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Identifying the multi-ion effects on the phase flow, mass and heat transfer in amine absorption of CO_2

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ABSTRACT

Carbon dioxide mitigation strongly supports the greenhouse gas control. Amine absorption of CO_2, as a method to mitigate the CO_2, is a typical multi-ion system with obvious multi-ion effects. However, there is little information about the multi-ion effects on the phase flow, mass and heat transfer in amine absorption of CO_2. The multi-ion effects have previously to be neglected to simplify the absorption process description, which produces unknown deviations from the realistic absorption process. According to experiment data, a multi-ion mass transfer, heat transfer and phase flow model is here developed to describe the realistic amine absorption of CO_2. The turbulent diffusivity, turbulent thermal diffusivity, turbulent viscosity, CO_2 concentration, liquid temperature and velocity are analyzed under the multi-ion conditions. It was found that there is 6–22% CO_2 concentration difference between the multi-ion effects case and the neglect of the multi-ion effects (NME) case. The positive ions show the better synergy effects compared with the negative ions. Under the ion concentration of 0.001 kmol/m^3 to 0.02 kmol/m^3, 0.2 kmol/m^3 to 2 kmol/m^3 and 4 kmol/m^3 to 7 kmol/m^3, the multi-ion mass transfer, heat transfer and phase flow model provides an accurate description of the realistic CO_2 absorption against the NME case. Finally, Nusselt number and mass transfer coefficient models revised by synergy angles are developed to include the multi-ion effects for engineering application. Adding the amine salt and Na_2CO_3 respectively reduce the liquid film thickness and liquid film depth, which increases the Nusselt number by 9.5% and 9.3%, respectively. Adding the metal Cu increases the Nusselt number by 11.57%, which helps to reduce the energy consumption by 7.8%.

1. Introduction

Carbon dioxide (CO_2) emission from the industry has produced the serious environment issue, which is now an urgent mission for the world [1,2]. In order to control the CO_2 emission, amine absorption of CO_2 is developed as an effective technical route [3,4]. However, the high energy penalty for regeneration of the CO_2 by heating has reduced the efficiency of the amine method significantly. The potential way is to design an alternative amine mixture to reduce the energy cost [5,6]. During the amine mixture absorption of CO_2, the multi-ion effect is a quite typical phenomenon. However, it is not well understood due to the complexity of the amine mixture and CO_2 system in the packed column [7,8].

In the previous researches, the multi-ion effects are neglected and they are assumed as a single ion effect or an average ion effect to simplify the two phase flow model [9–11]. The multi-ion effects on the phase flow, heat transfer and mass transfer are still not understood clearly. Thus, it is important to characterize the multi-ion effects mechanism, which will probably offer new insights on how to intensify the CO_2 capture process by controlling the ion species and ion motion in the packed column.

The multi-ion transports are the dominant multi-ion effects in the amine mixture absorption of CO_2 and thus the two film theory is usually used to determine the transport phenomenon [12]. In the two film theory, ions transports in the film regions are the key steps to describe the interface characteristic between gas and liquid two phases. Taking the aqueous amines and CO_2 as the electrolytes, Nernst-Planck equations are normally used to determine the ion transport mechanism in the film region [13]. Compared with Fick's law, the Nernst-Planck equations fully characterize the diffusion, ion transport and convection between film region and interface [14]. During the CO_2 absorption by amines, multi-ion diffusion is a common process. However, the different ion diffusivities are assumed to be the same or to be substituted by the

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Nomenclature

A	concentration variance
B	thermal diffusivity, m^2/s
c_p	heat capacity, J/g K
C	concentration, $kmol/m^3$
d_l	liquid film depth, m
d_g	gas film depth, m
D	diffusivity, m^2/s
E	Enhancement factor
F	Faraday constant
F_a	electrostatic force, $kg/m^2\ s^2$
F_b	body force, $kg/m^2\ s^2$
F_d	drag force, $kg/m^2\ s^2$
F_g	gravity, $kg/m^2\ s^2$
G	electrostatic potential gradient, V/m
h	liquid volume fraction
H	Henry's constant, $MPa/kmol/m^3$
I	unit tensor
k	turbulent kinetic energy, m^2/s^2
k_2	reaction rate, $m^3/kmol\ s$
K, k_g	mass transfer coefficient, m/s
l	liquid film direction coordinate or liquid film thickness, m
l_c	liquid film thickness by mass transfer coefficient, m
L	characteristic length, m
M	molecular weight, g/mol
m	loading, mol/mol
N	mass transfer amount, $kg/m^3/s$
N_{ci}	convective flux, $kmol/m^3/s$
n	total number of the ion components
P	pressure, MPa
p	partial pressure, MPa
Pr	Prandtl number
Q,Q_a	heat transfer amount and additional electrostatic energy, $kJ/m^3/s$
r_i	reaction rate for ion component i, $kmol/m^3/s$
R	ideal gas constant
RN	Reynolds number
Sc	Schmidt number
T	temperature, K
U	velocity, m/s
w	film width, m
X	dimensionless variable
z	ion charge
ε	turbulent dissipation rate, m^2/s^3
ε_C	concentration dissipation rate, 1/s
ε_t	dissipation rate for temperature fluctuation, 1/s
α	thermal diffusivity, m^2/s
ρ	density, kg/m^3
μ	viscosity, Pa s
γ, β	synergy angle, degree
$\aleph$	thermal conductivity, W/m/K

Subscript

g	gas or gas phase
i,j	ion species index
m	multi-ion effects
t	turbulent state

minimum ion diffusivity. The errors caused by these assumptions are significant, especially in the multi-amine and CO_2 system [7,8,15,16], which are generated by the obvious electrostatic potential gradients in the multi-ion system [15]. However, the errors are not quantified exactly in the previous work. The objective of this work is to determine how the multi-ions affect the CO_2 absorption by amine solutions.

Amines absorption of CO_2 is a typical two phase flow, heat transfer and mass transfer process [4,17]. As for MEA absorption of CO_2, the CFD model is used to describe the gas and liquid phase flow [18], which uses the gas and liquid phase flow to intensify the mass transfer. In these researches, Billet and Schultes model is suitable to describe the MEA and DEA and Rocha model is proper for AMP and MDEA [19–21]. The diffusion term, convection term, accumulation term and other source terms offer the possibility to determine the phase slip phenomenon [16,22]. Thus, it is feasible to study how the multi-ion affects the phase flow, heat transfer and mass transfer in the amine absorption of CO_2, which is simply described in Fig. 1. This may also provide interesting information for the reactor design.

Considering the complexity of the amine absorption of CO_2, the field synergy theory is extended to describe the synergy effects between multi-ion diffusion, phase flow and heat transfer. This is feasible due to that the field synergy theory has been used successfully in the multi-field analysis of the CO_2 capture process [18,23–24]. After the synergy effects are identified, the ion concentrations and ion species may be determined correctly for when the multi-ion effects must be considered rather than being neglected.

2. Multi-ion mass transfer, heat transfer and phase flow model

In order to develop the multi-ion mass and heat transfer and phase flow model, the assumptions are made as follows.

(1) The gas and liquid two phases are continuous phases in the packed column.
(2) The gas and liquid films exist in the interphase.
(3) The multi-ion charge follows the electroneutrality rule.
(4) The turbulent flow affects the diffusion and thermal diffusion.
(5) Turbulent dissipation occurs in the gas and liquid phases.

Here, the multi-ion mass transfer, heat transfer and phase flow model is divided into multi-ion film model, multi-ion two phase model and multi-ion synergy model.

2.1. Multi-ion film model

Based on the assumptions above, the multi-ion effect in the liquid film is considered on steady conditions. The partial differential equation for each ion is developed as

$$D_i\frac{\partial^2 C_i}{\partial l^2} - z_i D_i \frac{RT}{F}\frac{\partial G C_i}{\partial l} + N_{ci} + r_i = 0 \tag{1}$$

where N_{ci} is the convective flux [14]. The reaction rate r_i is calculated by the reaction set and equilibrium data, which has been successfully used in the blended amines absorption of CO_2 [9].

G indicates the electrostatic potential gradient, which correlates the multi-ion diffusion. Here, G is correlated with the ion concentration and ion diffusivities by using the electroneutrality characteristic [15], which is given as

$$G = \frac{F}{RT}\frac{\sum_{j=1}^{n} z_j D_j \frac{\partial C_j}{\partial l}}{\sum_{j=1}^{n} z_j^2 D_j C_j} \tag{2}$$

The static electroneutrality condition is used to keep the charge balance in the mass transfer, heat transfer and phase flow zones.