Assess proper drag coefficient models predicting fluidized beds of CLC reactor by utilizing computational fluid dynamic simulation

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ABSTRACT:

A two dimensional simulation fluidized beds of CLC reactor were carried out by using Eulerian-Eulerian multi phase flow approach in the OpenFOAM v2.1.1 CFD software package. Data obtained from simulation part compared with the fuel reactor of a pilot CLC rig at the Vienna University of Technology. Different drag correlation were tested for varying size of particles: Ergun, Gibilaro, Gidaspow, WenYu, SchillrNaumann , in order to find the model that exhibit flow behavior of gas and particles in the fuel reactor precisely. Slightly discrepancy between these models were detected, however the Gidaspow model captured experimental trend accurately more than the other models for the all range of particles size.

1. Introduction

According to the Statistics from IPCC, the last decade is ranked among warmest years recorded since 1850[1]. One of the main causes of this Global Warming is Greenhouse gases (GHG) like: H_2O, CO_2, CH_4, N_2O, CFC's and SF_6. Among these gases, CO_2 is considered making largest contribution to the GHG effect, since it represents the largest emissions of the global anthropogenic GHG emissions, and also it has a high residence time in atmosphere. CO_2 emission attribute to human activity as a result of the dependency on fossil fuels for energy production. Until now, intensive investigations have been performed in order to reduce net CO_2 emission, in instance a) increasing the efficiency of conversion of fuel to energy b) substituting the fossil fuel with renewable energy or nuclear energy c) utilizing techniques for capturing CO_2 from exhaust gas and storing it. It appears that Carbon Capture and storage (CCS) is one of the promising approaches for reducing concentration of CO_2 in atmosphere and as a consequence mitigating GHG effects.

Three main methods have been considered to industrial and power plant for sequestering CO_2 from exhaust gas: post-combustion systems, oxy-fuel combustion, and pre-combustion systems[2]. All of these technologies have been reached to a good progress, and they can be available in commercial scale. The foremost drawback of these techniques is, they contain a high energy penalty, which has effects on efficiency of the whole process. Therefore, great efforts have been carried out to eliminate this defect, Chemical Looping Combustion (CLC) is an alternative that can reduce the cost of CO_2 capturing significantly[1]. CLC has not been attained to maturity but it has experienced a great development. Typical CLC system is made from two fluidized bed reactors, oxidizer for combustion process is provided indirectly by means of oxygen carrier materials in absence of air. The solid particles that contain oxygen require for combustion lose their oxygen in fuel reactor, the oxygen depleted particles must re-generated before beginning new cycle, and this can be carried out in the second reactor through passing air among solid particles. Through this procedure the exhaust gases in fuel reactor are just H_2O and CO_2, hence energy demand for separating these two gases from each other reduces considerably.

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The efficiency of chemical-looping system is dependent on flow behavior of oxygen-carrier from one reactor to other one and awareness of it affects on scaling and designing steps[3]. CFD depicted that it can provide a precious insight into the system behavior. For simulating CLC, different techniques can be applied, among them multiphase fluid dynamic models supply more satisfactory level of details as result. In this method the solid and fluid phases are modeled in the framework of the coupled Navier-Stokes equations through spatially and temporally averaged quantities[4]. Since gravity and drag forces play great roles in fluidized bed system (bed expansion, distribution of particles in vessel), so it require more consideration. Kinetic Theory of Granular Flows (KTGF) is a promising approach for simulating gas-particle systems. The properties of solid phase like pressure and viscosity are derived from KTGF[5].

This study is investigated on various drag models and compared the results in order to obtain best model that predict the behavior of fluid and particles in CLC system.

2. Simulation

2.1. Model Equation

In this study, it was assumed that an isothermal fluid passing through particles and no reaction occurred so the energy equation has not been included among conservation equations. In Eulerian-Eulerian multiphase framework separate conservation equations in combination with various constitute models as complementary are calculated for the gas and the solids phases. A brief outline is provided as follow.

2.2. Conservation equations

The continuity equations for both phases are solved as follow:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g\right) + \nabla \cdot \left(\alpha_g \rho_g v_g\right) = \alpha_g S_g \qquad (2\text{-}1)$$

$$\frac{\partial}{\partial t}\left(\alpha_s \rho_s\right) + \nabla \cdot \left(\alpha_s \rho_s v_s\right) = \alpha_s S_s \qquad (2\text{-}2)$$

Right hand terms in both equations are source terms and account for mass transfer according to reaction but since there is no reaction in this study, their values will be equal to zero.

Momentum conservation for the gas is provided as

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g \vec{v}_g\right) + \nabla \cdot \left(\alpha_g \rho_g \vec{v}_g \vec{v}_g\right) = -\alpha_g \nabla p + \nabla \cdot \bar{\bar{\tau}}_g + \alpha_g \rho_g \vec{g} + K_{sg}\left(\vec{v}_s - \vec{v}_g\right) + S_g \qquad (2\text{-}3)$$

And for solid as

$$\frac{\partial}{\partial t}\left(\alpha_s \rho_s \vec{v}_s\right) + \nabla \cdot \left(\alpha_s \rho_s \vec{v}_s \vec{v}_s\right) = -\alpha_s \nabla p - \nabla \mathrm{p_s} + \nabla \cdot \tau_s + \alpha_s \rho_s \vec{g} + K_{gs}\left(\vec{v}_g - \vec{v}_s\right) + S_s \qquad (2\text{-}4)$$

Where K is the interfacial momentum exchange or drag, τ is stress-strain tensor. Similar to continuity equation, source terms in momentum equations are also zero. In KTGF the random motion of granular particles are addressed to gas molecules motion where kinetic theory of gas will be applied. Through this analogy fluid properties as previously mentioned can be determined, the granular temperature is written in conservation form as follow[6]:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\alpha_s \rho_s \Theta_s\right) + \nabla \cdot \left(\alpha_s \rho_s \vec{\mathrm{v}}_s \Theta_s\right)\right] = \left(-p_s \bar{\bar{I}} + \bar{\bar{\tau}}_s\right) : \nabla \vec{v}_s + \nabla \cdot \left(K_{\Theta_s} \nabla \Theta_s\right) - \gamma_{\Theta_s} + \emptyset_{gs} \qquad (2\text{-}5)$$

Further details about conservation and constitute equations can be found in[7].

3. Drag models

The most drag models use values of Reynolds number, phase fraction, relative velocity between phases, and drag coefficient. Also various expressions are used for calculating C_d depending on the Reynolds number. For dispersed multiphase flow different drag correlations can be utilized. Some of them are investigated in this section.

3.1. Schiller Naumann drag model

There is a transitional region between Stoke drag and Newtonian drag, where predicting analytical solution for a falling sphere is so sophisticated. For tackling this obstacle, empirical expressions are applied to compute drag in this regime. Schiller Naumann drag model is one such equation.

$$\boldsymbol{F = C_D \rho_f \frac{U^2}{2} A} \quad \textbf{(3-1)}$$

$$\boldsymbol{C_D = \frac{24}{Re}(1 + 0.15 Re^{0.687})} \quad \textbf{(3-2)}$$

3.2. Wen Yu drag Model (Densely Distributed Solid Particles)

This model has similarity form as Schiller Naumann, just with one modification in Reynolds number and power law correlation. Both of them are functions of the continuous phase volume fraction r_c [6].

$$\boldsymbol{C_D = r_c^{-1.65} max\left(\frac{24}{Re}(1 + 0.15 Re'^{0.687}), 0.44\right)} \quad \textbf{(3-3)}$$

$$\boldsymbol{Re' = r_c Re} \quad \textbf{(3-4)}$$

$$\boldsymbol{K_{sg} = \frac{3\rho_g \alpha_g (1-\alpha_g)}{4 d_p} C_D |\vec{u}_s - \vec{u}_g| \alpha_g^{-2.65}} \quad \textbf{(3-5)}$$

3.3. Gidaspow drag model

This model is a combination of Wen Yu correlation for low solid volume fraction, and Ergun's law for larger solid volume fractions[6].

Ergun equation is shown as follow[8]

$$\boldsymbol{K_{sg} = 150 \frac{\mu_g (1-\alpha_g)^2}{\alpha_g (d_s \emptyset)^2} + 1.75 \frac{\rho_g (|\vec{u}_g - \vec{u}_s|)(1-\alpha_g)}{d_s \emptyset}} \quad \textbf{(3-6)}$$

The constant ϕ is a shape factor for particles.

So Gidaspow drag model is like

$$\boldsymbol{K_{sg} = \begin{cases} K_{sg}(Wen\ Yu) & \alpha_g \geq 0.8 \\ K_{sg}(Ergun) & \alpha_g \leq 0.8 \end{cases}} \quad \textbf{(3-7)}$$

4. Simulation

4.1. Geometry and boundary conditions

3D Cylindrical fuel reactor had to be simulated on 2D plane due to computational effort (computational cost) required. Reactor diameter is 0.16 m and height is 4.1, tangential and normal velocity of gas phase are set to zero at the wall of reactor (no-slip), the gas outlet from top of reactor is defined as pressure outlet, and the gas inlet is specified as velocity inlet. The particle size is investigated in two diameters 120, 290μm[9].

4.2. Solver setting

OpenFOAM v2.1.1 CFD software package was used as solver. This software allows implementation of extra equation and boundary conditions according to the requirements of the problems in comparison to other software like Fluent, which make this software more flexible. Mesh generation was accomplished with "blockMesh" Utility[4]. A summary of solver setting provided in Table 1.

Table 1: Summary of solver setting

Temperature	1173 (K)
Superficial gas velocity	1.8 (m/s)
Particle diameter	120, 290 (μm)
Particle density	2800 (kg/m^3)
Static bed height	0.6 (m)
Gas viscosity	1.789×10^{-5} (kg/m.s)
Restitution coefficient	0.9
Specularity coefficient	0.5

5. Result and discussion

Four sets of numerical experiments were performed; in the first three the effects of different drag models on hydrodynamic behavior of the system were investigated. Finally, the proper drag model was selected for comparing behavior of two sizes of particles. Solids volume fraction and solids axial velocity as a function of dimensionless lateral distance were utilized for comparing different models. Data of Volume fraction and axial velocity of particles were collected from 0.5 m and 1.5 m, vertical levels of fuel reactor. The results were depicted in Figure 1, and Figure 2. As the graphs show, the Gidaspow and Wen Yu drag model lines are in the vicinity of each other in comparison to Schiller Naumann, which can be referred to that Gidaspow model originated from Wen Yu. In addition, by contrasting the data gained through simulation (following graphs) and ref [3, 5], it can be deduced that by implementing Gidaspow drag model in gas-particle momentum exchange equation, more precisely results can be achieved.

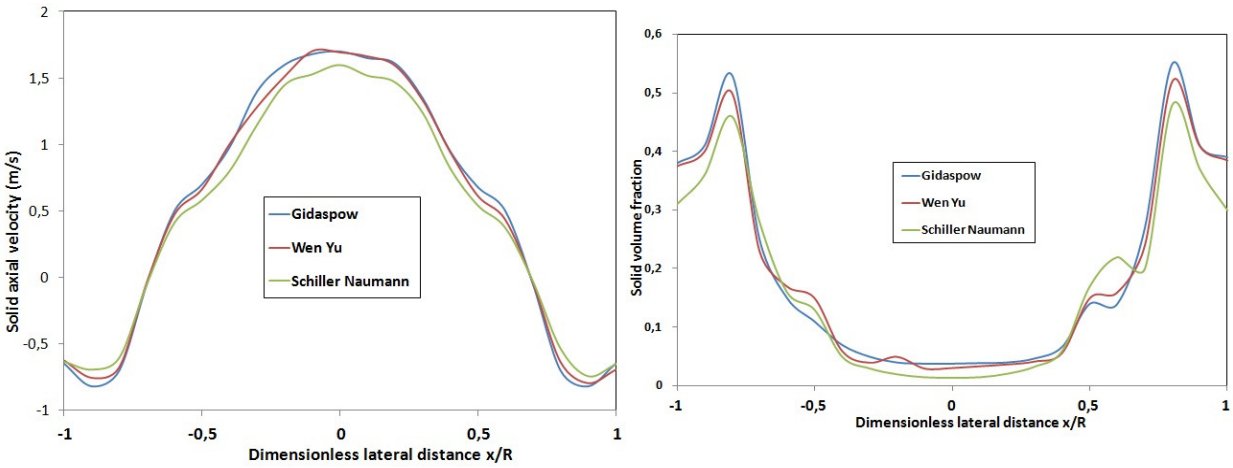

Figure 1: Solids axial velocity and volume fraction along the diameter of the reactor at axial position 0,5m for three drag models: Gidaspow, Wen Yu, and Schiller Naumann

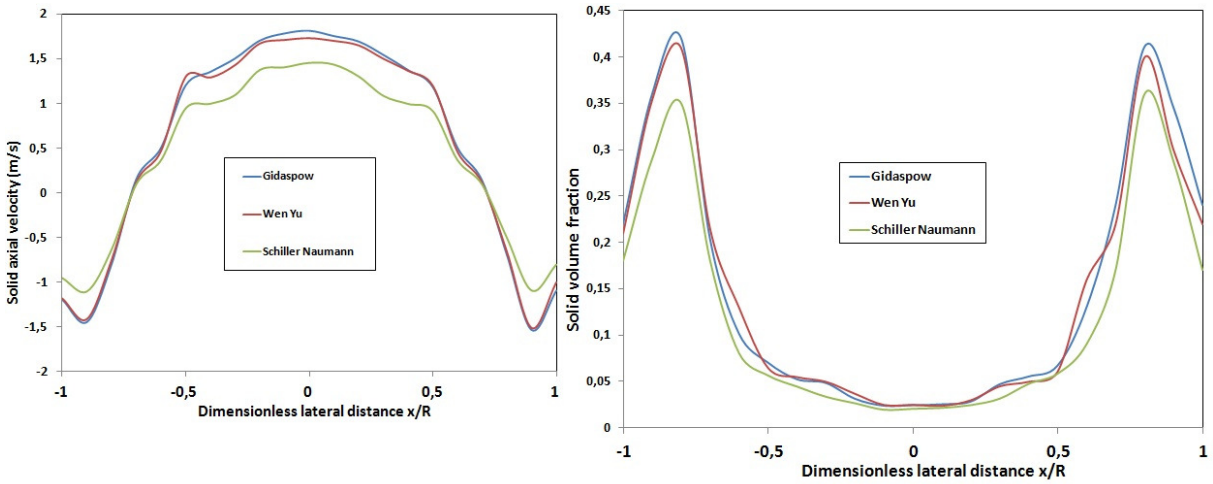

Figure 2: Solids axial velocity and volume fraction along the diameter of the reactor at axial position 1,5m for three drag models: Gidaspow, Wen Yu, and Schiller Naumann

In Figure 3, the time averaged volume fraction of particles with two sizes was compared with each other. The particles concentration for fine particles is higher near to the wall but particles with bigger scale size distributed more uniformly along width of reactor, just like in the real flow, the particle concentration is highest at the bottom and on average the solid particles rise in the middle and come down as clusters near the walls[10].

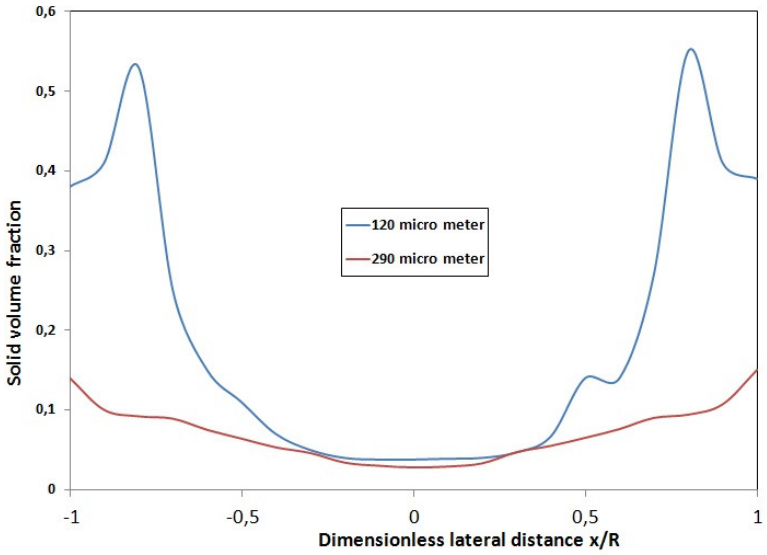

Figure 3: Particles volume fraction along the diameter of the reactor at axial position 0,5m acquired from Gidaspow drag models

6. Conclusion

Various drag models are examined in 2 dimensional CFD simulation for a fuel reactor of a CLC system, the distribution of concentration of particles and their velocities are obtained, the computed results are also compared with experimental data[5, 11] that depict similar behaviors for the particles along height of the column in this paper and [5], the Gidaspow model gives better agreement with experimental data, even if there is a negligible differences between these models. Particularly, Gidaspow drag model is applied for two particle sizes, and it demonstrates that at the height of 0.5 m from bottom of the reactor the volume fraction of large particles are fewer than small ones which is in agreement with real experiments.

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