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3D modeling of hydrodynamics and physical mass transfer characteristics of liquid film flows in structured packing elements

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ABSTRACT

Post-combustion CO_2 capture by chemical absorption in structured packed columns has been technically and commercially proven as a viable option to be deployed for carbon emissions mitigation. In this work, a three dimensional CFD model at small scale for hydrodynamics and physical mass transfer in structured packing elements is developed. The results from the present model are validated with theory and reported experimental data. For hydrodynamics, the liquid film thickness and wetted area are calculated whereas for mass transfer, the Sherwood number and concentrations of dissolved species are predicted. The CFD results match reasonably with experimental and theoretical data. Furthermore, the influence of texture patterns and the liquid phase viscosity on the wetted area is studied. It is found that both parameters have a strong influence on the results. For physical mass transfer, the study of the transient behavior and the impact of the liquid load on the absorption rate is assessed. It is observed that lower liquid loads maximize mass transfer coefficients but also enhance liquid misdistribution (i.e. with the possibility of hindering mass transfer). An optimum liquid load is found where the effect of liquid misdistribution can be avoided, maximizing gas absorption.

1. Introduction

Human activity in the last centuries has increased the amount of greenhouse gases, including CO_2, in the atmosphere, contributing to anthropogenic climate change (IPCC, 2001). One of the most important sources of CO_2 is fossil fuel power plants. Emissions can be reduced by applying carbon capture and storage (Abu-Zahra et al., 2007). Carbon capture and storage (CCS) is a technology that deals with the capture of CO_2, its transportation, and its storage, e.g. injection into geological formations or to perform enhanced oil recovery (Razi et al., 2012). This work focuses in the first part of the CCS process (i.e. carbon capture). Three different technologies exist to avoid the release of power plant generated CO_2 into the atmosphere (Figueroa et al., 2008): pre-combustion, oxy-fuel technology and post-combustion. Pre-combustion techniques remove CO_2 after gasification of coal (i.e. before the combustion of syngas takes place). In oxy-fuel combustion almost pure oxygen is combined with the fuel, and the flue gases contain mainly water vapor and CO_2. The latter can be easily removed by condensation. In post-combustion, CO_2 is scrubbed from the flue gas stream after combustion is carried out in the conventional way. Among these techniques, post combustion method via chemical absorption by means of reactive amine solutions in packed columns has been identified to have a high potential of being applied in a commercial scale due to the possibility of being retrofitted to existing coal or gas power plants, the existence of high values of effective mass exchange areas, and the capability of treating large amounts of flue gas with a relatively low pressure drop (Mangalapally et al., 2012; Hosseini et al., 2012). The high regeneration cost of the amine solutions, which accounts approximately for 60–80% of the total operating cost, is one of the drawbacks (Mores et al., 2012; Raynal et al., 2011). In a post-combustion CO_2 scrubbing facility by chemical absorption, the solvent enters the absorber at the top of it whereas the flue gas from the power plant is injected at the bottom of the reactor. In the literature, various solvents including aqueous solutions of MEA (monoethanolamine, C_2H_7NO), MDEA (methyldiethanolamine, $C_5H_{13}NO_2$) or TEA (triethanolamine, $C_6H_{15}NO_3$) have been tested to increase capture efficiency and to reduce regeneration costs. After the chemical reaction is produced, the output is CO_2-free flue gas and a solvent mixture rich in CO_2. Regeneration of the rich solvent into a CO_2-free stream takes place in the regenerator, where hot steam is applied to decrease the carbon dioxide partial pressure, to break the weak bonds between CO_2 and the amine solution, and to heat the solvent.

In recent years CFD has become an indispensable tool for the study of multiphase flows within complicated geometries since it helps to reduce the number of experiments and the cost of design

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Nomenclature

Latin symbols

a	area per unit volume (m^{-1})
C	total concentration ($kg\,m^{-3}$)
D	mass diffusivity ($m^2\,s^{-1}$)
d	liquid inlet thickness (m)
F	volume fraction (−)
g	acceleration of gravity ($m\,s^{-2}$)
k	mass transfer coefficient ($m\,s^{-1}$)
L	distance traveled by liquid film (m)
P	pressure (Pa)
S	mass source term ($kg\,s^{-1}\,m^{-3}$)
t	time (s)
v	velocity ($m\,s^{-1}$)
X	inclined plate length (m)
y	mass fraction (−)
z	coordinate along film thickness (m)

Greek symbols

β	plate inclination angle (−)
ρ	density ($kg\,m^{-3}$)
μ	dynamic viscosity (Pa s)
δ	liquid film thickness (m)
σ	surface tension coefficient ($N\,m^{-1}$)
θ	contact angle between liquid and solid wall (−)
τ	exposure time (s)
κ	surface curvature (m^{-1})

Subscripts

avg	averaged
e	effective
g	gas phase
i	interface
inj	injection
l	liquid phase

Dimensionless numbers

Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
We	Weber number

and optimization (Fernandes et al., 2009; Hosseini et al., 2012). Also, the difficulty to insert probes to measure velocity, temperature or pressure profiles within the falling liquid film in a structured packed column makes numerical studies significant in this field (Adachi, 2013).

Due to the current computational capacity available, it is impossible to perform simulations of the entire absorbing column focusing in every physical phenomenon therein (i.e. hydrodynamics, mass transfer, and chemical reactions). Thus, numerical studies on absorption columns are often investigated in three different scales including micro-scale, meso-scale and macro-scale (Raynal and Royon-Lebeaud, 2007; Sun et al., 2013). In micro-scale, the hydrodynamics (i.e. liquid holdup and liquid misdistribution) and the reactive mass transfer characteristics of liquid films in a small element of packing material are studied using the VOF method. Micro-scale simulations normally consist of millimeter or centimeter-sized computational domains with cell sizes about the order of the micron. Hoffmann et al. (2005) studied the gas–liquid flows on an inclined plate using both experimental and numerical simulations. They reported a good agreement of surface velocities and wetted area results obtained from experiments and numerical simulations. Haelssig et al. (2010) studied mass transfer for an ethanol–water mixture in simple 2D geometries. Haroun et al. (2010) studied the interfacial mass transfer in falling liquid films by 2D direct numerical simulations using a VOF solver (JADIM code). They compared the Sherwood number calculated from simulations and Higbie penetration theory and concluded that a good agreement was achieved between numerical studies and theoretical predictions. Iso and Chen (2011) and Iso et al. (2013) reported an increase in the wetted area when textured plates are employed (i.e. instead of smooth surfaces) for liquid film flows. In small-scale hydrodynamics liquid misdistribution is one of the key aspects affecting the performance of a structured packed column. Although the purpose of a structured packing is to accomplish a substantial amount of surface per unit volume of packing, not all this surface is normally wetted by the liquid. As a result, the amount of surface available for absorption is less than expected, and this reduces the quantity of absorbed CO_2. Fourati et al. (2012) visualized this effect by means of gamma-ray tomography, showing a heterogeneous concentration of liquid phase at small-scale. They reported that the presence of this heterogeneous concentration field is mainly due to the liquid misdistribution phenomenon. The authors also found that this effect is more pronounced in the lower part of the reactor than in the zone closer to the liquid injection region.

Meso-scale studies involve the flow of gas phase between metal sheets, which gives the dry pressure drop in the packed column. In this approach, a set of representative elementary units stands for the entire structured packed column (Larachi et al., 2003; Said et al., 2011). Correction factors are applied to dry pressure drop in order to obtain wet pressure drop as a function of liquid holdup (Fernandes et al., 2009). Chen et al. (2009) presented a 3D two-phase flow VOF model using ANSYS® FLUENT in an actual representative elementary unit (REU) of packing material (Mellapak® 350Y), analyzing wetted area and mass transfer performance. To validate mass transfer, the results for the concentration of the species being transferred at the liquid outlet were used. van Baten and Krishna (2002) studied the mass transfer between phases within KATAPAK-S® sandwich structures using ANSYS® CFX version 4.2. Numerical results for Sherwood number as a function of gas velocity were compared with the results from Subawalla et al. (1997).

Macro-scale approach utilizes the pressure drop correlations obtained from meso-scale studies as an input to determine the flow patterns inside the absorbing column, and the influence of walls, injectors, etc. on them. Raynal et al. (2009) implemented pressure drop correlations obtained at meso-scale in a full-scale reactor to check velocity patterns for three different geometrical configurations: no gas distributor, vertical pipe distributor, and vertical pipe with impact plate distributor. Asendrych et al. (2013) presented an Euler–Euler model for reactive mass transfer within a 1.5 m-long porous region that simulated a structured packed column, obtaining results for pressure drop, gas velocities, liquid velocities, volume fraction and CO_2 concentration along the reactor. Fourati et al. (2013) developed 2D, axi-symmetric simulations of a porous domain to reproduce the liquid spreading results previously studied by means of gamma-ray tomography. In their work, the structured packed zone was treated as a porous zone where the advection–diffusion equation (Edwards et al., 1999) is solved. Lappalainen et al. (2009, 2011) used the same approach to study the radial spreading phenomenon of liquid flow in trickle bed reactors.

As a conclusion, even though some studies on hydrodynamics of liquid misdistribution along with mass transfer have been reported at various scales in the literature, the relationship between both features still needs to be understood thoroughly at small-scale.

In this work, the hydrodynamics and physical mass transfer characteristics of liquid film flows on an inclined metallic plate are studied using 3D CFD simulations. The numerical results from the present model are validated to ensure their reliability. For