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A Comparison study of Drag correlations for a Dispersed Multiphase flow in a Fluidized bed

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ABSTRACT

The present study compares different drag models like Syamlal O'Brien, Gidaspow Ergun WenYu (GEW), and Gidaspow Schiller Naumann (GSN) in modeling fluidized-bed. With the help of the open-source CFD software OpenFOAM, timeaveraged particle velocity components were calculated at five lateral locations of the fluidized bed for inlet gas velocities of 2.19m/s and 3.28 m/s. Later these values were used for validation against experimental data generated by the National Energy Technology Laboratory (NETL). The Eulerian-Eulerian approach is adopted for the present 2D computational study with closures from the Kinetic Theory of Granular Flow (KTGF). The study identified the Syamlal O'Brien drag closure to be reliable in modeling the interfacial momentum transfer phenomenon between the phases. Thus, it accurately predicted the particle velocity distribution at different lateral locations of the fluidized bed. It was found that the velocity distribution is sensitive to the Specularity coefficient. It was also observed that the accuracy of the predictions made by GEW drag closure reduced significantly as the inlet gas velocity increased from 2.19 m/s to 3.28 m/s. Despite being least accurate in predicting particle velocities, GSN drag correlation provided valuable insights about its applicability for fixed bed applications.

Keywords: OpenFOAM, CFD, Fluidized bed, Multiphase

1. INTRODUCTION

Research on sustainable technologies has burgeoned in the 21st century to tackle environmental degradation occurring at every stage of any industrial process. Fluidized bed technology is one such potential deployment into the category of sustainable technologies, widely used in the pharmaceutical, petroleum, chemical, and many other industries and has been at a focal point of research.

With the primary function of making a solid-fluid mixture behave as a fluid, this technology can reduce the harmful gas emissions from industries without compromising the efficiency of results like combustion, catalytic cracking, and other chemical processes. For further advancement and proliferation of this technology, research into Computational models capable of accurately predicting the flow structure inside the Fluidized Bed is of vital interest. This study analyses the reliability of various drag correlations in modeling the interfacial momentum

transfer between the current phases in a Fluidized-bed phenomenon.

2. LITERATURE REVIEW AND OBJECTIVE

Systematic validation and uncertainty quantification of CFD models for Multiphase flows have been the fundamental objective of the small-scale challenge put forth by NETL in 2013 [1]. As a part of this challenge, the experimental data obtained by measuring the pressure drop and the particle velocities at various locations of a rectangular bed were made available to the research community for validation purposes. A low frequency (1 Hz) and a high frequency (1kHz) pressure transducers extract the pressure drop data. Parallelly, Highspeed Particle Image Velocimetry is used to obtain the particle velocity at the desired locations [2]. Considering that the interfacial momentum transfer phenomena between the phases in a Multiphase flow simulation is essential in obtaining accurate results, neglecting this can introduce relative errors as large as 30% into the typically obtained results [3]. Hence, it is essential to investigate the factors contributing to the momentum transfer between phases in a Multiphase Flow. A detailed formulation of these factors is provided in Enwald et al. (1996) [4]. In the case of a solid-fluid dispersed flow, the generalized drag force term in the Reynolds averaged momentum equation predominantly contributes to the interfacial momentum transfer, unlike separated flows, where factors like interfacial pressure difference and combined interfacial shear play a significant role. Thus, evaluating the drag correlations available in the literature to model the Fluidized bed phenomenon has been a crucial aspect of the present research. Although multiple pieces of literature discussed various drag closures that can be implemented in OpenFOAM, studies [4] and [5] provided a comprehensive overview of the physics behind each drag closure and its operational phase fraction ranges. Present research involves comparing the CFD results obtained for three drag correlations against the experimental data to quantify the uncertainties of each drag closure. Considering the possibility of a drastic variation in phase fraction values at the interface of both the phases, the drag closures were chosen such that their operating ranges can accommodate both low and high-phase fraction regimes. The original Syamlal O'Brien drag closure in OpenFOAM was tuned based on the value of minimum fluidization velocity obtained from the experiment [1]. This

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step ensures that the computationally modeled drag force accurately mimics the experimental drag force.

Similarly, the Specularity coefficient value, which indicates the wall roughness, is found iteratively for the inlet gas velocity of 2.19 m/s and is adapted from Lungu et al. (2016) [6] for 3.28 m/s case. The present study also focuses on the performance of the GSN drag model in modeling interfacial momentum transfer due to the scarcity in previous research conducted on it. Particles belonging to Geldart group D are considered the particulate phase in this study, which is fluidized by gas at ambient conditions. Eulerian – Eulerian approach is chosen for this study due to its relative computational inexpensiveness compared to other approaches. The fluidized bed being a dispersed system, multi-fluid modeling is used where both phases are treated as interpenetrating continua.

3. MATERIALS AND METHODS

The geometry, dimensions, and boundaries of the 2D fluidizedbed used for this study are shown in fig. 1. The geometric data used from [1], fig. 1 shows the parts of a Fluidized bed. The lateral locations where the particle velocities were measured compared with the experimental data produced by the National Energy Technology Laboratory (NETL) are also shown. Crucial parameters considered in the study, like the superficial gas velocity at the inlet, the initial phase fraction of the dispersed phase (particles), are mentioned in table 1. An initial phase fraction of 0.58 means that 58% of the static bed is occupied with the dispersed phase (particles) and the remaining 42% with the continuous phase (liquid). An entire domain is 2806 quadrilateral elements. discretized into twoPhaseEulerFoam solver from OpenFOAM software is used for running the simulations.

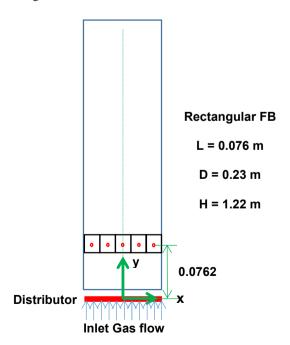


Figure 1: Schematic diagram of the set-up with dimensions [1]

Table 1: Parameters used in this study

Parameters	Value
Superficial Gas Velocities	2.19 m/s & 3.28 m/s
Minimum Fluidization Velocity	1.03 m/s
Static Bed Height	0.173 m
Initial phase fraction (α_i)	0.58
Gas density (ρ_g)	1.204 kg/m ³
Mean Particle diameter (d_p)	3256 μm
Particle density (ρ_p)	1131 kg/m ³
Specularity Coefficient (Φ)	0.125 & 0.05

3.1 Governing Equations

Multiphase flows can be numerically modeled using different approaches such as:

- a) Direct Numerical Simulation (DNS)
- b) Eulerian Langrangian approach
- c) Eulerian Eulerian approach

Eulerian – Eulerian approach is further classified based on the phase morphology into separated and dispersed systems [4]. For a dispersed system like the fluidized bed, multi-fluid modeling is used, where both phases are considered as interacting and interpenetrating continua, therefore, share the same continuity and momentum equations for each phase individually as shown in Eqs. (1), (2), and (4). For the solid phase, the Kinetic Theory of Granular Flow (KTGF) [7] was adopted for closure which considers the conservation of Solid Fluctuation Energy. KTFG approach extends the classical kinetic theory of gases to dense granular flows, where the fluctuation energy is described using the granular temperature (θ).

Three important assumptions made in this study for simplification are:

- i. Both solid and liquid phases are isothermal.
- There is no interphase mass transfer between both phases.
- iii. Solid particles are of pure spherical configuration with a mean diameter and density as mentioned in table 1.
 - Conservation of Mass (k = f for fluid phase, s for solid phase)

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \frac{\partial}{\partial x}(\alpha_k \rho_k \boldsymbol{u}_k) = 0 \tag{1}$$

• Conservation of Momentum (fluid phase)

$$\frac{\partial}{\partial t} (\alpha_f \rho_f \mathbf{u}_f) + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f \mathbf{u}_f) =$$

$$\alpha_f \nabla \cdot \mathbf{\tau}_f + \alpha_f \rho_f \mathbf{g} - \alpha_f \nabla p - \mathbf{F}_{df} - \mathbf{F}_{vm}$$

$$- \mathbf{F}_{lf}$$

$$(2)$$

 ${\it F}_{df}$, ${\it F}_{lf}$, ${\it F}_{vm}$ is the drag force, lift force, and virtual mass force respectively in Eqs. (2) and (4). Since drag force contributes predominantly to the momentum exchange between the fluid and particulate phases, it is given more importance in this study.

$$\bar{\boldsymbol{\tau}}_f = \mu_f \left[\nabla \boldsymbol{u}_f + \left(\nabla \boldsymbol{u}_f \right)^T \right] - \frac{2}{3} \mu_f (\nabla \cdot \boldsymbol{u}_f) \bar{\boldsymbol{I}}$$
 (3)

The stress tensor of the liquid phase from Eq. (2) is expanded in Eq. (3) where μ_f is the combined turbulent and laminar viscosity for the fluid phase. Further, $k-\varepsilon$ turbulence model is used in the study for the fluid phase.

• Conservation of Momentum (solid phase)

$$\frac{\partial}{\partial t} (\alpha_s \rho_s \mathbf{u}_s) + \nabla \cdot (\alpha_s \rho_s \mathbf{u}_s \mathbf{u}_s) =$$

$$-\alpha_s \nabla p - \nabla p_s + \nabla \cdot \mathbf{\tau}_s + \alpha_s \rho_s \mathbf{g} + \mathbf{F}_{df} + F_{pm} + F_{lf}$$

$$(4)$$

The solid phase stress tensor is expressed in terms of bulk solid viscosity ξ_s , and shear solid viscosity μ_s in Eq. (5).

Conservation of Solid Fluctuation Energy

$$\frac{3}{2} \left[\frac{\partial}{\partial t} (\alpha_s \rho_s \theta) + \nabla \cdot (\alpha_s \rho_s \theta) \mathbf{u}_s \right] =$$

$$\left(-\nabla p_s \mathbf{I} + \mathbf{\tau}_s \right) : \nabla \mathbf{u}_s + \nabla \cdot (k_s \nabla \theta) - \gamma_s - 3\beta\theta + D_{l_s}$$
(5)

$$\theta = \frac{1}{2} \left(\langle v_x^2 \rangle + \langle v_y^2 \rangle + \langle v_z^2 \rangle \right) \tag{6}$$

The random oscillations of particles in the gaseous medium generate wall-shear causing the random kinetic energy per unit mass, Eq. (6), in simple terms granular temperature, to rise in the near wall region. Analogous to the thermal diffusion in gases, this granular temperature drives the particle movement. Granular temperature is determined by the complex interaction between the viscous and inertial forces exerted on a particle by its local gas and particle environment. It is not a thermodynamic quantity but a steady state constant [10].

3.2 Drag Correlations

Numerous drag correlations are available [4] and [5] that can model the mechanism of interfacial momentum transfer majorly caused due to drag force between the phases. A thorough literature study was performed to identify such drag correlations that could model the flow for all phase fraction regimes, individually or as a combination of two. A drag

correlation must predict the flow at all phase fraction regimes accurately. Because the probability of a cell in a domain, especially at the interface, to overshoot the maximum phase fraction of the domain can never be neglected and must be taken into account. Also, the correlations adopted must be applicable for a multi-particle system to consider the effect of other particles' presence. After considering such fundamental factors, three drag correlations were chosen to model the two-phase flow inside a fluidized bed.

a) Gidaspow Ergun WenYu:

It is a combination of the Ergun drag correlation applicable for dense systems and the Wen Yu correlation that can model a dilute flow where viscous forces are dominant, accurately.

This correlation uses the Ergun equation, Eq. (7), for $\alpha_p \ge 0.2$ and the Wen–Yu equation, Eq. (8) for $\alpha_p \le 0.2$, where K is defined as the drag function for each correlation. Drag force in the Ergun correlation is calculated based on pressure drop per unit length, Eq. (9), unlike the Wen Yu correlation that considers the drag coefficient on a single particle, Eq. (10).

$$K = 150 \frac{\mu_g}{d_p} \frac{\alpha_p^2}{(1 - \alpha_p)^2} + 1.75 \frac{\rho_g U_r}{d_p} \frac{\alpha_p^2}{(1 - \alpha_p)^2}$$
(7)

$$K = \frac{3}{4d_p} C_{DS} \alpha_p (1 - \alpha_p) \rho_g U_r (1 - \alpha_p)^{-2.65}$$
(8)

$$\frac{\Delta p}{L} = 150 \frac{\mu_g U_r}{d_p g} \frac{\alpha_p^2}{(1 - \alpha_p)^3} + 1.75 \frac{\rho_g U_r^2}{d_p g} \frac{\alpha_p}{(1 - \alpha_p)^3}$$
(9)

$$C_{DS} = \begin{cases} \frac{24}{\text{Re}} (1 + 0.15\text{Re}^{0.687}), \text{Re} \le 1000\\ 0.44, & \text{Re} > 1000 \end{cases}$$
 (10)

b) Gidaspow Schiller Naumann:

This drag correlation is capable of calculating the drag in a multi-particle system, unlike the Schiller-Naumann correlation, which is restricted to a single particle system only. The drag function for this correlation is defined in Eq. (11). Schiller-Naumann drag coefficient, Eq. (12), is used by replacing the Re with $(1-\alpha_p)$ Re, as shown in Eq. (12) below.

$$K = \frac{3}{4d_p} C_{DS} \alpha_p (1 - \alpha_p) \rho_l U_r (1 - \alpha_p)^{-2.65}$$
 (11)

$$C_{Ds} = \begin{cases} \frac{24}{(1-\alpha_p)\text{Re}} \left(1 + 0.15 \left((1-\alpha_p)\text{Re} \right)^{0.687} \right), \text{Re} \le 1000 \\ 0.44, & \text{Re} > 1000 \end{cases}$$
(12)

c) Syamlal O'Brien

This drag correlation is based on the primary assumption that the Archimedes number remains the same for terminal settling velocity for both single and multi-particle systems [4]. 480 M. S. Karthikeya et al.

It uses the expression, Eq. (13), to relate the settling velocity and the void fraction, where Re_s is the Reynolds number for a single particle and V_r , the ratio of terminal settling velocity in a multi-particle system to that of a single particle system.

$$\frac{V_r - A}{B - V_r} = 0.06 \text{Re}_s \tag{13}$$

$$V_r = 0.5(A - 0.06\text{Re} + \sqrt{(0.06\text{Re})^2 + 0.12\text{Re}(2B - A) + A^2})$$
(14)

$$A = (1 - \alpha_p)^{4.14} \tag{15}$$

$$B = \begin{cases} \mathbf{C}_1 (1 - \alpha_p)^{1.28}, \alpha_p \ge 0.15\\ (1 - \alpha_p)^{\mathbf{C}_2}, \alpha_p < 0.15 \end{cases}$$
 (16)

Eq. (14), (15), and (16) are obtained by solving Eq. (13) after replacing Re_s with Re/ V_r . Drag coefficient proposed by Dallavalle, Eq. (17), is used here to obtain the final drag function in Eq. (18), where \mathbf{U}_r is the relative interstitial velocity, $\mathbf{U}_q - \mathbf{U}_p$.

$$C_{DS} = \left(0.63 + \frac{4.8}{\sqrt{\text{Re}_s}}\right)^2 \tag{17}$$

$$K = \frac{3\alpha_p (1 - \alpha_p)\rho_g}{4V_r^2 d_p} \left(0.63 + 4.8 \sqrt{\frac{V_r}{Re}} \right)^2 |\mathbf{U}_r|$$
 (18)

The coefficients \mathbf{C}_1 and \mathbf{C}_2 in Eq. (16) are unique to a problem statement and depend on the parameters like Archimedes number, minimum fluidization velocity, and other physics properties of the individual phases. In our case, $\mathbf{C}_1 = 0.88$ and $\mathbf{C}_2 = 2.04$. Existing Syamlal O'Brien drag closure was tuned with the new coefficients by creating a new drag model with the name newSyamlalObrien.

3.3 Boundary Conditions

In a granular flow case, the particles neither stick to the wall nor slip freely on it. Thus, a wall boundary condition introduced by Johnson and Jackson [8] is implemented to the field variables of particles in the simulation. The boundary conditions are summarized in Tables 2 and 3.

Specularity coefficient (ϕ_s) is defined as the fraction of particle tangential momentum transferred to the wall through collisions. It indicates the wall's roughness, which is affected by the superficial gas velocity and the particle size.

 $(\phi_s) = 1 \Rightarrow$ Zero tangential velocity, maximum hindrance

 $(\phi_s) = 0 \Rightarrow$ Free slip along the wall, minimum hindrance

In this study, the specularity coefficient was considered as 0.05 for 3.28 m/s gas velocity [6] and 0.125 for 2.19 m/s gas velocity, which yielded more accurate results.

Table 2: Velocity boundary conditions considered in this study

Boundary	$u_f(m/s)$	u_s (m/s)	
Inlet	2.19 and 3.28	Fixed Value	
Outlet	Pressure Inlet Outlet	Fixed Value	
Walls	noSlip	JohnsonJacksonParticleSlip	

Table 3: Pressure boundary conditions considered in this study

Boundary	p_rgh
Inlet	fixedFluxPressure
Outlet	prghPressure
Walls	fixedFluxPressure

4. RESULTS AND DISCUSSION

Post-processing of the results was carried out in ParaView, open-source visualization software, and MS Excel. Particle velocity at different lateral locations was obtained by plotting the entire transient simulation over time for each lateral location to extract the velocity data at every time step for an overall time interval of 50 seconds. The extracted data was time-averaged in the interval 15-50 seconds, after a bubbling fluidization flow regime is established, as shown in fig. 2, which is sustained till the end of the simulation. The results are then validated against the experimental data generated by National Energy Technology.

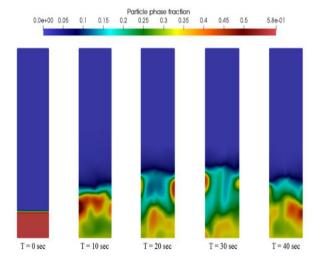


Figure 2: Contours of particle phase fraction (α_p) at five different timestamps

4.1 Case 1: Superficial Gas Velocity of 2.19 m/s

The time-averaged axial velocity data of the particles at different lateral locations of the fluidized bed is plotted in fig. 3 for various drag correlations. Experimental data generated by NETL for the same is included for comparison with the CFD results. The Syamlal O'Brien drag closure accurately predicts the axial particle velocity at all the lateral locations, followed by GEW. The trend of experimental results is followed by both Syamlal O'Brien and GEW but not GSN. The time-averaged axial velocity is the highest at the central location for all correlations except GSN.

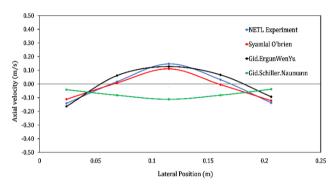


Figure 3: Axial velocity vs Lateral position plot for various drag correlations (U_a = 2.19 m/s).

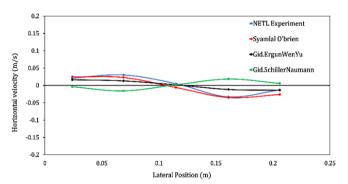


Figure 4: Horizontal velocity vs Lateral position plot for various drag correlations (U_g = 2.19 m/s).

The results obtained for horizontal velocity distribution, fig. 4, further strengthen our inference from the axial velocity results about the accuracy of the Syamlal O'Brien correlation because of its overlapping with the experimental results. However, the GEW closure is nearly as accurate as of the Syamlal O'Brien closure for the first case. Similar to the axial velocity distribution, the GSN correlation fails to follow the trend of the experimental plot and overpredicts at most of the lateral positions.

4.2 Case 2: Superficial Gas Velocity of 3.28 m/s

Interesting behavior was observed in the axial velocity distribution when the superficial gas velocity was increased from 2.19 m/s to 3.28 m/s, as shown in fig. 5. Syamlal O'Brien's closure again proved to be accurate, among others. The direction of velocity at the five lateral locations for both GEW and Syamlal O'Brien

closure happens to be the same as that of experimental observations, which is not the case with GSN. Though GEW closure has managed to follow the trend of experimental results successfully, it overpredicts the axial velocity at the center of the bed. The deviations observed in GSN closure have significantly increased from case 1 to case 2.

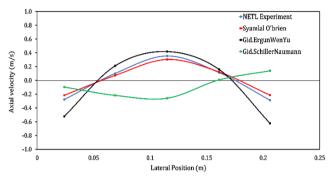


Figure 5: Axial velocity vs Lateral position plot for various drag correlations (U_a = 3.28 m/s).

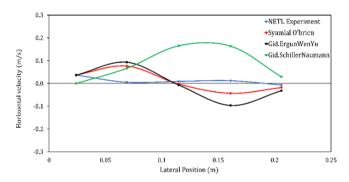


Figure 6: Horizontal velocity vs Lateral position plot for various drag correlations (U_g = 3.28 m/s).

The drag closures predict an opposite horizontal velocity trend from the experimental observations for case 2, as depicted in fig. 6. The experimentally obtained velocity profile also seems to reverse from case 1 due to the downward shift of the center of counter-rotating circulation cells [6].

The first significant inference from the results is the GSN closure that poorly predicted particle velocity distributions for gas velocity cases. Despite being developed to account for the particle-particle interactions by including the voidage function [4], it was the least accurate for both the velocity cases. It can be attributed to the fact that it was primarily developed for packed bed applications where the gas velocity is relatively low, restricting the flow regime to a fixed bed. The increase in relative error as the gas velocity is raised from 2.19 m/s to 3.28 m/s for the GSN closure reinforces our inference about the better performance of the model at low fluid velocities and dilute particle concentrations.

At first, a notable deviation was observed in the axial velocity plots at the central location for different drag closures

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compared with the experimental counterpart. Changing the specularity coefficient from 0.5 to 0.125 for cases 1 and 0.5 to 0.05 for case 2 provided the required bump in the axial velocity at the central location was observed for both GEW and Syamlal O'Brien drag correlations. Low values of specularity coefficient produce high particle velocities in the bed due to less loss of tangential momentum to the walls [6].

Finally, Syamlal O'Brien's drag correlation was most accurate in replicating the experimental results for both cases. This realistic behavior could be because of considering the clustering effect [9] of particles in the model, unlike other correlations. GEW drag correlation performed on par with the Syamlal O'Brien model at lower gas velocity. As the gas velocity increases to 3.28 m/s, the horizontal and axial velocities trend was replicated precisely; a higher relative error than the Syamlal model makes it unsuitable at higher velocities.

5. CONCLUSIONS

- This study was performed to identify the most reliable drag correlation for computational modeling of dispersed multiphase flows in a fluidized bed by validating against experimental data generated by NETL.
- Syamlal O'Brien drag correlation outperformed others for both the cases of superficial gas velocity, 2.19 m/s and 3.28 m/s, by accurately predicting the mean eulerian particle velocity distributions at various lateral locations of the fluidized bed.
- ➤ The Gidaspow Ergun WenYu correlation's predictions were on par with Syamlal O'Brien for the lower gas velocity of 2.19 m/s but are only satisfactory for the 3.28 m/s gas velocity case.
- The Gidaspow Schiller Naumann correlation was least accurate among the three in predicting the velocity profile but has given valuable insights about the better performance of the model for packed bed applications with low gas velocities.
- Specularity coefficient affects the particle velocity distribution mainly in providing the required maxima for the axial velocity at the central location of the bed for both the cases of inlet gas velocity.

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NOMENCLATURE

и	Velocity	[m/s]
F_{df}	Drag Force	$[kg/m^2-s^2]$
F_{lf}	Lift Force	$[kg/m^2-s^2]$
F_{vm}	Virtual Mass Force	$[kg/m^2-s^2]$
α	Phase fraction	
ho	Density	$[kg/m^3]$
C_D	Drag coefficient	

μ	Dynamic Viscosity	[kg/m-s]
θ	Granular Temperature	$[kg/m-s^2]$
K	Drag Function	
Φ	Specularity Coefficient	
Re	Reynolds Number	
V_r	Terminal Settling Velocity ratio	

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