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CFD modelling of multiphase flow distribution in trickle beds

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ABSTRACT

Multiphase flow in trickle-bed reactors (TBR) is known to be extremely complex and depends on a multitude of effects including the physico-chemical properties of both gas, liquid and solid phases, the ratio of column diameter to particle diameter and most importantly the gas and liquid superficial velocities. Despite several works devoted to the experimental investigation of liquid distribution, there is yet no universal agreement on the influence of interstitial phenomena on overall TBR hydrodynamics.

Consequently, a Eulerian multiphase model was developed to predict the liquid holdup and pressure drop in the trickling flow regime with a 3D computational grid. The multiphase model was optimized in terms of mesh density and time step for the successful hydrodynamic validation activities. The model predictions correctly handled the effect of different numerical solution parameters. Afterwards, particular attention is paid to the consequences on flow development and hydrodynamic parameters of imposing liquid maldistribution at the bed top with three types of liquid distributors. Several computational runs were carried out querying the effect of gas and liquid flow rate on overall hydrodynamics. Computational fluid dynamics (CFD) predictions demonstrated that liquid flow rate had a prominent effect on radial pressure drop profiles at the higher values whereas the gas flow rates had it major outcome at lower regimes. Regarding the liquid holdup predictions, several time averaged for radial and axial profiles illustrated that a five times increase on liquid flow rate cannot be matched by an equivalent change on gas flow rate. The increase in both flow rates was found to smooth the oscillatory behaviour of local phenomena, but the gas flow rate had an outstanding consequence on both hydrodynamic parameters. Finally, CFD simulations at atmospheric conditions were compared with the pressurized ones. Liquid holdup fluctuations of about 25% between the liquid-rich and the gas-rich zone can be smoothened as long as the operating pressure is increased until 30 bar.

1. Introduction

A trickle-bed reactor (TBR) is a packed bed in which gas and liquid flow co-currently downwards. Several aspects of hydrodynamics including flow patterns, pressure drop, gas and liquid holdup, wetting efficiency, heat and mass transfer, etc. were extensively studied and reviewed by Satterfield and co-workers [1–6]. TBRs have been commonly used in the petroleum industry for many years and are now gaining widespread use in several other fields from bio and electrochemical industries to the remediation of surface and underground water resources, being also recognized for its applications in advanced wastewaters treatments [7].

For a concurrent downflow trickle-bed reactor, four different flow patterns exist: the gas-continuous or trickle flow at low liquid and gas rates, pulse flow at intermediate liquid and gas rates, liquid continuous or dispersed bubble flow at higher liquid rates. The main characteristic in trickling flow is that at a sufficiently low liquid flow, the catalyst particles will only be partially wetted (partial wetting regime). If the liquid flow rate is increased, the partial wetting regime will gradually change to a complete wetting regime [8]. According to this flow map regime, the TBR selection choice is mainly motivated by hydrodynamic considerations in where one or more liquid–solid catalytic reactions occur. Liquid phase maldistribution is then an important factor in the design and scale-up of trickle-bed reactors so that one of the major challenges in its operation is the prevention of liquid flow maldistribution which causes portions of the bed to be incompletely wetted by the flowing liquid. Hence, the catalyst bed is underutilized and reactor performance and productivity is reduced, particularly for liquid limited reactions at low liquid mass velocities.

The research on liquid flow maldistribution is often dedicated in the experimental liquid distribution studies carried out in laboratory scale units using a collector at the outlet of the bed. Recently, several groups had emphasized the use of tomographic and video imaging techniques, which provides the flow distribution infor-

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Nomenclature

$C_{1\varepsilon}$, $C_{2\varepsilon}$	k–ε model parameters: 1.44, 1.92
d_p	particle nominal diameter (m)
E_1, E_2	Ergun's constants
$\vec{F}_i$	interphase momentum exchange term of ith phase
$\vec{g}$	gravitational acceleration, 9.81 s^2
G	gas mass flux (kg/m^2 s)
k	k–ε model kinetic energy
L	liquid mass flux (kg/m^2 s)
p	pressure (bar)
Δp	total pressure drop (Pa)
Re_i	Reynolds number of ith phase $[\rho_i u_i d_p/\mu_i]$ (dimensionless)
$\vec{u}$	superficial vector velocity (m/s)

Greek letters

α_i	volume fraction of ith phase
ε	k–ε model dissipation energy
ε_L	liquid holdup
ε_G	gas holdup
ε_S	solid volume fraction
μ_i	viscosity of ith phase (Pa s)
ρ_i	density of ith phase (kg/m^3)
σ_k, σ_ε	k–ε model parameters: 1.2, 1.0
$\hat{\tau}_i$	shear stress tensor of ith phase (Pa)

Subscripts

G	gas phase
i	ith phase
L	liquid phase
S	solid phase

mation more quantitatively [9–12]. The flow pattern and liquid maldistribution have been found to be dependent not only on the physico-chemical properties of the liquid (density, viscosity, surface tension), liquid and gas flow rates [13,14] but also on the ratio of reactor diameter to catalyst particle diameter [3,14,15], wettability [16], and shape and orientation of catalyst particles [8,17]. And ineffective liquid inlet distributor may also lead to poor liquid distribution due to large non-wetted regions of the packed bed.

Consequently, the assumption of uniform wetting efficiency throughout the reactor made in conventional reactor models is found to overpredict the reaction rate [18]. The solution to this problem requires a deep understanding of interstitial flow in trickle beds. A number of models of the liquid distribution have been developed in the past two decades based on different concepts or governing principles [19–24]. Sáez and Carbonell developed a model based on concept of relative permeability [25] whereas slit models proposed by Holub et al. and Iliuta et al. are based on phenomenological principles [26,27]. In this model the local flow of liquid and gas around the particles is modelled by assuming flow in rectangular inclined slits of width related to void fraction of the medium. The interfacial force model presented by Attou and Ferschneider takes into account the drag force on each phase with the contribution from the particle–fluid interaction as well as from the fluid–fluid interaction [28]. Recently, and with the increasing computational power and development of efficient computational fluid dynamics (CFD) algorithms multiphase flow in TBR has been modelled in a fashionable manner accounting for a new methodology for liquid flow distribution studies by means of numerical simulations. In this category, Souadnia and Latifi and Atta et al. have used the porous media model [29,30] and Jiang et al. and Gunjal et al. investigated the TBR hydrodynamics through the k-fluid model [31,32].

In the present work, the Eulerian framework is applied here to describe the multiphase flow in a three-dimensional geometry which allows the capture of interstitial flow in the packed bed. The Euler model is based on a set of continuity and momentum equations of each fluid phase with appropriate closures for the interaction forces. The individual drag forces are related with the flow velocities and volume fractions of each phase and to the physical properties of the gas, liquid and solid phases obtained from the fluid–fluid interfacial force model [28]. First, several computational runs were performed for the purpose of hydrodynamic model validation either in terms of liquid holdup or two-phase pressure drop. Afterwards, the quantitative understanding of flow maldistribution at the catalyst scale in the trickle bed is accomplished through the evaluation of time averaged axial and radial profiles for both hydrodynamic parameters. The influences of liquid distributor geometry as well as the effect of gas and liquid flow rates are investigated in the trickling flow regime.

2. CFD modelling

2.1. Euler–Euler momentum equation

Multiphase flow in the trickle-bed reactor was modelled using a multifluid CFD Euler–Euler two-fluid model implemented in commercial software FLUENT 6. In the Eulerian two-fluid approach, the gas and liquid phases are treated mathematically as interpenetrating continua. The derivation of the conservation equations for mass, momentum and energy for each of the individual phases is done by ensemble averaging the local instantaneous balances for each of the phases. At the subgrid scale, the two-fluid phases are described by the corresponding volume fractions and the pressure constrains the velocity field to ensure that the sum of the phase volume fractions equals unity. Fluids, gas and liquid, are treated as incompressible, and a single pressure field is shared by all phases.

FLUENT uses phase-weighted averaging for turbulent multiphase flow, and then no additional turbulent dispersion term is introduced into the continuity equation. The mass conservation equation for each phase is written in Eq. (1).

$$\frac{\partial}{\partial t}(\rho_i\alpha_i) + \nabla\cdot(\alpha_i\rho_i\vec{u}_i) = 0 \qquad (1)$$

where ρ_i, α_i and $\vec{u}_i$ represent the density, volume fraction and mean velocity, respectively, of phase i (L or G). As referred, the liquid phase L and the gas phase G are assumed to share space in proportion to their volume such that their volume fractions sums to unity in the cells domain:

$$\alpha_L + \alpha_G = 1 \qquad (2)$$

The momentum conservation equation for the phase i after averaging is written in Eq. (3).

$$\frac{\partial}{\partial t}(\rho_i\alpha_i\vec{u}_i) + \nabla\cdot(\rho_i\alpha_i\vec{u}_i\vec{u}_i) = -\alpha_i\nabla p + \nabla\cdot\bar{\bar{\tau}}_{eff} + \rho_i\alpha_i\vec{g} + \sum_{p=1}^{n}\vec{F}_{ij}(\vec{U}_{ij} - \vec{U}_{ji}) \qquad (3)$$

p is a pressure shared by the two phases and $\vec{F}_{ji}$ represents the interphase momentum exchange terms. The Reynolds stress tensor $\bar{\bar{\tau}}_{eff}$ is related to the mean velocity gradients using a *Boussinesq* hypothesis as expressed in Eq. (4).

$$\bar{\bar{\tau}}_{eff} = \alpha_i(\mu_{lam,i} + \mu_{t,i})(\nabla\vec{u}_i + \nabla\vec{u}_i^T) - \frac{2}{3}\alpha_i(\rho_i k_i + (\mu_{lam,i} + \mu_{t,i})\nabla\cdot\vec{u}_i)\bar{\bar{I}} \qquad (4)$$