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Energy Procedia 00 (2016) 000–000

Energy Procedia

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The 8th International Conference on Applied Energy – ICAE2016

CFD study of hybrid membrane contactors for absorption and stripping of carbon dioxide

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Abstract

Carbon capture and storage (CCS) has been identified as an essential technology to meet the internationally agreed goal of limiting the temperature increase to 2°C. Compared to traditional gas-liquid contactors, the membrane contactors provide many beneficial features, including the high specific area, independent gas and liquid flows, modular units and easy to include internal heat exchange. The solvent carbon dioxide absorption processes employing membrane contactors is an important technology. Limited by the low partial pressure of carbon dioxide, physical absorption is not a feasible technology for post-combustion flue gas treatment. However, chemical absorption technology is high energy consumption. In this study, an innovative hybrid absorption/stripping membrane contactor (HASMC) for physical solvent carbon capture is proposed. The simultaneous absorption and stripping can enhance the effectiveness of carbon capture. The device can raise the feasibility of applying physical solvent technology to the treatment of gases with low carbon dioxide partial pressure. In this paper, computational fluid dynamics simulation of the concentration profiles and mass fluxes for parallel-flow and cross-flow modules are presented.

Selection and/or peer-review under responsibility of ICAE

Keywords: Carbon Capture; Solvent Absorption; Membrane Contactor; Absorption; Stripping

1. Introduction

Carbon capture and storage (CCS) has been identified as an essential technology to meet the internationally agreed goal of limiting the temperature increase to 2°C. The state of the art CO_2 capture (CC) technology, amine absorption technology, will cause the cost of electricity (COE) to increase 75%. Compared to traditional gas-liquid contactors, the membrane contactors provide many beneficial features, including the high specific area, independent gas and liquid flows, modular units and easy to include internal heat exchange. The solvent carbon dioxide absorption processes employing membrane contactors is an

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important technology for reducing COE. Limited by the low partial pressure of carbon dioxide, physical absorption is not a feasible technology for post-combustion flue gas treatment. However, chemical absorption technology is high energy consumption.

This paper presents an innovative hybrid absorption/stripping membrane contactor (HASMC) for physical solvent carbon capture. The simultaneous absorption and stripping can enhance the effectiveness of carbon capture. The device can raise the feasibility of applying physical solvent technology to the treatment of gases with low carbon dioxide partial pressure.

Computational fluid dynamics (CFD) simulation has been used to investigate the flow phenomena and separation performance of membrane modules which involves vapor and liquid phases, such as membrane distillation [1,2]. In this study, CFD simulation is employed to study the mass transfer boundary layer and the transmembrane mass flux of HASMC. Two configurations, parallel-flow and cross-flow, are simulated. The absorbent is propylene carbonate.

2. Module Concept and Modeling

The parallel-flow and cross-flow configurations of HASMC are depicted in Fig. 1. In the parallel-flow module, as shown in Fig. 1(a), the liquid absorbent channel is placed between the flue gas channel and the stripping channel. Carbon dioxide is transferred across the absorption membrane into the liquid and the carbon dioxide dissolved in the liquid is transferred across the stripping membrane into the stripped gas channel, which can be operated under vacuum condition or using a sweeping gas. In the cross-flow module, the absorption membrane and the stripping membrane are next to each other and allocated on the same side of the liquid channel. As shown in Fig. 1(b), multiple sets of gas channels can be placed on both sides of the liquid channel.

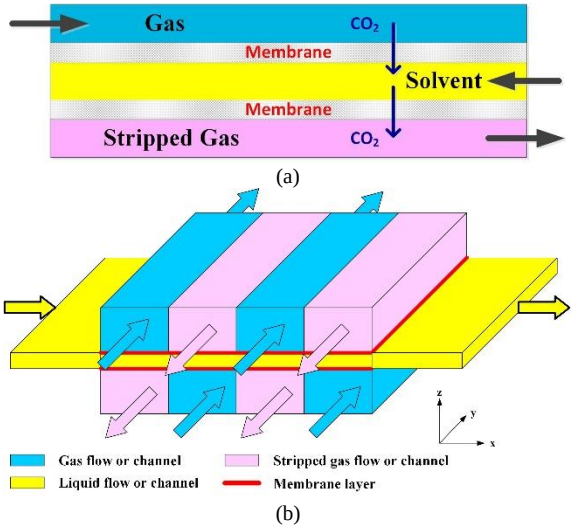


Fig. 1. HASMC configurations (a) Parallel-flow; (b) Cross-flow

The laminar flow model of the FLUENT software was employed for the CFD simulation. User defined functions were developed to account for the trans-membrane heat and mass transfer using the information of the cells adjacent to the membrane [2,3]. For the membrane layer, the mechanisms of heat transfer (heat

conduction) and mass transfer (Knudsen diffusion, molecular diffusion and viscous flow) were taken into account to calculate the fluxes. The physical properties needed for the simulation include the solubility and diffusion coefficient of carbon dioxide in the propylene carbonate solvent and the heat capacity, thermal conductivity, viscosity and density of all species in the gas and liquid phases.

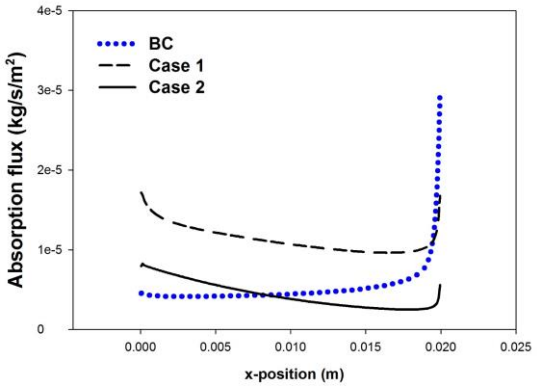
Grid independent analysis was carried out to determine the grid sizes by examining the trans-membrane mass flux. In addition to the momentum, energy and mass, the trans-membrane mass flux was included in the convergence criteria. The Poly (ether ether ketone) (PEEK) membrane used has a permeation coefficient of 1000 GPU (1 GPU=1 x 10^6 cm^3 (STP)/cm^2/s/cmHg) [4]. The model is verified using the experimental data from Dindore et al. [5].

3. Results and discussion

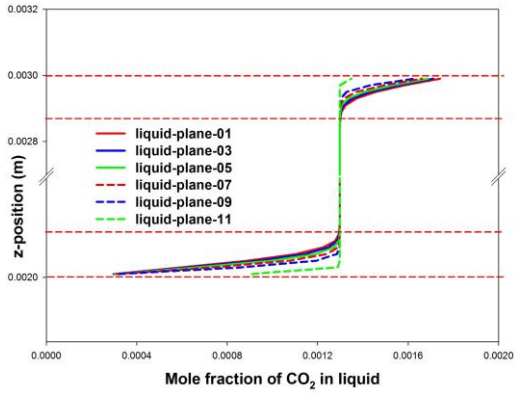
For the cross-flow HASMC module, three cases were simulated with the operation conditions listed in Table 1. The trans-membrane carbon dioxide mass flux profiles along the length of the module are shown in Fig. 2(a). For all the cases, mass flux at both ends of the modules, where the liquid and gas enter, are higher, in particular in BC, the mass flux at liquid entry end is very high and followed by rapid decrease because of the saturation of carbon dioxide in liquid. For Case 1, the carbon dioxide diffusion coefficient in the liquid is increase by 10 times, the mass flux along the entire module length is much higher than BC, except at the liquid inlet (which is also the gas outlet) end. The higher mass flux of Case 1 results from the more effective concentration penetration of carbon dioxide into the bulk liquid because of the higher diffusivity. The concentration penetration can be observed from Fig. 2(b), which is the region between two dotted lines. For Case 2, the height of the liquid channel is reduced by half. Because the liquid velocity is the same, the liquid flow rate is also reduced by half, the mass flux is lower than BC. These analysis results lead to the conclusion that parallel-flow HASMC cannot realize the advantage anticipated, which is simultaneous stripping the liquid for enhancing the absorption. The reason is that the concentration penetration thickness is too small and cannot extent from the absorption membrane layer to the stripping membrane layer.

Table 1. Cases of parameter study for parallel-flow HASMC

Parameters	BC	Case 1	Case 2
Gas side inlet temperature (K)	298.16	298.16	298.16
Gas side inlet velocity (m/s)	0.018	0.018	0.018
Gas side inlet CO_2 mass fraction in N_2	0.217	0.217	0.217
Gas side outlet pressure (Pa)	100,000	100,000	100,000
Vacuum side inlet temperature (K)	298.16	298.16	298.16
Vacuum side outlet pressure (Pa)	4000	4000	4000
Liquid side inlet velocity (m/s)	0.02	0.02	0.02
Liquid side inlet temperature (K)	298.16	298.16	298.16
Liquid side inlet CO_2 mass fraction	0.00026	0.00026	0.00026
Liquid side outlet pressure (Pa)	100,000	100,000	100,000
Liquid side diffusion coefficient (m^2/s)	1×10^{-9}	**1×10^{-8}**	1×10^{-9}
Liquid channel height (mm)	1	1	**0.25**



(a)



(b)

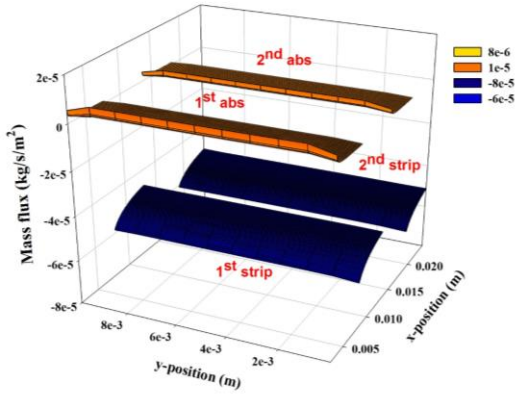
Fig. 2. Parallel-flow HASMC (a) absorption flux; (b) liquid layer concentration profiles (liquid entrance at x=0.02 m and liquid-plane-11)

For the cross-flow HASMC, the simulation cases are listed in Table 2, which include the base case and the cases with different liquid flow rate, carbon dioxide diffusion coefficient in the liquid, and gas concentration. The trans-membrane mass flux profiles of the two absorption sections and the two stripping sections are shown in Fig. 3(a). The mass fluxes of the first absorber and the first stripper are both higher than the second ones. However, the extents of decrease are not large, which means the interlaced arrangement of absorption and stripping on the same side of the liquid channel can provide the refreshing effect of the absorbent liquid. In Fig. 2(b), it is shown that the average cross-section carbon dioxide concentration in liquid increases in the absorption section and decreases in the following stripping section. Although the concentrations of the second absorption and stripping sections are both higher than the first ones, the follow-up of stripping after absorption does supply lower-concentration liquid for the second absorption operation. Figs. 2(c)-(f) show the concentration penetration in the liquid channel and similar profiles are obtained for the first set and the second set of the configuration. The effects of operation parameters are summarized in Fig. 2(b). The decrease of liquid flow rate or increase of gas concentration

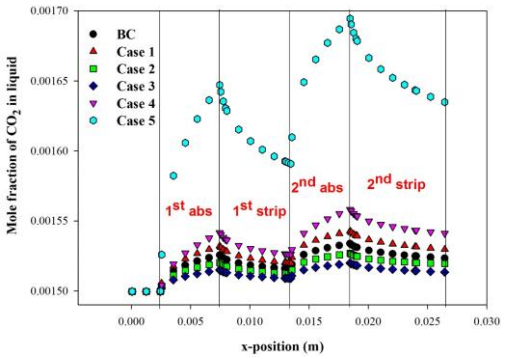
will result in higher liquid concentration. The increase of carbon dioxide diffusion coefficient will raise the concentration penetration and the absorption, hence the liquid concentration will increase.

Table 2. Cases of parameter study for cross-flow HASMC

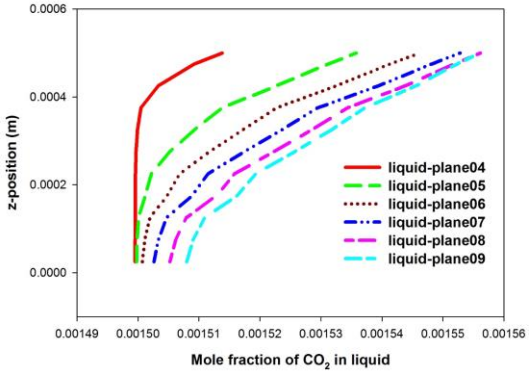
Parameters	BC	Cases 1-3	Case 4	Case 5
Gas side inlet temperature (K)	298.16	298.16	298.16	298.16
Gas side inlet velocity (m/s)	0.018	0.018	0.018	0.018
Gas side inlet CO_2 mass fraction in N_2	0.217	0.217	0.217	**0.362**
Gas side outlet pressure (Pa)	100000	100000	100000	100000
Vacuum side inlet temperature (K)	298.16	298.16	298.16	298.16
Vacuum side outlet pressure (Pa)	10000	10000	10000	10000
Liquid side inlet velocity (m/s)	0.01	**0.005/0.02/0.04**	0.01	0.01
Liquid side inlet temperature(K)	298.16	298.16	298.16	298.16
Liquid side inlet CO_2 mass fraction	0.000647	0.000647	0.000647	0.000647
Liquid side outlet pressure (Pa)	100,000	100,000	100,000	100,000
Liquid side diffusion coefficient (m^2/s)	1×10^{-9}	1×10^{-9}	$\mathbf{1\times10^{-8}}$	1×10^{-9}



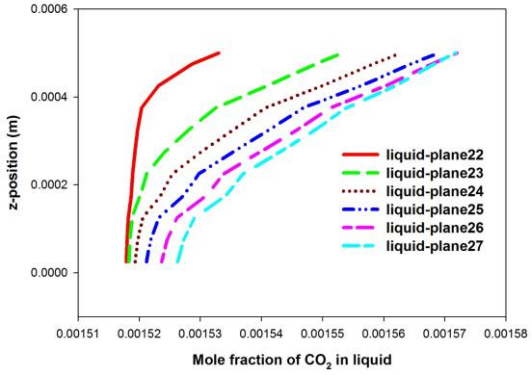
(a) mass flux



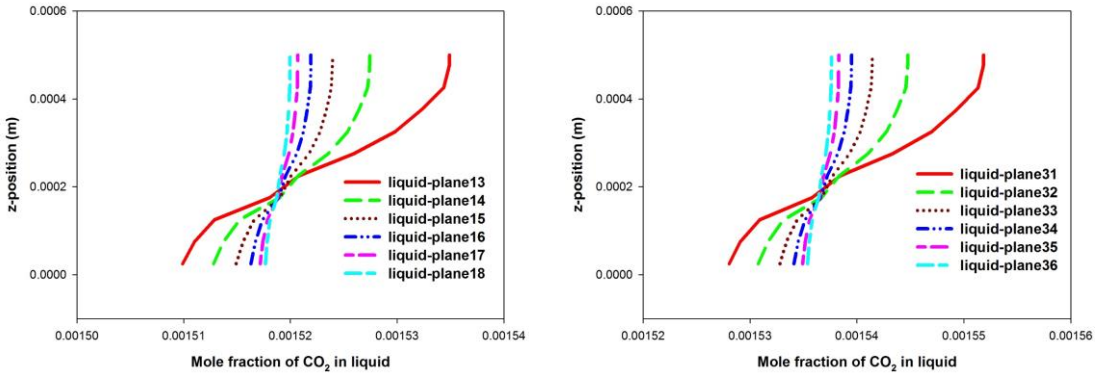
(b) y-z plane average CO_2 concentration in liquid



(c) first absorber



(d) second absorber



(e) first stripper (f) second stripper

Fig. 3. Cross-flow HASMC mass flux and liquid layer concentration profiles

4. Conclusions

An innovative hybrid membrane module for simultaneous absorption and stripping of carbon dioxide is proposed. For the physical absorbent of propylene carbonate, the concentration profiles and trans-membrane mass flux profiles in two configurations, parallel-flow and cross-flow, have been analyzed using CFD simulation. Because the concentration penetration thickness is too small, the parallel-flow configuration is not effective for reducing the concentration of carbon dioxide in the liquid. However, the cross-flow configuration, which adopts an interlaced arrangement of absorption and stripping sections on the same side of the liquid channel, is effective for refreshing the liquid concentration by the stripping operation following the absorption operation.

Acknowledgements

The authors gratefully acknowledge the sponsorship from the Ministry of Science and Technology of Taiwan (R.O.C.).

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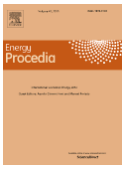

Biography

Hsuan Chang is a professor in the Department of Chemical and Materials Engineering, Tamkang University, Taiwan. She received her Ph.D. from the Department of Chemical Engineering of Ohio State University, USA. Her research interest is in the simulation and design of chemical and energy processes.