3D Modeling and Simulation of a Two-Phase Mixing Jet Flow

Jaci C. S. C. Bastos¹, Udo Fritsching² and Milton Mori*¹

¹University of Campinas, Campinas, São Paulo, Brazil
²University of Bremen, Institut für Werkstofftechnik, Bremen, Germany

Abstract

Gas-solid mixing jet flows are an essential feature of typical chemical engineering processes. A proper analysis of the mixture flow optimizes process qualities and efficiencies. In this contribution, a numerical study of the solids dispersion in a two-phase jet flow is presented. The mathematical model treats the gas and the solid phases with an Eulerian approach. Radial profiles of the solid-phase mean velocity were computed on five axial levels, subdivided in five cases, in the mixing jet flow using a two-phase 3D computational fluid dynamics model. The computed solids velocities were compared with experimental data on a jet with an internal diameter of 12mm, at different inlet conditions of solid mass load for rates (3 to 7) and velocities (8 to 16m/s). The mean particle diameter used was 50µm and a density of 2500kg/m³. Three different drag models were applied to evaluate the solids dispersion. Wen and Yu [1], Gidaspow [2] and Massarani [3] correlations, the latter being a continuous one. The two-equation (k-ε) turbulence model was employed to describe the gas-phase, while the zero-equation (kinematic viscosities analogy) turbulence model describing the solid-phase in a jet flow. The mathematical model predicts a developed flow regions similar to that found experimentally.

Keywords: Gas-solid flows; Two-phase jet; Computational Fluid Dynamics (CFD)

Introduction

Two-phase jet flows are extensively used in a variety of engineering application sectors; more precisely, fluid flows containing solid particles, such as chemical, pharmaceutical, healthcare, biomedical, fuel, personal products, minerals industries and new materials. In all these applications, a fundamental understanding of how particles interact with fluid flows is necessary to allow the use of computational fluid dynamics (CFD) models in the optimization and performance improvement of existing equipment and processes; the identification and solution of operating problems; the evaluation of retrofit options and the design of new equipment, systems and plants including process scale-up [4].

The dynamic behavior of a gas-solid jet is defined by the complex interaction between its individual phases. Previous research indicates that in this type of flow the effects of entrainment and mixture of large quantities from the jet outer boundaries in a direction to the jet core are observed. The radial flow is defined as having a dense central solids region with high velocities for both phases and a low solids concentration near the boundaries. Furthermore, coherent structures are responsible for transport of significant mass, heat and momentum without being highly energetic, typical structures in shear flow are originated from some flow instabilities, mainly in the case of free shear layers (Decker et al. [5]).

Hardalupas et al. [6] investigated the velocity and particle flux characteristics of a turbulent particle-laden jet and found that the mass mixture ratio has a little effect on the particle concentration distribution. Hadinoto et al. [7] investigated a downward flow of glass bead particles in a vertical pipe for different Reynolds numbers and a constant particle loading with two particle sizes. For the 70µm particles, the authors observed that the presence of the particles damped the gas-phase turbulence intensity for smaller Reynolds numbers. Then, these results were compared with the single-phase flow for the same Reynolds numbers. As a consequence, it was observed an enhancement of the turbulence intensity at higher Reynolds numbers for the two-phase flow.

Multiphase flow equations have been developed and analyzed by many researchers, such as He and Rudolph [8], Theologos and Markatos [9] and Ali and Rohani [10]. However, Soo [11] is credited with the mathematical approach to this type of flow. Rietema and van der Akker [12] presented a detailed derivation of the momentum equations for disperse two-phase systems.

Currently, two of the most well-known methods for the mathematical modeling of the solid-phase in numerical simulations of gas-solid flows are the discrete particle simulation and the two-fluid approach. In both approaches gas-phase is described as a local average and the Navier-Stokes equation for the gas phase (Fairweather and Hurn [4]).

However, due to the large number of particles, the resultant number of equations would be too large to allow a direct solution, at least with the computer capacity currently available. Thus, the solid-phase is also treated as a continuous-phase, exposed to the analogous conservation equations for the fluid phase. The Eulerian-Eulerian approach proved

*Corresponding author: Milton Mori, University of Campinas, Department of Chemical Processes, School of Chemical Engineering, P.O. Box 6066, 13083-970 Campinas, SP, Brazil, Tel: +55 19 3521 3963; Fax: +55 19 3521 3910; E-mail: mori@eq.unicamp.br

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to be capable of predicting the gas-solid flow, as seen in the research conducted by Meier and Mori [13], Alves et al. [14] and Bastos et al. [15] and it was used in this study.

The specific interest in the present research is flow simulations containing a particle-laden jet. Researchers have shown that the gas-phase and the solid-phase axial and radial distribution can be computed using the two-equation and zero-equation respectively, based on multiphase models. In general, the performance of the current models critically depends on the accuracy of the drag force formulation, which has been extensively analyzed in the studies of Gidaspow [2], Meier and Mori [13], Alves and Mori [14], Meier and Mori [16], Alves et al. [17], Bastos et al. [15]. However, as the drag force is described by empirical models, it is of extreme importance to evaluate them in accordance with the equipment employed. Due to this criterion, it was chosen the gas-solid flow jets to study the influence of loading particles in the mixture on its fluid dynamics.

The turbulent regime in studying is mainly dependent on momentum conservation. This enables us to consider separately the influence of particles in the flow behavior through models for the turbulent viscosity. The effect of turbulence on particle motion in gas-solid suspension was analyzed by Yoshida and Masuda [18], Crowe [19], Alves et al. [17] and Zhang and Reese [20].

Mathematical Model

The equations used for the gas and solid phases, which are included in the description of the mathematical model, were developed with the Eulerian-Eulerian phenomenological approach. Differential equations in the balance are formulated for mass and momentum; treating the gas-phase and the kinematic viscosities analogy model on the solid-phase. The specific interest in the present research is flow simulations conducted by Meier and Mori [13], Alves et al. [14], Bastos et al. [15]. However, as the drag force is described by empirical models, it is of extreme importance to evaluate them in accordance with the equipment employed. Due to this criterion, it was chosen the gas-solid flow jets to study the influence of loading particles in the mixture on its fluid dynamics.

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Momentum and continuity conservation equations

The momentum and continuity conservation transient equations for each phase are as follows:

- **Continuity equation, gas-phase**

\[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g V_g \right) + \frac{\partial}{\partial x} \left( \alpha_g \rho_g V_{g,x} \right) + \frac{\partial}{\partial y} \left( \alpha_g \rho_g V_{g,y} \right) + \frac{\partial}{\partial z} \left( \alpha_g \rho_g V_{g,z} \right) = \mathbf{S}_g^\rho
\]

- **Continuity equation, solid-phase**

\[
\frac{\partial}{\partial t} \left( \alpha_s \rho_s V_{s,x} \right) + \frac{\partial}{\partial x} \left( \alpha_s \rho_s V_{s,x} \right) + \frac{\partial}{\partial y} \left( \alpha_s \rho_s V_{s,y} \right) + \frac{\partial}{\partial z} \left( \alpha_s \rho_s V_{s,z} \right) = \mathbf{S}_s^\rho
\]

Where \( \alpha_g \) and \( \alpha_s \) are the volume fractions; \( \rho_g \) and \( \rho_s \) are the density of both phases; \( V \) is the velocity vector, which can be decomposed into \( v_x, v_y, \) and \( v_z \), and \( S^\rho \) represents the source term of continuity for each phase.

In the particular case of this research, the mass source terms are null due to the assumption of no mass transfer between phases.

\[
\mathbf{S}_g^\rho = \mathbf{S}_s^\rho = 0
\]

- **Momentum equation, gas-phase (x direction)**

\[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g \mu_g V_{g,x} \right) + \frac{\partial}{\partial x} \left( \alpha_g \rho_g \mu_g v_{g,x} V_{g,x} \right) + \frac{\partial}{\partial y} \left( \alpha_g \rho_g \mu_g v_{g,y} V_{g,x} \right) + \frac{\partial}{\partial z} \left( \alpha_g \rho_g \mu_g v_{g,z} V_{g,x} \right) = \mathbf{S}_g^{\mu_x}
\]

- **Momentum equation, gas-phase (y direction)**

\[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g \mu_g V_{g,y} \right) + \frac{\partial}{\partial x} \left( \alpha_g \rho_g \mu_g v_{g,x} V_{g,y} \right) + \frac{\partial}{\partial y} \left( \alpha_g \rho_g \mu_g v_{g,y} V_{g,y} \right) + \frac{\partial}{\partial z} \left( \alpha_g \rho_g \mu_g v_{g,z} V_{g,y} \right) = \mathbf{S}_g^{\mu_y}
\]

- **Momentum equation, gas-phase (z direction)**

\[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g \mu_g V_{g,z} \right) + \frac{\partial}{\partial x} \left( \alpha_g \rho_g \mu_g v_{g,x} V_{g,z} \right) + \frac{\partial}{\partial y} \left( \alpha_g \rho_g \mu_g v_{g,y} V_{g,z} \right) + \frac{\partial}{\partial z} \left( \alpha_g \rho_g \mu_g v_{g,z} V_{g,z} \right) = \mathbf{S}_g^{\mu_z}
\]

Where \( \mu_g \) is the viscosity and \( S_g^{\mu} \) represents the momentum transformation of the gas-phase. Analogous equations can be written for the solid-phase, where \( S_s^{\mu} \) represents the momentum transformation in the solid-phase.

- **Momentum equation, solid-phase (x direction)**

\[
\frac{\partial}{\partial t} \left( \alpha_s \rho_s \mu_s V_{s,x} \right) + \frac{\partial}{\partial x} \left( \alpha_s \rho_s \mu_s v_{s,x} V_{s,x} \right) + \frac{\partial}{\partial y} \left( \alpha_s \rho_s \mu_s v_{s,y} V_{s,x} \right) + \frac{\partial}{\partial z} \left( \alpha_s \rho_s \mu_s v_{s,z} V_{s,x} \right) = \mathbf{S}_s^{\mu_x}
\]

- **Momentum equation, solid-phase (y direction)**

\[
\frac{\partial}{\partial t} \left( \alpha_s \rho_s \mu_s V_{s,y} \right) + \frac{\partial}{\partial x} \left( \alpha_s \rho_s \mu_s v_{s,x} V_{s,y} \right) + \frac{\partial}{\partial y} \left( \alpha_s \rho_s \mu_s v_{s,y} V_{s,y} \right) + \frac{\partial}{\partial z} \left( \alpha_s \rho_s \mu_s v_{s,z} V_{s,y} \right) = \mathbf{S}_s^{\mu_y}
\]

- **Momentum equation, solid-phase (z direction)**

\[
\frac{\partial}{\partial t} \left( \alpha_s \rho_s \mu_s V_{s,z} \right) + \frac{\partial}{\partial x} \left( \alpha_s \rho_s \mu_s v_{s,x} V_{s,z} \right) + \frac{\partial}{\partial y} \left( \alpha_s \rho_s \mu_s v_{s,y} V_{s,z} \right) + \frac{\partial}{\partial z} \left( \alpha_s \rho_s \mu_s v_{s,z} V_{s,z} \right) = \mathbf{S}_s^{\mu_z}
\]
\[ S_{s,y}^m = \beta_{gs}^m (v_{g,y} - v_{s,y}) + \alpha_s \rho_s g_y - \frac{\partial p}{\partial y} \]  
\[ (14) \]

- Momentum equation, solid-phase (z direction)
\[ \frac{\partial}{\partial t}(\alpha_s \rho_s v_{s,z}) + \sum_{z=x,y,z} \left[ \alpha_s \rho_s v_{s,z} v_{s,z} - \alpha_s \rho_s \mu_s \left( \frac{\partial v_{s,z}}{\partial z} + \frac{\partial v_z}{\partial z} \right) \right] = S_{s,z}^m \]  
\[ (15) \]

The exact determination of the effective viscosity of the solid-phase is fundamental in attaining the radial distribution of the particles, and consequently, all the fluid dynamics variables [13]. In this research, the dynamic viscosity of the solid-phase is used due to viscous considerations.

The dispersed-phase zero-equation model consists in an analogy for the kinematic turbulent viscosities of the gas and solid phases; Equation (23) shows the expression for the solid phase:
\[ v_{s,z} = \frac{V_{g,z}}{\omega} \]  
\[ (22) \]

Where \( \omega \) is constant turbulent with a value of 10, relating the dispersed-phase kinematic turbulent viscosity \( (\mu_s/\rho_s) \) to the gas-phase kinematic turbulent viscosity \( (\mu_g/\rho_g) \).

### Constitutive equations

#### Continuity between the phases:
\[ \sum_i a_i = \alpha_g + \alpha_s = 1 \]  
\[ (23) \]

#### Interphase momentum exchange: The coefficients of drag between \( \frac{\Delta p}{Ax} = \frac{\alpha_g^3}{\alpha_s^3} \left( \frac{d_p^3}{d_p^3} \right) + 1.75 \frac{U^2 \alpha_s^2 \rho_s}{\alpha_g^2} \]  
\[ \frac{\Delta p}{Ax} = \frac{150 \alpha_g^3 \mu_g U}{\alpha_s^3} + 1.75 \frac{U^2 \alpha_s^2 \rho_s}{\alpha_g^2} \]  
\[ (25) \]

Where \( U \) is the superficial velocity, \( U = a_g (v_g - v) \) and \( \theta_s \) is the particle sphericity; in particular cases, \( \theta_s = 1 \) was used.

A comparison of Equations. (24) and (25) shows that for dense regimes (with \( a < 0.8 \)), the momentum transfer coefficient between gas phase and particles are in accordance with the following equation:
\[ \rho_{gs}^m = \frac{150 \alpha_g^3 \mu_g U}{\alpha_s^3} + 1.75 \frac{U^2 \alpha_s^2 \rho_s}{\alpha_g^2} \]  
\[ (26) \]

where \( d_p \) is the particle diameter.

For porosities higher than 0.8, the expression for pressure drop results in the following equation for the interphase momentum transfer coefficient (Crowe [22]); this was also proposed by Gidaspow [2] and used in the simulation of Meier and Mori [13], Meier et al. [16], Alves et al. [14,17] and Bastos et al. [15] with a good agreement. In the Wen and Yu proposal the particles populational effect is desconsiderated, while Gidaspow and Ettehadieh (Gidaspow, [2]), the term \( f^{2.65} \) indicates the presence effect of the others particles in the fluid and actsuates as a correction of usual Stokes law for the pressure drop of a simple particle.
\[ \rho_{gs}^m = 3 \frac{C_d}{4} \frac{f_s - \rho_s}{\alpha_g \rho_g} \]  
\[ (27) \]
The drag coefficient, $cd$, applied to Equation (27), is a function of the Reynolds number and behaves according to Equation (28), with a modified particle Reynolds number, and a power law correction, both functions of the continuous-phase volume fraction $α_g$.

$$Cd = \alpha_g^{-1.65} \max \left[ \frac{24}{Re_p^2 \alpha_g} \left(1+0.15(Re_p \alpha_g)^{0.687}\right) \right]$$

(28)

For particle Reynolds numbers above 1,000 (turbulent flows), Equation (29) which is sufficiently large for inertial effects to dominate viscous effects (the inertial or Newton’s regime), the drag coefficient becomes independent of Reynolds number:

$$Cd = 0.44$$

(29)

This uses the Wen and Yu correlation for low solid volume fractions $α_s < 0.2$, and switches to Ergun’s law for flow in a porous medium for larger solid volume fractions.

Note that this is discontinuous at the cross-over volume fraction.

In order to avoid subsequent numerical difficulties, it modifies the original Gidaspow model by linearly interpolating between the Wen and Yu and Ergun correlations over the range $0.7 < α_s < 0.8$. The Reynolds equation for the particle is given by

$$Re_p = \frac{|v_s - v_g| \rho_s \mu_p}{\rho_g \mu_g}$$

(30)

Massarani (Massarani, [3]) proposed a modification in the drag coefficient correlation ($Cd$). This modification cover all values of Reynolds for the particle, thus avoiding possible discontinuities in the calculation caused by the change of the flow regime due to axial velocity increase. Two new constants were introduced, particle sphericity functions, presented in Equation (31).

$$Cd = \left[ \frac{24}{K_1 \cdot Re_p} \right]^{0.85} + K_2^{0.85}$$

(31)

where $K_1$ and $K_2$ are model constants and expressed by correlations, Equations 32 and 33:

$$K_1 = 0.843 \log_{10} \left( \frac{\theta}{0.065} \right)$$

(32)

$$K_2 = 5.31 - 4.880/\alpha_s$$

(33)

where $θ$ is the particle sphericity.

Simulation

The simulated model consists basically of a turbulent jet flow, where two phases enter into contact. The gas-phase is formed by air and the solid-phase composed of catalysts. The particles are considered inviscid, smooth, spherical and inelastic, with a mean diameter of 50µm and a density of 2500kg/m³. Three different drag models were used in these cases (Wen and Yu [1], Gidaspow [2] and Massarani [3]) in order to evaluate which one better represents the jet flow dynamics. Due to gas-phase forces, which are responsible for the effective solid-phase distribution, the particles accelerate and move in the direction of the flow, characterizing the particle-laden jet regime in a short period of time. Measurements were taken at five axial levels of 120, 150, 180,210 e 240mm at the jet center, which has an internal diameter of 12mm, for Test and five cases with different initial conditions of velocity and solid mass loading rates, being all cases at its respective radial position in accordance with the data of Decker et al. [5].

Boundary conditions

At the entrance, all velocities and concentrations of both phases are specified. At the walls, the gas-phase velocity is zero and the solid-phase velocity has a free-slip condition. The incompressible gas-phase pressure was defined at the exit, assuming atmospheric pressure. At the mesh boundaries, the opening condition was used. As inlet conditions for the Test case and other five cases of interest, the gas velocity (8 to 16m/s), the solid mass loading ratio (3 to 7) and the Reynolds number (5500 to 11000) are specified for each case and presented in Table 1.

Mesh and computational code

The non-structured mesh was composed of 170,000 control volumes. The details of the geometry and mesh are presented in Figure 1. The time step was on the order of 10⁻¹ for the first second and on the order of 10⁻² thereafter. Adaptation of the mathematical model for generation of the numerical model was achieved using the ANSYS CFX 12.0 commercial simulator, which is based on the finite volume method.

Results and Discussion

Mesh tests

The radial profiles of the solid-phase mean velocity for the two-phase jet flow were analyzed, using the proposed conditions by

<table>
<thead>
<tr>
<th>Cases</th>
<th>$U_i$ (m/s)</th>
<th>$\eta$</th>
<th>Re</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Case</td>
<td>11.13</td>
<td>4.5</td>
<td>7485</td>
</tr>
<tr>
<td>Case 1</td>
<td>8.25</td>
<td>6.34</td>
<td>5543</td>
</tr>
<tr>
<td>Case 2</td>
<td>9.64</td>
<td>5.41</td>
<td>6471</td>
</tr>
<tr>
<td>Case 3</td>
<td>11.78</td>
<td>4.26</td>
<td>7911</td>
</tr>
<tr>
<td>Case 4</td>
<td>13.23</td>
<td>3.69</td>
<td>8884</td>
</tr>
<tr>
<td>Case 5</td>
<td>15.83</td>
<td>3.09</td>
<td>10627</td>
</tr>
</tbody>
</table>

Table 1: Inlet flow conditions.

Figure 1: Geometry and Mesh details.
Decker et al. [5]. Eight meshes in two distinct configurations were tested, considering the jet nozzle into (Figure 2) and out the mesh, with different numbers of control volumes. Each pair consisted of approximately 100,000, 130,000, 170,000 and 200,000 control volumes.

These meshes were tested and the one that was the best behavior for standard flow would be used to begin the simulations of the real process. In evaluating the dependence of flow on numerical mesh, it is known that the appropriate number of control volumes is of extremely important to avoid numerical errors, which is not possible with coarser meshes. The one-phase model was used for the tests, subjected to equations of continuity and momentum.

As a result, a mesh composed of 170,000 control volumes was chosen. This was shown to be in accordance with the established standards for both configurations used. Figure 3 shows these results for the Test case in both mesh configurations at z/D 12.5 and 15.0 without jet nozzle into the mesh (num’), jet nozzle into the mesh (num**) and experimental data, using Gidaspow drag correlation.

The simulations with different meshes resulted in the following observations:

In each one of the transversal sections, there are two distinct zones: a primary zone (where the particle velocities are high and quasi-constant), which extends from the radial center (r/R = 0) to approximately r = 0.007m, and a secondary zone (where the particle velocities are intermediary and decrease moderately), which is located at r = 0.007m to r = 0.02m (end of measurement line) for the two different configurations, in the two measured transversal sections [z/D = 12.5 and 15.0]. In the axial direction a single zone was observed, whereas for the same configuration in distinct sections overlap (Figure 3).

- Jet nozzle out the mesh

The velocity axial and radial profiles only reproduced the fluid dynamics behavior at the internal diameter of the jet nozzle (r = 0.006m), after this limit all results were underestimated compared to experimental results, due to not add to the calculations the effects of the jet outer boundaries in a direction to the jet core.

- Jet nozzle into the mesh

The velocity axial and radial profiles reproduced completely the flow behavior as much quantitative as qualitatively.

- Axial dependency: There is not a significant influence on the mesh refinement in the axial direction. However, a slight variation was verified in the less refined mesh on the first and second cross sections (z/D 12.5 and 15.0).

- Radial dependency: In all cross sections the flow radial behavior was analogous compared to the experimental results for the Test case, according to Decker et al. [5], except for the coarser mesh.

Figure 4 shows the respective measurement lines, in the center and line jet, and mainly the flow vectors, which indicates the influence of the effects of the jet outer boundaries in the direction to the jet center (jet into the geometry).

Dispersion model verification

Different simulations were accomplished to evaluate the flow dynamics in terms of the dispersion model used for the solid-phase. Among three drag correlations Wen & Yu symbolized by TCW, Gidaspow by TCG and Massarani by TCM.

Figures 5a and 5b (close up), Figures 6a and 6b (close up) show the
results of radial profiles of the solid-phase mean velocity for the Test case at z/D 12.5 and 15.0 compared to the experimental data of Decker et al. [5]. All the three models used showed good agreement with the experimental data. The drag models of Wen and Yu and Gidaspow showed similar results overlapped. However, the Massarani (TCM10) model showed a better tendency than them, what can be better observed in Figures 5b and 6b. Due to proximity of these results, it was chosen the last one to be closer to the experimental data and also the advantage of being continuous for the following five study cases.

**Radial Profiles of the Solid-Phase Mean Velocity**

The radial profiles of the solid-phase mean velocity were computed numerically at 7s of real time, using a complete mathematical model with Massarani drag correlation, k-ε turbulent model for the gas-phase, kinematic turbulent viscosities analogy for the solid-phase and the time averaging procedure at each time step.

Figures 7 and 8 shows the obtained simulation results for cases 1, 2, 3, 4 and 5 at the closer cross sections z/D 12.0 and 12.5, respectively (Figure 4). Although the simulated results under predicted the solid-phase mean velocity in the near the jet boundaries, one can see that the profiles in Figure 7 show the tendency of the experimental data. In Figure 8 this can only be observed for case 5, however more attenuated. Cases 1,2,3 and 4 showed good agreement between numerical and experimental data.

It is possible to observe the same behaviors, both quantitative and qualitative, at different radial and axial positions. The solid-phase velocity tends to remain similar in all planes and in all cross-sections near the central jet. However, this velocity, whether near or far from jet limit decreases axially and radially. It can be observed in each plane there are variations in that solid-phase velocity at the boundary of the jet, especially at the higher velocities (cases 4 and 5) and in the end of measurement line.
The simulated results for the other three cross sections ($z/D$ 15.0, 17.5 and 20.0) for five interest study cases presented complete agreement between numerical and experimental data. Figures 9, 10 and 11 show these results. It is possible to observe the same behaviors, both quantitative and qualitative, at different radial and axial positions. The solid-phase velocity tends to remain similar in all cross-sections in the center jet and near the jet boundaries. It can be observed in all cross-sections investigated, as in Test case, two distinct zones that extend at same radial points (0 to approximately 0.007 and 0.007 to 0.02m). Also, in the axial direction a single zone was observed. The solid-phase velocity was for the five cases, in fact, higher in the primary zone than in the second zone at all axial positions, in agreement with experimental data (Decker et al. [5]) and as seen in Yan et al. [23].

**Conclusions**

The objectives of this research was analyzing the influence of the different mathematical models of drag for the gas-solid jet flow prediction and confirm the turbulence models for each phase, in special the kinematic turbulent viscosities analogy for jet flow. Numerical radial profiles of the solid-phase mean velocity were analyzed for all experimental measured positions and the results were compared. The simulation results obtained regarding drag and solid-phase dispersion correlations dependence on the three different drag correlation used in this work were analyzed. The predicted radial profiles of the solid-phase mean velocity showed excellent agreement with the measurements in the flow cross sections for the Test case and five study cases in a jet.

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