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Investigation of liquid maldistribution in trickle-bed reactors using porous media concept in CFD

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Abstract

A *three-dimensional* CFD model for simulating two-phase flow in trickle-bed reactors (TBRs) is presented. Based on porous media concept, a two-phase Eulerian model (rather than computationally demanding traditional three-phase Eulerian model) describing the flow domain as porous region is presented to understand and forecast the liquid maldistribution in TBRs under cold-flow conditions. The drag forces between phases have been accounted by employing the relative permeability concept [Sàez, A. E., Carbonell, R. G., 1985. Hydrodynamic parameters for gas–liquid cocurrent flow in packed beds. A.I.Ch.E. Journal 31, 52–62].

The model predictions are validated against experimental data reported in literature, notably using the liquid distribution studies of Marcendelli [1999. Hydrodynamique, Transfert de Chaleur Particule-Fluide et Distribution des phases dans les Reacteurs a lit Fixe a Ecoulement a Co-courant Descendant de Gaz et de Liquide. Doctoral Thesis. INPL, Nancy, France]. Various distributor configurations reported therein have been recreated in the CFD model and sensitivity studies have been performed. Good agreement is obtained between the reported experimental results and this proposed first-principle based CFD model.

Finally, the concept of distribution uniformity is discussed and applied to the CFD model predictions. The CFD model is subjected to a systematic sensitivity study in order to explore better liquid distribution alternatives.

Keywords: Trickle-bed; Porous media; Liquid distribution; CFD; two-phase flow

1. Introduction

Three-phase reactors (G-L-S) comprising a fixed bed of catalyst with flowing liquid and gaseous phases have various applications, particularly in the petroleum industry for hydroprocessing of oils (e.g. hydrotreating, hydrocracking). Trickle-bed reactors (TBR) are one of the most extensively used three-phase reactors. With a view towards developing more efficient TBR units in the future, for meeting stringent environmental and profitability targets, it is crucial that we develop the know-how for tailoring the flow patterns in them to optimally match the demands made by the kinetics of these reaction processes.

One of the critical issues in the efficient use of TBRs is the understanding and prediction of liquid maldistribution. With current interest in technologies of 'deep' processing, such as deep hydrodesulfurization, the need to be able to predict liquid maldistribution accurately is even more important, since small variations in liquid distribution can cause significant loss in activity in trickle-bed reactors operating close to 100% conversion (see for example, Harter et al., 2001). Regions of the TBR those are dosed by more than the required amount of liquid reactant and insufficient gas phase reactant may lead to under-utilization of the catalyst, while regions which have less than required amount of liquid may have both under-utilization of catalyst as well as formation of local hot spots (particularly in the case of highly exothermic reactions). Added to those are negative effects like coking of catalyst (particularly in petroleum refining applications), in regions of the TBR which are not exposed to the right amount of gas phase and liquid phase reactant. Liquid distribution also has a sharp impact on pressure drop, which may add significantly to the long-term operating cost of a TBR unit.

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Table 1
Recent investigation of liquid distribution in trickle-bed reactor

Investigator	Techniques of measurement	Experimental conditions	Observations/conclusion
Sapre et al. (1990)	Heater probe technique	Large scale commercial TBRs	(i) Maldistribution can occur above liquid mass flux of $4\,\mathrm{kg\,m^{-2}\,s^{-1}}$ (ii) Flow nonuniformity increase moving down the reactor
Lutran et al. (1991)	Computer assisted tomography	Square cross section (0.0603 m, $l=$ 0.1905 m, $d_p=3$–6 mm)	(i) Nonprewetted bed—filament flow (ii) Prewetted bed—film flow (iii) Large particle—film flow (iv) Low particle size—more pockets
Reinecke and Mewes (1996)	Capacitance tomography	$D_c=120\,\mathrm{mm}$	(i) Increasing the liquid flow rate make the liquid distribution uniform (ii)Wall effect is more in small diameter column but is less in industrial columns
Saroha et al. (1998)	Liquid collector six zones	$l=0.152\,\mathrm{m}$; Flow rate range $L=1.46$–$7.31\,\mathrm{kg\,m^{-2}\,s^{-1}}$ $G=0-0.043\,\mathrm{kg\,m^{-2}\,s^{-1}}$	(i) Increase in liquid or gas flow, improves the liquid distribution (ii) Decrease in liquid density and surface tension reduces the wall flow
Marcandelli et al. (2000)	Pressure drop measurement, RTD method, heat transfer sensor, capacitive tomography, and liquid collector nine zones.	$l=1.3\,\mathrm{m}$, $D_c=0.3\,\mathrm{m}$, 2 mm glass beads and polylobe extrudates three types of distributors (a) multi-orifice (b) bi-orifice (c)mono-orifice	(i) Maldistribution depends significantly on initial distribution (ii) Distribution is improved due to the presence of gas (iii) RTD is good method to determine the maldistribution as pressure drop can determine but cannot quantify it. Thermal sensors and tomography are too local and not realistic for every reactor
Li et al. (2000)	Liquid collector 64 cups	121 tubes 2 mm inside dia $l=$ 100–300 mm d_p=1.6 mm trilobe particles	(i) Randomly packed bed with spherical and trilobe packings shows relatively uniform distribution (ii) Orientation effects in trilobe packing are canceled due to random packing (iii) The bed height improves the uniformity of the random packed bed (iv) Effect of gas velocity is not significant
Kundu et al. (2001)	Liquid collector six zones	$l=0.152\,\mathrm{m}$ Flow rate range $L=1.46$–$7.31\,\mathrm{kg\,m^{-2}\,s^{-1}}$ $G=0$–$0.043\,\mathrm{kg\,m^{-2}\,s^{-1}}$	(i) Decrease in surface tension and density reduces the wall flow (ii) Distribution improves with velocities (iii) Significant effect of particle geometry and orientation in case of cylindrical and other non-spherical shapes
Sederman and Gladden (2001)	Magnetic resonance imaging	$u_l=0.5$–$5.8\,\mathrm{mm\,s^{-1}}$ $u_g=66$–$356\,\mathrm{mm\,s^{-1}}$ $d_p=5\,\mathrm{mm}$ $D_c=40\,\mathrm{mm}$	(i) Wetting efficiency increases with liquid flow rate (ii) No effect of gas flow rate on distribution (iii) Extreme liquid maldistribution in non-prewetted bed (iv) Start up procedure affects the final operating characteristics of TBR
Boyer and Fanget (2002)	Gamma-ray Tomography	$l=60\,\mathrm{cm}$ $d_p=1.66\,\mathrm{mm}$ $\varepsilon=0.36$	(i) Flow is non axi-symmetric in several zones. This difference is attributed to bed structure (ii) Advocated the use of gamma ray tomography to study flow distribution in trickle-bed reactors

Table 1. (*Continued*)

Investigator	Techniques of measurement	Experimental conditions	Observations/conclusion
Tsochatzidis et al. (2002)	Conductance probe	$l = 0.14\,\text{m}$ $d_p = 1.6\,\text{mm}$ spherical packing	(i)Starting from maldistribution, an adequate liquid distribution is established at about 80 cm below the top of the bed (ii) Increasing the size of the packing particles (for the same shape), radial liquid distribution improves (iii) For the same size, spherical particles "perform" better than cylindrical ones
Gunjal et al. (2003)	Conductivity probe	$l = 1\,\text{m}$ $D_c = 0.1\,\text{m}$	Non uniform liquid distribution at inlet causes a major maldistribution in bed

The history of research in maldistribution effects is perhaps as old as the technology of TBRs itself. Table 1 summarizes the efforts made in this direction since last decade. Most of the experimental liquid distribution studies were carried out in laboratory scale units using a collector at the outlet of the bed (below the lowermost plane of catalyst packed into the bed) due to the simplicity of the technique. While easy to implement and relatively simple in construction, in this technique there are chances of flow redistribution at the exit of the bed. To overcome this drawback, recent studies by several groups had emphasized the use of tomographic and video imaging techniques, which provides the flow distribution information more quantitatively (e.g. Reinecke and Mewes, 1996; Sederman and Gladden, 2001; Harter et al., 2001; Boyer and Fanget, 2002).

Maldistribution of liquid is principally thought to depend on the ratio of reactor diameter to catalyst particle diameter (Herskowitz and Smith, 1978; Al-Dahhan and Dudukovic, 1994; Saroha et al., 1998), physicochemical properties of the liquid (e.g. density, viscosity, surface tension of liquid), liquid and gas flow rates (Onda et al., 1973; Saroha et al., 1998), wettability (Schwartz et al., 1976), shape and orientation of catalyst particles (Ng and Chu, 1987; Kundu et al., 2001). Initial liquid distribution is supposed to determine the extent of maldistribution in that a poor distribution of liquid established at the top of the bed is, at least partly, likely to propagate down the length of the bed. There is however, some debate in the literature about the role of initial liquid distribution.

Some of the authors had reported that a uniform distribution was achieved regardless of the feed arrangement (Herskowitz and Smith, 1978). Jiang et al. (1999) described that effect of initial distribution is significant in the upper half of the reactor. Marcandelli et al. (2000), Boyer and Fanget (2002) and Gunjal et al. (2003) used different inlet flow profiles and advocated the need of uniform initial liquid distribution.

Since the flow in TBRs is so complex and depends in a arguably non-linear and unknown fashion on a multitude of effects such as the geometry of bed and inlet, physical properties of the solid particles and fluid, and multiphase flow phenomena, there is as yet no universal agreement on what the right way of modeling the flow phenomena is. Consequently, there is also no universally valid approach towards the design of liquid distributors and in many cases, the industry practice, depends on application-specific experience and heuristics. Some of the important models of TBR hydrodynamics are reported in Table 2. Many of the earlier models are phenomenological, i.e., they assumed a simple picture of the microscale flow pattern (such as the "slit models"), and then integrated this picture to envisage the entire bed (Holub et al., 1992; Iliuta et al., 2000). More recently, computational fluid dynamics (CFD) based approaches have become popular (Jiang et al., 2002a,b; Gunjal et al., 2003, 2005; Atta et al., 2007) and the use of CFD-based models to simulate the flow in TBR is a promising methodology for exploring the problem of large scale liquid maldistribution effects, and its impact on the reaction performance of trickle-beds. While these models have tried to resolve the existing complexities of the TBRs up to a great extent, considerable debate still persists on the exact nature of equations (in particular, the drag force model) to be solved.

In the final analysis, the test of any model is in its ability to correspond with the experimental observations. In particular for the case of TBRs, liquid distribution is an important global measure of performance and hence any model, CFD or otherwise, must be tested against this important measure of performance. Experimental results available on distribution studies for randomly packed beds (Saroha et al., 1998; Marcandelli et al., 2000) showed that liquid distribution is not symmetric in axial direction, so 2-D models would be incapable of producing a satisfactory picture for liquid distribution.

In this present contribution, we have extended our previous approach (Atta et al., 2007) i.e., porous media model using relative permeability concept (Sáez and Carbonell, 1985), to predict liquid maldistribution in TBR. With this approach, the trickle-bed is envisaged as one pseudo-homogeneous porous media through which two-phase gas–liquid flow occurs. Though this formalism makes the complex flow patterns tractable, it may lose out on the ability to describe fine scale interactions at the pellet level (including particle wetting (partial or total), rivulet formation, etc.) between the three phases with complete fidelity. However, in our previous communication (Atta et al., 2007)

Table 2
Various models proposed for trickle-bed reactor

Earlier models		
Diffusion model	Stanek and Szekely (1974)	The model is formulated to solve the equations of flow and diffusion, but effect of gas–liquid interactions is neglected
Model based on concept of relative permeability		
The relative permeability model	Saez and Carbonell (1985)	Drag force is calculated by using the concept of relative permeability of each phase
Slit models		
Single slit model	Holub et al. (1992)	Local flow of liquid and gas around the particles is modeled by assuming flow in rectangular inclined slits of width related to void fraction of the medium
Double slit model	Iliuta et al. (2000)	Holub's model is extended to allow for a distribution of slits that are totally dry in addition to slits that have liquid flow along the wall
The interfacial force model		
The fluid–fluid interfacial force model	Attou et al. (1999)	The drag force on each phase has contribution from the particle–fluid interaction as well as from the fluid–fluid interaction
Recent 'CFD-based' models		
Porous media model	(1) Anderson and Sapre (1991) (2) Souadnia and Latifi (2001) (3) Atta et al. (2007)	The drag exchange coefficients are obtained from the relative permeability concept developed by Saez and Carbonell (1985)
k-fluid model	(1) Jiang et al. (2002a,b) (2) Gunjal et al. (2003, 2005)	The drag exchange coefficients are obtained from the fluid–fluid interfacial force model

we had discussed the ability and accuracy of this approach to predict reactor scale hydrodynamics of TBR with less computational efforts. The success of that effort provides encouragement in favor of widening this promising model to foresee macro-scale flow distribution effects.

In this paper, a 3-D CFD-based porous media model to study the effect of initial feed distribution on liquid distribution in TBRs, has been developed. Numerical simulations (using commercial CFD code solver, FLUENT 6.2; ANSYS, Inc.) have been carried out and verified with the experimental studies by Marcandelli et al. (2000) ($D/d_p = 150$, i.e., a relatively large diameter column) for liquid flow distribution in TBR. Note that for large diameter columns the wall effect is relatively less. For small diameter columns (i.e., columns with D/d_p of 20 or less), porosity oscillations near wall about the cross-sectionally averaged voidage are more pronounced (see for example, the work of Mueller, 1991, 1992; Martin, 1978; Bey and Eigenberger, 1997; Yin et al., 2000; de Klerk, 2003; Li et al., 2006), causing relatively larger impact on the wall flow of liquid. In view of this, some attempts have also been made for simulating small diameter columns and in this case, the results presented here have been verified with the experimental studies by Herskowitz and Smith (1978) ($D/d_p \approx 18$).

Thus, the modeled set-ups are of two different geometries. The main simulation study has been performed on a 0.3 m ID column of 1.3 m height with three different distributor designs (Marcandelli et al., 2000) used to vary the quality of inlet liquid distribution. The gas in all the distributors was fed through four chimneys, while the liquid was injected through a perforated plate with either (a) 25 10 mm ID orifices (Multi-orifice) (b) two 25 mm ID orifices (Bi-orifice) or (c) one 25 mm ID orifice (Mono-orifice) (Fig. 1a, adapted from Marcandelli et al., 2000). The liquid distribution had been quantified using a collector at the bottom of the reactor. This collector is shown in Fig. 1b. The outlet liquid flow was divided into nine equal area zones and the flow rate through each zone was determined by averaging the flux of outlet liquid across the cross-section of each zone.

In addition, a small diameter column of 0.114 m diameter and 0.7 m height with point source feed inlet and four section concentric annular collector has also been considered (for details, please refer to Herskowitz and Smith, 1978). While this study is an addendum to our extensive set of simulations validated with the work of Marcandelli (1999,2000), it does demonstrate the efficacy of our modeling approach even in smaller diameter packed beds. Thus, to some extent we are also addressing the issue of scale.

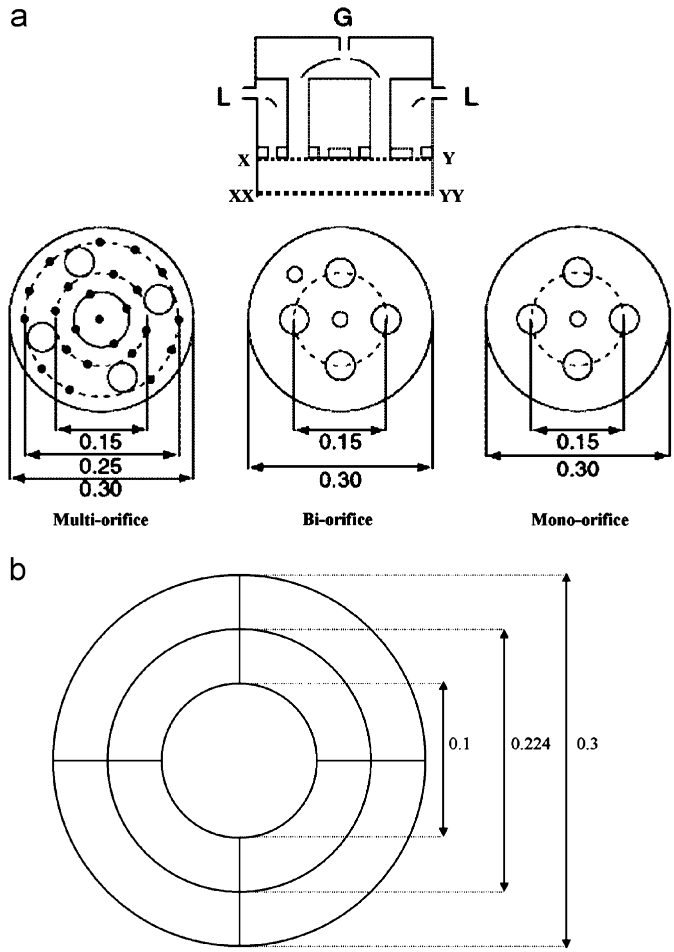

Fig. 1. Distributors and collector used by Marcandelli et al. (2000) (i.e., 1a and 1b).

2. Model equations

The model equations describing the gas and liquid two-phase flow through the packed bed are based on the phasic volume fraction concept. Volume fractions represent the space occupied by each phase, and the laws of conservation of mass and momentum are satisfied by each phase individually.

The volume-averaged equations for each flowing phase can be written as

Continuity equation:

$$\frac{\partial(\varepsilon\rho_\alpha s_\alpha)}{\partial t}+\nabla.(\rho_\alpha u_\alpha)=0,\qquad \alpha=g,l. \tag{1}$$

Momentum balance equation:

$$\rho_\alpha\left(\frac{\partial u_\alpha}{\partial t}+u_\alpha.\nabla u_\alpha\right)=-(\nabla p_\alpha-\rho_\alpha g)+\nabla.(\tau_\alpha+R_\alpha)+F_\alpha, \tag{2}$$

where F_α is the total drag force per unit of bed volume exerted by the phase α, τ_α and R_α are, respectively, the volume averaged viscous stress tensor and the turbulence stress tensor of phase α. Inter-phase coupling terms accounted by Eq. (2) are based on relative permeability concept developed by Sáez and Carbonell (1985) which states that

$$\frac{F_\alpha}{\varepsilon_\alpha}=\frac{1}{k_\alpha}\left[A\frac{Re_\alpha}{Ga_\alpha}+B\frac{Re_\alpha^2}{Ga_\alpha}\right]\rho_\alpha g, \tag{3}$$

where A and B in Eq. (3) are the Ergun equation coefficients for single-phase flow in the packed bed (Ergun, 1952). The Reynolds and Galileo numbers are defined as

$$Re_\alpha=\frac{\rho_\alpha u_\alpha d_e}{\mu_\alpha(1-\varepsilon)},$$

$$Ga_\alpha=\frac{\rho_\alpha^2 g d_e^3\varepsilon^3}{\mu_\alpha^2(1-\varepsilon)^3},$$

$$d_e=\frac{6V_p}{A_p}. \tag{4}$$

Since the Ergun's equation has been modified by relative permeability parameter which has been incorporated to accommodate the presence of a second phase, essentially it will be a function of phase saturation or holdup of that corresponding phase. To determine the dependence of the relative permeability on the saturation for each phase Sáez and Carbonell (1985) analyzed different data sets for liquid holdup and pressure drop over a wide range of Reynolds and Galileo numbers in packed beds available in the literature till that time. Finally they reported a set of empirical correlations for liquid and gas phase permeabilities as

$$k_l=\delta_l^{2.43},$$

$$k_g=s_g^{4.80}, \tag{5}$$

where $s_g=1-\varepsilon_l^0/\varepsilon$ and $\delta_l=\varepsilon_l-\varepsilon_l^0/\varepsilon-\varepsilon_l^0=$ ratio of effective volume of flow of the liquid phase to the available volume of flow.

The static liquid holdup (ε_l^0) can be calculated by the following correlation given by Sáez and Carbonell (1985)

$$\varepsilon_l^0=\frac{1}{(20+0.9Eo^*)}\quad\text{where } Eo^*=\frac{\rho_l g d_p^2\varepsilon^2}{\sigma_l(1-\varepsilon)^2}. \tag{6}$$

More detailed derivation and discussions of these equations can be found elsewhere (Sáez and Carbonell, 1985; Atta et al., 2007).

3. Model setup and numerical solution procedure

The primary objective in the current study is to quantify the liquid maldistribution due to inlet feed effect of a cylindrical packed bed with monodisperse spherical particles by porous media CFD model. The column dimensions are 1.3 m in length and 0.30 m in diameter. The glass particle diameter is 2 mm, and the column-to-particle diameter ratio is 150. These operational conditions are based on the experimental work of Marcandelli (1999). To simplify as well as to make this whole modeling approach flexible and tractable, we have divided the total setup in two parts of numerical simulation (Fig. 2). In the first section, we have recreated the various distributor geometries used by Marcandelli (1999) (i.e., mono, bi and multi-orifice, Fig. 1) in preprocessor GAMBIT and then simulated by using two-phase Eulerian approach to obtain a steady velocity profile of gas and liquid at a plane of 5 cm below the liquid and gas inlet (i.e *XX–YY* plane in Fig. 2a). Subsequently these velocity profiles of gas and liquid are set as the inlet boundary condition (at plane *XX–YY* in Fig. 2b) for the cylindrical geometry of 1.3 m which has a collector plate of nine equal area zones at the bottom as pressure outlet. The aforementioned model equations were solved for this zone (i.e., Fig. 2b) describing the bed as porous zone and no slip boundary condition was used for the impermeable wall.

It is known that in packed beds, the void fraction variation and packing configuration near the walls is distinctly different from the corresponding pattern in the bulk of the bed (e.g. Mueller, 1991). This effect needs to be incorporated into our model as well, however since our model is based on a porous media concept (which does not recognize the solid phase to be made up of discrete particles but only an effective phase with a stated void fraction), there is no readily obvious method for doing this. We have adapted the modified correlation of Vortmeyer and Schuster (1983) proposed by Sun et al. (2000), to define the porosity profile inside the bed as a user defined function

$$\varepsilon = 1 - (1-\varepsilon_b)\left\{1 - \exp\left(-2\left(\frac{R-r}{d_p}\right)^2\right)\right\}. \tag{7}$$

This equation predicts that the porosity will significantly increase near the wall and reaches 1 at the wall.

However, for the small diameter column, due to large oscillation of porosity inside the bed, we have characterized the bed voidage by the correlation presented by Cohen and Metzner (1981):

$$\begin{aligned}
&\frac{1-\varepsilon}{1-\varepsilon_b} = 4.5\left(y - \frac{7}{9}y^2\right), \quad y \leqslant 0.25,\\
&\frac{\varepsilon-\varepsilon_b}{1-\varepsilon_b} = a_1 \mathrm{e}^{-a_2 y}\cos(a_3 y - a_4)\pi, \quad 0.25 < y < 8,\\
&\varepsilon = \varepsilon_b, \quad 8 \leqslant y < \infty,
\end{aligned} \tag{8}$$

where y is the distance from the wall non-dimensionalized with respect to the particle diameter. The values of the constants are

$$a_1 = 0.3463; \quad a_2 = 0.4273; \quad a_3 = 2.4509; \quad a_4 = 2.2011.$$

In order to solve the governing equations for the cylindrical bed section the assumptions taken in this model are:

1. There is no inter-phase mass transfer.
2. Both the flowing fluids are incompressible.
3. Capillary pressure force can be neglected. This means that we assume same pressure for both phases at any point in time and space.
4. The contribution of the turbulent stress terms to overall momentum balance equation (2) is not significant. This assumption has also been used by other authors (e.g. Jiang et al., 2002a).

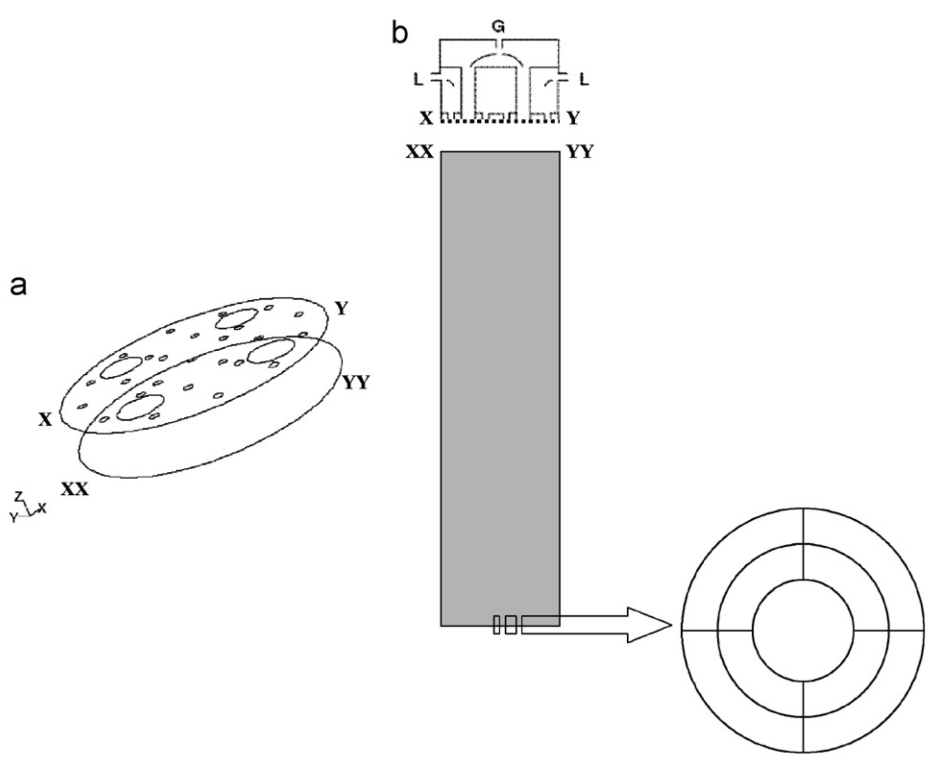

Fig. 2. Representative geometry created: (a) distributor section; (b) packed bed section.

Experiments with prewetted and non-prewetted bed (Jiang et al., 2001) also indicated that the macro-scale effects of capillary pressure are negligible when the particles are completely wetted.

A commercial CFD package, FLUENT 6.2 (ANSYS Inc., USA) has been used as the simulation platform where the above mentioned porosity profile (Eq. (7) for large diameter column and Eq. (8) for small diameter column) has been incorporated as user defined function (UDF). The time step for the unsteady state simulation of both the parts (i.e distributor and porous cylindrical bed) was chosen to be three orders of magnitude smaller than the respective mean residence time. In order to accurately implement the porosity profile (which is a sharply oscillatory function of the radial position), refined grid spacing has been used near the wall. Sensitivity to the grid spacing and time step were checked in the initial numerical experiments. Furthermore, the numerical computation was assumed to be converged by checking mass residual (less than 10^{-4}) at different plane along the length.

4. Results and discussion

With a particular set of flow velocities (gas and liquid), flow rate maps were obtained at the bottom of the cylindrical porous bed (Fig. 2b) for three different types of inlet velocity profile which can be found at the 5 cm below of the gas and liquid distributor plate (plane *X–Y* in Fig. 2a). These flow maps were then compared with the experimental observations of Marcandelli (1999). The example of such kind of comparison is demonstrated in Fig. 3 for liquid and gas superficial velocities of $0.003\,\mathrm{m\,s^{-1}}$ and $0.051\,\mathrm{m\,s^{-1}}$, respectively. Marcandelli (1999) proposed two different ways to quantify the liquid flow distribution for the different type of distributors as shown in Fig. 1a. According to their study, maldistribution was calculated:

- By measuring the volume fraction of liquid flowing through each of the zone in collector, divided into nine equal area compartments (Fig. 1b). This is a spatially averaged measurement, averaged over the dimensions of each cell.
- Using the maldistribution factor, M_f, (originally outlined by Hoek et al., 1986) defined as

$$M_f = \sqrt{\frac{1}{N(N-1)} \sum \left(\frac{Q_{Li} - Q_{\mathrm{mean}}}{Q_{\mathrm{mean}}} \right)^2}, \tag{9}$$

where Q_{Li} is the liquid flow rate through zone i, N is the number of zones (nine in this case) and Q_{mean} is the mean flow rate through all zones ($=Q_L/N$). The maldistribution factor, as defined, can vary from 0 (for ideal distributor) to 1 (all liquid goes through one single zone out of nine). Thus, a low value of maldistribution factor qualifies a better distribution.

Fig. 3 is based on the observed flow rate maps of way to quantify maldistribution. It can clearly be seen that multi-orifice is the most efficient one among these three types of distributor configuration, in terms of effecting a uniform liquid distribution

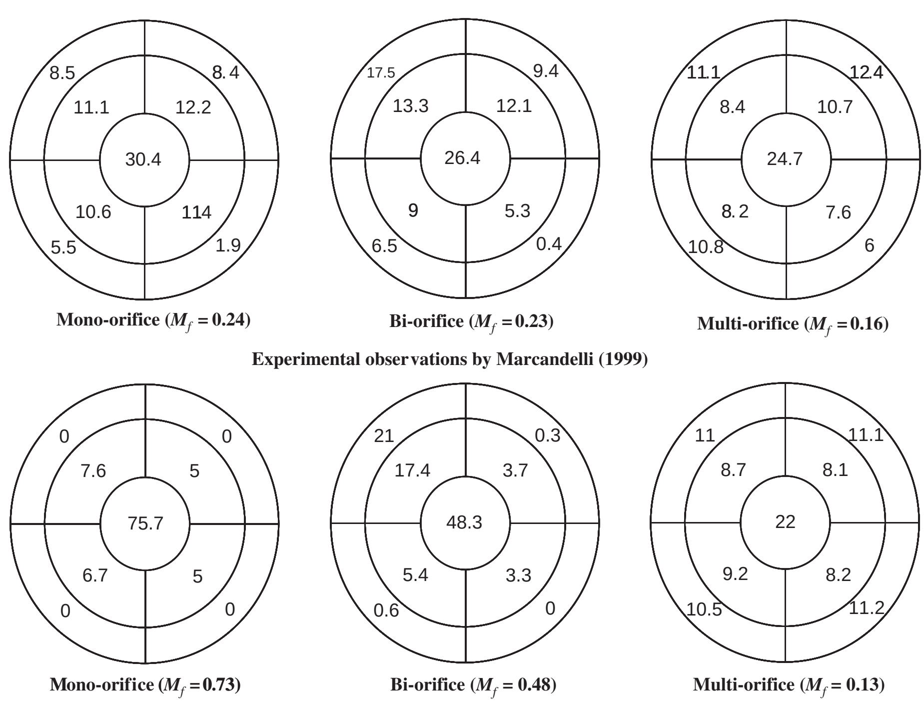

Fig. 3. Comparison of flow maps obtained with the collector at the bottom of the column for three different (mono, bi and multi-orifice) distributors ($u_l = 0.003\,\mathrm{m\,s^{-1}}$; $u_g = 0.051\,\mathrm{m\,s^{-1}}$).

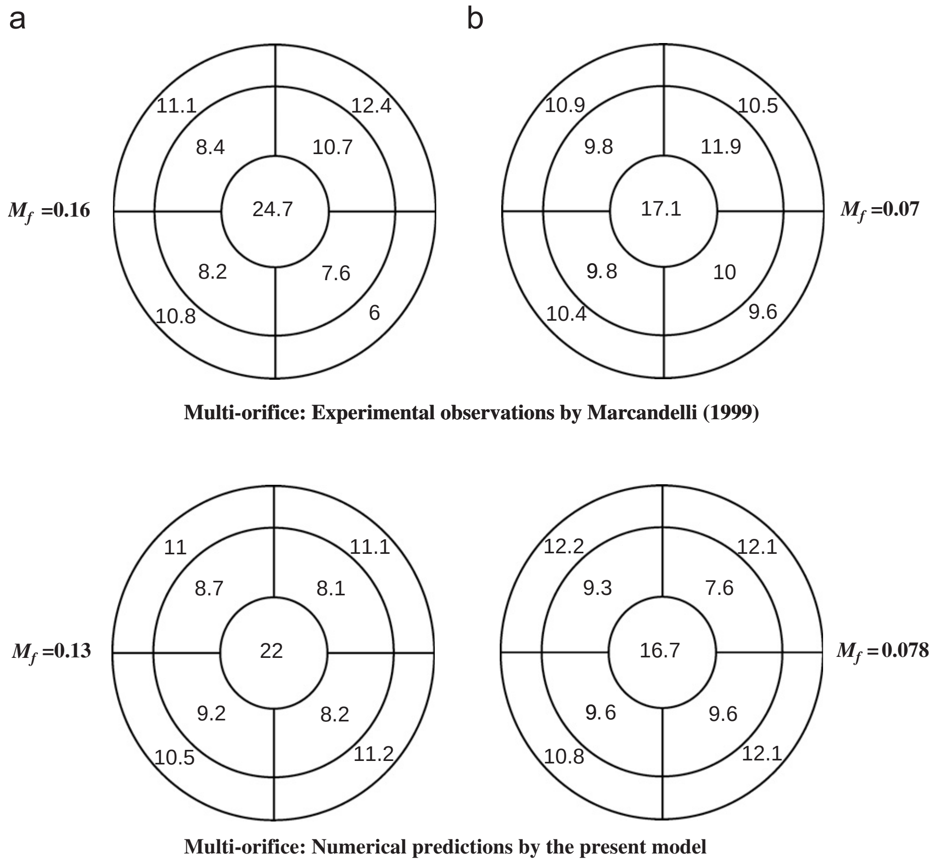

Fig. 4. Comparison of flow maps obtained with the collector at the bottom of the column for multi-orifice distributor: effect of liquid velocity (a) $u_l = 0.003\,\mathrm{m\,s^{-1}}$; $u_g = 0.051\,\mathrm{m\,s^{-1}}$ (b) $u_l = 0.006\,\mathrm{m\,s^{-1}}$; $u_g = 0.051\,\mathrm{m\,s^{-1}}$.

across the cross-section. Being axisymmetric in nature, mono-orifice distributor seems to perform better than the asymmetric bi-orifice distributor. With this understanding, in further studies we have considered only the most efficient distributor i.e., multi-orifice distributor, to observe the effect of liquid and gas velocities on maldistribution which is by far significantly better in providing a good liquid distribution.

The effect of liquid velocity and its comparison with the experimental results has been shown in Fig. 4. The comparisons between the experimental and predicted results show reasonable agreement in quantifying liquid maldistribution and also predict in line with the experimental results that increase in liquid velocity improves the liquid distribution in TBR. Further, the maldistribution index (M_f) was computed for different set of flow variables and then compared with the experimental results of Marcandelli (1999). The effect of gas velocity on liquid distribution (Fig. 5) is typical of this kind of quantification. It is evident from Fig. 5 that with the increase in gas velocity, the liquid distribution becomes more uniform. It must be noted that there could be possibility of experimental error in measurement of the liquid distribution, because introduction of a collector apparatus almost always leads to some discrepancy in such a measurement. What is however, much more reliable, is the metric of overall maldistribution (M_f), and in this comparison both the experimental and modeling results agree quite well (Fig. 5).

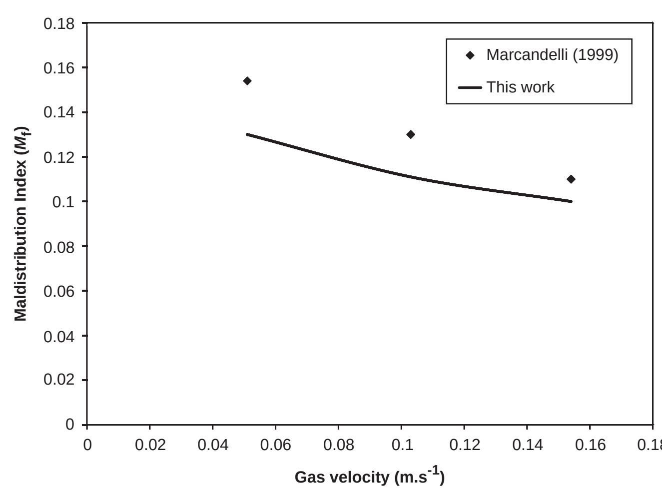

Fig. 5. Comparison of Maldistribution index (M_f) for Multi-orifice distributor as a function of the gas velocity ($u_l = 0.003\,\mathrm{m\,s^{-1}}$).

However, at the same point one needs to be careful about the significant increase in pressure drop with the increase in gas velocity (Fig. 6). The comparison of our simulated results with the experimental measurement of pressure drop (Fig. 6) shows that the modeling results systematically overpredict the experimentally observed values by almost a factor of 1.5 at all conditions. This seems to indicate that while our porous media

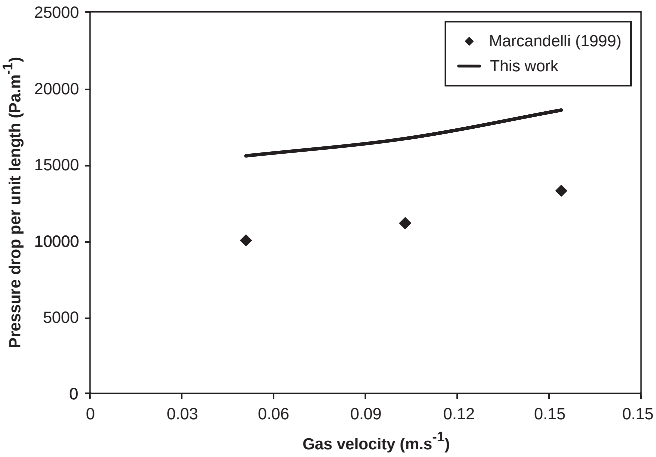

Fig. 6. Comparison of pressure drop for Multi-orifice distributor as a function of the gas velocity.

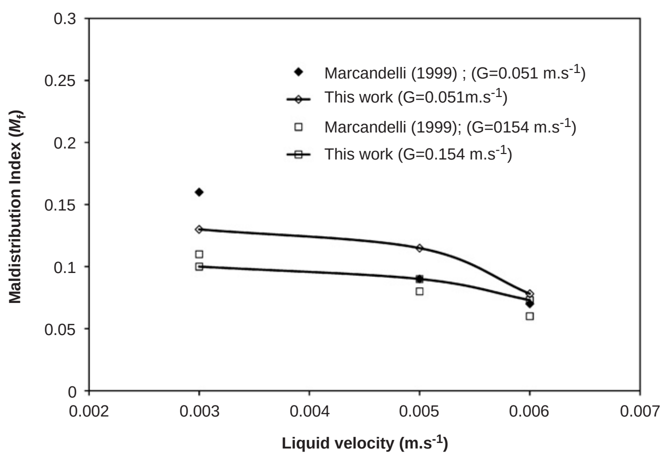

Fig. 7. Comparison of Maldistribution index (M_f) for Multi-orifice distributor as a function of the gas and liquid velocities.

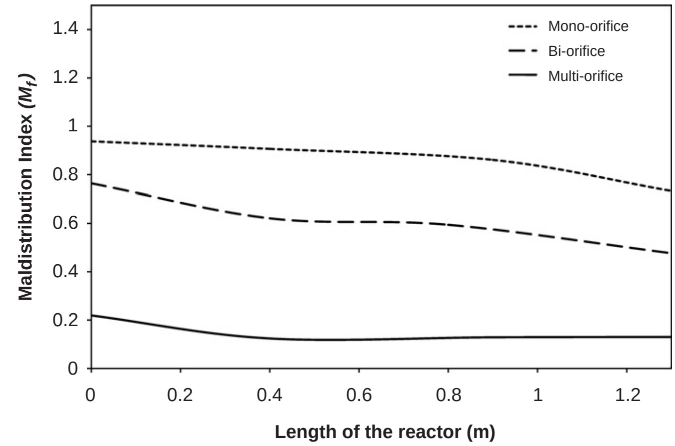

Fig. 8. Prediction of Maldistribution index (M_f) for different distributors along the length of the reactor from the inlet for $u_l = 0.003\,\mathrm{m\,s^{-1}}$; $u_g = 0.051\,\mathrm{m\,s^{-1}}$.

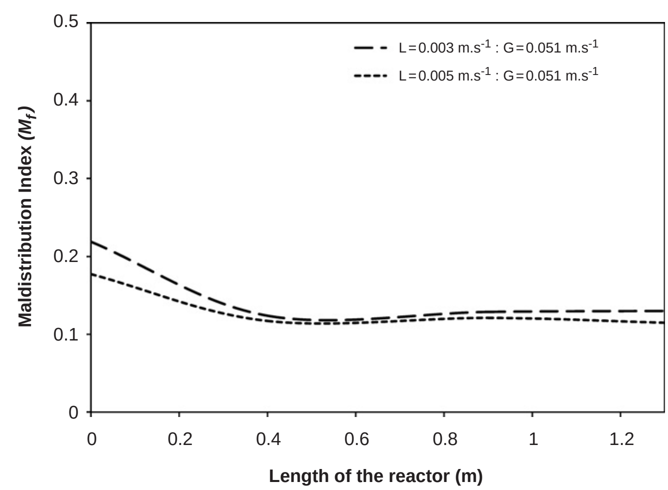

Fig. 9. Prediction of maldistribution index (M_f) for multi-orifice distributor along the length of the reactor from the inlet as a function of liquid velocity.

approach seems to be reasonably accurate in predicting the distribution results qualitatively, there is still significant scope for improvement in the closures for interphase interactions (which are important contributors to interphase friction and hence pressure drop).

We have also verified our model with the experimental observations for two distinctly different set of gas velocities ($u_g = 0.051$ and $0.154\,\mathrm{m\,s^{-1}}$). Fig. 7 shows the proposed model predictions holds fairly good agreement with the experimental results. Nevertheless, it is interesting to note that for higher liquid velocities, liquid distribution appears to be independent of gas velocity. This probably occurs because at higher liquid superficial velocities, all the points in the cross-section are fairly well irrigated by the larger liquid flows. Thus the dimensionless maldistribution index (which represents the dimensionless deviation from the mean distribution) does not show any appreciable variation with further increase in total liquid flow (or, liquid superficial velocity).

Armed with a fairly predictive and validated model, we have made an effort to explore the variation of maldistribution along the length of the reactor for different distributors. Fig. 8 points out the trend that after certain length, fairly uniform flow distribution can be achieved in case of multi-orifice distributor. However, in the case of mono-orifice and bi-orifice distributors, the flow uniformity continues to improve along the length of the reactor but is distinctly poorer in quality compared to the multi-orifice distributor. The sensitivity analysis (Fig. 9) of the multi-orifice distributor for the different liquid inlet velocity with constant gas velocity indicates that good initial distribution is being transmitted down the length of the reactor and reaches almost a steady value. Further down the reactor, the value of M_f does not seem to change appreciably. This may be an indication of essentiality for re-distributor to achieve the uniform distribution at its maximum value (i.e., lowest M_f value).

For the small diameter column (setup of Herskowitz and Smith, 1978), the collector is of different kind, with clearly demarcated concentric circles (Fig. 10a, details may be found

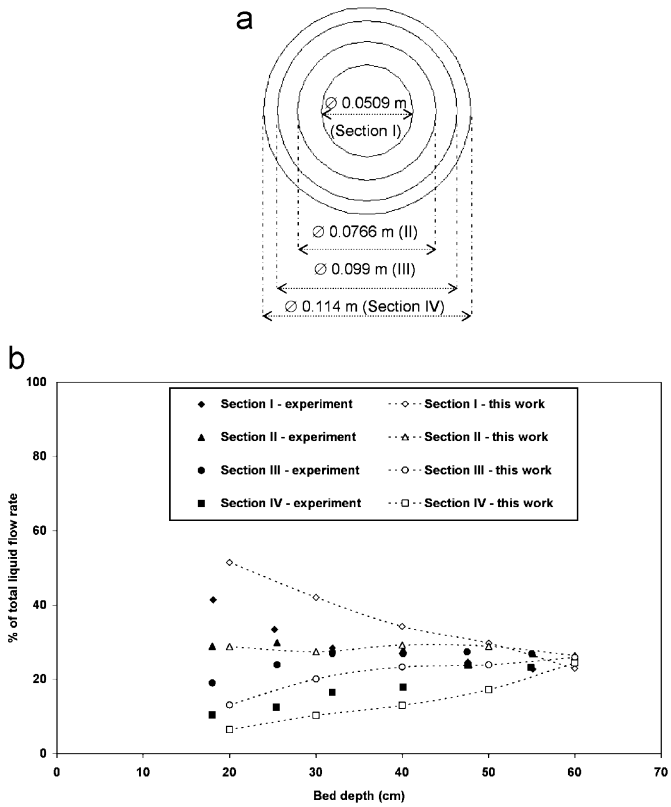

Fig. 10. (a) Collector used in case of Herskowitz and Smith (1978) ($D/d_p \approx 18$), (b) Comparison of liquid distribution for point source feed inlet at various bed depth with Herskowitz and Smith (1978).

in the aforementioned publication). For this chosen set of experiments, Fig. 10b represents the comparison of prediction of our model with the reported experimental dataset for point source feed inlet with ceramic balls (of 0.635 cm dia.) packed inside the bed. Again, it exhibits fairly good agreement with the experimental observations and endorses the fact that at low bed depth where liquid is spreading out from point source, the change in distribution with bed depth is more rapid for inner part of the bed. However, as the bed depth increases, the outer peripheries of the bed collect more liquid, relatively and everywhere the distribution tends to the cross-sectional average. This effect is clearly captured by our model with fidelity. Note that in this unit, there is a larger contribution of wall flow (because of more porosity oscillation), and this effect is also captured by our model.

It has been observed that for large diameter column, at higher liquid flow rates the simulated values of the flow distribution are in good agreement with the experimental results. However, at lower liquid flow rates we have observed a deviation in our CFD predictions and the experimental results. This deviation may be because of not taking into account the details of wetting phenomena in the model which usually dominates in large diameter column as there is more partially wetted particles due to low flow rates of liquid and gas velocities (with some sections of the bed potentially not receiving any liquid at all and particles getting only internally wetted due to capillary effects).

5. Summary and conclusions

In this communication, we have carried out 3-D CFD simulations in pilot scale trickle-bed reactor (TBR) using porous media flow concept for predicting the meso-scale liquid maldistribution. The porous media model is advantageous to handle gas–liquid interaction terms due to its ability to lump the adjustable parameters as compared to the conventional treatment of the problem.

Numerical simulations were carried out for water/air system with several initial liquid distributions and over the liquid superficial velocity range of 0.001–0.006 $\mathrm{m\,s^{-1}}$ and gas superficial velocity range of 0.02–0.154 $\mathrm{m\,s^{-1}}$. The simulation studies suggest that for low liquid and gas velocities, the details of particle wetting phenomena seems to have more significant effect in case of large diameter column rather than in a smaller diameter column. However, for higher flow velocities this CFD-based porous media model can forecast the reactor scale maldistribution in TBR with high degree of confidence in all cases. Nonetheless, considering the physical influences of the collector device for experiments with low flow rates, we can claim our model to be good enough to predict overall liquid distribution in TBR at the present form for a wide range of flow velocities. At the same time, it also pioneers an immense scope for the researchers to find out the possible thread to incorporate the effect of micro-scale details in this macro-scale model for better predictions. Furthermore, in this contribution we have attempted to quantify the large scale liquid maldistribution with help of porous media concept (developed by Sáez and Carbonell, 1985). In this work as well as in a previous contribution (Atta et al., 2007), we have shown this to be a very useful method for developing CFD models for trickle-beds, treating it as a system of gas–liquid flow through a porous medium.

Validation of our model was also performed with a smaller diameter laboratory-scale TBR (from the experimental data of Herskowitz and Smith, 1978), in which the liquid distribution from a single inlet has been tracked along the bed depth. Again, our model works quite remarkably in being able to predict the experimental results with acceptable accuracy.

Further, we have employed this duly validated model to establish the efficacy of the three distributors and make a relative comparison between them down the length of the reactor. We also investigated the effect of liquid flow on how the quality of liquid distribution varies along the length of the reactor and indicated the need for liquid redistributors. In fact, posed thus, this model can be employed to establish the length in a column after which re-distributors (and other internals like wall wipers) may be installed for better utilization of the trickle-bed.

This work opens up exciting possibilities of harnessing the relatively less computational requirements of this method (while maintaining the richness of information that is available from a CFD model), to explore the hydrodynamic behavior of larger scale pilot plant and industrial scale process units. Indeed, some of our future contributions will be addressing some of these pressing issues.

Notation

A	constant in the viscous term of the Ergun type equation
A_p	particle surface area, m^2
B	constant in the inertial term of the Ergun type equation
d_e	equivalent particle diameter, $6V_p/A_p$, m
d_p	particle diameter, m
D_c	column diameter, m
Eo^*	modified Eötvos number, $\rho_l g d_p^2 \varepsilon^2/\sigma_l(1-\varepsilon)^2$
F_α	drag force on the α phase per unit volume, $kg\,m^{-2}\,s^{-2}$
g	gravitational acceleration, $m\,s^{-2}$
G	gas phase loading, $kg\,m^{-2}\,s^{-1}$
Ga_α	Galileo number of the α phase, $\rho_\alpha^2 g d_e^3 \varepsilon^3/\mu_\alpha^2(1-\varepsilon)^3$
k_α	relative permeability of α phase
l	length of the reactor, m
L	liquid phase loading, $kg\,m^{-2}\,s^{-1}$
M_f	Maldistribution index, as defined by Eq. (9)
p	pressure, Pa
r	radial distance from the centre of the bed, m
Re_α	Reynolds number of the α phase, $\rho_\alpha u_\alpha d_e/\mu_\alpha(1-\varepsilon)$
s_α	saturation of the α phase
u_α	superficial velocity of the α phase, $m\,s^{-1}$
V_p	particle volume, m^3
y	distance from the wall nondimensionalized with respect to particle diameter

Greek letters

δ_l	reduced saturation of liquid phase, $\varepsilon_l - \varepsilon_l^0/\varepsilon - \varepsilon_l^0$
ε_l^0	static liquid hold up
ε	bed voidage
ε_α	hold-up of α phase
μ	viscosity, Pa s
ρ_α	density of α the phase, $kg\,m^{-3}$
σ	surface tension, $N\,m^{-1}$

Subscripts

b	bulk
α	gas/liquid phase
g	gas phase
l	liquid phase

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