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Modification of Ergun equation for application in trickle bed reactors randomly packed with trilobe particles using computational fluid dynamics technique

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Abstract−Based on a slit model, a pellet scale model has been developed for calculation of drag force imposed on trilobe catalyst particles in a packed bed reactor. The drag coefficient for single gas phase flow in a porous media has been calculated by CFD simulation and the results compared to the Ergun equation. The results show that the drag coefficient predicted by Ergun equation should be modified for various bed porosities, particle aspect ratio and gas densities. Therefore, a correction factor has been proposed to correct the Ergun equation constants in various conditions for trilobe particles. Comparison between the proposed corrected Ergun equation results and experimental data indicates considerable agreement.

Key words: Trickle Bed Reactor, Drag Coefficient, Computational Fluid Dynamics (CFD), Ergun Equation, Pellet Scale Model

INTRODUCTION

Multiphase flow systems, in which gas and liquid flow concurrently downward through a packed bed, are extensively applied in processing of fuels and chemicals such as desulfurization, hydrogenation, absorption, distillation and filtration. Although a considerable amount of research has been conducted for more than three decades [1-4], the methodology adopted for the design of such multiphase systems still relies on simplified empirical models rather than on a theoretical basis, mainly due to lack of knowledge about the detailed flow picture in trickle bed reactors (TBR), from which a physical model of the multiphase flow could be established.

One of the effective hydrodynamic parameters of packed beds which should be considered in studying of such reactors is the particle shape. In previous studies, Ahmadi Motlagh and Hashemabadi [5] studied wall effects on flow pressure drop through the randomly packed bed of cylindrical particles. Their results show that the modified Ergun equation, which takes into account the wall effects, obtains better results in comparison with other methods. Moreover, as the flow Reynolds number increases, hydrodynamic analysis of flow pattern around a quadralobe catalyst shows an increase in drag coefficient in comparison with cylindrical particles [6,7]. Up until now, many different shapes of particles have been used in the TBRs. Trilobes are one of the useful catalyst particles that are widely used in industry, since they provide higher surface/volume ratios than spherical particles at the same specified pressure drop. However, only a very few studies have been reported on the effect of trilobe particle on the hydrodynamics of a TBR. Nemec and Levec [8] studied the effect of particle shape on pressure drop of a single phase flow through the trickle bed reactors. Based on experimental data, they found that the original Ergun constants are only able to accurately predict the pressure drop of a single phase flow over spherical particles. Therefore, they modified Ergun constants for cylindrical and other shape of particles. In another study, in a small diameter column, Nemec and Levec [9] concluded experimentally that particle shape does not have any effect on liquid holdup. Gunjal and Ranade [10] modified the Ergun constants to simulate the tickle bed reactor with trilobe catalyst particles using CFD technique. Lebigue et al. [11] investigated empirically the effect of particle shape on wetting efficiency. Nguyen et al. [12] used magnetic resonance imaging (MRI) to determine the effect of fluid dynamics on hydrodesulfurization (HDS) reactions of diesel oil in bench scale reactors. They also quantified the porosities and liquid saturations of trilobe particles catalyst beds.

Drag force or inter-phase momentum exchange is one important hydrodynamics term of TBRs which should be modeled correctly for accurate design and scale up of this type of reactor [13,14]. In the Ergun equation, drag force is usually expressed as the sum of viscous and inertial terms [15]. Among various approaches that have been adopted to calculate the drag force term in momentum balance equation, four distinct and important models can be identified. The relative permeability model [9,16], single slit model [17,18], double slit model [19] and finally, the two-fluid model [20-24] which drag exchange coefficients are obtained from the fluid-fluid interfacial force. In slit models the local flow of liquid and gas around the particles is modeled by assuming the flow between two parallel inclined plates that their gap is related to void fraction of the medium. While these approaches are all based on spherical shape and a single parameter (equivalent diameter, which is used to represent the packing shape effect for non spherical particles). In this study, a pellet scale model is presented to investigate the effect of shape and bed porosity of trilobe particles and physical properties of fluid on the interphase momentum term. The proposed model simulates trickle bed reactors based on the slit model using CFD technique. The results have been compared with the two-fluid model and experimental data. Using the proposed model, the effect of some variables on

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Ergun constants of two-fluid model for trickle bed with trilobe particles have been studied.

GOVERNING EQUATIONS

The continuity and momentum equations can be written, respectively, as below:

$$\frac{\partial \rho_G}{\partial t} + \nabla \cdot (\rho_G u_G) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho_G u_G) + \nabla \cdot (\rho_G u_G u_G) = -\nabla p + \nabla \cdot (\mu_G \nabla u_G) + \rho_G g + F_{GS} \tag{2}$$

Where F_{GS} is the momentum exchange between gas and solid phases. In the two-fluid model [20,21], it is assumed that trickle flow can be idealized as an annular flow in which the gas and liquid phases are completely separated by a smooth interface [24]. Therefore, each fluid behaves as a continuous medium which Ergun equation can be applied to predict the momentum exchange term. The Ergun equation calculates the particle-gas drag force per unit volume of bed void space as follows:

$$F_{GS} = \frac{E_1(1-\varepsilon)^2 \mu_G u_G}{\varepsilon^3 d_p^2} + \frac{E_2(1-\varepsilon)\rho_G u_G^2}{\varepsilon^3 d_p^2} \tag{3}$$

Where E_1 and E_2 are Ergun constants which their value is subjected to change with any alteration in the conditions of trickle bed (such as size and shape of particles, operating conditions, fluids properties, particles arrangement or bed tortuosity). Macdonald et al. [25] recommended experimentally values of 180 and 1.8 for E_1 and E_2 respectively. But these values are not fixed and they will change in various conditions, particularly for various particle shapes.

CFD SIMULATION BASED ON PELLET SCALE MODEL

To develop a pellet scale model, the slit model was used [17,18] to determine the distance between particles in the bed. The slit model considers an opening between two particles which fluid passes according to Fig. 1. Two parameters, W (slit half-void thickness) and S (slit half-wall thickness) can be obtained as follows:

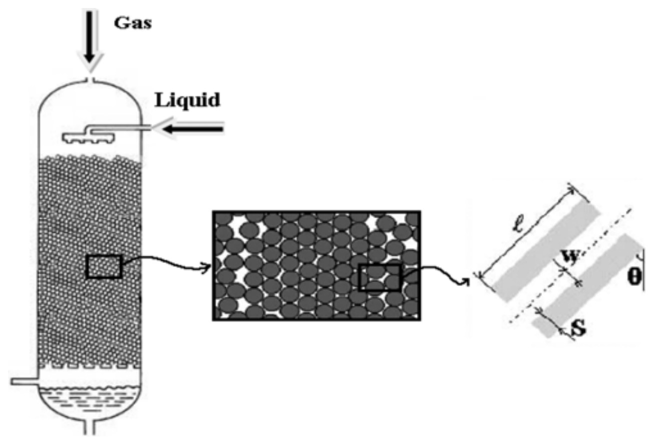

Fig. 1. Sketch of trickle bed reactor and geometrical configuration in slit model.

$$S = \frac{1-\varepsilon}{a} \tag{4}$$

$$\frac{W}{S} = \frac{\varepsilon}{1-\varepsilon} \tag{5}$$

In the proposed pellet scale model, the distance between two trilobe particles is 2W. Fig. 2(a) depicts the cross section of hydrodesulfurization (HDS) trilobe catalyst taken by Philips XL30 scanning electron microscope (SEM). There are two methods of catalyst loading: sock loading and dense loading. In sock loading, a canvas tube conveys the catalyst from the reactor inlet to the bottom of the catalytic reactor. Fig. 2(b) illustrates the actual arrangement of the hydrodesulfurization trilobe catalyst loaded bed using sock method. Dense bed packing is done with the help of a mechanical device. The advantages of dense loading include increased density, capacity, run

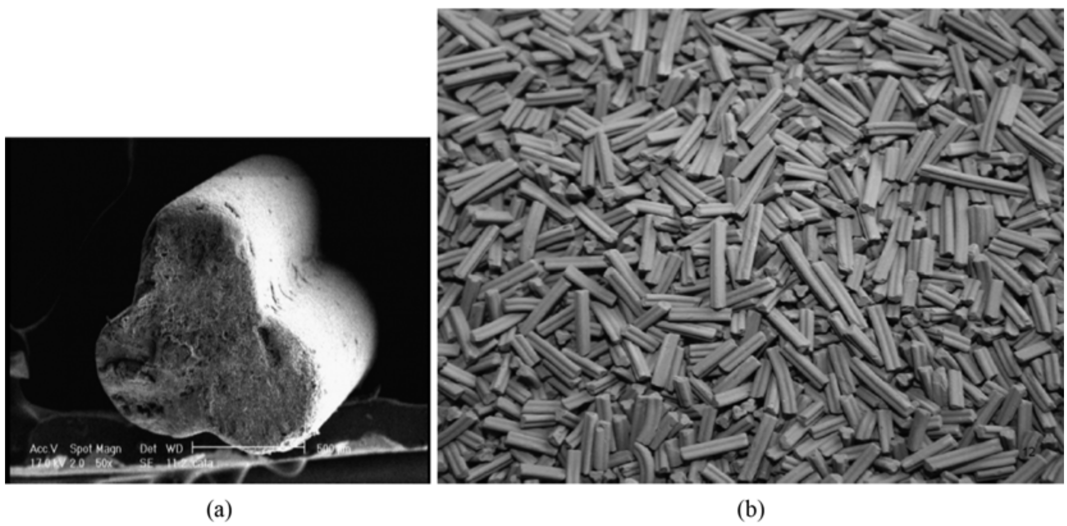

Fig. 2. (a) Scanning Electron Microscopy of trilobe catalyst of hydrodesulphurization (HDS) process (b) Photo of hydrodesulphurization (HDS) trilobe catalyst bed (sock loading).

length and reactor integrity. Due to mechanical stability, in dense loading, particles are arranged horizontally in pellet scale model. The trilobe particles have symmetry axis and can be arranged either in upward or downward orientation in reactor and, thus, the actual tortuosity of the bed is represented by the arrangement of particles. Due to the low Reynolds number flow, the particle end effects can be assumed negligible [26,27], so a two-dimensional simulation was performed. Due to flow symmetry, a solution to this problem is to use periodic boundary conditions (PBC). When using PBC, three particles are enclosed in a box, and we can imagine that this box is replicated to infinity by rigid translation in all the three Cartesian directions, completely filling the space. Fig. 3 depicts a square arrangement of trilobe particles in accordance with the pellet scale model.

Figs. 4(a), 4(b) and 4(c) represent grid and boundary conditions of the proposed model for cylindrical, upward and downward trilobe particles, respectively. Velocity inlet is subjected to inlet boundary, and pressure outlet is used as outlet boundary condition. Moreover, a symmetrical boundary is used for both sides. A refined triangular mesh, which its structure was tuned along the walls, was used to accurately predict drag force imposed on particle wall. The governing equations were discretized by finite volume approach [22]. First-order upwind differencing method was used for discretization of convection terms, and the SIMPLE algorithm was applied for solution of the pressure velocity coupled equations [28].

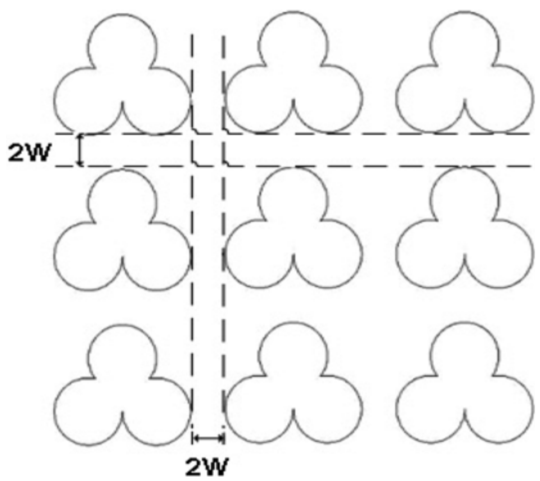

Fig. 3. Pellet scale model for trilobe particles in square arrangement.

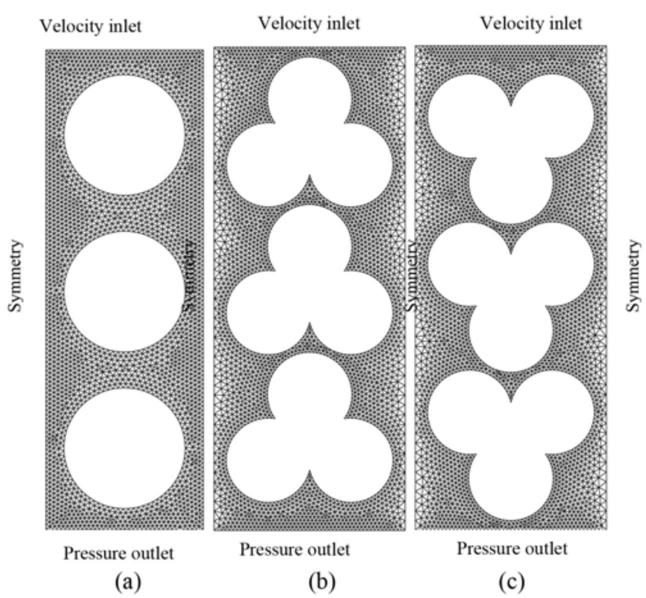

Fig. 4. Mesh generation and boundary conditions used in the proposed pellet scale model (a) Cylindrical particle (b) Upward trilobe particle (c) Downward trilobe particle.

EXPERIMENTAL SETUP

Fig. 5 illustrates a schematic of the experimental setup for studying two-phase liquid/gas flow hydrodynamics in trickle bed reactors. This setup has been applied in this work for experimental study of gas flow pressure drop through the trilobe particle packed bed. The diameter and height of column are 15 cm and 100 cm, respectively. The bed was loaded with industrial trilobe catalyst with 1 mm diameter and average length of 4.2 mm, which is commonly used in hydrodesulfurization (HDS) of diesel (Fig. 2(a)). In our experi-

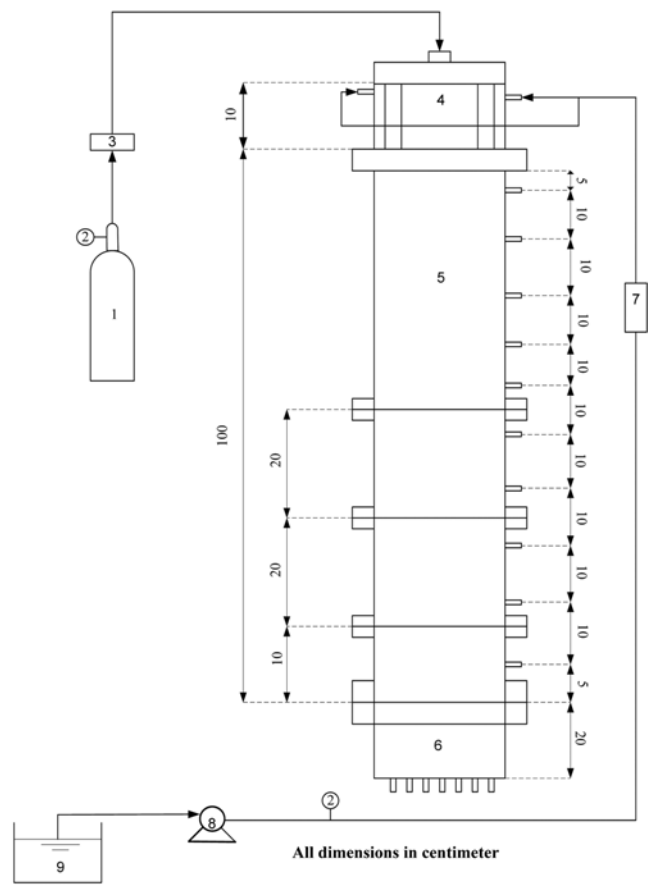

Fig. 5. Experimental flow loop for trickle bed reactor with trilobe particles.

1. Gas cylinder
2. Pressure gauge
3. Gas mass flow meter
4. Bed distributor
5. Trickle bed reactor
6. Bed collector
7. liquid flow meter
8. Liquid pump
9. Liquid storage tank

ments, catalyst dense loading method was applied which naturally has a higher loaded density (up to 20%) and improved homogeneity in fixed bed axial flow reactors compared to the sock loading method. The bed porosity was calculated using the ultra porosimetry technique. Measurements were conducted with single phase flow of the nitrogen. Gas superficial velocity range was between 0.01 to 0.15 m/s. The gas was distributed homogeneously over the bed cross-section from a distributor installed at the top of the reactor. A DWYER Gas Mass Flow Control connected to digital indicators and control system was used to accurately control gas flow rate up to 150 lit/min. The bed pressure drop was measured by means of a precise (DWYER HM35 Love) differential pressure transducer (DPT) with the accuracy of 0.1 Pascal. The pressure profile was measured longitudinally at 10 points, equally spaced from the top to the bottom of the bed.

RESULTS AND DISCUSSION

1. Model Validation

For evaluating the validity of two dimensional CFD simulations, some 2D and 3D numerical investigations was performed for single particle as well as a particle which is located in porous media according to pellet scale model. Preliminary calculations were carried out to obtain grid-independent results under different operating conditions. Furthermore, the results indicate that number of particles does not have any effect on the drag force value imposed on the middle particles. Therefore, the pellet scale model is considered with three particles, and drag force on the middle particle has been reported. Fig. 6 shows the comparison of two-dimensional CFD simulation results with Cox equation predictions [29] along with empirical drag coefficient [30] for a single cylindrical particle (aspect ratio L/d is 2). It can be seen that considerable agreement exists between experimental data and Cox equation predictions, especially in higher Reynolds number. Fig. 7 shows the comparison of drag coefficients predicted by two- and three-dimensional CFD simulation for different length to diameter ratio of cylindrical particle placed in porous media according to pellet scale model (Fig. 4(a)). The results imply that the difference between the predicted drag coefficients in two- and three-dimensional CFD simulations are minor and therefore end effects are negligible in this range of Reynolds number (up to 60). Obviously, this difference decreases in higher particle aspect ratios (L/d). Therefore, the 2D simulation was performed to obtain lower computation time and complexity.

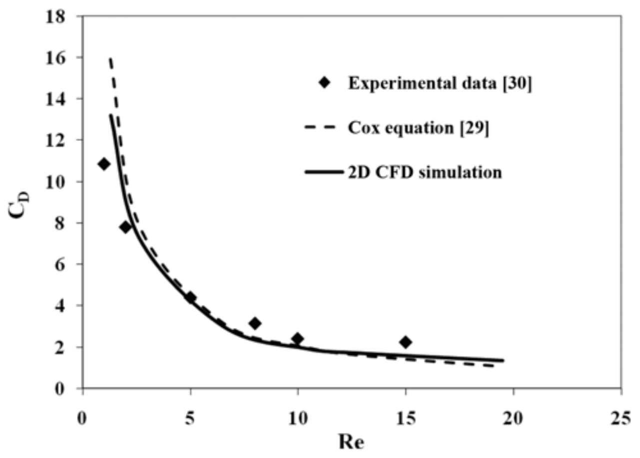

Fig. 6. Comparison of empirical drag coefficient for single cylindrical particle [30] with 2D CFD simulation (this work) and Cox Equation [29].

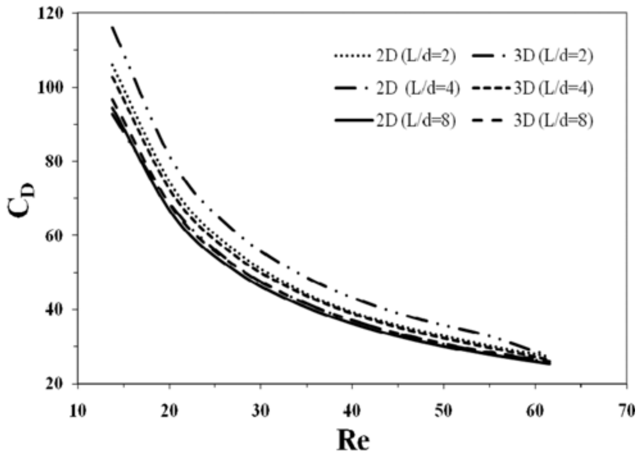

Fig. 7. Comparison of 2D and 3D predicted drag coefficient for particles with different L/D in pellet scale model.

2. The Effect of Particle Arrangement

Figs. 4(b) and 4(c) illustrate a pellet scale model for upward and downward orientations. The bed porosity is 0.4, diameter and length of trilobe particles is 1 and 4 millimeters, respectively. The simulation results show that the drag coefficients for both orientations are nearly equal (Fig. 8). Fig. 9 shows the velocity contours of upward and downward arrangements and the maximum velocities observed in two sides of particles are the same. Therefore, the particle orientation in the pellet scale model has no significant effects.

3. The Effect of Reynolds Number

Fig. 10 shows the drag coefficient vs. Reynolds number for Ergun equation and pellet scale model simulation results. The Ergun equation shows under-prediction in comparison with the pellet scale model. One possible explanation is that the reactor beds with trilobe particles have a more tortuous structure compared to reactor beds with spherical particles. As a result, the original Ergun constants should be modified based on the pellet scale model. For this purpose, a

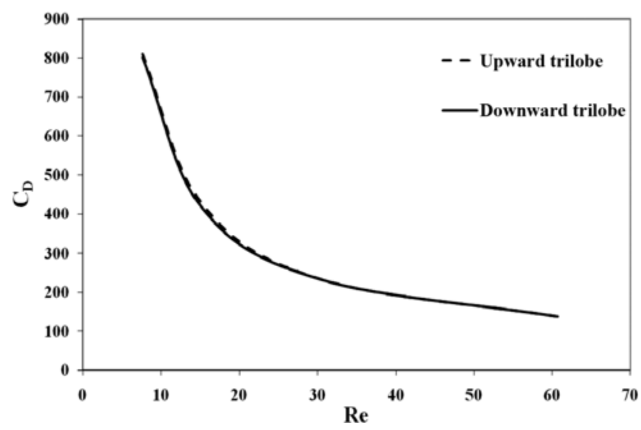

Fig. 8. Comparison of drag coefficient predicted by pellet scale model for upward and downward orientations (e=0.4).

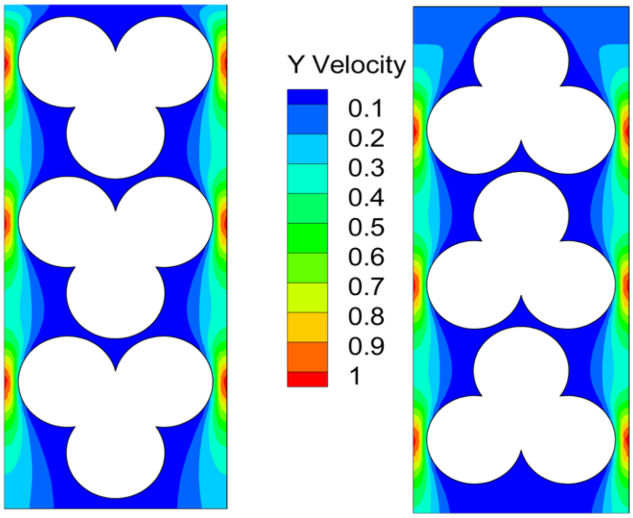

Fig. 9. Velocity contour for up and down ward configuration.

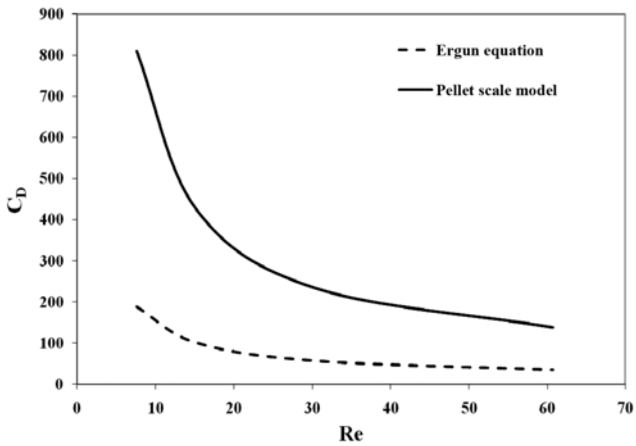

Fig. 10. Comparison of drag coefficient predicted by pellet scale model and Ergun equation (e=0.4).

correction factor (CF) was defined as follows:

$$CF = \frac{(C_D)_{CFD}}{(C_D)_{Ergun}} \tag{6}$$

4. The Effect of Porosity

One of the most effective parameters on drag force imposed on particles in trickle bed reactors is bed porosity. In this study, the governing equation for flow over trilobe particles with 1 mm diameter and 4 mm length in pellet scale model was solved numerically in various porosities (from 0.35 till 0.55) at constant gas velocity (0.1 m/s, Re=16.6). Fig. 11(a) shows considerable difference between the proposed model and Ergun equation predictions in lower porosities, and the correction factor (CF) approaches to one for higher porosities.

5. Influence of Particles Aspect Ratio

To study the effect of aspect ratio (length to diameter ratio, L/d), trilobe particles with different lengths and diameters were considered. Fig. 11(b) shows the influence of particle aspect ratio on proposed correction factor (Eq. (6)). For particles with the same diameter, decreasing the length increases the equivalent diameter. Besides,

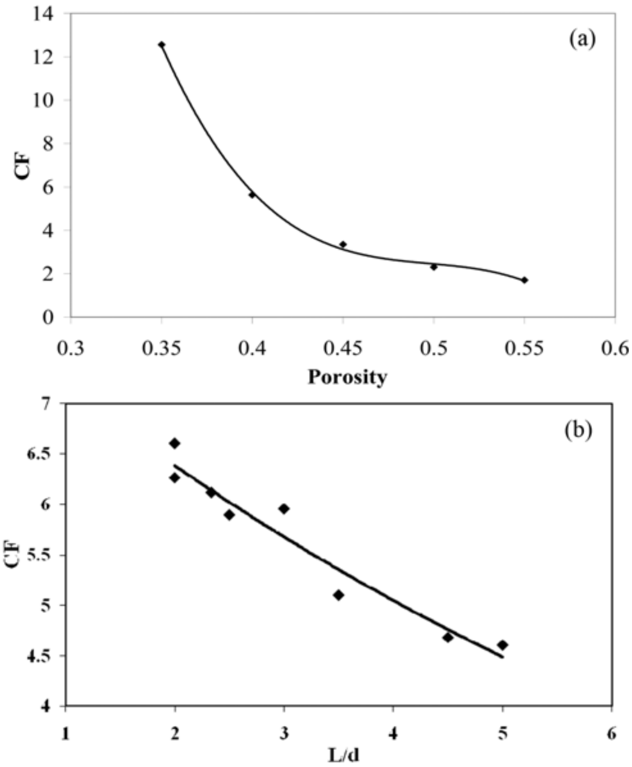

Fig. 11. Variations of correction factor (at constant Re=16.6) with (a) Porosity (b) Aspect ratio (e=0.4).

equivalent diameter is inversely proportional to packing specific area, and also according to Eqs. (4) and (5) packing specific area is oppositely proportional to values S and W. Therefore, by decreasing the length of particle, the value of W is reduced and this causes promotion of drag coefficient in relation to pellet scale model. The Ergun equation also indicates a similar trend but with lower severity especially for lesser L/d, hence the correction factor is greater than unity and increases at lower value of L/d.

6. The Pressure Effect

Prediction of flow hydrodynamics in pressurized packed beds has been the subject of many researches [31-33]. Density and viscosity of gas phase are two effective parameters on drag coefficient and pressure drop in trickle bed reactors which are included in the Ergun equation. Increasing of pressure results in higher gas density and drag forces. However, since the fluid kinetic energy variation is greater than the promotion in drag force imposed on the particles, so the drag coefficient decreases. According to our investigations, the original Ergun equation could not precisely demonstrate the effect of density for TBR with trilobe particles and the Ergun equation underpredicts the pressure drops. Fig. 12(a) shows the variation of correction factor versus gas density. It can be seen that increasing gas density would result in a decrease in correction factor. Therefore, original Ergun constants are more suitable for higher densities or higher pressures. Along with Fig. 12(b), the gas viscosity does not have a significant effect on the correction factor.

7. The Correction Factor for Ergun Equation

In accordance with the above-mentioned investigation on the effective parameters, it is possible to modify the Ergun constants by using a correction factor which includes all parameters. The following

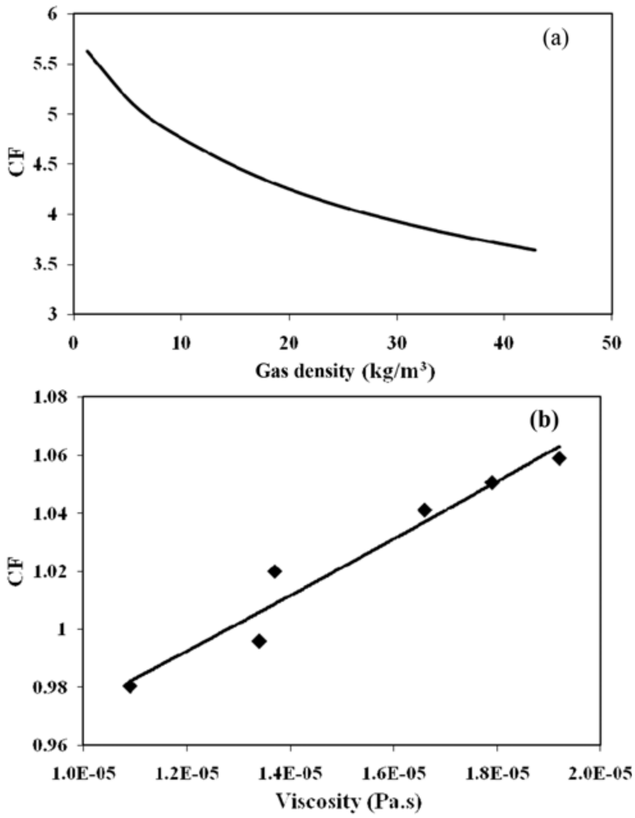

Fig. 12. Variations of correction factor with (a) Gas density (b) Gas viscosity (e=0.4, gas velocity of 0.1 m/s).

equation can be proposed for correction of the Ergun equation constants for trilobe particles in trickle bed reactor in various conditions:

$$\mathrm{CF}=\frac{0.133}{(\mathrm{L}^*)^{0.214}\varepsilon^{4.38}(\rho^*)^{0.123}} \tag{7}$$

Where L^* is the particle aspect ratio, ρ^* is the ratio of fluid density to air density at 15 °C and 1 bar (i.e. 1.225 kg/m^3). Whereas, Reynolds number effects are represented by two terms (Re and Re^2) in original Ergun equation [8] and, thus, the Reynolds number has not been considered in the proposed correction factor (Eq. (7)).

8. Accuracy of Correction

The correction accuracy was validated by comparison of the prediction of corrected Ergun equation for reported empirical data [8] and experimental data of this study. Experimental results of Nemec and Levec [8] are based on a trilobe catalyst with diameter and length of 1.03 and 5.5 mm, respectively, that conclude the bed porosity is 0.466, 10-bar nitrogen as gas phase. Fig. 13 compares the calculated pressure drop by original Ergun equation, Nemec and Levec modified model, corrected Ergun equation (with correction factor, Eq. (7)) and experimental data of Nemec and Levec [8]. It can be seen that our proposed correction improves agreement with experimental data, while much difference is shown with original Ergun equation. The corrected Ergun equation in this work can predict more accurately even in comparison with Nemec and Levec modified model [8]. Fig. 14 also compares the experimental bed pressure drop results of this study with above-mentioned corrected Ergun equation predictions. In this case, the nitrogen gas pressure, and the

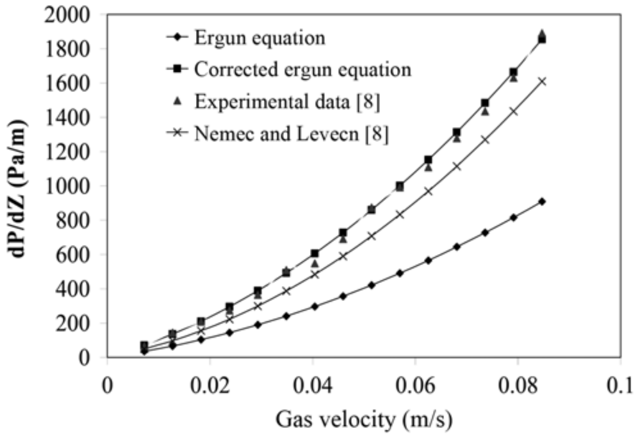

Fig. 13. Pressure drop prediction by Ergun equation, Nemec and Levec model [8], corrected Ergun (This work) and experimental data [8], P=10 bars, L/d=5.35, e=0.466.

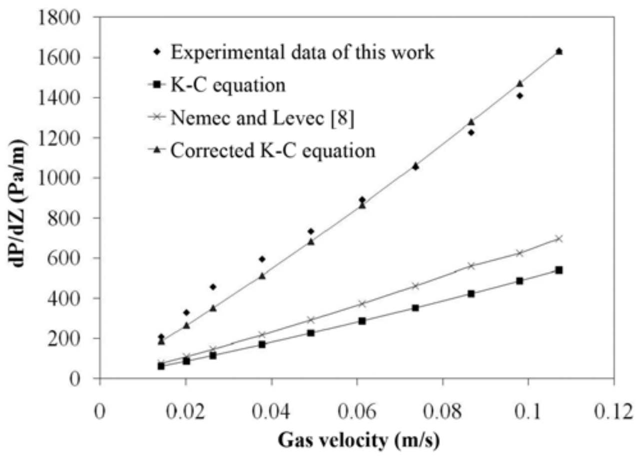

Fig. 14. Comparison predicted pressure drop by Ergun equation, Nemec and Levec model [8], corrected Ergun equation and experimental data (this work), P=1 bar, L/d=4.2, e=0.46.

length to diameter ratio of trilobe catalyst and the bed porosity were 1 bar, 4.2 and 0.46, respectively. The results show that the corrected Ergun equation which was modified by Eq. (7) has better agreement with experimental data, and in this case the original Ergun equation and Nemec and Levec modified model underpredicts the pressure drop.

CONCLUSION

Studying the hydrodynamics of trickle bed reactors (TBRs) with trilobe catalyst, which are widely used in refining and petrochemical industries, is a matter of great importance. In this study, the effect of catalyst shape on hydrodynamic of TBRs in Reynolds number range up to 60 was investigated. A pellet scale CFD model is proposed in order to predict the drag force imposed on trilobe catalyst. The 2D and 3D simulation results showed that for this range of Reynolds number, the end effects of particles are negligible and, thus, only 2D simulations in various conditions have been performed in order to correct the Ergun equation. A correction factor that considers different parameters such as gas properties, bed porosity and length to diameter ratio of the particles has been proposed for using the Ergun equation for single phase pressure drop prediction through the trilobe trickle bed reactors. The results show the gas viscosity variation has not considerable effects. This corrected model shows a very good agreement with experimental data of this work and another gathered set of experimental data from literature.

NOMENCLATURE

a : packing specific area [m^2/m^3]
C_D : drag coefficient
CF : correction factor [-]
d : diameter [mm]
d_P : equivalent diameter=($6V_p/S_p$) [mm]
E_1 : Ergun equation constant (Eq. (3))
E_2 : Ergun equation constant (Eq. (3))
F_D : drag force [N/m^3]
F_{GS} : gas-solid momentum exchange [N/m^3]
L : particle length [mm]
g : gravity acceleration [m/s^2]
p : pressure [pa]
Re : Reynolds number $Re=\rho u d_p/\mu$
S : Slit half-wall thickness [mm]
t : time [s]
u : velocity [m/s]
W : Slit half-void thickness [mm]
z : bed height [m]

Greek Symbol

ρ : density [Kg/m^3]
μ : viscosity [kg/ms]
ε : porosity [-]

Subscripts

G : gas
S : solid
L : piquid

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