Numerical Modelling of isothermal Gas-Solid Flow Development in the Riser of a Pilot-Scale Circulating Fluidised Bed (CFB) Reactor

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Abstract
Numerical simulations of isothermal turbulent gas-solid flow in the riser of a pilot-scale circulating fluidised bed (CFB) reactor has been carried out using FLUENT CFD software. An Eulerian-Eulerian multiphase flow model was used. The constitutive equations in terms of the granular temperature based on the kinetic theory of granular flow (KTGF) were used to determine the solids pressure, shear and bulk viscosity. The granular temperature is determined using both the algebraic and differential transport models. The $k\!-\!\varepsilon$ model is used for the gas phase turbulence. The predicted particle velocity and concentration are compared with experimental data collected by (Huang et. al., 2007) in a riser of 15.10 m in height and 0.10 m in diameter with particles of d_p, 67.0 μm mean diameter. In general, the measured trends are well predicted by both the models of granular temperature. However, the predictions obtained using the differential transport model for the granular temperature are in a better agreement with data compared with those obtained using the algebraic model. Advance studies are been initiated which includes other granular constants like steady state transport (SST), Lagrangian, Gidaspow, Arastoopour etc.

Keywords: *CFD modelling, gas-solid, CFB, KTGF and predictions*

1. Introduction

Circulating fluidised bed (CFB) reactors are widely used in the industry to carry out a variety of multiphase gas-solid catalytic and non-catalytic reactions including coal combustion and gasification, fluid catalytic cracking (FCC) of heavy oil fractions for the production of gasoline, LPG and middle distillates, and Fischer-Tropsch synthesis of hydrocarbons. In the riser of a CFB, gas flows through granular solids at a high velocity which entrains the solids and transports them out of the riser. Three distinct fluidisation regimes have been identified in the riser Levenspiel, (1999), namely turbulent fluidisation, fast fluidisation and pneumatic conveying. However, most risers in industrial CFB reactors operate in the turbulent and fast fluidisation regimes Grace, (2000), (Jiradilok et. al., 2006), which are not fully understood (Jiradilok et. al., 2006), (Du et. al., 2003) and phenomenological flow models are not well developed Levenspiel, (1999). Consequently, uncertainty exists in the design, scale-up and performance prediction of such reactors. In recent years, there have been significant advances in computational fluid dynamics (CFD) modelling of improved understanding of the riser hydrodynamics and to facilitate the reactor design and the selection of appropriate operating conditions to achieve the desired fluidisation regime. However, multiphase CFD models require validation against data from large-scale experimental rigs before they can be used with confidence for the above mentioned purposes.

A large number of CFD modelling studies of gas-solid flows through the riser of CFB reactors have been reported in the literature Ranade, (2002), Almuttahar and Taghipour (2007). However, it appears that no systematic approach has been used to select models for the gas phase (such as laminar or turbulent) and for the solid phase (such as empirical constitutive relations or models based on the kinetic theory of granular flow) and the parameters of the constitutive equations (such as the values of restitution and specularity coefficients, and interphase drag coefficients) to simulate gas-solid flow in riser systems Ranade, (2002), Almuttahar and Taghipour (2007). Although multiphase flows in riser reactors generally occur at high Reynolds numbers associated with high levels of turbulence, many previous CFD studies have treated flows as laminar, in some cases (Almuttahar and Taghipour (2007) with satisfactory agreements between the predictions and experimental data. The riser flows are also three-dimensional, yet in many studies the flow has been treated as two-dimensional in order to reduce the computational demand. This has lead to discrepancies between the predictions and measurements.

In the present study, gas-solid flow behaviour in the riser section of a pilot-scale CFB investigated experimentally by (Huang et. al., 2007) has been simulated using a proprietary CFD code, ANSYS FLUENT. Calculations were carried out using an Eulerian-Eulerian multiphase flow model. The solids pressure, shear and bulk viscosity were obtained in terms of the granular temperature using the constitutive equations derived from the kinetic theory of granular flow (KTGF). The granular temperature was determined using both the algebraic and differential transport models. The gas phase turbulence was represented by the k–ε model. The CFD predictions are compared with the measured radial distributions of particle mean axial velocity and concentration at different locations along the height of the riser.

1.1 Problem Statement

The depletion in the ozone layer has resulted due to increase in human activities globally, which caused global warming. This resulted in the emission of certain hydrocarbons (HCs) and their sister pollutants from the petroleum industry possess serious threat to the survival of human and other lives on the planet earth. Therefore, the hydrodynamic study of the CFB as the parent cycle to FCC reactor to arriving at a better flowing regime is the crux of the subject.

1.2 Significance of the Study

An excellent performance of CFB/FCC riser systems is subject to quality flowing regime. Good mixing flowing regime with the required heat transfer contributes to effective distribution of reactants, whereas sufficient mixing with poor heat distribution can lead to incomplete combustions, these pose a serious threat. Therefore, adequate understanding of the dynamic behaviours is very important to ensure a high combustion efficiency and quality control of emissions.

2. Mathematical Model

An outline of the multiphase CFD modelling methodology for the gas-solid turbulent flows through the riser is given here; full details may be found in Idris, (2010). An Eulerian-Eulerian multiphase flow modelling approach with the KTGF was used. A set of the mass

and momentum equations was solved for each phase, where the momentum equations were coupled by an interphase exchange term.
The Reynolds-averaged continuity and momentum equations for the gas phase are given by (Almuttahar and Taghipour (2007) :

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right)+\nabla.\left(\varepsilon_g \rho_g \vec{v}_g\right)=0 \qquad (1)$$

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

The continuity and momentum equations for the solid phase are:

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s\right)+\nabla.\left(\varepsilon_s \rho_s \vec{v}_s\right)=0 \qquad (3)$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s \vec{v}_s\right)+\nabla \cdot\left(\varepsilon_s \rho_s \vec{v}_s \vec{v}_s\right)=-\varepsilon_s \nabla p- \nabla p_s+\nabla \cdot \bar{\bar{\tau}}_s+\varepsilon_s \rho_g \vec{g}+K_{gs}\left(\vec{v}_g-\vec{v}_s\right) \qquad (4)$$

where $\vec{v}_g$ and $\vec{v}_s$ are the gas and solid velocity vector, respectively; p and p_s are the fluid and solids pressure, respectively; g is the gravitational acceleration, K_{gs} is the gas-solid momentum exchange coefficient which is obtained from the drag model of (Gidaspow, D., et. al., 1992); $\bar{\bar{\tau}}_g$ and $\bar{\bar{\tau}}_s$ are the gas and solid phase stress tensors, respectively; ρ_g and ρ_s are the gas and solid density, respectively; and ε_g and ε_s are the volume fraction of gas and solid. In addition, the volume fractions add up to unity:

$$\varepsilon_g + \varepsilon_s = 1 \qquad (5)$$

The gas phase turbulence is represented by the widely used k–ε turbulence model. The turbulence quantities of the solid phase are predicted using the dispersed turbulence modelling approach ANSYS Fluent (2015). The solids stress tensor is given by:

$$\bar{\bar{\tau}}_s=\varepsilon_s \mu_s\left(\nabla.\vec{v}_s+\nabla.\vec{v}_s{}^T\right)+\varepsilon_s\left(\lambda_s-\frac{2}{3} \mu_s\right) \nabla.\vec{v}_s \bar{\bar{I}} \qquad (6)$$

Constitutive equations Gidaspow, D. (1994) for the solids pressure (p_s), solids bulk (λ_s) and shear (μ_s) viscosity are derived from the KTGF (for details, see Gidaspow, D., et. al., (1992)) in terms of the granular temperature defined as:

$$\Theta_s=\frac{1}{3} \overline{u_s'^2} \qquad (7)$$

The granular temperature, which is a measure of the kinetic energy due to the fluctuating velocities of the particles (u_s'), can be determined by solving a differential transport equation or from an algebraic equation resulting from neglecting the convection and diffusion terms in the transport equation.

3. Application of the Model

3.1 The Experimental Case

In this study, the experiments carried out by (Huang et. al., 2007) in a pilot-scale CFB system were simulated. Fig. 1 is a schematic diagram of the riser section of the CFB consisting of a cylindrical vessel with 0.10 m in diameter and 15.1 m in height, which provided a sufficiently long distance for flow development. The solids used in the riser were FCC particles of 67 µm mean diameter having a density of 1500 kg/m^3. The solid mass flow rate (G_s) was varied between 50 and 200 kg/m^{2}s. Air at ambient conditions was used in the experiments with a superficial velocity (U_s) varying between 3.5 and 8.0 m/s.

Measurements of the solid concentration and mean axial velocity distributions along the radius of the riser at eight locations along the height, at z = 0.95, 2.59, 4.51, 6.34, 8.16, 10.0, 12.28 and 14.08 m (where *z* is the distance from the riser inlet), were reported. The operating conditions of the experimental cases simulated in this study are given in Table 1.

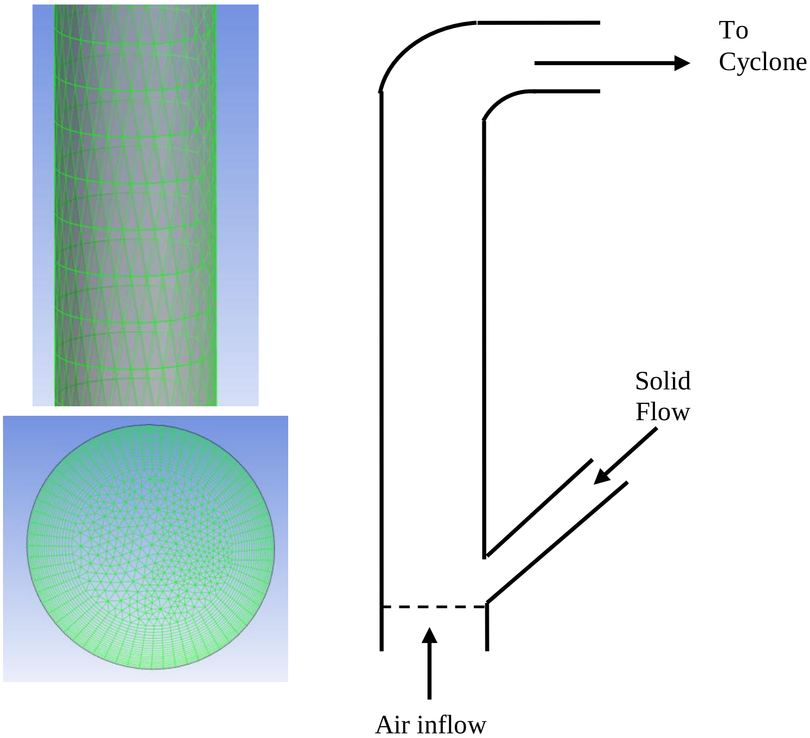

Fig. 1: Schematic of the riser section of CFB and the computational mesh

Table 1: Experimental condition

Operating conditions	Unit	Case 1	Case 2	Case 3	Case 4
G_s	kg/m^{2}s	100	50	100	200
U_g	m/s	3.5	5.5	5.5	8.1

3.2 Computational Details

Three-dimensional, transient calculations were performed on an unstructured mesh consisting of 5.78×10^{-5} cells. Four mesh sizes ranging from 1.34×10^{-5} to 7.38×10^{-5} cells were tested in order to examine the influence of the mesh size and its distribution on the predictions. The test calculations show that the selected mesh size is adequate to provide acceptable mesh independent solutions. The input parameters for the flow simulations are summarised in Table 2. The conservation equations were discretised using the finite volume method. A second order upwind discretisation scheme was used for the convection terms.

At the inlet of the riser, the velocities and volume fractions of gas and solid were specified. At the outlet, the pressure was assumed atmospheric. At the walls, the no-slip boundary condition was specified for the gas phase.

The wall boundary condition developed by Johnson and Jackson (1987), was used for the solid phase. The discretised momentum and pressure correction equations, together with the equations for turbulence model quantities, were solved iteratively using FLUENT CFD code. Transient computations were performed using zero initialisation for a real time of 5 s, with a time step of 1×10^{-4} s. The target value of the normalised residual for each variable was 1×10^{-4}. For a converged solution, the overall mass conservations for the gas and solid phases were typically within 0.002 and 0.15%, respectively. The typical computational time for the transient simulation was 10-13 days on a 4 GHz processor.

Table 2: Input parameters for the simulation

S/No.	Parameters	Values	Units
1.	Density of air (ρ_g)	1.185	kg/m^3
2.	Density of solid (ρ_s)	1500	kg/m^3
3.	Viscosity of air (μ_g)	1.831×10^{-5}	kg/m.s
4.	Particle diameter	67.00	µm
5.	Particle-particle restitution coefficient	0.99	dimensionless
6.	Particle-wall restitution coefficient	0.60	dimensionless
7.	Specularity coefficient	0.60	dimensionless

4. Results and Discussion

In order to establish the potentials and limitations of the multiphase CFD modelling methodology, the model was evaluated for all the experimental conditions given in Table 1 ranging from a low to a high density flow. However, simulation results for the experimental case 1 (G_s = 100 kg/m^{2}s and U_s = 3.5 m/s) are presented here as page limitation precluded coverage of all the cases.

The comparison between the measured and predicted solid velocity profiles using the differential transport equation (referred to as the transport-KTGF) and the algebraic equation (referred to as the algebraic-KTGF) modelling approaches for the granular temperature are shown in Fig. 2 only at z = 2.59, 8.16 and 14.08 m due to the space limitation. A scrutiny of the simulation results at all the measurement locations reveals that the general measured trends are reasonably well reproduced in the predictions obtained using both the modelling methods for the granular temperature.

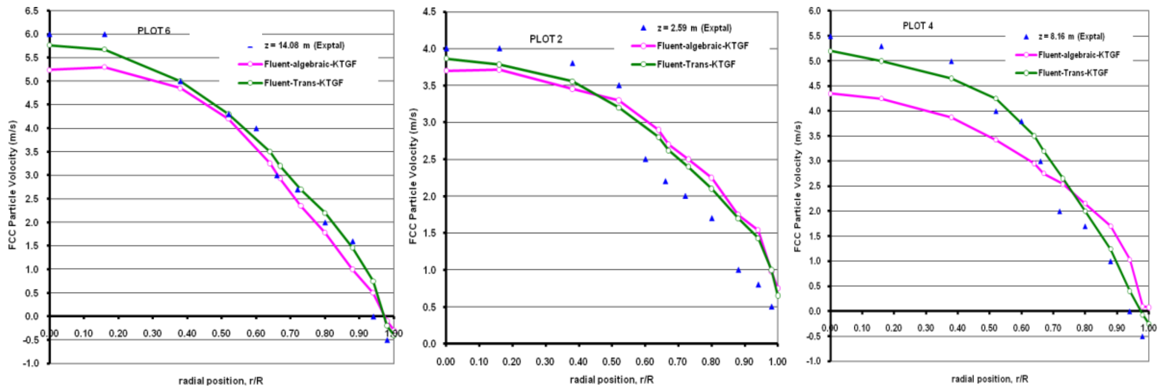

Fig. 2: Predicted and measured (Huang et. al., 2007) solid velocity distributions

However, there are discrepancies between the predictions and measurements and also between the two sets of predictions. The solid velocity at and around the riser axis is underpredicted at all the locations except at z = 0.95 (not shown here). The algebraic-KTGF model for the granular temperature consistently under-predicts solid velocity in this region compared with the transport-KTGF model.

However, as can be seen in Fig. 2, the quality of the predictions improves and the difference between the two sets of predictions reduces significantly in the region further away from the axis. An important feature of the solid flow in the riser observed in previous experimental studies including that of (Huang et. al., 2007) is the down flow of solids along the wall. This is evident at z = 8.16 and 14.08 m in Fig. 2. In fact, the experimental data show the reverse flow of solids close to the wall at all measurement locations between z = 4.51 and 14.08 m. This feature of the solid flow is well captured qualitatively in the predictions obtained using the transport-KTGF model, although the maximum reverse velocity of solids is underpredicted. However, in the case of the algebraic-KTGF model, the down flow of solids was predicted only near the top region of the riser at z = 10.0 and 14.08 m.

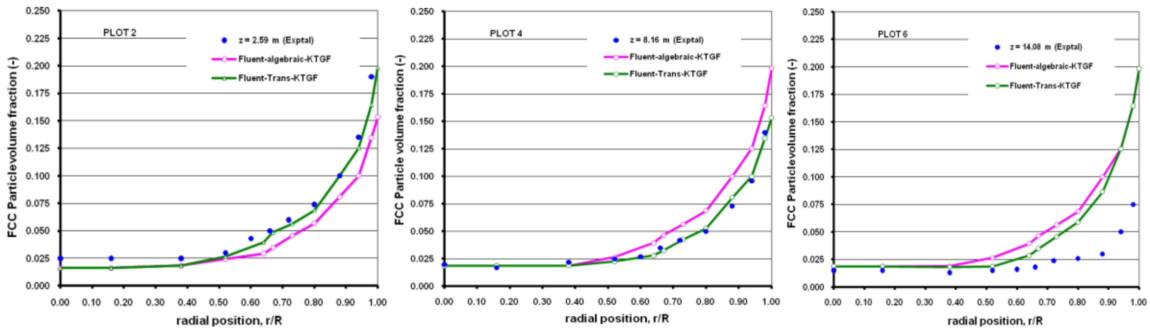

Fig. 3: Predicted and measured (Huang et. al., 2007) solid concentration distributions

Fig. 3 shows the comparison between the measured and predicted (using the algebraic-KTGF and transport-KTGF models) volume fraction of solids at the corresponding locations. Again, the measured trends are generally well reproduced in the predictions. As can be seen in the figure, the solid concentration is low in the central region and high near the wall of the riser at all measurement locations conforming core-annulus flow behaviour observed in previous studies. Such a significant deviation of catalyst distribution from a plug-flow profile in a FCC riser reactor will adversely affect the cracking reaction process. As for the quality of the predictions, both the models for the granular temperature accurately predict the solid concentrations in the central region of the riser. In the region near the wall the transport-

KTGF model generate better predictions compared with the algebraic-KTGF model at z = 2.59 and 8.16 m. However, both models significantly overpredict the solid concentration near the exit at z = 14.08 m

5. Conclusions

An Eulerian-Eulerian multiphase CFD modelling methodology imbedded in FLUENT was used to simulate isothermal gas-solid flows in the riser section of a pilot-scale CFB reactor (Huang et. al., 2007). The predicted solid velocity and concentration profiles obtained using the two approaches to calculate the granular temperature, namely the differential transport equation model and the algebraic equation model, are compared with measurements at different locations along the height of the riser. The overall agreement between the predictions and the reported experimental data is reasonably good. However, there are differences in the predicted and measured solid velocity models, whereas the algebraic-KTGF model is able to capture this feature of the flow close to exit. The profiles in the central region of the riser and in the solid concentration profiles near the wall, the down flow of particles along the wall were correctly predicted by the transport-KTGF. Overall, the former model for the granular temperature performs better than the latter model.

Notations

A	*Area, (m^2)*
c	*Coefficient of Restitution*
C	*Courant number*
D	*Diameter, (m)*
d_p	*Particle diameter, (m)*
$\bar{\varepsilon}_g$	*Averaged voidage (volume fraction) in the reactor*
$\bar{\varepsilon}_s$	*Local solids holdup (volume fraction) in the FCC reactor*
g	*Acceleration due to gravity, (9.81 m/s^2)*
h	*mesh spacing*
L	*Length of the riser pipe (m)*
P	*pressure (N/m^2)*
t	*time, (s)*
Δt	*Time step (s)*
T	*Temperature, (K)*
$\vec{T}_s$	*Stress tensors in solid medium*
u_i	*Mean velocity (m/s)*
ρ_g	*Density of gas (Kg/m^3)*
ρ_s	*Density of solids catalyst (Kg/m^3)*
μ	*Gas viscosity, (Pa.s)*
$\sigma_k, \sigma_k, \sigma_\varepsilon$	Constant
y_i	Weight fraction of component i
z	Axial position, (m)

Recommendations

Efforts toward carrying out simulation using other granular constants like SST, algebraic, Gidaspow correlations, Lagrangian etc. to study the flowing phenomena would be instituted.

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