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NOTE

Simulation Studies on H_2S Absorption in Potassium Carbonate Aqueous Solution Using a Membrane Module†

MAHMOUD REZA SOHRABI[1], AZAM MARJANI[2,*], SADEGH MORADI[3], MEHRAN DAVALOO[1] and SAEED SHIRAZIAN[2]

[1]Department of Applied Chemistry, Faculty of Science, Islamic Azad University Tehran-North Branch, Tehran, Iran
[2]Department of Chemistry, Islamic Azad University, Arak Branch, Arak, Iran
[3]Department of Chemical Engineering, Arak University, Arak, Iran

*Corresponding author: E-mail: a-marjani@iau-arak.ac.ir

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Removal of H_2S from H_2S/N_2 gas mixture using a hollow-fiber membrane module is studied theoretically in this work. The absorption medium is aqueous solution of potassium carbonate. A mathematical model was developed to describe absorption of H_2S in the module. Laminar parabolic velocity profile was used for the gas flow in the tube side; whereas, the liquid flow in the shell side was characterized by Happel's free surface model. The effect of various operating conditions on H_2S removal is examined. The operating conditions examined included the gas flow rate, the liquid flow rate and the liquid concentration. The model was found to be efficient in prediction of membrane performance in gas absorption.

Key Words: Gas absorption, H_2S, Hollow fiber, Mathematical model, Simulation.

Hydrogen sulfide (H_2S) is a toxic gas and is also one of the major causes for environmental problems in chemical or petrochemical industries. It also has serious health effects associated with exposure of H_2S[1]. The current H_2S separation processes are based on physical and chemical processes including absorption, adsorption, cryogenic and membrane processes[2]. The separation of H_2S through ordinary processes experiences a number of shortcomings such as channeling, flooding, entraining, foaming and also high capital and operating costs[3,4]. Recently, the gas-liquid hollow-fiber membrane contactors as gas absorption devices have become a subject of great interest[4-8].

The main purpose of this study is to simulate H_2S absorption through a hollow-fiber membrane contactor. The simulations are based on computational fluid dynamics of mass and momentum transfer in the liquid and gas phases.

Simulation of H_2S absorption

Formulation of mass transfer and absorption: The model is developed for a segment of a hollow fiber, as shown in Fig. 1, through which the gas mixture flows with a fully developed laminar parabolic velocity profile. The fiber is surrounded by a laminar liquid flow in an opposite direction. Hydrogen sulfide gas is removed from the gas mixture by diffusing through the membrane and then absorption and reaction with the solvent.

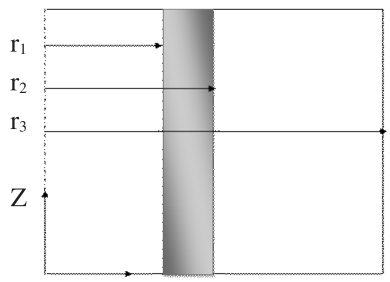

Fig. 1. Model domain

The continuity equation for each species in a reactive absorption system can be expressed as[9]:

$$\frac{\partial C_i}{\partial t} = -(\nabla.C_i V) - (\nabla.J_i) + R_i \quad (1)$$

where C_i, J_i, R_i, V and t are the concentration, diffusive flux, reaction rate of species i, velocity and time, respectively. Either Fick's law of diffusion or Maxwell-Stefan theory can be used for the determination of diffusive fluxes of species i.

†This work is results of Azam Marjani's Ph.D. Thesis in Islamic Azad University, Tehran North Branch.

Reaction rate for H_2S absorption into K_2CO_3 aqueous solution: When the potassium carbonate is dissolved in water it is ionized into the potassium ion and carbonate ion. The bicarbonate ion and hydroxyl ion are then generated by the reactions in following reaction scheme.

$$HCO_3^- + OH^- \leftrightarrow CO_3^{2-} + H_2O \quad (2)$$

$$2H_2O \leftrightarrow H_3O^+ + OH^- \quad (3)$$

The COMSOL multiphysics software is used to solve the differential equations set, by the finite element method and the direct linear system solver UMFPACK.

Effect of gas and liquid flow rates on the removal of H_2S: The per cent H_2S removal for different values of gas flow rates (the effect of convection term) is presented in Fig. 2. The increase in the gas flow rate reduces the residence time in the module, which in turn reduces the removal rate.

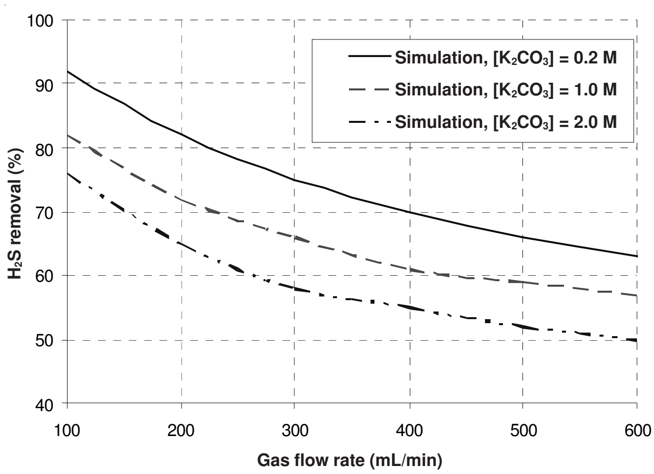

Fig. 2. Simulation results for different values of absorbent concentration as function of gas flow rate

The convective term in the shell has an opposite effect. Increasing liquid flow rate increases the removal rate (Fig. 3). As the solvent moves faster, the gas concentration at the outer surface of the fiber along the length of the contactor becomes less, resulting in higher concentration gradient at the interface and thus higher H_2S removal rate. Furthermore, the figures clearly shows that increasing of absorbent concentration from 0.2-2.0 M decreases the per cent H_2S removal because the solubility of H_2S in the solvent decreases from 2.31 to 0.39.

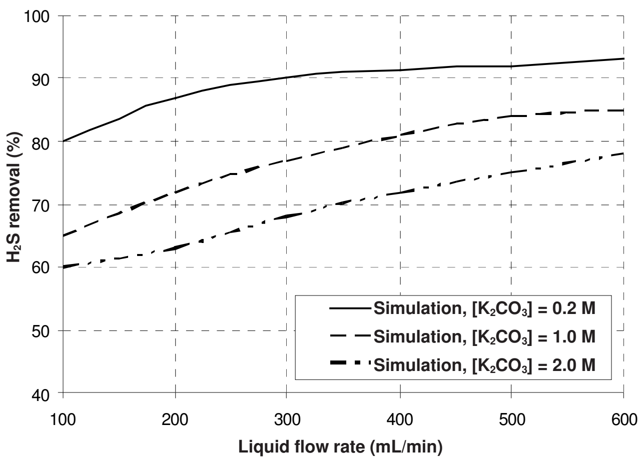

Fig. 3. Simulation results for different values of absorbent concentration as function of liquid flow

Conclusion

In this work, the absorption of H_2S in aqueous solution of potassium carbonate using a hollow-fiber membrane module was studied. A mathematical model was developed to describe absorption of H_2S in the module. The hollow-fiber membrane module was found to be efficient in purification of gas streams containing soluble toxic gases. The simulation results for the absorption of H_2S in liquid solvent indicated that the removal of H_2S increased with increasing liquid velocity in the shell side.

Nomenclature

A : Cross section of tube (m^2)
C : Concentration (mol/m^3)
D : Diffusion coefficient (m^2/s)
J_i : Diffusive flux of any species (mol/m^2 s)
k : Reaction rate coefficient of H_2S with absorbent (m^3 /mol s)
P : Pressure (Pa)
T : Temperature (K)
u : Average velocity (m/s)
V : Velocity in the module (m/s)
z : Axial coordinate (m)

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