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Hydrodynamics of the rivulet flow over corrugated sheet used in structured packings

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ABSTRACT

A key factor influencing the overall efficiency in a structured packed column, such as used for solvent absorption, is wetting of the corrugated sheets. Computational fluid dynamics modeling of solvent absorption is a multi-scale problem with flow over a corrugated sheet providing a relatively simple setup to investigate the microscale flow phenomena present in these complex systems. Accordingly, multiphase flow simulations of rivulet flow over a corrugated sheet were systematically carried out over a wide range of solvent physical properties and contact angles using the volume of fluid method. A scaling analysis for wetted and interfacial areas was performed on the simulation results, and a theory for interfacial area in terms of Kapitza number is proposed. The advantage of the Kapitza number is that it only depends on fluid properties and is independent of flow parameters. The results show that the interfacial area of the rivulet decreases as the Kapitza number increases for a given contact angle and flow rate. The effects of the corrugation angle on the interfacial area were also extensively investigated. The interfacial area shows non-monotonic variation with increasing corrugation angle, i.e, it first increases until 45° and then it decreases. Hence, 45° can be considered the optimum corrugation angle for enhanced interfacial area in this setup.

1. Introduction

Carbon dioxide (CO_2) and other greenhouse gases emissions are the primary source of global warming (IEA, 2008). One of the major sources of CO_2 emissions that must be mitigated is fossil fuel power plants as they contribute to roughly 40% of the emissions worldwide (Chu, 2009). Post-combustion carbon capture by chemical absorption is an efficient technology used to reduce CO_2 emissions in industry and is being explored for its potential use in power plants (Spiegel and Meier, 2003). The conventional process for chemical absorption involves countercurrent gas–liquid flow through a packed column. Structured packing provides a large surface area for mass transfer between the phases and produces a minimum pressure drop across the column (Mackowiak, 2010). This packing is generally made of corrugated sheets arranged in a crisscross fashion that are combined to form a single layer of the packing element. The column is then filled with many layers of these packing units rotated with respect to one another. The liquid distribution in the packing unit plays a key role in the efficiency of the column. For example, two columns may exhibit different absorption rates even at the same liquid holdup for a given liquid flow rate (Eldridge, 2005) due to differences in the liquid flow pattern and resulting interfacial area. When the liquid distribution becomes especially uneven (i.e., liquid maldistribution) it may result in unacceptable operation (Lockett and Billingham, 2003). Therefore, accurate column design requires knowing such hydrodynamic characteristics of the packing system.

A structured packed column exhibits a wide disparity in length scales: column dimension ($\sim$5–10 m and $H \sim$ 20–30 m), characteristic dimensions of packing unit ($\sim$20 cm), and film thickness ($<$1 mm). These scales cannot be resolved simultaneously within a single computational model. Accordingly, a multiscale (i.e., micro, meso, and macro) modelling approach could be used to resolve these differences in scale (Raynal and Royon-Lebeaud, 2007). Computational fluid dynamic (CFD) simulations of rivulet flow over corrugated sheets can provide useful insights into the packing unit's microscale hydrodynamics, such as, interfacial area and film thickness.

Over the past several decades, CFD has shown promise and gained acceptance for studying flow characteristics in structured packings. CFD simulations using the volume of fluid (VOF) method were conducted of film flow over an inclined plate in an effort to explain the

Abbreviations: CFL, Courant–Friedrichs–Lewy; CSF, Continuum surface force; AMP, 2-aminomethylpropanol; MDEA, *N*-methyldiethanolamine; MEA, Monoethanolamine; MPZ, 1-methylepiperazine; PISO, Pressure implicit with split of operators; PLIC, Piecewise linear interface calculation; VOF, Volume of fluid

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Nomenclature

A	Area
B	Base of channel
CO	Courant number
D	Hydraulic diameter
F	Surface tension force per unit volume
f	Volume fraction
g	Gravitational acceleration
h	Height of channel
h_L	Liquid holdup
H	Height of column
Ka	Kapitza number
n	Unit normal vector
p	Pressure
Q	Solvent flow rate
Re	Reynolds number
S	Side of channel
t	Time
u	Velocity vector
W	Sheet width
We	Weber number
x	Mole fraction

Greek symbols

α	Corrugation angle
δ	Film thickness
ϕ	Column diameter
γ	Contact angle
∇	Gradient operator
Δt	Time step
κ	Interface curvature
μ	Dynamic viscosity
ν	Kinematic viscosity
θ	Crimp angle
ρ	Density
σ	Surface tension

Subscripts

av	Average
f	Projected
g	Gas
In	Normalized interfacial
in	Inlet
l	Liquid
wn	Normalized wetted
w	Wetted
P	Total

Superscripts

*	Normalized value
T	Transpose

hydrodynamics in a packed column (Iso et al., 2013; Singh et al., 2016; Hoffmann et al., 2006; Ataki and Bart, 2004; Singh et al., 2017). These works are based on relatively simple setups and flow patterns compared to the complexity of geometry and flow that exists in an actual structured packing column. As such, it is unlikely that these studies' results will fully capture that which occurs under more realistic conditions. Structured packings have been more specifically targeted by a number of 2D VOF simulation studies that examined film flow over wavy plates in either stagnant air conditions (Gu et al., 2004), or for co-current (Raynal et al., 2004; Fernandes et al., 2009) or countercurrent (Hosseini et al., 2012; Szulczewska et al., 2003) gas–liquid flow. In several of these CFD studies, film thickness predicted by simulation or computed based on simplifying assumptions (e.g., uniform film thickness) was first used to derive liquid holdup. Calculations were then made to determine the wet pressure drop in structured packings via a pseudo single phase CFD model (Raynal et al., 2004; Fernandes et al., 2009; Hosseini et al., 2012). Szulczewska et al. (Szulczewska et al., 2003) studied the effect of flow rate on the interfacial area and used the VOF model to predict the value of liquid flow rate needed to achieve fully wetted packing. Haroun et al. (Haroun et al., 2010) conducted 2D simulations to study mass transfer and liquid hold-up in structured packings and observed that interfacial mass transfer is affected by the interface shape and flow conditions that control exposure time at the interface. Still, the knowledge gained from such studies must be carefully considered given their 2D nature and simplification of the flow/geometry. Flow effects and events such as film rupture and rivulet flow cannot be captured by 2D simulations and require a 3D simulation for investigation (Hoffmann et al., 2005).

Various 3D CFD studies of gas-liquid flow in geometries of varying complexity that are representative of different structured packings have also been performed. Owens et al. (2013) performed single phase flow simulations through single and multiple half elements of Mellapak N250.Y packing and found that the CFD-predicted pressure drop matched well with experimental results. Li et al. (2015) studied liquid flow behavior on a sheet of corrugated SiC-foam using the VOF method and the CFD results for wetted area matched well with experimental observations. Subramanian et al. (2012) used the VOF method to examine both rivulet flow on a single corrugated sheet using a single liquid inlet, and wetting behavior on two corrugated sheets using multiple liquid inlets. Although different fluids and contact angles (γ) were involved in the simulation, the effect of solvent properties was not the focus of their study. Instead, the authors were interested in the influence of surface structure and perforations on wetting and wetting efficiency.

As noted earlier, interfacial area is the critical component for absorption efficiency, and numerous experimental and computational efforts have been reported. Using high resolution tomography Janzen et al. (2013) reported enhanced interfacial area with increasing viscosity (ranging from 1 to 20 mPas) at different liquid loads on MellapakPlus 752.Y packing. In contrast, using absorption measurements Tsai et al. (2011) reported negligible effect of solvent viscosity (ranging from 1 to 15 mPas) on interfacial area at different liquid loads on three structured packings. The influence of surface tension (σ) was found to be more significant and depend on the packing. Rizzuti and Brucato (1989) observed non-monotonic variation of the interfacial area with increasing viscosity (interfacial area increases and then decreases) based on absorption data in a Raschig ring packed column for varying liquid flow rates. In this case the range of viscosity explored was limited: ~1.23–2.3 mPas. As indicated, the effect of solvent properties on interfacial area is not entirely clear, and so is an area more extensively investigated herein.

More recent experimental studies using x-ray tomography have shown a complex inter-dependency of liquid load and viscosity on liquid holdup in structured packings (Bradtmöller et al., 2015). The authors identified three flow patterns in their investigation, including film flow, which is generally considered the most important when considering interfacial area. Under film flow, the authors observed non-monotonic variation in liquid holdup with liquid load (i.e. first increases then decreases) for a highly viscous liquid ($\mu \geq 20$ m Pas). However, for two lower viscosity liquids the liquid holdup always increased with liquid load although the increase became less significant at