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HYDRODYNAMICS MODELING OF A BENCH SCALE TRICKLE BED REACTOR USING CFD

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Abstract

Trickle bed reactors are commonly used in chemical industries. Scale-up of trickle bed reactors is difficult and simple scaling rules often lead to poor design. Fluid dynamics of the trickle bed reactors is complex and sensitive to the scale of the reactors. Flow mal-distribution, channeling, wetting of catalyst and local temperature variation are some of the important parameters which controls the overall performance of the trickle bed reactors. Two-phase pressure drop and liquid holdup are two important hydrodynamic parameters which should be considered while analysing and designing a trickle bed reactor. By using computational fluid dynamics, we can understand fluid dynamics and its interactions with chemical reactions. In this study a computational fluid dynamic model based on Eulerian multiphase 2D model has been developed for simulating two phase flow in a trickle bed laboratory scale reactor.The porous media concept was used to model solid packings in the reactor. Model predictions were evaluated by comparing them with published experimental data. Pressure drop and liquid hold up along the bench scale reactor were obtained and were in good agreement with experimental data.

Keywords: Trickle bed; CFD; Hydrodynamics; bench scale; Two phase Eulerian model; Porous media; Relative permeability.

1. Introduction

Trickle-bed reactors (TBRs) are packed beds of solid catalysts with concurrent downward flow of gas and liquid reactants. In the field of petroleum refining industry, more specifically in the hydroprocessing of crude oil derivatives (e.g. hydrotreating, hydrocracking), these types of reactors have widespread applications. For conventional hydrocracking reactions, fall in effective reaction rate along the reactor length is observed because of reduction in hydrogen partial pressure, as well as because of possible inhibition by a product species like H_2S. In addition, high temperature results in gas phase expansion and in turn impedes the gaseous reactant from dissolving sufficiently into the liquid phase. To avoid these kinds of difficulties, trickle-bed reactors in a refinery are generally operated at high pressures up to about 20–60MPa to provide sufficient numbers of hydrogen molecules, to improve the solubility of the gaseous reactant and therefore to attain high conversion [1], and also to slow down catalyst deactivation. The design and scale-up of trickle bed reactors depend on key hydrodynamic variables such as liquid volume fraction (liquid saturation),particle scale wetting and overall gas–liquid distribution. These variables are difficult to determine experimentally and interactions between these are as yet poorly understood [2].

Numerous authors have studied and reported experimental data on pressure drop and liquid saturation in trickle-bed reactors (e.g. Specchia and Baldi, [3]; Rao *et al.*, [4]; Szady and Sundaresan,[5]; Al-Dahhan *et al.*, [6]). The attempts for describing trickle bed hydro-dynamics can be categorized mainly into two different classes of work [2]. The classical approach is empirical wherein correlations are developed to fit the experimental data (e.g. Larkins *et al.*, [7]; Ellman *et al.*, [8,9]; Larachi *et al.*, [10]). Another approach is to describe hydrodynamics in phenomenological manner, i.e., assuming a simple picture of the microscale flow pattern, and then integrate that depiction to address the entire bed (e.g. Holub *et al.*, [11]; Iliuta *et al.*, [12]).

At present Computational Fluid Dynamics (CFD) has allowed applications of numerical simulations to the modeling of multiphase flow in TBR (e.g. Attou and Ferschneider, [13]; Propp *et al.*, [14]; Souadnia and Latifi, [15]; Jiang *et al.*, [16,17]; Gunjal *et al.*, [18,19]; Atta

et al., [2]; Rodrigo J.G. Lopes *et al.*, [20]). There are two approaches for modeling trickle bed reactors by using CFD method. The porous media and packed bed concepts.

Most of the literature available (Jiang *et al.*, [16,17]; Gunjal *et al.*, [18,19]; Rodrigo J.G. Lopes *et al.*, [20]) dealing with packed bed flow simulations by use of a three-phase Eulerian model in which the solid velocity is identically set to zero. Such a calculation is nevertheless computationally demanding. Some of the literature [2] dealing with porous media concept which is less computationally intensive and use two phase Eulerian model in which the solid phase is defined as porous zone.

The independent experimental data sets reported by Szady and Sundaresan [5]; Gunjal et *al.* [19], are selected in the present work to validate the predictions. In addition, we compare our results with the numerical simulation of Gunjal *et al.* [19], which is based on a three phase Eulerian concept, and the work of Atta et al. [2], which is based on a two phase Eulerian model and the porous media concept.

Then, the obtained model will be used to simulate commercial scale reactor.

2. Modeling

Validation of CFD model is performed using experimental data sets of pressure drop and liquid saturation reported by Szady and Sundaresan [5] and Gunjal *et al.* [19]. Characteristics of the beds are shown in Table1.

Table1 Experimental parameters and operating conditions

	Bed diameter(m)	Bed length(m)	Particle diameter(m)	Bed porosity	Gas velocity(m/s)	Liquid velocity(m/s)
Szady *et. al.*	0.165	1.49	0.003	0.37	0.22	0.002-0.008
Gunjal *et. al.*	0.114	1	0.003	0.36	0.22	0.003-0.007

There are two approaches for CFD modeling of multi phase flows in trickle bed reactors. Fluid-fluid interaction model and porous media concept. fluid-fluid interaction model, use inter phase drag forces to define the interaction between phases but in porous zone the relative permeability concept is used to specify the effect of phases on each other. Because of being less computationally intensive the porous media approach is more suitable for commertial scale reactors. The model presented here to describe the multiphase flow is based on the Eulerian framework, which consists of continuity and momentum equations of each phase with appropriate closures for evaluating the influence of porous media on two phase flow. The approach which is used in this work is based on the assumption that flow domain (fixed bed with catalyst particles) can be described as porous media. The closures used in this model are the relative permeability equations which have been developed by Saez and Carbonell [21], to relate the drag forces with the flow velocities and volume fractions of each phase, and to the physical properties of the gas, liquid and solid phases.

The continuity equation for each phase is:

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla.\left(\alpha_k \rho_k \overrightarrow{U_k}\right) = 0 \qquad (1)$$

Where $\overrightarrow{U_k}$ is the velocity and α_k is the volume fraction of each phase.

Momentum balance equation is:

$$\frac{\partial}{\partial t}\left(\alpha_k \rho_k \overrightarrow{v_k}\right) + \nabla\left(\alpha_k \rho_k \overrightarrow{v_k}\overrightarrow{v_k}\right) = -\alpha_k \nabla P + \nabla \overline{\overline{\tau_k}} + \sum_{p=1}^{n} \overrightarrow{R_{PK}} + \alpha_k \rho_k g - \frac{\Delta P}{l} \qquad (2)$$

Where R_{PK} is the fluid-fluid drag force.

$$F_{drag,PK} = \overrightarrow{R_{PK}} = \beta_{PK}\left(U_P - U_K\right) \qquad (3)$$

Where β_{PK} is the fluid-fluid drag coefficient.

The term $\frac{\Delta p}{l}$ (two phase pressure drop) in Eq.(2) is the effect of porous media on each phase pressure drop which is based on relative permeability concept developed by

Saez and Carbonell [21]. The two-phase flow pressure drop can be represented in dimensionless form with the help of Reynolds and Galileo numbers.

$$\left(\frac{\Delta p}{l}\right)=\frac{F_k}{\alpha_k}=\frac{1}{k_k}\left[A\frac{\mathrm{Re}_k}{Ga_k}+B\frac{\mathrm{Re}_k^2}{Ga_k}\right]\rho_k g \tag{4}$$

$$\mathrm{Re}_k=\frac{\rho_k u_k d}{\mu_k(1-\varepsilon)} \tag{5}$$

$$Ga_k=\frac{\rho_k^2 g d^3 \varepsilon^3}{\mu_k^2(1-\varepsilon)^3} \tag{6}$$

The constants *A* and *B* in Eq. (4) are the Ergun equation coefficients for single-phase flow in the packed bed. ε is the bed porosity.

In order to consider the microscopic/local configuration of the second fluid and to define the ability to flow of one fluid in presence of other fluid, the term relative permeability (k_k) was introduced. Since the relative permeability parameter 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 [2]. To determine the dependence of the relative permeability on the saturation for each phase Saez and Carbonell [21], analyzed different data sets for liquid holdup and pressure drop over a wide range of Reynolds and Galileo numbers. They made the hypothesis that liquid relative permeabilities are only a function of reduced saturation (δ_l) which is represented by the ratio of effective volume of flow of the liquid phase to the available volume of flow considering that the static liquid holdup ($\alpha_{l,stat}$) represents a portion of the void fraction occupied by stagnant liquid.

$$\delta_l=\frac{\alpha_{l,dyn}}{\varepsilon-\alpha_{l,stat}} \tag{7}$$

The gas phase relative permeability was correlated as a function of the gas phase saturation. The empirical correlations were reported to be [21]:

$$k_l=\delta_l^{2.43} \tag{8}$$

$$k_g=S_g^{4.8} \tag{9}$$

Where $s_g=1-\frac{\alpha_l}{\varepsilon}$ is the gas saturation.

The static liquid holdup can be calculated by the following correlation given by Saez and Carbonell [21].

$$\alpha_{l,stat}=\frac{1}{(20+0.9Eo)} \tag{10}$$

$$Eo=\frac{\rho_l g d^2 \varepsilon^2}{\sigma_l\left(1-\varepsilon^2\right)^2} \tag{11}$$

In order to solve these equations the assumptions taken in this model are:

1. Both the flowing fluids are incompressible.
2. The porous medium is taken to be isotropic, i.e., permeabilities are independent of direction.
3. The porosity is uniform and constant.
4. The bed is pre-wetted so capillary pressure force can be neglected.
5. The flow is laminar within the porous zone. At inlet and outlet of the bed realizable k-e turbulence model is used.

The transform equation for turbulent kinetic energy is:

$$\frac{\partial}{\partial t}\left(\rho_g\lambda_g\right)+\nabla.\left(\rho_g\vec{U}_g\lambda_g\right)=\nabla\left(\frac{\mu_{t,f}}{\sigma_\lambda}\nabla\lambda_g\right)+G_{\lambda,g}-\rho_g\varphi_g \tag{12}$$

The equation of disipation rate of turbulent kinetic energy is :

$$\frac{\partial}{\partial t}\left(\rho_g\varphi_g\right)+\nabla.\left(\rho_g\vec{U}_g\varphi_g\right)=\nabla\left(\frac{\mu_{t,f}}{\sigma_\varphi}\nabla\varphi_g\right)-C_2\rho_g\frac{\varphi_g^{\ 2}}{\lambda+\sqrt{\nu\varphi_g}} \tag{13}$$

CFD modeling involves three main steps:
(1) Creating the model geometry and grid,
(2) Defining the appropriate physical models and
(3) Defining the boundary and operating conditions.

The governing conservation equations of mass, momentum and energy and physical models involved in the process are discretized over control volumes and solved by finite volume method. CFD modeling of bench scale reactors was carried out in 2D dimension and it's results were validated by use of experimental and simulated data of Szady and Sundaresan [21]; Gunjal *et al.*[19], Atta [2]. The geometry of reactor consists of cylindrical pipe that is filled with solid packing (Fig1).

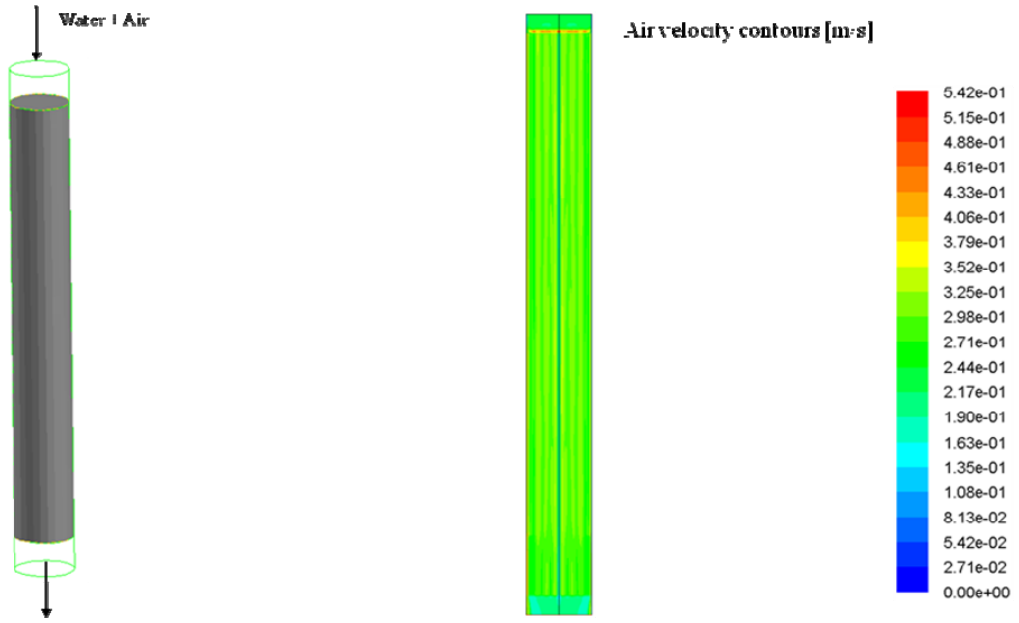


Fig.1. Contours of air velocity magnitude through porous media

Boundary conditions for 2D dimensional bench scale reators are same as table1. For Gunjal et al.[19], data, the porosity distribution near the wall was considered which was calculated by Eqs. (14)-(16) proposed by J. Theuerkauf *et al.* [22].

$$\varepsilon = 2.14x^2 - 2.53x + 1 \qquad x \le 0.637 \qquad (14)$$

$$\varepsilon = \bar{\varepsilon} + 0.29\exp(-0.6x)\cos[2.3\pi(x-0.16)] + 0.15\exp(-0.9x) \qquad x > 0.637 \qquad (15)$$

$$x = (R-r)/d_p \qquad (16)$$

The porosity distribution is shown in Fig. 2.

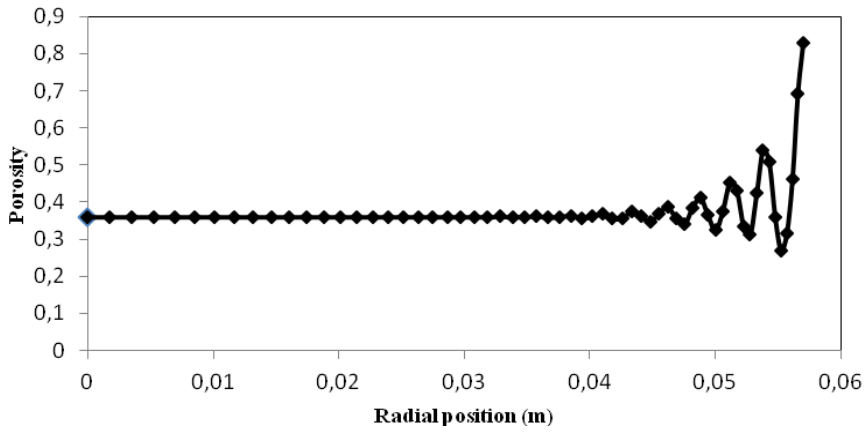
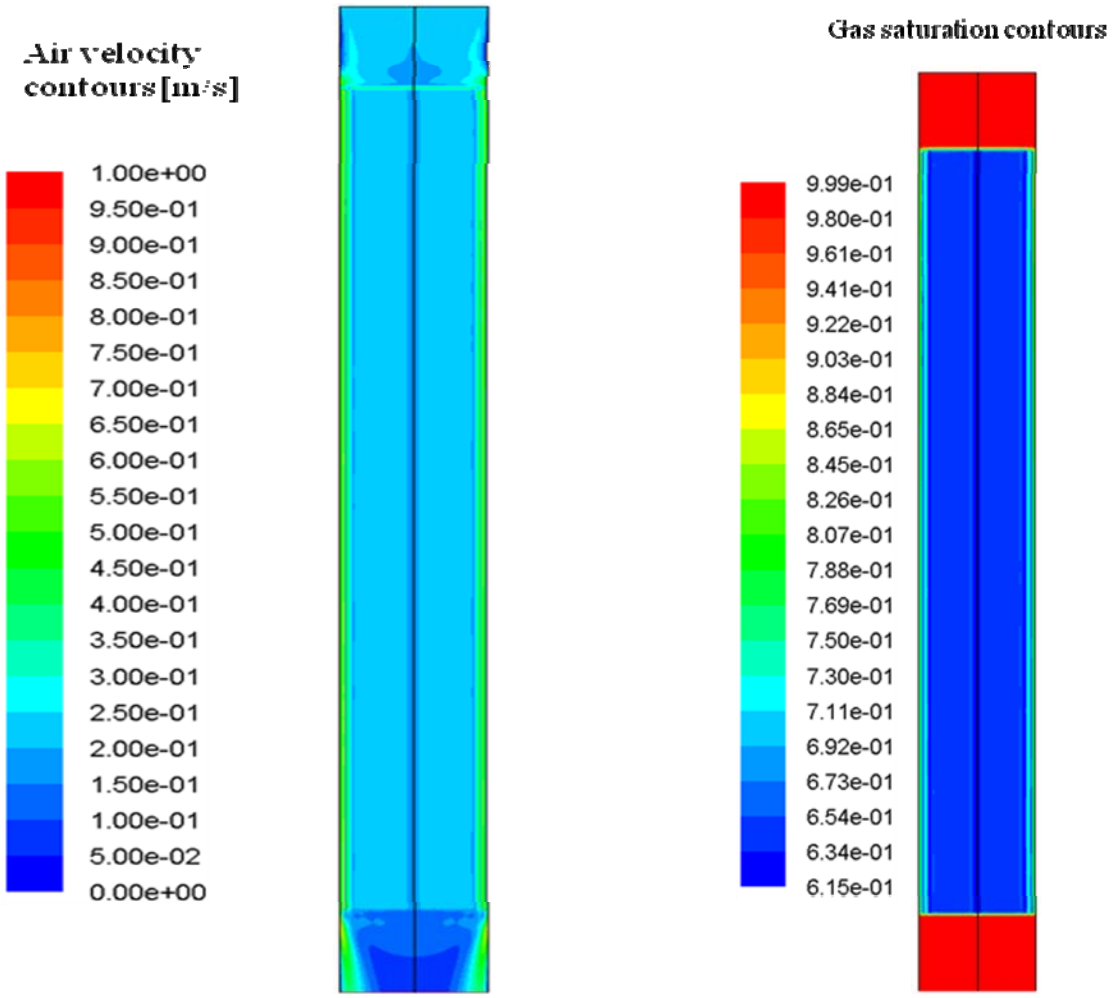


Fig. 2. Radial porosity distribution

Air velocity contours for Gunjal reactor with porosity distribution is depicted in Fig.3



(a) (b)

Fig.3 (a)Air velocity contours (b)Air saturation contours through porous media with porosity distribution

As can be seen from Fig.3 the more porosity near the reactor wall leads to deviate air strean from the center to near the reactor wall and therefore, can reduce the gas-liquid contact which is the drawback of porosity distribution near the wall.

3. Results and Discussion

Presssure drop per unit length and mean liquid saturation of the bench scale reactors are obtained from 2D axisymmetric CFD modeling. The experimental values and the relevant CFD results are compared and discussed hereinafter. In Fig.4 and Fig.5 comparison between CFD results and experimental data of Szady and Sundaresan [5], and numerical prediction of Atta [2], for pressure drop per unit length of the bed and mean liquid saturation versus liquid superficial velocity is depicted. Numerical modeling of Atta has been carried out based on porous media concept. The gas superficial velocity is constant and equal to 0.22 (m/s). As shown in Figs. 4,5 the pressure drop and liquid saturation are increased with increasing liquid superficial velocity, this is due to the trickling flow regime which the interaction between liquid and gas is low. By increasing gas and liquid flow rates, the pulsing flow regime occurs. This regime is characterized by the successive passage of liquid-rich and gas-rich regions through the bed. In pulsing flow regime pressure drop and liquid holdup are depend only on the gas flow rate and independent of the liquid flow rate (Boelhouwer [23]). The over prediction of pressure drop in Fig.4 may be related to Ergun's constants in Eq (6) which are selected based on Atta et al. A=180, B=1.8,.

In Fig. 6 and Fig. 7 the CFD results of pressure drop and liquid saturation are compared with experimental and numerical results of Gunjal et al. [19], for different liquid superficial velocities. It is noteworthy that Gunjal's simulation is based on three-phase Eulerian model in which the interaction between phases is defined by Attou and Ferschneider [13], drag force model which is developed for the regime in which liquid flows in the form of film.

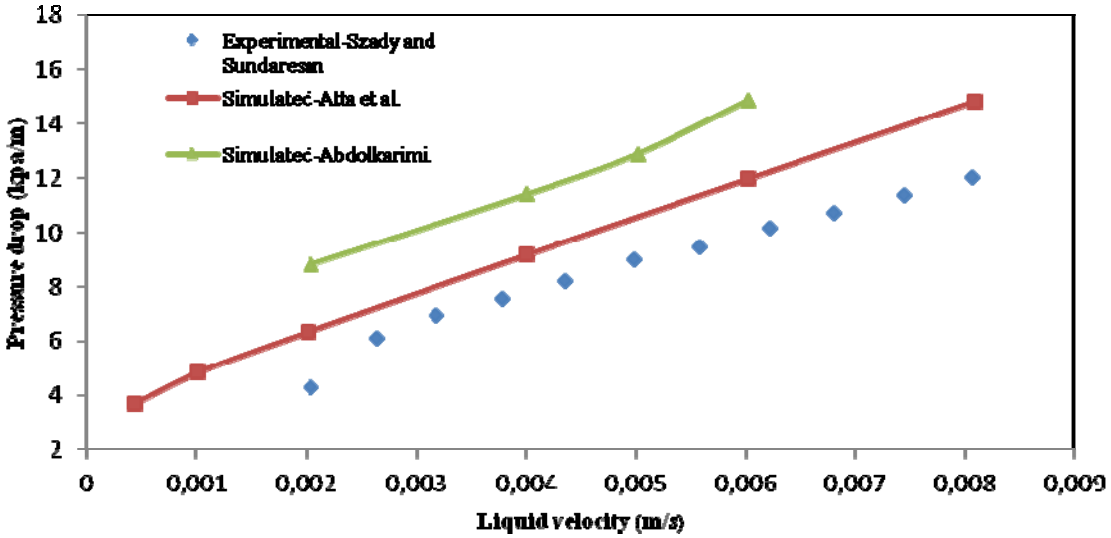


Fig. 4. Comparison of simulated results of pressure drop with data of Szady and sundaresan

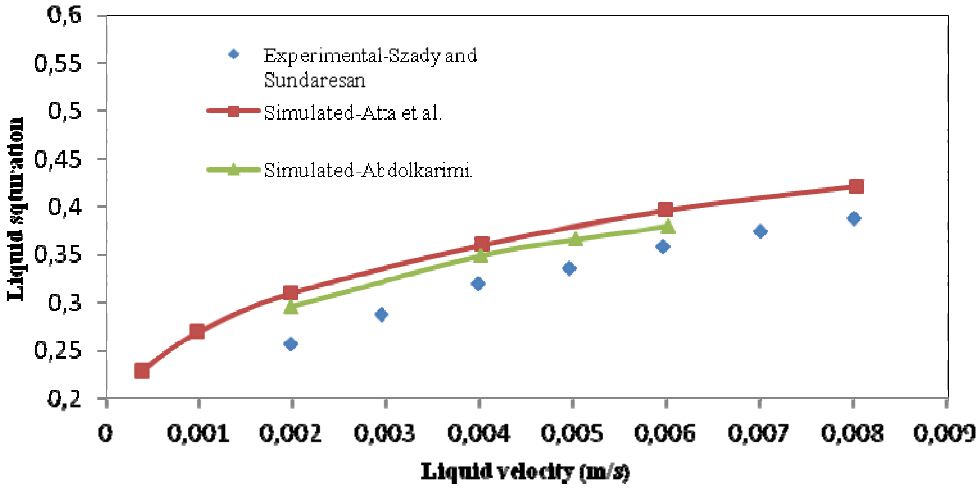


Fig. 5. Comparison of simulated results of mean liquid saturation with data of Szady and sundaresan

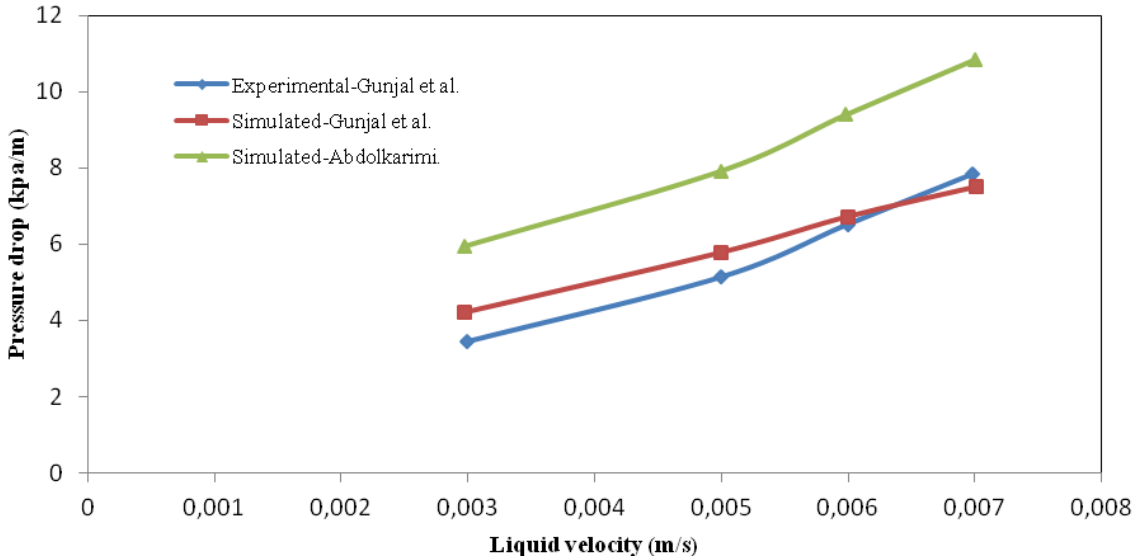


Fig. 6. Comparison of simulated results of pressure drop with data of Gunjal et al.

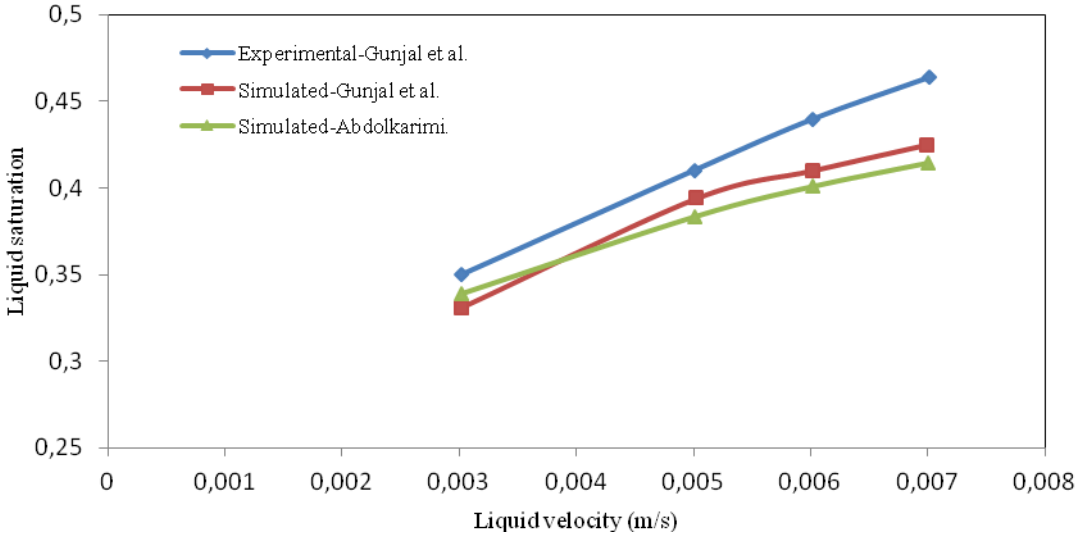


Fig. 7. Comparison of simulated results of mean liquid saturation with data of Gunjal et al.

4. Conclusions

In this study, we have developed a two-phase Eulerian CFD model based on porous media concept to simulate two dimensional gas–liquid flow through packed beds in the bench scale. With regard to importance of the uniform distribution of the gas and the liquid flows over catalytic bed, it is necessary to have an insight about how reactor internals affect the gas and the liquid distribution which is done by three dimensional CFD modeling of the flow field.

The closures which have been used in this model are the relative permeability model developed by Saez and Carbonell [21]. The predicted results are verified for different sets of independent experimental data (Szady and Sundaresan, [5]; Gunjal *et al.*, [19]). The predicted results are also compared with the numerical results of Atta et al. [2] which is based on the two-phase Eulerian model and Gunjal *et al.* [19], which is based on the three-phase Eulerian simulation.

We can propose this model for future studies on prediction of hydrodynamic and reaction parameters in the commercial scale trickle beds, because the use of porous media concept for modeling two phase flow in catalytic beds is computationally less demanding in contrast with using three phase Eulerian model.

Nomenclature

ρ_k	Phase density (kg.m^{-3})	s_g	Gas saturation
α_k	Phase volume fraction	d	Particle diameter (m)
U_k	Velocity vector for each phase (m.s^{-1})	σ_l	Liquid surface tension (N.m^{-1})
τ_k	Stress tensor for each phase (N.m^{-2})	λ_g	Turbulent kinetic energy of gas phase (m^2.s^{-2})
R_{PK}	Drag force between two phases (N.m^{-3})	φ_g	Turbulent dissipation rate of gas phase (m^2.s^{-2})
β_{PK}	Inter phase drag coefficient (Kg.m^{-3}.s^{-1})	σ_λ , σ_φ	Turbulent Prandtl number
k_k	Relative permeability for each phase	$G_{\lambda,g}$	Generation of turbulence kinetic energy due to the mean velocity gradients (Kg.m^{-1}.s^{-3})
δ_l	Liquid saturation	ν	Kinematic viscosity (m^2.s^{-1})
ε	Void fraction		

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