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CFD investigation of coal gasification: Effect of particle size

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Abstract - *The present work studies the effect of different particle size diameter on fluidised bed hydrodynamics with different fluidization velocity. This study of operational parameters of hydrodynamics can form a basis for integration of kinectic into CFD model. The contours of solid volume fraction at different velocity with two particle size are shown. A range of velocity between minimum fluidization velocity and terminal velocity are studied to see the repeatability and observed that at high velocity there is no significant effect of particle size other than height of bed expansion for larger paricle diameter.*

Key Words: Coal gasification, fluidised bed, coal particle size, CFD

1. INTRODUCTION

Energy crisis is the major threat the entire world is facing today, depletion of the fossil fuel being the major reason. Among the variety of fossil fuel present coal is said to be the clean energy of the future. Fluidised bed coal gasification is one of the potential sources for the production of clean and eco friendly fuel. In coal gasification instead of burning fossil fuel it is chemically transformed to syngas which is a combination of hydrogen, carbon monoxide and very less carbon di oxide. The syngas produced has variety of applications ranging from use in fertilizers to production of electricity. The fluidized bed technology allows efficient gas–solid contact; therefore it is widely used in covering particles, drying, granulation, blending, combustion and gasification processes [1].In this type of flow understanding the process and insight of the gasifier is a complex phenomenon due to particle-particle interaction and chemical reactions. So there is need of mathematical models that develop better understanding of the processes. Mathematical modeling of gas flow in fluidised bed began in 60s with Kunni and Levenspiel [2] being the major pioneer to analyze bubble motion, system instability and mass transfer.

Computational fluid dynamics is a branch of fluid mechanics which is widely used to predict the physical and chemical processed inside a fluidised bed technology.CFD uses mathematical models based on mass, momentum and energy equations along with empirical and theoretical correlations which give better understanding, requires supercomputers and is less time consuming. In coal gasification efficiency is mainly concerned with chemical reactions and energy transfer, therefore a hydrodynamic study is important to improve the process as it gives insight of distribution of phases and species involved. Xi-Zhong Chen [3] studied the effect of distributor shape, solid particle size, and operational gas velocity and feed manner on the flow behavior in the polymerisation reactor. Caterina Goncalves Philippsen [1] also presented a review on fluidised bed technology giving importance of hydrodynamics. Process parameters play an important role in improving efficiency and the effect of one such parameter i.e. coal particle size is being studied in the present work. An Eulerian Eulerian CFD model with kinectic theory of granular flow is being used in this study

2. EQUIPMENT AND MATERIAL

2.1 Fluidised Bed

The simulated case is a bubbling fluidised bed coal gasifier designed and built for studying the gasification of Columbian coal [3]. The schematic view of the gasifier is shown in Fig-1 the reactor has an internal diameter of 0.22 m and a height of 2m. A uniform velocity is assumed at the air and the steam inlet. The geometry for the model is created in ANSYS FLUENTdiscretized into 9981 quadrilateral cells as shown. The air and the steam flow into from the bottom of the gasifier. The outlet pressure is fixed at atmosphere. The bed is initially assumed to be filled with coal particles up to 1m with a solid volume fraction of 0.48[4]

2.2 Materials

Two coal particles size is used in the present study in the size range of 0.00062m and 0.01m. The density of the particles (coal) was taken to be 1250 kg/m3. The value of particle sphericity was assumed to be equal to one

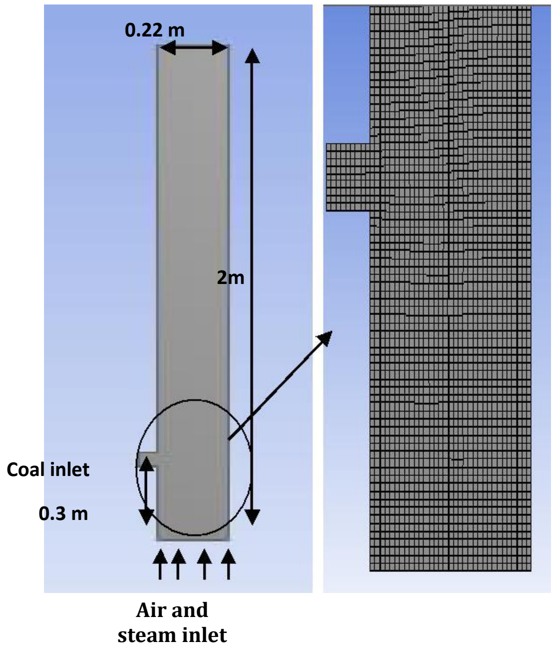

Fig -1: Geometry and Mesh

2.3 CFD model

This section describes the modeling equations employed in the present Euler–Euler two-fluid CFD model.

The volume fraction of the phases sum to one, i.e.

$$\varepsilon_g + \varepsilon_s = 1$$

The continuity equation for gas and solid phases are described below

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla(\varepsilon_g \rho_g u_g) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla(\varepsilon_s \rho_s u_s) = 0 \quad (2)$$

The conservation of momentum for the gas and solid phases are described below

$$\frac{\partial}{\partial t}(\rho_g \varepsilon_g u_g) + \nabla(\rho_g \varepsilon_g u_g u_g) = -\varepsilon_g \nabla p + \nabla \tau_g + \rho_g \varepsilon_g g + F_{i,g} \quad (3)$$

$$\frac{\partial}{\partial t}(\rho_s \varepsilon_s u_s) + \nabla(\rho_s \varepsilon_s u_s u_s) = -\varepsilon_s \nabla p + \nabla \tau_s + \rho_s \varepsilon_s g + F_{i,s} \quad (4)$$

Where the terms $F_{i,g}$ and $F_{i,s}$ of the above momentum equations represent the interphase momentum exchange for gas phase and solid phase respectively

Thus the gas solid interface drag force is expressed as

$$F_{D,gs} = K_{gs}(u_g - u_s) \quad (5)$$

Here τ is Reynolds stress tensor, g is gravitational force, and ($-\varepsilon_s \nabla p + K_{gs}(u_g - u_s)$) is an interaction force (drag and buoyancy forces) depicting the momentum transfer between gas and solid phases.Gidaspow [5] drag model, has been used in the present work.

Gidaspow Drag Model

When $\varepsilon_g > 0.8$

$$K_{gs} = \frac{3}{4} C_D \frac{\varepsilon_g \varepsilon_s \rho_g |u_g - u_s|}{d_p} \varepsilon_g^{-2.65} \quad (6)$$

When $\varepsilon_g \leq 0.8$

$$K_{gs} = 150 \frac{\varepsilon_s (1-\varepsilon_g) \mu_g}{\varepsilon_g d_p^2} + 1.75 \frac{\varepsilon_s \rho_g |u_g - u_s|}{d_p}, \quad (7)$$

Where

$$C_D = \frac{24}{\varepsilon_g Re_p}[1 + 0.15(\varepsilon_g Re_p)]^{0.687} \quad (8)$$

The particle Reynolds number is defined as follows:

$$R_{ep} = \frac{\rho_s d_p |u_g - u_s|}{\mu_g} \quad (9)$$

Using this equation momentum exchange can be calculated at any point in bed.

2.4 Kinectic theory of granular flow

The kinetic theory of granular flow (KTGF) is basically an extension of the classical kinetic gas theory and it has been utilised to interpret the random granular motion of particle collision in fluidized bed. In the KTGF, the rheology of fluidized particles is dominated by the fluctuating motion and local concentration of solids. The KTGF expresses the particle collision using two parameters, the solid phase stresses and viscosities, which are represented in turn as a function of granular flow temperature. This study adopts the equation as described in this equation

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \Theta) + \nabla.(\varepsilon_s \rho_s \Theta) u_s\right] = (-\nabla p_s I + \tau_s):\nabla u_s + \nabla.(k_s \nabla \Theta) - \gamma_s + \Phi_s + D_{gs} \quad (10)$$

In Equation (10), the two terms on the left hand side account for the accumulation and convection of kinetic fluctuation energy separately. The first term on the right hand side depicts the production of kinetic fluctuation energy due to irreversible deformation of the solid phase velocity field, while the conductive transport of kinetic fluctuation energy is described by the second term. The third term is used to model the dissipation of the fluctuation energy resulted from the inelastic inter-particle interactions. The fourth term indicates the exchange of the fluctuation energy owing to the Interphase momentum transport. The interaction between the fluctuating superficial gas velocity and the fluctuating particle velocity represented by the last term is usually neglected due to the complete suppression of gas phase turbulence in bubbling gas-solid fluidized beds

2.5 Strain Tensors

Constitutive equations are required to close the governing relation. The equations are as follows -

The terms τ_g and τ_s are the stress-strain tensors of gas and solid phase in the below equations

$$\tau_g = \varepsilon_g \mu_g (\nabla u_g + \nabla u_g^T) + \varepsilon_g (\lambda_g - \frac{2}{3}\mu_g) \nabla u_g I \quad (11)$$

$$\tau_s = \varepsilon_s \mu_s (\nabla u_s + \nabla u_s^T) + \varepsilon_s (\lambda_s - \frac{2}{3}\mu_s) \nabla u_s I \quad (12)$$

2.6 Solid shear stresses

These contain shear and bulk viscosities arising from particle momentum exchange due to translation and collision

$$\mu_s = \mu_{s,col} + \mu_{s,kin} + \mu_{s,fr.} \quad (13)$$

Where $\mu_{s,col}$ is the collision viscosity [5] and is described as

$$a)\mu_{s,col} = \frac{4}{5}\varepsilon_s \rho_s d_s g_{o,ss}(1+e_{ss})(\frac{\Theta_s}{\pi}) \quad (14)$$

Where $\mu_{s,kin}$ is the kinetic viscosity [6]and is described as

$$b)\ \mu_{s,kin} = \frac{\varepsilon_s \rho_s d_s \sqrt{\Theta_s \pi}}{6(3-e_{ss})}[1 + \frac{2}{5}(1+e_{ss})(3e_{ss}-1)\varepsilon_s \quad (15)$$

c). $\mu_{s,fr.}$ is the frictional viscosity [7] and is written as

$$\mu_{s,fr.} = \frac{p_s \sin\emptyset}{2\sqrt{I_{2D}}} \quad (16)$$

d)Bulk viscosity

The bulk viscosity account for the resistance of the granular particle to compression and expansion given by [8]

$$\lambda_s = \frac{4}{3}\varepsilon_s \rho_s d_s g_{o,ss}(1+e_{ss})(\frac{g\Theta_s}{\pi})^{\frac{1}{2}} \quad (17)$$

2.7 Radial Distribution Function

The radial distribution function, go is a correction factor that modifies the probability of collision of solid granular phase [9] and is expressed as follows

For one solid phase

$$g_o = [1 - (\frac{\varepsilon_s}{\varepsilon_{s,max}})^{\frac{1}{3}}]^{-1} \quad (18)$$

2.8 Solid Pressure

For granular flow in the compressible regime (i.e. where the solid volume fraction is less than its maximum allowable value), a solid pressure is calculated independently. The solid pressure [8] is composed of a kinetic term and a secondary term due to particle collisions and is expressed as follow

$$P_s = \varepsilon_s \rho_s \Theta_s + 2\rho_s(1+e_{ss})\varepsilon_s^2 g_{o,ss}\Theta_s \quad (19)$$

2.9 Granular Temperature

The granular temperature for solids phase is proportional to the kinetic energy of particles for its random motion. The transport equation derived from kinetic theory takes the following form

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \Theta_s) + \nabla.(\varepsilon_s \rho_s \vec{v}\Theta_s\right] = (-P_s I + \tau_s) : \nabla \cdot \vec{V_s} + \nabla \cdot (K_{\Theta_s}\nabla \cdot \Theta_s) - Y_{\Theta_s} + \Phi_{gs} \quad (20)$$

Where K_{Θ_s} the diffusion coefficient for granular energy is defined as [6]

$$K_{\Theta_s} = \frac{15\varepsilon_s \rho_s d_s \sqrt{\Theta_s \pi}}{4(41-33\eta)}\left[1 + \frac{12}{5}\eta^2(4\eta-3)\varepsilon_s g_{o,ss} + \frac{16}{15\pi}(41 - 33\eta)\eta\varepsilon_s g_{o,ss}\right] \quad [21]$$

Where

$$\eta = \frac{1}{2}(1+e_{ss}) \quad [22]$$

The collision dissipation of energy is expressed as follows [8]

$$Y_{\Theta_s} = \frac{12(1+e_{ss}^2)g_{0,ss}}{d_s\sqrt{\pi}} \cdot \rho_s \varepsilon_s^2 \Theta_s^{\frac{3}{2}} \quad [23]$$

The transfer of the kinectic energy is written as

$$\emptyset_{gs} = -3K_{gs} \quad [24]$$

2.8 CFD modeling strategy

A commercial grid-generation tool, Ansys ICEMCFX (of Fluent Inc., USA) was used to create the 2D geometry with 9981 quadrilateral cells. Standard k–ε model was used. “SIMPLE” scheme for pressure–velocity coupling was used. The wall was modeled using no-slip boundary conditions for both phases. The bottom of the bed was defined as velocity inlet to specify a uniform gas inlet velocity. Pressure boundary conditions were employed at the outlet .The bed was considered 2m deep and initial solids volume fraction was defined as 0.48 with a maximum packing of 0.63[4] Constitutive equations for the particulate phase properties such as solid pressure, solid bulk viscosity and the solid shear viscosity were derived from the KTGF. Models of Lun et al. [8] were used for solid pressure and granular bulk viscosity. Model of Syamlal et al.[6]was used for solid shear viscosity. Similarly, Radial distribution function of Sinclair and Jackson [10] was used, as it approaches the correct value of one as the solids volume fraction tends to zero. Model of Schaffer [7] was used for frictional stress. The two-dimensional steady-state solvers, used in the computational model, along with their characteristics are shown in Second-order upwind method has been used for discretization and first order implicit for transient formulation.

3.0 RESULTS AND DISCUSSION

CFD simulations of fluidized bed were done with two coal particle size 0.001m (dp_b) and 0.00062 m (dp_s) in order to see the effect of it on solids and gas distribution inside the gasifier. Particle size 0.00062 m is the coal particle size which has been reported in several literatures [4]

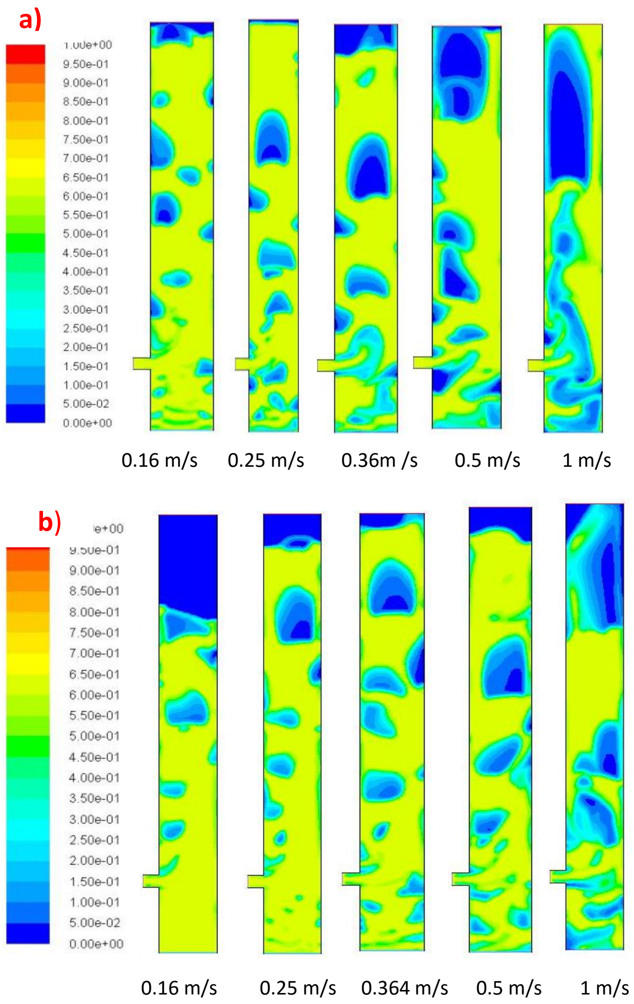

Fig 2: Simulation results for different coal particle size for Gidaspow drag model (a) 0.00062m (dps) (b) 0.001m (dpb) for fluidization velocity range.

an obvious gradient of solid holdup can be observed with the fluidization proceeding. In addition, it also shows that with the increase of the solid particle diameter, the total amount of bubbles becomes less and the size of bubbles becomes larger at same velocity, therefore, the bed expansion ratio becomes smaller. As a whole, it proves that it spends less time to arrive at the fluidization state for the smaller particles in the bed From Fig 2(a) it is clearly seen particle tend to flow easily due to smaller particle size and has better solid distribution and Figure 2(b) outlines that the larger particle has more residence time inside the gasifier and as we go on a higher side with inlet velocity the flow changes to slug. In practice, with the decrease of the particle size, the drag force acting on the particles increase, it leads to the easy generation of bubbles in the bed and then the flow of smaller particles toward the top is easy, which leads to the decrease of fluidization time and the increase of bed height Fig 3shows velocity vectors overlapped with axial velocity of air for both particle size giving a more clear picture of the scenario inside the gasifier for 0.16 m/s air velocity.

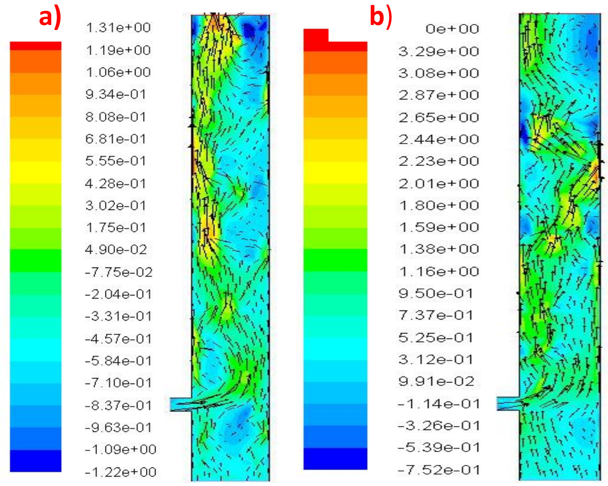

Fig.3 velocity vectors of axial air vlocity for 0.16m/s.

4.0 CONCLUSION

A two-dimensional Eulerian granular is developed to understand the hydrodynamics of a gas–solid fluidized bed satisfactorily Accordingly, based on the above simulated results, one can obtain that it is necessary to consider the size distribution in the fluidized bed .It can also be concluded that high velocity the particle size do not have much effect on the distribution other than expansion in bed height.

NOMENCLATURE

ρ Density of fluid kg/m^3
u Velocity m/s
p Pressure ,Pa
g Acceleration due to gravity m/s^2
F Force
d Diameter, m
ε Volume fraction
μ Viscosity, Pa S
K_{gs} Fluid–solid and solid–solid exchange coefficient
I_{2D} Second invariant of the deviatoric stress tensor
Re Reynolds number
e_{ss} Coefficient of restitution
$g_{o,ss}$ Radial distribution coefficient
C_D Drag coefficient
Θ_s Solid phase granular temperature, m^2/s^2
μ_s Solid shear viscosity, Pa S
$\mu_{s,col}$ Collision viscosity, Pa S
$\mu_{s,kin}$ Kinetic viscosity, Pa S

$\mu_{s,fr.}$ Frictional viscosity, Pa S
λs Bulk viscosity, Pa S
ø Angle of internal friction, deg
Θ_s Diffusion coefficient
$Y_{\Theta s}$ Collisional dissipation of energy, kg/s^3m
Φ_{gs} Energy exchange of solid phase, kg/s^3m
η Rate exponent
$\vec{v}_s$ Phase-weighted velocity
∇ Gradient
KTGF Kinetic theory of granular flows

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