CFD-DEM and TFM Simulations of Spouted Bed

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This research compared TFM and CFD-DEM models for simulation of a slot-rectangular spouted bed. Limits, drawbacks and benefits of the models were discussed and compared. Results of the two models were compared with available experimental data in literature. Axial distributions of the axial component of particle velocity and solids hold-up at the center of the spout, as well as the radial distributions of the axial component of particle velocity at four heights were found and compared with experimental data. Similar increasing-constant-decreasing trends were observed for both axial velocity and hold-up distributions in CFD and CFD-DEM simulations. Decreasing-constant trends were observed for radial distributions of particle velocity at all heights in CFD and CFD-DEM simulations. Simulation times were also compared at equal condition for the two models. It was found that for all the studied velocity and voidage distributions, CFD-DEM model shows better accuracies.

1. Introduction

Several researches have been conducted on the simulation of multiphase flow systems and various models have been proposed. Among all the proposed models, Eulerian two fluid model (TFM) and Eulerian-Lagrangian computational fluid dynamics – discrete element method (CFD-DEM) have attracted attentions of majority of the researchers and have been used for simulation of different gas-solid contactors, especially fluidized beds and spouted beds. In this research, a slot-rectangular spouted bed was utilized as the case study to compare TFM and CFD-DEM models. Spouted beds are gas-solid contactors which are being used in various industries such as gasification, pyrolysis, drying and coating. Spouted beds have special advantages comparing to other types of gas-solid contactors, including the ability to work with large distribution of particle size.

Several researchers have been conducted investigations on the simulation of multiphase flow systems using TFM. Du et al. (2006a) studied the effect of different drag coefficient correlations on the simulation of spouted beds. In a similar research effects of frictional stress, maximum packing limit and coefficient of restitution of particles have been studied using TFM simulations (Du et al., 2006b). It was found that frictional stress only influences the annulus region in the simulation of large particles. On the other hand, changing the maximum packing limit showed significant impact on the radial distribution of the solids hold-up. Lan et al. (2012) studied influence of solid-phase wall boundary condition on the simulation of a spouted bed. Other researchers used TFM for simulation of spouted beds with and without draft tubes (Azizi et al., 2010, Wang et al., 2006).

CFD-DEM, as a novel model, has attracted attention of many researchers in the field of multiphase flow simulation. CFD-DEM was utilized to study the gas-solid hydrodynamics of rectangular spouted bed (Saidi et al., 2015). Yang et al. (2013) used CFD-DEM to study the effects of operating conditions, flow regime and presence of draft tube on the hydrodynamics of spouted beds. Salikov et al. (2015) studied hydrodynamics of a prismatic spouted bed with two gas inlets using CFD-DEM simulations. Rong and Zhan (2010) proposed an improved CFD-DEM model and validated the model by simulation of a spouted bed.

Despite all the conducted researches on proposing improved models and studying the effects of different parameters by means of TFM and CFD-DEM simulations, little has been published on the comparison of the mentioned models. This work compared TFM and CFD-DEM in simulation of a slot-rectangular spouted bed. Simulation results were compared with experimental results to evaluate the accuracy of each model. Required simulation times for different condition were compared for different models and some recommendations were...
provided to choose the best method for other simulations. Limitations, drawbacks and benefits of the models in the simulation were also discussed.

2. Model

2.1 CFD (TFM)

Two fluid model (TFM) was used for simulation of the spouted bed. In this paper, this model is referred to as CFD. Governing equations of the TFM can be found in literature (Ueyama, 2012). For calculation of the gas-solid drag coefficient, the model proposed by Gidaspow et al. (2003) was used which considers a combination of Ergun and Wen-Yu models:

\[ \beta = (1 - \varphi_g) \beta_{\text{Ergun}} + \varphi_g \beta_{\text{Wen-Yu}} \]  

in which:

\[ \beta_{\text{Ergun}} = 150 \frac{\alpha_g \mu}{\alpha_p d_p^2} + 1.75 \frac{\alpha_g \rho_g}{d_p} \left( \frac{v_p - u}{d_p} \right)^{-1} \alpha_s \leq 0.8 \]  

\[ \beta_{\text{Wen-Yu}} = \frac{3}{4} C_D \frac{\alpha_p \alpha_g \rho_g}{d_p} \left( \frac{v_p - u}{d_p} \right)^{-2.65} \alpha_s > 0.8 \]

\[ C_D = \begin{cases} 24 \alpha_s \rho_p \left( 1 + 0.15 (\alpha_s \text{Re}_p)^{0.687} \right), & \text{Re}_p < 1000 \\ 0.44 & \text{Re}_p \geq 1000 \end{cases} \]

\[ \varphi_g = \frac{\arctan[150 \times 1.75(0.2 - \alpha_g)]}{\pi} + 0.5 \]

OpenFOAM® software was used for the CFD simulation in this work.

2.2 CFD-DEM

CFD-DEM model initially solves the local-averaged Navier-Stokes equation in the gas phase. After reaching convergence, the calculated drag force is used in the DEM part. DEM part solves the equation of motion for all the particles in the system. After calculation of the new position of particles in the bed, the voidage distribution is found and used in the next CFD iteration. It should be mentioned that a soft-sphere model is used based on Hertzian contact model in this research. The governing equations of CFD-DEM are shown in Table 2. Detailed information about the governing equations can be found in literature (Golshan et al., 2017). An open-source CFD-DEM code (Goniva et al., 2012) was used for CFD-DEM simulation in this research. Parameters which were used for the CFD and CFD-DEM simulation are shown in Table 1.

3. Result and discussion

In this work, we compared the simulation results with available experimental data of Zhao et al. (2008a and 2008b) to find and compare the accuracies of the models. Schematics and dimensions of the bed are illustrated in Figure 1 and other details can be found in literature (Zhao et al., 2008b). Particle used in the simulations were glass beads with diameter of 1 mm. Properties of particles and bed where chosen based on the values used by Zhao et al. (2008a and 2008b). Particles were initially inserted into the bed without any gas flow in both CFD and CFD-DEM simulations and after finishing the insertion step the gas flow was inserted into the bed. Sensitivity analysis were performed on the mesh size to find the suitable mesh size in both CFD and CFD-DEM simulations. Four mesh sizes \((d_m/d_p = 2, 3, 4, 5)\) were used to find the effect of mesh size on the simulation results. The largest mesh size with no significant effect of decreasing the size on the results \((d_m/d_p = 3)\) was chosen for both CFD and CFD-DEM simulations.
Table 1: CFD-DEM governing equations.

**CFD**

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \mathbf{u}) = 0
\]

\[
\frac{\partial}{\partial t} (\rho \varepsilon \mathbf{u}) + \nabla \cdot (\rho \varepsilon \mathbf{uu}) = -\varepsilon \nabla P + \nabla \cdot \left( \varepsilon \mathbf{e} \right) + \rho \varepsilon \mathbf{g}
\]

**DEM**

\[
m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \left( \mathbf{F}_{ij}^N + \mathbf{F}_{ij}^T \right) + m_i \mathbf{g}
\]

\[
I_i \frac{d\omega_i}{dt} = \sum_j \mathbf{M}_{ij}^T + \mathbf{M}_{ij}^\mu
\]

\[
\mathbf{F}_N = \left( -\frac{4}{3} E_{eff} \sqrt{R_{eff} \sigma_N^{1/2}} \right) \left( \eta_o \sigma_N^{1/2} \mathbf{v} \right) n_{ij}
\]

\[
\mathbf{F}_T = -\frac{16}{3} G_{eff} \sqrt{R_{eff} \sigma_N^{1/2}} \sigma_{ij}
\]

Table 2: CFD and CFD-DEM simulation parameters.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>e</td>
<td>0.9</td>
</tr>
<tr>
<td>(\mu)</td>
<td>0.3</td>
</tr>
<tr>
<td>(\mu_r)</td>
<td>0.03</td>
</tr>
<tr>
<td>E (GPa)</td>
<td>200</td>
</tr>
<tr>
<td>(\nu)</td>
<td>0.3</td>
</tr>
<tr>
<td>(\Delta t_{DEM}) (s)</td>
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</tr>
<tr>
<td>(\Delta t_{CFD}) (s)</td>
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</tr>
<tr>
<td>(\rho_p) (kg/m(^3))</td>
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</tr>
<tr>
<td>(\rho_g) (kg/m(^3))</td>
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</tr>
<tr>
<td>T.I.</td>
<td>0.06</td>
</tr>
<tr>
<td>(\mu_g) (Pa.s)</td>
<td>1.7894×10(^{-5})</td>
</tr>
<tr>
<td>(U) (m/s)</td>
<td>1.58</td>
</tr>
<tr>
<td>(t) (s)</td>
<td>5</td>
</tr>
</tbody>
</table>

Figure 1: Schematics and dimensions of the simulated spouted bed.
Both CFD and CFD-DEM simulations were performed on seven CPUs (3.30 GHz). Required simulation time for CFD and CFD-DEM simulations were approximately 92 and 31 h. Both CFD and CFD-DEM models demonstrate some benefits and limitations during simulation which are discussed here. Both models are dependent on the mesh size, consequently performing a sensitivity analysis on the effect of mesh size is inevitable. As mentioned earlier required simulation time for the CFD-DEM simulation was considerably (approximately one third) less than CFD for this case. The required simulation time increases exponentially with the number of particles in the bed (Norouzi et al., 2016). In cases with low number of particles (similar to the case study in this research) CFD-DEM simulations are more computationally efficient. As the number of particles increases, required simulation time for CFD simulations become less than CFD-DEM. Additionally, input parameters of CFD-DEM simulations are more than CFD, which means more accurate information about the particle and bed properties should be known for a CFD-DEM simulation. However the accuracy of CFD-DEM simulation is significantly higher than CFD which will be discussed in details. Moreover, some post-simulation analysis can be performed only in CFD-DEM simulations such as calculation of solids circulation time and rate using the method used by Golshan et al. (2016).

![Figure 2: Axial distributions of (a) the axial component of particle velocity and (b) solids hold-up at the center of the spout (r = 0) in CFD and CFD-DEM simulations.](image)

![Figure 3: Radial distributions of particle velocity at (a) z = 3.04 cm, (b) z = 4.56 cm, (c) z = 6.08 cm and (d) z = 9.12 cm in CFD and CFD-DEM simulations.](image)

At \( t = 0 \) s, gas was inserted to the bed and opened its way to the bed surface. By reaching to the bed surface the spout region was observable in the bed. Particles which were initially located on the gas way, were
entrained with the gas to the surface. The gas jet scattered the particles over the annulus and stable spouting began. Axial distributions of the axial component of the particle velocity and solids hold-up for CFD and CFD-DEM simulations are illustrated in Figure 2. It can be observed that the axial distribution of particles velocity consist of three distinct increasing-constant-decreasing parts. Particles accelerate at lower heights due to high gas velocity. As the height increases, particles reach the maximum velocity (constant part in Figure 2a) and decelerate afterwards. CFD-DEM simulation predicts the mentioned trend (experimental trend) with high accuracy, however CFD results underestimate experimental results. The solids hold-up distribution results are also compared for CFD and CFD-DEM simulations with experiments. A similar increasing-constant-decreasing trend is also observed for the hold-up distribution. It should be mentioned that CFD-DEM simulations have better prediction of experimental results comparing to CFD simulations. Figure 3 shows radial distribution of the axial component of particle velocity at four heights ($z = 3.04, 4.56, 6.08$ and $9.12$ cm). A decreasing-constant trend is observed for the radial distributions. As the height increases, the accuracy of simulation decreases. It also can be observed that CFD-DEM simulation illustrate better predictions of experimental results similarly.

4. Conclusions

CFD (two fluid model) and CFD-DEM simulations of a slot-rectangular spouted bed were performed and compared with available experimental results. Axial distributions of axial component of particle velocity and solids hold-up and radial distributions of particle velocity at four heights were found and compared with experimental data. It was reported that both CFD and CFD-DEM could successfully predict the increasing-constant-decreasing trends of axial velocity and hold-up distributions as well as decreasing-constant trends of radial particle velocity at all four heights. Results also show that CFD-DEM provides more accurate results comparing with CFD simulation. Required simulation time for CFD and CFD-DEM simulations were approximately 92 and 31 h, respectively. For cases with low numbers of particles (such as case study in this research) CFD-DEM requires less time comparing to CFD. However as the number of particles increases in a system, the required time for CFD-DEM simulation increases exponentially and CFD becomes the efficient model. Other limitations, benefits and drawbacks of each model are discussed in this research.

Nomenclature

\[ C_D = \text{drag coefficient, dimensionless} \]
\[ d_p = \text{diameter of particles, mm} \]
\[ E = \text{Young's modulus, Pa} \]
\[ e = \text{coefficient of restitution, dimensionless} \]
\[ F_{ij}^N = \text{normal force, N} \]
\[ F_{ij}^T = \text{tangential force, N} \]
\[ G = \text{shear modulus, Pa} \]
\[ g = \text{gravity acceleration, m/s}^2 \]
\[ H_s = \text{static bed height, mm} \]
\[ I = \text{moment of inertia, kg.m}^2 \]
\[ M_{ij}^T = \text{tangential torque, N.m} \]
\[ M_i^R = \text{rolling friction torque, N.m} \]
\[ m = \text{mass of particle, kg} \]
\[ n_{ij} = \text{normal vector, dimensionless} \]
\[ P = \text{pressure, Pa} \]
\[ R_{ef} = \text{effective diameter, m} \]
\[ Re_p = \text{particle Reynolds number, dimensionless} \]
\[ T.I. = \text{turbulent intensity, dimensionless} \]
\[ t_i = \text{tangential vector, dimensionless} \]
\[ U = \text{minimum spouting velocity, m/s} \]
\[ u = \text{gas velocity, m/s} \]
\[ v_p = \text{velocity of particle, m/s} \]
\[ z = \text{height, cm} \]

Greek letters:

\[ \alpha_g = \text{gas volume fraction, dimensionless} \]
\( \alpha_p \) = particle volume fraction, dimensionless
\( \beta \) = gas/solid momentum exchange coefficient, kg/m\(^3\)s
\( \Delta t_{\text{CFD}} \) = CFD time step, s
\( \Delta t_{\text{DEM}} \) = DEM time step, s
\( \delta \) = overlap of particles, m
\( \varepsilon \) = voidage, dimensionless
\( \eta_\alpha \) = damping coefficient, kg/s.m\(^{0.25}\)
\( \mu \) = friction coefficient, dimensionless
\( \mu_g \) = gas viscosity, Pa.s
\( \mu_r \) = rolling friction factor, dimensionless
\( \nu \) = Poisson's ratio, dimensionless
\( \nu_{\text{RN}} \) = relative velocity of particle in normal direction, m/s
\( \rho_p \) = density of particles, kg/m\(^3\)
\( \rho_g \) = density of gas, kg/m\(^3\)
\( \phi_{gs} \) = switch function in the Gidaspow model, dimensionless
\( \omega \) = angular velocity of particle, rad/s

Reference