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Mathematical modeling of CO_2 absorption into novel reactive DEAB solution in hollow fiber membrane contactors; kinetic and mass transfer investigation

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ABSTRACT

In this study, 4–diethylamino–2–butanol (DEAB) has been applied as a novel amino alcohol absorbent in a gas–liquid hollow fiber membrane contactor (HFMC) for CO_2 separation from a CO_2/N_2 gas mixture. A comprehensive 2–D mathematical model based on the finite element method (FEM) was developed to solve the applied partial differential equations for the shell, tube and membrane sides of a gas–solvent HFMC. The proposed model was validated using the available experimental data in the literature and the modeling results were in consistent with the experimental data. To investigate the influence of solvent on separation performance of a non–wetted mode of HFMC, the absorption of CO_2 using DEAB is compared with other common industrial solvents such as monoethanolamine (MEA), diethanolamine (DEA), triethanolamine (TEA) and methyldiethanolamine (MDEA). Under moderate operating conditions, the impact of parameters such as liquid and gas flow rates, concentration, temperature and CO_2 partial pressure on the performance of a HFMC have been examined. Sensitivity analysis of operating conditions reveals that mass transfer resistance of gas phase is more significant than mass transfer resistance of liquid phase and the major mass transfer resistance is located in the gas phase. The modeling results indicated that the percentage absorption of CO_2 into DEAB solution was competitive with MEA solution, however much higher than DEA, MDEA and TEA solutions in all range of liquid and gas flow rates and also partial pressure. It was concluded that increasing temperature, absorbent concentration, liquid flow rate and also decreasing gas flow rate enhance the removal of CO_2.

1. Introduction

Due to increased emission of CO_2 as the major contributor to global warming and climate change problems, CO_2 absorption into chemical solvents is one of the most promising technologies for capturing CO_2[1–3]. Currently the major strategies to decrease the penalty associated with CO_2 capture by amine scrubbing is the development of efficient processes and solvents with a better performance when compared to the common industrial solvents and processes [4–7]. The main drawbacks of gas–liquid absorption using amine solutions in packed columns as the most common industrial process are technical and economic constraints [3–5,8]. Also some operational limitations such as foaming, channeling, entraining and flooding are associated with this technology [4]. Recently, researchers have turned their attention to intensify the process by optimizing the process energy requirement and equipment size [9–12].

Nowadays, hollow fiber membrane contactor (HFMC) is introduced as an alternative technology for capturing CO_2, due to its promising intensification potential such as high surface to volume ratio (1500–3000 m^2/m^3), flexibility, modularity, compact size, easy installation and low cost [2,11,13–16]. HFMC contains two channels at the middle of which stands the membrane and fluids flow through the channels for separation. Since membrane is located between fluids as a solid phase, absorbent liquid and gas mixture are in contact with each other without getting mixed, so enhances in the fluid velocity through the channels will not lead to the common operational problems of absorption towers.

Choosing an effective amine solvent to ensure such benefits as fast reaction kinetics, high absorption capacity, low energy requirement for regeneration, low degradation rate, and low corrosiveness is another factor which plays an important role in performance of HFMC for capturing CO_2 [17–19]. Many theoretical and experimental studies are carried out for capturing CO_2 using different solvents in various HFMC types [16]. Rangwala [20] compared the absorption of CO_2 into water, sodium hydroxide and DEA solution through HFMC and traditional packed columns. He reported that using HFMC, the overall mass transfer rate per unit volume can be 3–9 times higher than traditional packed columns. In another related study, Kreulen et al. [21,22]

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Nomenclature

C	Concentration (mol m^{-3})
C_0	Initial concentration (mol m^{-3})
C_{CO_2e}	Equilibrium CO_2 concentration in the bulk of liquid (kmol m^{-3})
$C_{CO_2-membrane}$	CO_2 concentration in the membrane (mol m^{-3})
$C_{CO_2-shell}$	CO_2 concentration in the shell side (mol m^{-3})
C_{CO_2-tube}	CO_2 concentration in the tube (mol m^{-3})
Cp	Specific heat (J mol^{-1} K^{-1})
$D_{CO_2-membrane}$	Diffusion coefficient of CO_2 in the membrane (m^2 s^{-1})
$D_{CO_2-shell}$	Diffusion coefficient of CO_2 in the membrane (m^2 s^{-1})
D_{CO_2-tube}	Diffusion coefficient of CO_2 in the tube (m^2 s^{-1})
D_{w,co_2}	Diffusion coefficient of CO_2 in pure water (m^2 s^{-1})
H	Solubility of carbon dioxide in solution (kmol atm^{-1} m^{-3})
$\mathcal{H}$	Henry's constant
$k_{(R-1)}$	Forward rate constant of reaction (R–1) ($m^3 kmol^{-1} s^{-1}$)
$k_{-(R-1)}$	Backward rate constant of reaction (R–1) ($m^3 kmol^{-1} s^{-1}$)
$k_{(R-2)}$	Forward rate constant of reaction (R–2) ($m^3 kmol^{-1} s^{-1}$)
$k_{-(R-2)}$	Backward rate constant of reaction (R–2) (s^{-1})
K_i	Chemical equilibrium constant for reaction i
K_w	Chemical equilibrium constant for reaction (R–5).
L	Length of fiber (m)
m	Physical solubility (dimensionless)
$\mathcal{N}$	Molar flux
n	Number of fibers
Q_g	gas volume flow rate (mL min^{-1})
Q_l	liquid volume flow rate (mL min^{-1})
r_1	Inner tube radius (m)
r_2	Outer tube radius (m)
R	Inner shell radius (m)
T	Temperature (K)
V	Velocity (m s^{-1})
$V_{z,shell}$	Velocity in the shell side (m s^{-1})
$V_{z,tube}$	Velocity in the tube side (m s^{-1})
$\mathcal{Z}$	Height of the membrane contactor (m)

Greek symbols

ε	Porosity
ρ_G	Gas phase density (kg m^{-3})
ρ_L	Liquid phase density (kg m^{-3})
$\sigma_{CO_2-N_2}$	Lennardejones parameter ($\overset{0}{A}$)
χ	Thermal conductivity (W m^{-1} K^{-1})
Ω	Collision integrals
ΔHi	Heat of absorption (J mol^{-1})

indicated that the use of polypropylene HFMC can improve the absorption of CO_2 into water/glycerol mixtures with respect to bubble columns. Saidi et al. [3] and Lee et al. [23] investigated the CO_2 capture performance using potassium carbonate solution in the HFMC for determination of optimal absorbent flow rate. They reported that the CO_2 removal efficiency in HFMC enhances with increasing liquid velocity, number of fibers, temperature and also decreasing gas velocity in the membrane contactor. Dindore et al. [14] have examined the effect of aqueous carbonate potassium on the CO_2 and H_2S absorption in the case of a cross–flow membrane contactor. They observed that the CO_2 absorption flux is a strong function of the liquid velocity when the liquid velocity is relatively low. Contrary, at higher liquid velocities, the absorption rate is dominated by the chemical reaction rate and the liquid velocity has less influence on the average absorption flux [14]. CO_2 absorption in an aqueous potassium carbonate liquid membrane module with dense polymeric supporting layers was studied by Shalygin et al. [24]. Their results showed that increasing the concentration of potassium carbonate as well as the temperature led to large increases in the CO_2 removal. Keshavarz et al. [25,26] studied the effects of membrane wetting and fiber distribution in the module to analyze the acid gas absorption in HFMC. They concluded that membrane wetting by DEA solution could decrease the absorption flux significantly. In another related study, Mansourizadeh et al. [27] considered the CO_2 absorption with aqueous NaOH solution through porous polyvinylidene fluoride (PVDF) hollow fiber membranes. Their results indicated when water is used (physical absorption) for CO_2

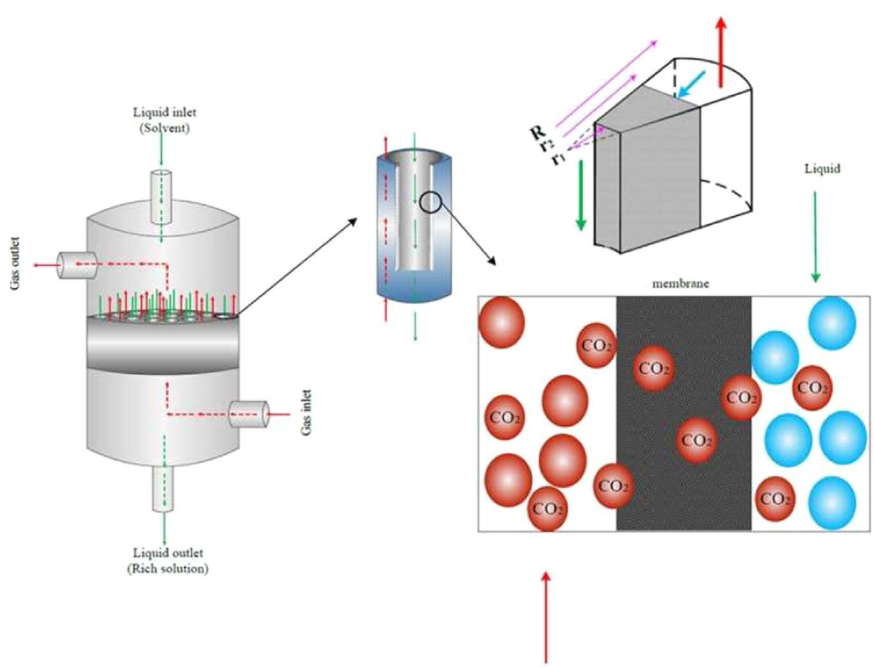

Fig. 1. Schematic diagram of a gas–liquid hollow fiber membrane contactor.