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Mathematical modeling of CO_2 absorption into reactive DEAB solution in packed columns using surface-renewal penetration theory

Majid Saidi

Faculty of Engineering, Shahrekord University, Shahrekord, Iran

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ABSTRACT

In this work, a comprehensive model has been developed for CO_2 absorption into 4-diethylamino-2-butanol (DEAB) as a reactive amino alcohol solution. The mathematical model is developed based on penetration theory by simultaneous considering of mass transfer phenomenon and chemical reactions. The penetration theory provides appropriate absorption rate and enhancement factor for the chemical absorption. A numerical analysis was performed to solve the applied partial differential equations for the liquid and gas phases simultaneously. The model results were validated using the available experimental data in literature. In this study, the absorption of carbon dioxide by monoethanolamine (MEA), diethanolamine (DEA), triethanolamine (TEA), methyldiethanolamine (MDEA) and DEAB solutions was compared theoretically in a packed column absorber. The impact of parameters such as DEAB concentration, temperature, liquid flow rate, CO_2 loading and CO_2 partial pressure on the performance of a split-flow absorber have been examined. The modeling results indicated that the overall mass transfer coefficient ($K_G a_v$) for CO_2 absorption into DEAB solution was lower than MEA and DEA solutions, however much higher than MDEA and TEA solutions in all range of CO_2 loading and partial pressure. Increasing the operating temperature, DEAB concentration and liquid flow rate enhanced the overall mass transfer coefficient.

1. Introduction

Nowadays due to development of industrial activities, the accumulative concentration of greenhouse gases has been mounting enormously in the atmosphere [1–4]. The environmental concerns related to the global warming and climate change motivate interest in the development of new technologies for controlling and preventing greenhouse gases emission [4–6]. CO_2 as one of the main greenhouse gases has been produced largely from burning different fossil fuels. CO_2 absorption by reactive solvents is one of the most interesting technologies for CO_2 absorption due to its maturity, cost effectiveness, and capability of handling large amounts of exhaust stream [7–9]. The main considerable factors to select effective solvent for CO_2 absorption include high absorption capacity and also, low degradation rate, corrosiveness and solvent lost due to vaporization [10,11]. Furthermore fast reaction kinetics, high mass transfer performance and low energy requirement for regeneration are other important parameters which should be considered.

Chemical absorption with alkanolamine solutions such as monoethanolamine (MEA), diethanolamine (DEA), triethanolamine (TEA), 2-amino-2-methyl-1-propanol (AMP) and methyldiethanol amine (MDEA) in absorption columns is a common industrial process [12–15]. Although MEA, DEA and TEA have high reaction rates with CO_2, their application in the CO_2 capture process is associated with a number of drawbacks including low absorption capacity, high-energy requirements for regeneration, and high corrosion rate. International Test Center (ITC) analyzes for CO_2 capture revealed that application of innovative amine solutions containing an amino alcohol group such as 4-diethylamino-2-butanol (DEAB) and diethylenetri-amine (DETA) instead of conventional amines can be improved CO_2 absorption and cyclic capacity. Also the required regeneration heat of DEAB as a representative of tertiary amines solvents is less than unhindered amines solvents such as AMP, MEA, and DEA [16,17].

Currently, packed-bed absorbers and strippers using aqueous amine solutions are applied extensively as a suitable, mature, and well-documented technology for CO_2 capture [18]. Reliable process modeling of packed-bed reactive absorption columns and also development of effective solvents is necessary for design, scale-up and optimization of CO_2 capture process [15,19]. The CO_2 absorption process in the packed-bed absorbers is influenced by mass and heat transfer limitations [20]. Mass transfer performance in packed-bed absorber towers depends on having efficient contact area between liquid and gas phase [21]. Structured and random packing, the most common types of packing column, are widely

E-mail addresses: m.saidi@eng.sku.ac.ir, majidsaidi65@gmail.com, m.saidi@eng.sku

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Nomenclature

av	specific surface area ($m^2\ m^{-3}$)
C_k	concentration of kth component ($kmol\ m^{-3}$)
C_{ke}	equilibrium concentration of kth component in the bulk of liquid ($kmol\ m^{-3}$)
C_{ki}	concentration of kth component at interface ($kmol\ m^{-3}$)
C_{p_G}	average molar specific heat of gas ($kJ\ kmol^{-1}\ K^{-1}$)
C_{p_K}	average specific heat of kth component ($kJ\ kmol^{-1}\ K^{-1}$)
C_{pL}	molar specific heat of liquid ($kJ\ kmol^{-1}\ K^{-1}$)
D	diffusivity ($m^2\ s^{-1}$)
D_{kj}	knudsen diffusivity of species j ($m^2\ s^{-1}$)
d_p	packing nominal size (m)
E	enhancement factor
G	molar velocity of gas ($kmol\ m^{-2}\ h^{-1}$)
$\hat{G}$	mass velocity of inert gas ($kg\ m^{-2}\ h^{-1}$)
H	solubility of carbon dioxide in solution ($kmol\ atm^{-1}\ m^{-3}$)
h	heat transfer coefficient in gas phase ($kJ\ m^{-2}\ s^{-1}\ K^{-1}$)
ΔH_{CO_2}	heat of reaction and absorption ofCO_2 ($kJ\ kmol^{-1}$)
ΔH_{H_2O}	heat of vaporization of water ($kJ\ kmol^{-1}$)
$k_{(R-1)}$	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_g	gas side mass transfer coefficient ($kmol\ h^{-1}\ m^{-2}\ atm^{-1}$)
K_i	chemical equilibrium constant for reaction i
$K_G a_v$	volumetric overall mass transfer coefficient ($kg\ mol/m^2\ s\ kPa$)
K_G	overall mass transfer coefficient ($kmol\ s^{-1}\ m^{-2}\ Kpa^{-1}$)
K_w	chemical equilibrium constant for reaction (R-5)
k_y	gas side mass transfer coefficient ($kmol\ s^{-1}\ m^{-2}$)
k_l	liquid side mass transfer coefficient ($m\ s^{-1}$)
k_g	gas side mass transfer coefficient ($m\ s^{-1}$)
L	molar velocity of liquid ($kmol\ m^{-2}\ h^{-1}$)
$\hat{L}$	liquid mass flow rate ($kg\ h^{-1}$)
Le	Lewis number
N_k	transfer flux of kth component ($kmol\ m^{-2}\ s^{-1}$)
P_k	partial pressure of kth component in gas phase (atm)
P_{k_e}	equilibrium vapor pressure of kth component in gas phase (atm)
P_{k_i}	partial pressure of kth component in the liquid–gas interface (atm)
r	reaction rate
R	universal gas constant ($m^3\ atm\ kmol^{-1}\ K^{-1}$)
T_g	gas temperature (K)
T_L	liquid temperature (K)
T	temperature (K)
x_k	mole fraction of kth component in the liquid phase
y_k	mole fraction of kth component in the gas phase
z	height of the column (m)

Greek symbols

μ_g	gas phase viscosity ($kg\ m^{-1}\ h^{-1}$)
μ_v	vapor phase viscosity ($kg\ m^{-1}\ h^{-1}$)
μ_L	liquid phase viscosity ($kg\ m^{-1}\ h^{-1}$)
ρ_g	gas phase density ($kg\ m^{-3}$)
ρ_L	liquid phase density ($kg\ m^{-3}$)
$\sigma_{CO_2-N_2}$	Lennardejones parameter ($\overset{0}{A}$)
Ω	collision integrals

used in CO_2 capture processes. In comparison, the structured packing column provides a certain gas and liquid path, ameliorated gas–liquid distribution, lower pressure drop across the column, lower liquid holdup, large surface area per volume ratio and higher production capacity [16,20,22].

Mathematical modeling of absorption of CO_2 into DEAB in structured packing requires a comprehensive model for liquid and gas flow in the bed. In this study, a mathematical model for CO_2 absorption process using DEAB solution in a structured packed bed column has been developed. The combined effect of mass transfer and chemical reaction was considered by surface-renewal penetration theory. The mass transfer performance was investigated in terms of overall mass transfer coefficient ($K_G a_v$). A numerical method was employed to solve the simultaneous nonlinear mathematical equations. The model results were used to compare the absorption performance of DEAB with conventional amines such as MEA, DEA, TEA and MDEA solutions. In addition, the effect of different parameters of the packed column, including gas flow rate, temperature, CO_2 loading, amine concentration and amine flow rate have been investigated and the design consequences of different options have been discussed.

2. Gas sweetening plant

A typical industrial split-flow absorber-stripper unit is shown in Fig. 1. The unit consists of two packed towers namely, the absorber and the stripper [15,20,23–25]. The feed gas is introduced at the bottom of the absorber generally at an elevated pressure, and contacts counter-currently the lean amine solutions from the striper tower, which enters at the top of absorber at temperatures varying between 30 and 50 °C [15,21]. The rich liquid loaded with CO_2 from the bottom of the absorber is first flashed nearly to 1.15 atm in a throttling valve and subsequently passes through the stripper where it is stripped counter-currently by the stream generated by boiling solution in the bottom of the stripper. A portion of the lean solution from the striper is cooled and fed into the top of the absorber while the major portion is added at a point below the top without any change in temperature. This simple modification, which is called split-flow process, raises the temperature of the rich liquid and lowers the amount of heat needed for heating the solution to the regeneration temperature [26]. The outlet stream from the top of stripper which is concentrated acid gas stream enters a flash drum at low temperature for recovering the steam and the vaporized amine. The condensate is refluxed to the top of the stripper. The stripper usually operates at low pressure (below 1 bar) and high temperature (100–120 °C) [26].

3. Reaction network and kinetic analysis

DEAB as a tertiary amine solvent reacts as a base catalyst for hydration of CO_2. The overall reaction of DEAB solvent for capturing CO_2 takes place as below reaction network [5,22,27,28].

$$CO_2 + DEAB + H_2O \overset{K_{R-1}}{\leftrightarrow} DEABH^+ + HCO_3^- \quad (R\text{–}1)$$

$$CO_2 + OH^- \overset{K_{R-2}}{\leftrightarrow} HCO_3^- \quad (R\text{–}2)$$