Chemical Engineering and Processing 111 (2017) 46–56

Contents lists available at ScienceDirect

Chemical Engineering and Processing: Process Intensification

journal homepage: www.elsevier.com/locate/cep

Carbon dioxide (CO_2) absorption and interfacial mass transfer across vertically confined free liquid film-a numerical investigation

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ARTICLE INFO

Article history:
Received 13 February 2016
Received in revised form 21 August 2016
Accepted 11 November 2016
Available online 11 November 2016

Keywords:
Confined free liquid film
Mass transfer
Vorticity
Computational fluid dynamics (CFD)

ABSTRACT

CO_2 absorption by a confined free film has been investigated using the CFD approach. Particular attention focuses on the relationship between mass transfer and flow behaviour of the confined free film. Simulation results show that the average K_L value grows 26.9% for the open window region and 17.4% for the lower-wall region, respectively, in comparison to the values in the upper-wall region, and the average K_L value of confined free film along the flow direction is about 19.2% higher than the value of wall-bounded film, which affirms that the use of an open window can significantly enhance mass transfer performance and such effect also has impact on the entire regions. It was revealed that there exist two types of vortices inside the film, inner vortices and interfacial vortices. In addition, a correlation coefficient $R_{\Omega c}$ is proposed to provide a quantitative measure to characterise the relationship between the local mass concentration profile and vorticity distribution of confined free film. Simulation shows that the average value of $R_{\Omega c}$ is 0.93, indicating that the two parameters are highly correlated. Furthermore, the cause of lower correlation coefficient value is discussed.

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1. Introduction

Besides the two commonly known types of liquid films: wall-bounded film, which is supported by a solid wall, and free film, which flows without contact with any solid frame and has two apparent interfaces. There is another type of film flow that is rarely reported in the open literature, namely confined free film, in which both wall-bounded film and free film coexist. The important feature that distinguishes confined free film from typical liquid films is that it not only presents two free surfaces, but it is also enclosed in a solid boundary and is in contact with the surrounding solid frames. Typical examples, as shown in Fig. 1, are disc-rotating reactors and some structured packings.

The flow hydrodynamics of confined free film on a vertically aligned plate with an open window were investigated by Hu et al. [1] using the CFD modelling approach. In this research, particular interest is focused on the mass transfer process of vertically confined free film together with the interaction between the liquid film flow behaviour and the species transport inside the liquid film.

The earlier study that demonstrates the differences of mass transfer behaviour of wall-bounded film and confined free film probably can be traced back to Eckert's [2] study, who employed carbon dioxide and sodium hydroxide system to measure the mass transfer efficiency of several ring-type packings including Raschig Ring (unperforated) and Pall Ring (perforated) over a wide range of loading (24.4–48.8 $m^3/(m^2\,h)$). The results demonstrated that the mass transfer coefficient of the perforated packing (Pall Ring) is 25.0%–57.6% higher than the unperforated one (Raschig Ring) of the same size (25.4–50.8 mm). Fair et al. [3] investigated the effect of perforation on capacity of the 400 m^2/m^3 size packings. Their experimental results clearly indicate that the perforated sheet metal packing has a larger mass transfer capacity compared with that of the unperforated one of the same size. They suggested that the perforated surface has a high percentage of open area which allows the gas to escape to the neighbouring channels when local liquid overload occurs. Hu et al. [4] employed a novel structured plate with windows for CO_2 to be absorbed by highly concentrated DEA solutions. The absorption experimental results showed that when the liquid viscosity is lower than 5.8 mPa s, a mass transfer intensification of 30%–40% can be obtained for a plate with large size windows. Under the conditions of higher viscosity and lower liquid load, the mass transfer intensification may be attained up to 60%–70% and the maximum value can even reaches 100%. Hu et al.

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http://dx.doi.org/10.1016/j.cep.2016.11.002
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Nomenclature

c Concentration of a species in the aqueous phase (mol/m^3)
D Liquid side diffusion coefficient (m^2/s)
F_{VOL} Surface tension source term
g Gravitational acceleration (m/s^2)
h Local film thickness (m)
h_0 Nusselt film thickness (m)
K_L Liquid side mass transfer coefficient (m/s)
n Surface normal
Re Reynolds number
We Weber number
u Streamwise velocity; (m/s)
u_0 Average velocity; (m/s)
v Perpendicular velocity; (m/s)

Greek letters
α Volume fraction
κ Curvature of free surface
ρ Density; (kg/m^3)
μ Viscosity; (kg/(m s))
σ Surface tension; (N/m)
Ω Vorticity; (1/s)

Subscripts
g Vapour phase
L Liquid phase
in Inlet

[5] have recently developed a novel structured packing with vertical packing sheets perforated by large size windows for viscous absorbents, desorption of oxygen from water was carried out in a packed column operating under the liquid load of 10–38 m^3/(m^2 s) and F factor of 0.2–3.2 Pa$^{0.5}$. Experimental results have indicated that by adopting this kind of packing geometry, an enhanced mass transfer efficiency by 35%–45% can be obtained even comparing with currently used commercial structural packings. Though a solid substrate with holes or open windows has been widely recognised to be able to achieve better mass transfer performance, understanding of the mechanism of the mass transfer intensification by employing such structure is still not fully understood. To investigate the differences of surface renewal frequency between the confined free film and wall-bounded Deng and Dai [6] proposed a novel model to study the surface renewal in a rotating disc reactor with open windows by CFD method. The results showed that the renewal frequency of the film in the open window region is 40% faster than that of the film in the solid wall region, and it was also shown that the renewal frequency of the confined free film on round window was 34% faster than that on fan-shaped window.

It becomes quite clear that the hydrodynamic behaviour of a falling film plays an important role in enhancing and improving mass and heat transfer performance. To predict the effect of wavy interface on the enhancement of mass transport rates, various experimental methods have been attempted in previous studies [7–11], the experimental results revealed that the wave regimes and the wave parameters (e.g. wave frequency and wave amplitude) have a strong impact on mass transfer rate across the gas-liquid interface, and the mass transfer in wavy films is greater than those provided by the waveless flow. The use of the computational fluid dynamics (CFD) approach to study the hydrodynamics and mass transfer across the gas-liquid interface of thin liquid film flow has received great attention because it may be able to offer the details of hydrodynamics and mass transfer process occurring inside the film, which is still not easily acquired from the experiments. Hoffmann et al. [12] studied the complex flow behaviour of homogeneous and heterogeneous liquids on inclined plates by CFD method, it has been shown that flow behaviours like film break-up, rivulet and droplet flow can be represented as well as predicted by the numerical approach. Xu et al. [13,14] studied the liquid flow behaviour using a 3-D VOF model, the flow regimes and the transition conditions between droplet, rivulet and liquid film are especially investigated. Numerical results showed that the liquid rate is the most important factor affecting the liquid flow regimes. In addition, Many numerical studies [15–25] have focused on the relationship between the interfacial wave hydrodynamics and the corresponding mass transfer process. Recently, Hu et al. [26] studied the process of CO_2 absorption across a thin falling film gas-liquid interface. The mass transfer across the falling film interface is interpreted as the passive scalar entrapment and entrainment by the interfacial vortices. The numerical simulation reveals that mass transfer across the falling film is highly correlated with the interfacial vorticity. Nagaosa [27] used an extended concept of a two-compartment model to obtain details of the gas exchange mechanisms in the liquid phase. Particular attention is paid to the effects of the Schmidt number of the gas on the mass transfer rate at the interface. Cekic and Sisoev [28] focused on the mass transfer problem in a two-layer film flowing down a vertical plane. Based on an approximate long-wave model, they computed the nonlinear wavy regimes in the two-layer film flow and solved the gas absorption problem numerically. It has been shown that the absorption rate is promoted for wavy regimes in comparison with the waveless flow, and this amplification is much more obvious at the interface between the liquid as well as at the film surface. The largest local gas fluxes at the surface and interface can be observed at wave troughs where the local film thicknesses are minimum. Guo *et al.* [29] used LBM-FDM (Lattice-Bolzmann/finite-difference method) to investigate the temporal-spatial evolution of velocity and the transformation of mass transfer mechanism of the process of CO_2 absorption into solvents across a horizontal gas–liquid interface. The results showed that the Rayleigh convection can be considered as a special turbulent flow even that the whole domain remains quiescent, and convective mass transfer accounted for the dominant part of the mass flux in case of Rayleigh convection.

Though a solid substrate with holes or open windows has been widely recognised to be able to achieve better mass transfer performance, it seems that to the best of authors' knowledge, discussion in depth on the mass transfer mechanism of the free falling film in an open window is rarely found based on the research reported in the open literatures on gas absorption across a thin liquid film. To contribute the understanding of the problem concerned, on the basis of previous work [4,5,26], the present work aims at further illuminating the mass transfer behaviour of gas absorption into vertically confined free film. As the film hydrodynamics associated with the vorticity has a strong impact on the mass transfer across the gas-liquid interface, the current study will also seek the relationship between the mass transfer behaviour and the interfacial vorticity, in particular investigating CO_2 gas absorption into a falling confined free film. The paper is organized in such a way that mathematical modelling part describes the governing equations for interfacial mass transfer of CO_2 absorption into a falling confined free film and the numerical modelling together with the suitable boundary

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