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Numerical study of liquid coverage in a gas–liquid–solid packed bed

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A B S T R A C T

In this work, computational fluid dynamics (CFD) simulations using the volume-of-fluid (VOF) model were employed to investigate the effects of liquid properties, liquid and gas flow rates, and wettability of particles on liquid maldistribution at the microscopic level in a fixed bed reactor. The simulation results show that the number of wetted particles decreases with increasing gas velocity, consequently leading to lower liquid–solid contact areas. The radial liquid distribution is greatly enhanced by increasing the liquid flow rate, whereas the time for the liquid to pass through the whole bed is decreased, as expected. Based on simulation results, it was found that the liquid–solid contact area can be increased by using liquids of high viscosities and more wettable particles. However, the flow-through time increases with increasing liquid viscosity. An increase in the gas density showed a minimal impact on the liquid flow-through time, and the liquid density does not impact the radial liquid distribution or the liquid flow time within a range of liquid densities typically encountered in the petrochemical industry.

Introduction

Fixed bed reactors are widely used in various industrial applications, including petrochemical and chemical industries, waste water treatment, biochemical and electrochemical processing (Al-Dahhan, Larachi, Dudukovic, & Laurent, 1997; Larachi, Belfares, Iliuta, & Grandjean, 2003; Satterfield, 1975; Sobieszuk, Aubin, & Pohorecki, 2012). Different types of fixed bed reactors have been developed for different processes. For example, the trickle-bed reactor (TBR), in which gas and liquid reactants flow co-currently downward through the bed packed with solid catalyst particles, represents one widely-used type of multiphase flow reactor. The multiphase flow in a fixed bed is complex; different flow patterns can be found, including gas-continuous or trickle flow at low liquid and gas flow rates, pulse flow at intermediate liquid and gas flow rates, and liquid-continuous or dispersed bubble flow at higher liquid flow rates (Schwidder & Schnitzlein, 2012). Additionally, flow maldistribution, channeling, catalyst wetting, and local temperature variation may occur and significantly affect the overall reactor performance. Such phenomena may arise from systems with disparate parameters (Du, Feng, Xu, & Wei, 2013). Moreover, flow hysteresis, another undesirable flow phenomenon, caused by flow maldistribution in parallel channels in a TBR, is highly influenced by initial start-up conditions and tends to abate after the entire bed is fully wetted. However, the underlying mechanism is not clearly understood and flow hysteresis cannot be well interpreted from macro-scale analyses (Krieg, Helwick, Dillon, & McCready, 1995; Lin, Juang, Chen, & Chen, 2001; Urseanu, Boelhouwer, Bosmanand, & Schroijen, 2004). Therefore, attempts have been made to understand detailed flow behavior inside the flow channels between catalyst particles. Experimental studies (Wang, Mao, & Chen, 1992; Xiao, Zhu, Anter, Chen, & Yuan, 2000) have shown that liquid holdup could be directly linked to gas–liquid flow through the voidage based on an assumption of film flow on the surface of catalyst particles. However, this assumption is not always valid as varying channel sizes and other operating parameters could considerably alter the gas–liquid flow patterns between particles.

In addition to the experimental studies, computational fluid dynamics (CFD) is considered to be a powerful tool to investigate detailed flow behavior inside the flow channels between catalyst particles from a microscale perspective. In CFD simulations of packed-bed reactors, the discrete particle approach is largely adopted (Dixon, Nijemeisland, & Stitt, 2006), allowing simulation of an interstitial flow between particles accounting for the geometric complexity of the packing structure. In this method, a volume-of-fluid (VOF) model is incorporated into the Eulerian–Eulerian approach so that the surface between phases can be tracked in the simulations (Jiang, Khadilkar, Al-Dahhan, & Dudukovic, 2002a;

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Nomenclature

Bo	bond number ($(\rho_L - \rho_G)gd^2/\sigma$)
Ca	capillary number ($\mu_L U_L/\sigma$)
F	force (N)
G	gravitational constant (m/s^2)
n	surface normal, gradient of α
n_w	the unit vectors normal to the wall
p	pressure (N/m^2)
R	radii in orthogonal direction (m)
Re	Reynold number ($d_p U\rho/\mu$)
S	source term
t	time (s)
t_w	the unit vectors tangential to the wall
U	superficial velocity (m/s)
v	velocity (m/s)
We	Webber number ($\rho U^2 d_p/\sigma$)

Greek letters

α	volume fraction
θ_w	contact angle (°)
κ	curvature
μ	viscosity (Pa s)
ρ	density (kg/m^3)
σ	surface tension (dyn/cm)

Subscripts

1	phase 1
2	phase 2
G	gas
i	phase i
j	phase j
L	liquid
q	phase
w	wall

Jiang, Khadilkar, Al-Dahhan, & Dudukovic, 2002b; Lopes & Quinta-Ferreira, 2010a; Lopes & Quinta-Ferreira, 2010b). Great efforts have been made by Quinta-Ferreira and coworkers who use a high-resolution CFD simulation approach involving two moving phases (Lopes, Silva, & Quinta-Ferreira, 2007; Lopes & Quinta-Ferreira, 2010a; Lopes & Quinta-Ferreira, 2010b). In their work, a TBR was designed using regularly shaped catalyst particles in the simulation and the effects of the bed geometry on transport phenomena in the reactor were explored.

Recently, the gas–liquid flow maldistribution has been studied based on advances in CFD methodology and the multi-scale concept. Mousavi, Jafari, Yaghmaei, Vossoughi, and Sarkomaa (2006) investigated film flow, trickle flow, and spray flow behaviors in a packed bed and concluded that the liquid distribution and velocity distribution were mainly affected by liquid surface tension and the bed voidage. Jiang, Khadilkar, Al-Dahhan, and Dudukovic (2001) demonstrated that an unsteady-state operation ensured better uniformity in the liquid distribution. Boyer, Koudil, Chen, and Dudukovic (2005) found the capillary pressure term had a significant effect on predicting radial spreading of the liquid flow. Atta, Roy, and Nigam (2007) developed a three-dimensional two-phase model to predict liquid maldistribution in a TBR and found that significant liquid spreading only occurred where the ratio of the column diameter to the particle diameter was very small. Lopes and Quinta-Ferreira (2009) considered three types of liquid distributors in their CFD simulations and their results showed that the liquid distributor geometry had a major effect on hydrodynamic performance in low-interaction regimes.

Table 1
Summary of the volume fraction and momentum equations of the VOF model.

Continuity equation	
$\dfrac{\partial \alpha_q}{\partial t} + \vec{v} \cdot \nabla \alpha_q = \dfrac{S_{\alpha_q}}{\rho_q}$	(1)
$\sum_{q=1}^{n} \alpha_q = 1$	(2)
Mixture properties	
$\rho = \alpha_2\rho_2 + (1-\alpha_2)\rho_1$	(3)
$\mu = \alpha_2\mu_2 + (1-\alpha_2)\mu_1$	(4)
Momentum equation	
$\dfrac{\partial}{\partial t}(\rho\vec{v}) + \nabla \cdot (\rho\vec{v}\vec{v}) = -\nabla p + \nabla \cdot \left[\mu(\nabla\vec{v} + \nabla\vec{v}^T)\right] + \rho\vec{g} + \vec{F}$	(5)
Surface tension	
$p_2 - p_1 = \sigma\left(\dfrac{1}{R_1} + \dfrac{1}{R_2}\right)$	(6)
Volume force	
$F_{vol} = \sigma_{ij}\dfrac{\rho\kappa_i\nabla\alpha_i}{\frac{1}{2}(\rho_i + \rho_j)}$	(7)
Curvature	
$\kappa = \nabla \cdot \left(\dfrac{n}{\lvert n\rvert}\right)$	(8)
Wall adhesion	
$\hat{n} = \hat{n}_w \cos\theta_w + \hat{t}_w \sin\theta_w$	(9)

In the above-mentioned studies, the liquid maldistribution was mainly considered at a macroscopic level and was mainly seen to be affected by inlet liquid distribution, particle shape and size, fluid velocity, and the packing method. At the microscopic level, liquid maldistribution is believed to be closely associated with the physicochemical properties of the liquid (density, viscosity, surface tension), liquid and gas flow rates (Onda, Takeuchi, Maeda, & Takeuchi, 1973; Saroha, Nigam, Saxena, & Kapoor, 1998), wettability (Schwartz, Weger, & Dudukovic, 1976), shape and orientation of catalyst particles (Kundu, Saroha, & Nigam, 2001; Ng & Chu, 1987), and local packing structures. Our recent study (Du et al., 2013) has shown that the gas–liquid flow behavior around one spherical particle highly depends on the liquid velocity and liquid properties. The objective of this study is to understand which parameters influence liquid coverage and radial liquid distribution, especially at different locations in a TBR, which are of great importance to the reactor performance.

CFD simulation using VOF method

CFD model

In the present study, the VOF model was employed for numerical simulation of immiscible fluids. The key feature of this model is its ability to capture the effect of surface tension on the flow behavior of two immiscible phases in mini-channels.

The VOF model equations used in this study are summarized in Table 1, as provided in the FLUENT user's guide (2006). All variables and properties are shared by the two phases and represent volume-averaged values, as long as the volume fraction of each phase is known at each location. The tracking of the interface(s) between the two phases is accomplished by the solution of a continuity equation for the volume fraction of one (or more) of the phases (Eq. (1)). And the sum of the volume fractions for each phase is unity (Eq. (2)). The properties appearing in the transport equations are determined by the mixture of the component phases present in each control volume. In a gas–liquid two-phase system, for example, if the volume fraction is tracked, the density and dynamic viscosity in each cell are given by Eqs. (3) and (4). A single momentum equation, which is dependent on the volume fractions of both phases