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Effect of capillary pressure force on local liquid distribution in a trickle bed

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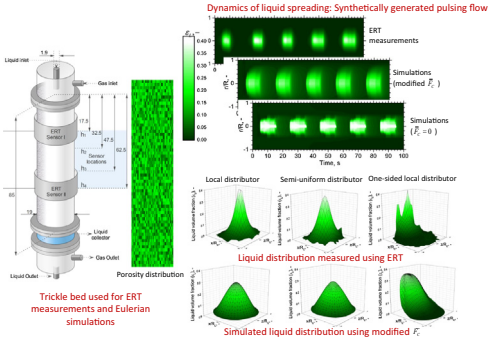
HIGHLIGHTS

- CFD simulations of local liquid distribution in trickle beds and verification using ERT measurements.
- Effect of capillary pressure force formulations on local liquid distribution evaluated.
- Roles of capillary pressure and mechanical dispersion forces analysed.
- Dynamics of local liquid spreading analysed using synthetically created pulsing flow.
- Modifications to capillary pressure force proposed.
- Ability of computational model to predict effects of liquid flow rates and liquid distributors verified.

GRAPHICAL ABSTRACT



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ABSTRACT

Accurate prediction of the local liquid volume fraction (ε_L) distribution, an important process parameter that governs the performance of Trickle Bed Reactors (TBRs), is still a challenge. In the present work, Eulerian multi-fluid simulations of local ε_L distribution were performed in a laboratory-scale pseudo-3D (rectangular) and cylindrical TBR and the predictions were compared with the Electrical Resistance Tomography (ERT) measurements of Singh et al. (2017). The effect of formulation of capillary pressure force ($\overline{F}_C$) was investigated and it was found that $-P_C\nabla\varepsilon_L$ definition of $\overline{F}_C$ preserved the functional relation between the capillary pressure (P_C) and ε_L, and that $\varepsilon_L\nabla P_C$ definition of $\overline{F}_C$ reversed the same. Through the simulations performed for the pseudo-3D column, we showed that the alteration in the functional relation severely affects the ability of $\overline{F}_C = \varepsilon_L\nabla P_C$ definition to predict the effects of particle diameter, gas and liquid flow rates. It was elucidated that such an alteration underpredicts $\overline{F}_C$ and could necessitate the inclusion of additional dispersion forces for particles with small diameters. $\overline{F}_C$ implemented as $-P_C\nabla\varepsilon_L$ provided satisfactory predictions of the steady-state local ε_L distribution for the bed pre-wetted with the pseudo-Kan pre-wetting method. However, the P_C model required an empirical correction ($[(d_P/d_{thr})(\varepsilon_S)^{0.6}]^{-13.957}$) to predict the steady-state local ε_L distribution in the bed pre-wetted using the Levec method. While the modified $\overline{F}_C$ predicted the time-averaged local ε_L distribution satisfactorily for different liquid flow rates and liquid distributor configurations, it was seen that further reduction in $\overline{F}_C$ was required to predict the dynamic liquid spreading behavior under synthetically created pulsing flow conditions.

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Notations

Symbols

a, b	model constants, –
C_μ	model constant (0.09), –
d_p	particle diameter, m
D/d_p	column to particle diameter ratio, –
d_{thr}	pore throat diameter, m
$\overline{F}_C$	capillary pressure force, kg/m^2 s^2
$\overline{F}_{ij}$	interaction force between phases i and j, kg/m^2 s^2
h	distance from the inlet, m
$J_0(x)$	zeroth order Bessel function.
P	pressure, kg/ms^2
P_C	capillary pressure, kg/ms^2
Q_i	mass flow rate of phase i per unit area, kg/m^2 s
r	radial coordinate, m
r^*	dimensionless radial coordinate, –
SD	standard deviation, –
V_i	volume of i, m^3
$\overline{U}_i$	mean (time averaged) velocity of phase i, m/s
k_i	turbulent kinetic energy of phase i, m^2/s^2
X_{ran}	random number, –

Greek letters

ε_b	bed porosity, –
ε_i	volume fraction of phase i, –
ε_i^*	turbulent dissipation rate of phase i, m^2/s^3
$\langle\varepsilon_L\rangle_{CS}$	cross-section average volume fraction of phase i, –
η_e	wetting efficiency, –
μ_i	viscosity phase i, kg/ms
π	constant (3.14), –
ρ_i	density of phase i, kg/m^3
σ	surface tension, kg/s^2

Subscripts

$i = L$	liquid
$i = G$	gas
$i = S$	solid
$i = B$	bed
$i = p$	particle

1. Introduction

Several applications in chemical process industry involve gas-liquid flow through packed beds. In a co-current down-flow TBR, gas and liquid reactants flow from the top of the column through a packed bed of solid catalyst. They find extensive applications in oil, petro-chemical and bio-chemical industries in general and in hydrotreating petroleum derivatives in particular, e.g. hydrodesulphurization of diesel. Since the local liquid distribution has a significant impact on their performance, better models are required for accurate prediction of local liquid distribution, which would significantly aid the predictions of local temperature and local concentration distributions, facilitating improved reactor design.

While measurements of parameters such as pressure drop, overall liquid hold-up, residence time distribution in a TBR are abundantly available in the literature, measurements of the local ε_L distribution in TBRs are rather limited. In the recent past, advanced non-intrusive techniques have been used to measure the liquid distribution in TBRs e.g. Magnetic Resonance Imaging, X-ray Tomography and Electrical Capacitance Volume Tomography. Nonetheless, these investigations are limited to ε_L distribution reported as cross-sectional averaged quantities or r-θ tomograms (Singh et al., 2017). Furthermore, radial ε_L distribution was investigated using the Gamma-ray Tomography (GRT) (Boyer et al., 2005; Schubert et al., 2008) at different Q_L and Q_G. Recently, Singh et al. (2017) used the Electrical Resistance Tomography (ERT) to measure local ε_L distribution over r-θ planes at different axial locations focusing on the influence of Q_L, Q_G, d_p and distributor configurations. Their spatially resolved (resolution $\approx$ 1 cm), and in some cases time-resolved (30 Hz) quantitative measurements of local ε_L distribution present a comprehensive data-set to validate computational fluid dynamics (CFD) based models for TBRs. Nevertheless, most of these experimental techniques pose practical limitations when employed in an industrial setting, thereby necessitating the development of computational models to predict the local liquid distribution in industrial-scale TBRs.

Primarily, the CFD models used to simulate liquid distribution in TBRs are developed based on two approaches: the porous media and the Eulerian multi-fluid; each differing solely on how the solid phase is modeled. Although both approaches have been used and shown to predict the overall pressure drop and overall liquid hold-up reasonably well, Martínez et al. (2012) have shown that the Eulerian multi-fluid approach led to better predictions of spatial liquid spreading. In the Eulerian multi-fluid framework, a common pressure is shared by the fluid phases. However, the interstitial capillary pores within trickle beds are of the length scales wherein the surface tension forces are significant and the assumption of a common fluid pressure breaks down. The difference in the pressures of the wetting and non-wetting phase in the trickle bed determined by the local curvature of the gas-liquid interface is defined as capillary pressure (P_C). This pressure difference drives liquid within the interstitial pores from a region of higher to lower liquid saturation and therefore it needs to be included in the Eulerian model. P_C can be predicted by different models with respect to the continuum framework. In the model proposed by Grosser et al. (1988), P_C was approximated to local liquid saturation through the well-known Leverett J function. They established the functional dependence of J function with liquid saturation based on the Leverett's experiments performed with sand samples. On the other hand, the model proposed by Attou and Ferschneider (1999) extends Young-Laplace's equation to the packed bed system, relating the orthogonal curvatures to d_p and local phase volume fractions. In the model proposed by Lappalainen et al. (2009b), P_C was determined based on the liquid saturation regimes, namely: pendular, funicular and capillary.

In order to account for the difference in pressure of the fluid phases, P_C predicted by these models must be included into the momentum conservation as a capillary pressure force ($\overline{F}_C$), typically into the liquid-phase momentum balance. Over the last decade, two different mathematical formulations have been used to define $\overline{F}_C$, which are: $\overline{F}_C = -P_C\nabla\varepsilon_L$ (Jiang et al. (2002), Boyer et al. (2005), Martínez et al. (2012), Jindal and Buwa (2017)) and $\overline{F}_C = \varepsilon_L\nabla P_C$ (Gunjal et al. (2005), Lappalainen et al. (2009a), Solomenko et al. (2015)). However, rigorous mathematical explanations for these definitions are limited. Nevertheless, the pressure difference drives liquid in the direction of decreasing liquid saturation; more precisely in the direction of the decreasing gradient of