimethylaniline as absorbent using alumina membrane contactor. The studies have focused on experiments and there is shortage of a comprehensive model for prediction of gas transport through ceramic membrane contactors [10].The main objective of the present study is to develop and solve a 2-dimensional mathematical model to predict the SO_2 absorption through a tubular ceramic membrane contactor.To insert images in Word, position the cursor at the insertion point and either use Insert | Picture | From File or copy the image to the Windows clipboard and then Edit | Paste Special | Picture (with “Float over text” unchecked).

II. Theory

A. Mass transfer model

The mass transfer model is developed for a tubular membrane, as shown in Fig. 1. The liquid absorbent flows with a laminar velocity in the tube and the gas mixture containing SO_2 and air flows counter currently through the shell side. So, the membrane contactor consists of three sections: tube side, membrane, and shell side. The steady state two-dimensional material balances are carried out for all three sections of the contactor.

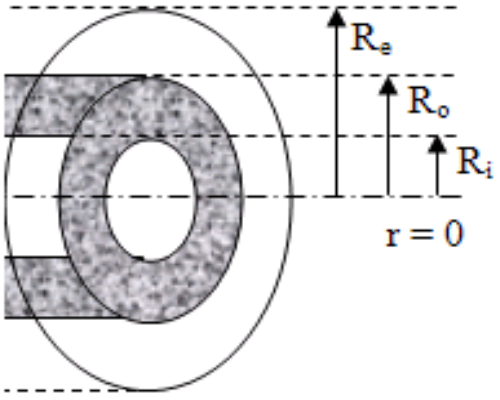

Fig. 1 Model domain for a tubular ceramic membrane

*Department of Chemistry, Arak Branch, Islamic Azad University-Arak-Iran
Corresponding author: a-marjani@iau-arak.ac.ir

The dimension of the free surface can be estimated by Happel's free surface model [11]:

$$R_e = \left(\frac{1}{1-\varphi}\right)^{1/2} R_o \quad (1)$$

φ is the volume fraction of the void. It can be calculated as follows [11]:

$$1-\varphi = \frac{nR_o^2}{R^2} \quad (2)$$

where n is the number of membranes and R is the module inner radius.

The continuity equation for steady state for **SO_2** transport in the shell side of the membrane contactor is obtained using Fick's law of diffusion for estimation of diffusive flux [12]:

$$-D_{SO2-air}\nabla.\left(\nabla C_{SO2-g}\right)+\nabla.\left(C_{SO2-g}V_{z-g}\right)=0 \quad (3)$$

In a laminar flow, Navier-Stokes equations can be applied for the shell side [12]:

$$\rho\frac{\partial V_{z-g}}{\partial t}-\nabla\cdot\eta(\nabla V_{z-g}+(\nabla V_{z-g})^T)+\rho(V_{z-g}.\nabla)V_{z-g}+\nabla p=F$$
$$\nabla V_{z-g}=0 \quad (4)$$

where V, p, ρ and η denote the velocity vector, pressure, density of the fluid, and the dynamic viscosity, respectively.

For the tube side, mass transfer equation (continuity equation) is:

$$-D_{SO2-L}\nabla.\left(\nabla C_{SO2-L}\right)+\nabla.\left(C_{SO2-L}V_{z-L}\right)=0 \quad (5)$$

The velocity distribution in the tube side is assumed to follow Newtonian laminar flow [12]:

$$V_{z-L}=2\overline{V_L}\left[1-\left(\frac{r}{R_i}\right)^2\right] \quad (6)$$

The steady-state continuity equation for the transport of SO_2 inside the membrane, which is considered to be due to diffusion alone, may be written as:

$$-D_{SO2-m}\nabla.\left(\nabla C_{SO2-m}\right)=0 \quad (7)$$

When the membrane is filled with gas phase (non-wetted mode), there are three mass transfer resistances for transport of **SO_2** from gas phase to the liquid phase. These mass transfer resistances include transfer of sulfur dioxide from the bulk gas to the membrane wall; diffusion across the pores of the membrane to the membrane–absorbent interface; and dissolution into the liquid, where a chemical/physical change takes place.

B. Physical properties and numerical solution of the equations

The dimensions of the membrane contactor used for the numerical simulation are the same as those in Ref. 9. The density and the viscosity data for gas phase are those of air because of low concentration of sulfur dioxide in the gas mixture. The inlet concentration of **SO_2** in the gas phase for all cases is 5 vol%. The model equations related to the tube side, membrane, and shell side with the appropriate boundary conditions were solved using COMSOL Multiphysics software, which uses finite element method (FEM) for numerical solution of differential equations. The finite element analysis is combined with adaptive meshing and error control using stationary nonlinear numerical solver.

III. Results and Discussion

*A. Concentration distribution of **SO_2** across the membrane*

Fig. 2 illustrates the distribution of **SO_2** concentration inside the ceramic membrane. The ceramic membrane used in the simulations is porous and is the most important part of the membrane contactor. The ceramic membranes for gas separation are very tortuous and can provide high concentration difference across the membrane. As the **SO_2** flows through the shell side, it is transferred towards the membrane pores due to the concentration gradient. Significant concentration change across the ceramic membrane shows that the main concentration change occurs in the membrane side, i.e. main mass transfer resistance is located in this part. It is due to high tortuosity of the applied membrane which provides a long path for transport of SO_2 through the membrane pores.

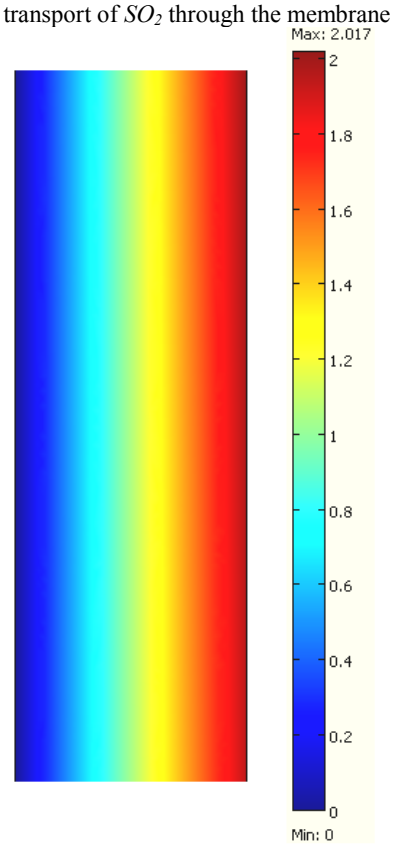

Fig. 2 Concentration distribution of SO_2 in the membrane. Gas flow rate = liquid flow rate = 1 L/min, T = 290K, Inlet SO_2 volume fraction = 5%.

B. SO_2 concentration distribution in the liquid phase

Fig. 3 indicates surface distribution of SO_2 concentration in the liquid phase. The concentration distribution is calculated through the developed model in the tube side of the membrane contactor where the liquid absorbent flows. The gas phase flows from one side of the membrane contactor where the concentration of SO_2 is the highest, whereas the absorbent flows from the other side where the concentration of SO_2 is assumed to be zero. At the membrane-liquid phase interface, the absorbed SO_2 is transferred through the boundary layer of liquid phase. The formation of boundary layer near the membrane can be observed from Fig. 3 clearly. In the regions near the membrane surface, concentration gradient is great. High mass transfer flux occurs in these regions of tube because of higher driving force.

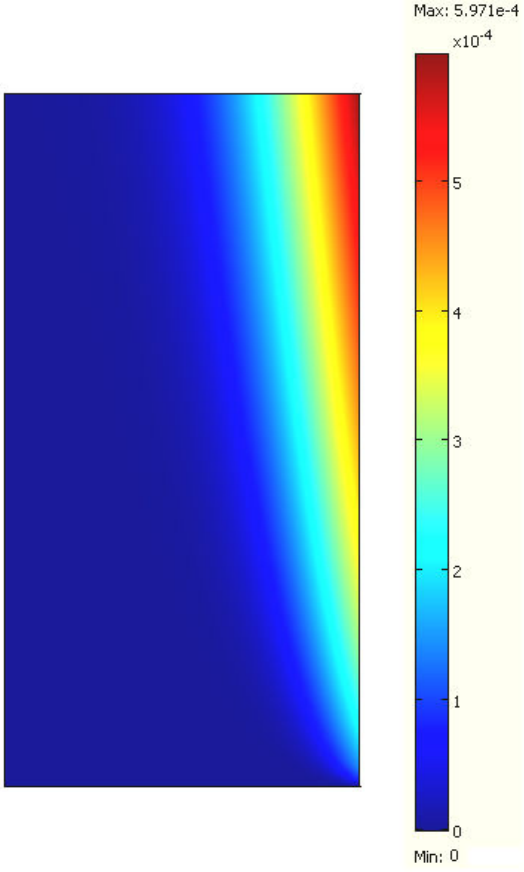

Fig. 3 Concentration distribution of SO_2 in the tube side. Gas flow rate = liquid flow rate = 1 L/min, T = 290K, Inlet SO_2 volume fraction = 5%.

C. Influence of liquid flow rate on SO_2 concentration profile in the liquid phase

Radial concentration profile of SO_2 in the tube side is shown in Fig. 4. At the zones near the tube center (r = 0), SO_2 concentration is zero. The concentration changes occur in the vicinity of the membrane wall. Fig. 4 also indicates the effect of liquid phase flow rate on the concentration profile of SO2. It is deduced that increasing liquid velocity, would make the concentration profile more flat in the liquid phase. By increasing liquid flow rate, the contribution of convective mass transfer to the total mass transfer increases and causes more uniform concentration profile. In fact, convective mass transfer tends to transfer the SO_2 toward the outlet of the membrane contactor.

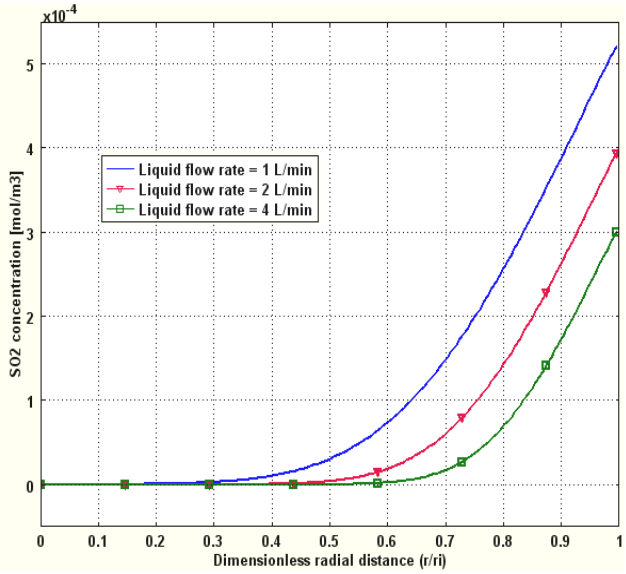

Fig. 4 Effect of liquid flow rate on SO_2 concentration profile in the tube side

IV. Conclusions

Separation of sulfur dioxide (SO_2) using ceramic tubular membrane contactors was studied in this work. A mass transfer model was developed to describe the transport of SO_2 through the membrane contactor. The model was based on solving the conservation equations for SO_2 in three sections of the contactor, i.e. shell, membrane, and tube. CFD was employed to solve the model equations. Effect of the operating parameters including liquid and gas flow rates on the removal of SO_2 was investigated. The simulation results indicated that the removal of SO_2 increased with either increasing the liquid velocity or decreasing the gas velocity in the membrane contactor. The model predictions also reveal that the main mass transfer resistances for transport of SO_2 are located in the membrane and gas phase. Ceramic membrane has the highest resistance because of its high tortuosity.

References

[1] Müller, H., 2005. Sulfur dioxide, in: Ullmann's Encyclopedia of Industrial Chemistry. Wiley-VCH Verlag GmbH & Co.:Weinheim.
[2] Bekassy-Molnar, E., E. Marki and J.G. Majeed, 2005. Sulphur dioxide absorption in air-lift tube absorbers by sodium citrate buffer solution. Chemical Engineering and Processing, 44: 1039–1046.
[3] VanDam, M.H.H., A.S. Lamine, D. Roizard, P. Lochon and C. Roizard, 1997. Selective sulphur dioxide removal using organic solvents. Industrial and Engineering Chemistry Research, 36: 4628–4837.
[4] Dutta, B.K., M. Shyamal and R.K. Basu, 1996. Absorption of sulfur dioxide in aqueous dispersions of dimethyl aniline. Canadian Journal of Chemical Engineering, 74: 339–346.
[5] Gabelman, A., S.T Hwang, 1999. Hollow fiber membrane contactors. Journal of Membrane Science, 159: 61–106.

[6] Qi, Z. and E.L. Cussler, 1985. Microporous hollow fibers for gas absorption. Journal of Membrane Science, 23: 321–345.
[7] Kreulen, H., C.A. Smolders, G.F. Versteeg and W.P.M. Van Swaaij, 1993. Microporous hollow fiber membrane modules. Industrial and Engineering Chemistry Research, 32: 674–684.
[8] Luis, P., A. Garea, A. Irabien, 2010. Modelling of a hollow fibre ceramic contactor for SO2 absorption. Separation and Purification Technology, 72: 174–179.
[9] Luis, P., A. Garea and A. Irabien, 2009. Zero solvent emission process for sulfur dioxide recovery using a membrane contactor and ionic liquids. Journal of Membrane Science, 330: 80–89.
[10] Shirazian, S., A. Moghadassi, S. Moradi, 2009. Numerical simulation of mass transfer in gas-liquid hollow fiber membrane contactors for laminar flow conditions. Simulation Modelling Practice and Theory, 17: 708-718.
[11] Happel, J., 1959. Viscous flow relative to arrays of cylinders. AIChE Journal, 5: 174–177.
[12] Bird, R.B., W.E. Stewart and E.N. Lightfoot, 2002. Transport Phenomena. 2nd edition, John Wiley & Sons: New York.