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CFD SIMULATION AND CO-VALIDATION OF A FLUIDIZED BED EXPERIMENT USING DIFFERENTS DRAG MODELS

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Abstract
The objective of this work is to perform a validation of the mathematical model applied by the software Star CCM + in applications involving fluidized bed and evaluate three drag models to fit with experimental data. This validation consists, primarily, on a study of the appropriate mesh size in order to describe the flow behavior, as well as an evaluation of the computational time required to describe the behavior of the bed through time-averages of the analyzed parameters. The reactor geometry based on experimental apparatus, particle properties and boundary conditions are maintained according to a previous study found on the literature. Also, the application of Arastoopour, Syamlal – O'Brien and Gidaspow drag coefficients are done for bed with Geldart B particles. The results show that a mesh approximately 10 times greater than the particle size, and a computational time of 20 seconds, can provide good results convergence compared to experimental data. Furthermore, it is possible to observe that both Gidaspow and Arastoopour drag models can provide results very close to those observed experimentally.

Keywords: *Fluidized bed, Drag coefficient, CFD, Multi-phase flow*

1. INTRODUCTION

The studies about fluidized bed systems in industry history began in 1922, when Fritz Winkler developed and obtained a patent for the particulate carbon gasification process. The first gasifiers have started production in Germany and Japan, in 1926, in order to supply energetically chemical industries. In the second war period, the countries involved started to search for fuel sources to supply their planes and tanks, so they needed to develop processes that would provide the fuel for their transports on a large scale. This process worked well to meet the demands of the time, and because it was highly demanded, many studies were done in the final years of the second war, with the intention of making production plants more compact, efficient and cheaper. Since then, many other fluidized bed systems, where high rates of heat transfer and chemical reaction are desired, have been developed for the most diverse applications, such as: pneumatic transport, gas phase polymerization, combustion, incineration, particulates, coating materials surfaces and drying (Kunii, D., Levenspiel, O., 1991).

In order to determine a bibliography destinated to fluidization applications, in the 50’s and 60’s, many researchers have worked hardly do develop technics to explain, based on fluid mechanical theories and empirical data, the fundamentals of fluidization. Then, Kunii and Levenspiel (1969), published a book compiling these variety of previous studies and correlations, making an approach of fluidization parameters, types of fluidization, heat transfer in fluidized beds, and so on Geldart (1973), brought in his study a classification for the particles and the types of fluidization based on a relation between particle size, particle density and fluidization media density. This classification has been used till today to determine the type of fluidization in each apparatus. As the applications of fluidized bed systems started to raise in many areas of industry, studies involving fluidization parameters variations raised as well. A mathematical model was proposed in a paper by Lun et al. (1984), which was based on the Kinetic Gas Theory, from Champan and Cowling (1961). From this Theory of Granular Kinetic Flow (KTGF), expressions of granular temperature and granular pressure emerged for application in Eulerian-Eulerian models. Subsequently, further studies were conducted, mainly by Gidaspow in the 1990s, to propose both expressions for viscosity and pressure of the solid medium with also adjustments in coupling models between phases. In order to determine the drag coefficient, equations and models were proposed by Syamlal, M. and O'Brien (1987), Arastoopour et al. (1990), and Gisdaspow et al. (1994). In other hand, Johnson, P.C., and Jackson, R.,1987, and Schaeffer, G. ,1987, proposed on their studies, models for frictional regime in particulate flows.

With the advancement of technologies for numerical simulations and the development of new numerical codes, softwares and supercomputers, many numerical studies started to be done and validated with experimental results. For example, Esmaili, E. and, Mahinpey, N., (2009), carried out an experimental and computational study of the fluid dynamics of a bubbling fluidized bed in the gas-solid phase iteration, in order to analyze the influence of different trawl correlations between phases, comparing the CFD results with the experimental one. The CFD simulation used the Eulerian-Eulerian model, with the Syamlal-O'Brien, Gidaspow and Wen-Yu correlations, simulating the transfer of momentum between the phases and analyzing which mathematical formulation would be ideal to represent the results obtained in the physical apparatus. The comparisons were made based on volume fractions, expansion and pressure drop within the fluidized bed at different gas surface velocities. Another recent work that intended to validate the interaction laws, was the study from Loha et al. (2012), employed in this present paper as a reference. In that work, the authors made a study of the hydrodynamics of a 2D fluidized bed, comparing the application of a k-ε turbulence model with the laminar model, applying to an Eulerian-Eulerian model combined with the Granular Flow Kinetic Theory. They evaluated and compared the parameters of velocity, particle volume fraction and granular temperature, varying four different types of trawl coefficients (Gidaspow, Syamlal-O'Brien, EMMS and McKeen) and verified that turbulent models do not bring any further information on the bed dynamics, and simulations could be performed more rapidly employing laminar flows, without loss of information.

Further, Loha et al did a variation of specularity coefficient and particle-particle restitution coefficient, in order to validate the experiment done by Jung et al., 2005. They observed that the specularity coefficient have influence on the results performed and should be carefully studied to represent the desired particles composing the bed, in order to promote the advantages and drawbacks of the tools for fluidized bed simulations. Khan et. al, 2014, performed a general review for CFD simulation application in fluid dynamics analysis in polymerization reactors in the production of polyolefins. That review brought studies that used CFD to determine bubble size, gas-solid bed behavior, bed expansion, particle volume distribution and fraction, as well as heat and mass transfer, among other parameters. important when analyzing the fluidization mechanism. The comparison between the commercially available software for this type of study, as well as the applicability of CFD in fluid bed olefin polymerization studies, were discussed in this paper.

Thus, the present work proposes a methodology for exploring the validity of Eulerian-Eulerian numerical schemes considering results presented in the literature. Validation of drag coefficients are explored based on comparison with other commercial codes data from the literature (from Loha et al., 2012) as well as experimental tests. The authors expect that the present work could point out direction on the application of numerical simulation methods for solving fluidized bed problems for application in future cases of industrial production processes.

2. MATHEMATICAL MODELING

Numerical simulation has been used in the fields of physics, mathematics and engineering to predict the behavior of biphasic flows in everyday applications. Thus, for numerical approximation of the results of this type of flow, two mathematical models to use for these determinations are highlighted: Eulerian-Eulerian, relating both phases (continuous and dispersed) as if they were continuous, and Eulerian-Lagrangian, where the fluid phase is treated as continuous and the dispersed phase is treated as discrete (Vegendla, 2011).

In this work, in order to obtain results of scalar parameters of a fluidized bed, it is used the Eulerian-Eulerian model. Then, it is necessary to apply the correlations of the Kinetic Theory of Granular Flow (KTGF), which is based on the kinetic theory of dense gases. The application of this equation serves to close the problem, considering the energy dissipation due to the collisions of the particles by means of the coefficient of restitution.

For a Eulerian-Eulerian biphasic (gas-solid in the present work) fluidization problem, where both phases behave as two distinct fluids, the equations of conservation of mass and momentum that govern the problem are presented in Eq. 3, 4 and 5 (Simcenter Star CCM +, 2019). Each phase occupies a part, within the domain of the problem, which is determined by the fraction of the total volume, ε_k, defined by Equation 3.

$$\varepsilon_k = \int_V V_k \, dV \qquad ; \qquad \sum_{k=1}^{N} \varepsilon_k = 1 \tag{3}$$

where V_k is the partial volume of phase k, ε_k is the volume fraction of phase k, and N is the number of phases. The mass conservation equation for each Eulerian phase is given by Equation 4:

$$\frac{\partial}{\partial t}\varepsilon_k\rho_k + \nabla.\varepsilon_k\rho_k\, u_k = \sum_{j\neq k}^{N}(\dot{m}_{jk} - \dot{m}_{kj}) + S_k^{\alpha} \tag{4}$$

where ρ_k is the density and u_k is the velocity The momentum balance equation for each Eulerian phase is given by Equation 5.

$$\frac{\partial}{\partial t}\varepsilon_k\rho_k u_k + \nabla.\varepsilon_k\rho_k u_k u_k = -\varepsilon_k\nabla p + \varepsilon_k\rho_k\vec{g} + \nabla.\varepsilon_k(\vec{\tau}_k + \vec{\tau}^t{}_k) + M_k \tag{5}$$

where $\dot{m}_{jk}$ and $\dot{m}_{kj}$ are the mass transfer from phase j to phase k, and vice-versa, and S_k^α is the mass source term, p is the pressure, $\vec{g}$ is gravity, $\vec{\tau}_k$ and $\vec{\tau}^t{}_k$ are the molecular and turbulent stress, respectively, and M_k is the sum of interfacial forces.

Particle-particle interactions are significantly relevant when there is a flow involving a fluid phase and a dense phase, and this granular phase requires its own set of models. Thus, a mathematical modeling is required to represent the interaction between these particles. This model is the Kinetic Theory of Granular Flow, proposed in a work by Lun et al. (1984), is based on the Kinetic Theory of Gases, by Champan and Cowling (1961). Analogously to the temperature of the gases, the granular temperature, θ_s, describes the energy resulting from the velocity fluctuation of the particles (turbulent kinetic energy of the granular phase), and it is determined according to Equation 6.

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s\rho_s\theta_s) + \nabla(\varepsilon_s\rho_s\vec{u}_s\theta_s)\right] = \left(-p_s\bar{\bar{I}} + \bar{\bar{\tau}}_s\right):\nabla\vec{u}_s + \nabla\left(k_{\theta_s}\nabla\theta_s\right) - \gamma_{\theta_s} + \varphi_{gs} \tag{6}$$

where $\left(-p_s\bar{\bar{I}} + \bar{\bar{\tau}}_s\right):\nabla\vec{u}_s$ is the energy resulting from the solid phase stresses, $\nabla\left(k_{\theta_s}\nabla\theta_s\right)$ is the term representing the diffusion of energy, γ_{θ_s} is the dissipation of energy through collisions, and φ_{gs} is the exchange of floating energy between phases. The determination of the diffusion coefficient between the phases is described in Equation 7.

$$k_{\theta_s} = k + \frac{3\mu_{pt}}{2} \tag{7}$$

Where k is the granular diffusion coefficient and μ_{pt} is the turbulent viscosity of the granular phase. The stress tensor equations for gas and solid phases are represented in Equations 8 and Equation 9, respectively.

$$\overline{\overline{\boldsymbol{\tau}_g}} = \varepsilon_g\mu_g\left(\nabla\vec{u}_g + \nabla\vec{u}_g{}^T\right) - \frac{2}{3}\varepsilon_g\mu_g\left(\nabla\vec{u}_g\right)\bar{I} \tag{8}$$

$$\bar{\bar{\boldsymbol{\tau}}}_s = \varepsilon_s\mu_s\left(\nabla\vec{u}_s + \nabla\vec{u}_s{}^T\right) - \varepsilon_g\left(\lambda_s - \frac{2}{3}\mu_s\right)(\nabla\vec{u}_s)\bar{I} \tag{9}$$

In these cases, μ_s is the solid shear viscosity, and λ_s is the bulk viscosity, which can be defined in Equation 10 and Equation 11, respectively.

$$\mu_s = \frac{4}{5}\varepsilon_s{}^2\rho_s d_p g_0(1-e)\left(\frac{\theta_s}{\pi}\right)^{\frac{1}{2}} + \frac{\varepsilon_s d_p\rho_s\sqrt{\pi\theta_s}}{6(3-e)}\left[1 + \frac{2}{5}(1+e)(3e-1)\varepsilon_s g_0\right] \tag{10}$$

$$\lambda_s = \frac{4}{3}\varepsilon_s{}^2\rho_s d_p g_0(1-e)\left(\frac{\theta_s}{\pi}\right)^{\frac{1}{2}} \tag{11}$$

Where e is the coefficient of restitution. The probability of particle collisions is characterized by the radial particle distribution function, g_0, defined in Equation 12.

$$g_0 = \frac{3}{5}\left[1 - \left(\frac{\varepsilon_s}{\varepsilon_{s,max}}\right)^{\frac{1}{3}}\right]^{-1} \tag{12}$$

The granular pressure is defined as the showed in Equation 13:

$$p_s = \varepsilon_s\rho_s\theta_s + 2\rho_s(1+e)\varepsilon_s{}^2 g_0\theta_s \tag{13}$$

The drag forces, $F_{D_{sg}}$, present in a fluidized bed, becomes one of the most important parameters for determination of the interaction between both phases involved in the problem. Many studies have been developed, over the time, to determine empirical correlations of these forces in different types of two-phase flows. The most traditional of them, already presented previously, the Ergun equation is one of those mathematical models obtained for determination of these parameters in a particulate bed. Among the studies developed for two-phase flows in the fluidized bed model are the Gidaspow (1994), Arastoopour (1990), and Syamlal-O'Brien (1989) models. The interaction between the two-participating means in these models is determined by the following relation of the drag coefficient between the phases, K_{sg}, presented in Equation 14.

$$F_{D_{sg}} = K_{sg}(\vec{u}_g - \vec{u}_s) \tag{14}$$

2.1. Gidaspow drag model

$$k_{sg} = \begin{Bmatrix} 150\frac{\varepsilon_s{}^2\mu_g}{d_s{}^2\varepsilon_g} + 1{,}75\frac{\varepsilon_s\rho_g|\vec{u}_s-\vec{u}_g|}{d_s} & \text{para } \varepsilon_s > 0{,}2 \\ \frac{3}{4}C_D\varepsilon_g\frac{\varepsilon_s\varepsilon_g\rho_g|\vec{u}_s-\vec{u}_g|}{d_s} & \text{para } \varepsilon_s \leq 0{,}2 \end{Bmatrix} \tag{15}$$

$$C_D = \begin{cases} \frac{24}{Re.\varepsilon_g} + (1 + 0{,}15(Re.\varepsilon_g)^{0{,}687}) & \text{para } Re.\varepsilon_s < 1000 \\ 0{,}44 & \text{para } Re.\varepsilon_s \geq 1000 \end{cases} \quad (16)$$

$$Re = \frac{\varepsilon_s d_p \rho_g |\vec{u}_s - \vec{u}_g|}{\mu_g} \quad (17)$$

2.2. Syamlal-O'Brien drag model

$$k_{sg} = \frac{3}{4}\frac{\varepsilon_s \varepsilon_g \rho_g}{v_{t,s}{}^2 d_p} C_d \frac{Re_s}{v_{t,s}} \left|\vec{u}_s - \vec{u}_g\right| \quad (18)$$

$$v_{t,s} = 0{,}5(\mathrm{A} - 0{,}06Re_s + \sqrt{(0{,}06Re_s)^2 + (0{,}12Re_s(2B - A) + A^2)} \quad (19)$$

$$\mathrm{A} = \varepsilon_g{}^{4{,}14} \quad (20)$$

$$B = \begin{cases} 0{,}8\varepsilon_g{}^{1{,}28}, & \varepsilon_g \leq 0{,}85 \\ 0{,}8\varepsilon_g{}^{2{,}65}, & \varepsilon_g \geq 0{,}85 \end{cases} \quad (21)$$

2.3. Arastoopour drag model

$$k_{sg} = \left(0{,}336 + \frac{17{,}3}{Re}\right) \frac{\varepsilon_s \rho_g |\vec{u}_s - \vec{u}_g|}{d_p} \varepsilon_g{}^{-2{,}8} \quad (22)$$

$$Re = \frac{d_p |\vec{u}_s - \vec{u}_g| \rho_g}{\mu_g} \quad (23)$$

3. EXPERIMENT SETUP AND CFD SIMULATION

In order to have a validation of the convergence parameters of the particulate bed fluidization problem, a computational experiment was performed based on a numerical analysis previously performed by Loha et al. (2012), and also an experimental study by Jung et al. (2005), respecting the same mesh and geometry parameters, the initial particle bed conditions, boundary conditions and mathematical models applied on his work. The purpose of this application is to validate the mathematical model applied by Star CCM +, commercial software used throughout the context of this work, compared to the mathematical model provided by the Ansys Fluent package, commercial software used by Loha et al., in order to have the same application to other subsequent problems in gas-solid two-phase flow in fluidized state, where the process conditions are similar to these studies.

The geometry of the problem was analyzed in 2D, which is a 400 mm high and 155 mm wide reactor, as shown in Figure 3.1, filled with solid spherical particles with a diameter of 530 µm and a density of 2500 kg/m³. The initial height of the particulate bed inside the reactor is 200 mm, with initial volume fraction equal to 0.4 and maximum volume fraction 0.6 (maximum compaction). The fluidizing media is air, with constant density and viscosity parameters, 1.188415 kg/m³ and 1.855e-5 Pas, respectively, and a constant and equally distributed velocity on the inlet of the reactor, of 0.587 m /s. The slip condition at the wall is defined as no-slip for the air and partial slip for the particles, with a specularity coefficient ∅ = 0.6. The restitution coefficients used, both for solid-solid and solid-wall, are equal to 0.99.

The equations, as shown previously, are solved on the commercial CFD software Star CCM+, using a SIMPLE phase couple algorithm. An implicit unsteady state formulation is selected, with a 2nd order convective terms and 2nd order time discretization, and a time step of 1x10e-3 seconds. The convergence criteria is based on the residuals, which must be smaller than 10e-4 for all continua parameters. Then, for this problem in Star CCM+, it is stablished 80 interactions per time step to achieve this convergence criteria. The mathematical model applied in this simulation is the Eulerian-Eulerian, combined with the Kinetic Theory of Granular Flow (KTGF). The Gidaspow correlation is used for the drag coefficient, in order to compare with based simulation by Loha et al., 2012. The analysis is made with laminar modeling, since for this case, Loha et al. have shown that there is no significant difference in the results in dense phase fluidized bed problems compared to the application of a k-ε turbulence model. In addition, the Kinetic Theory of Granular Flow presents the term of granular temperature, which considers the fluctuations of the particulate phase in relation to the fluid phase.

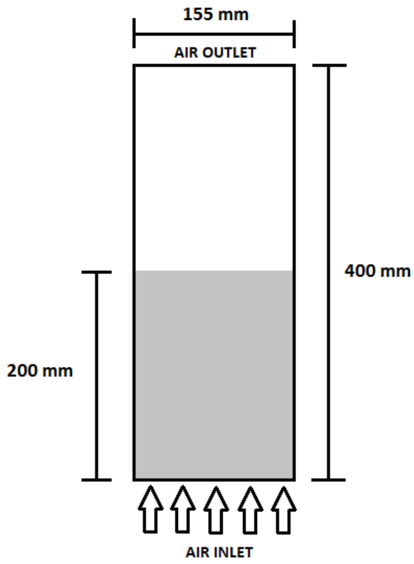

Figure 3.1. Geometry and initial conditions

The mesh used in this problem has tetrahedral geometry and it is uniformly disposed in the problem domain, having a size of 5 mm (30 x 80 volumes). This is determined due to a mesh independence study, analyzing three different mesh sizes. Among these meshes analyzed are: a coarser mesh, with 68 x 26 (1768 cells); a median mesh, with 80 x 30 (2400 cells); and a finer mesh, with 112 x 44 (4928 cells).

4. METHODOLOGY VALIDATION

The result of this study, it was found that the variation of the mean volumetric fraction in the central line of the problem, in the time of 30 s, did not change significantly, to the point of certifying that the 5 mm mesh brings convergent results for the presented case compared to the other meshes, as shown in Figure 4.1.

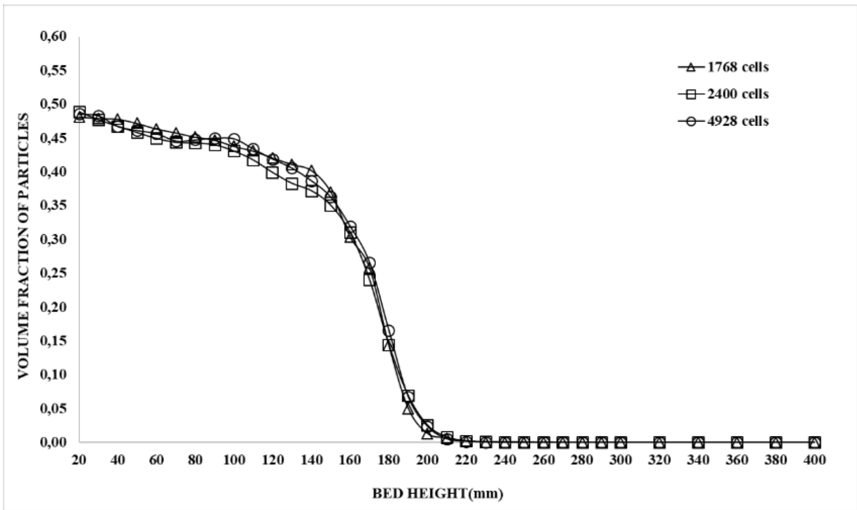

Figure 4.1. Study of a mesh independence among a coarser mesh, with 68 x 26 (1768 cells), a median mesh, with 80 x 30 (2400 cells), and a finer mesh, with 112 x 44 (4928 cells)

In order to employ only data for fluidized bed with recurrent behavior, a preliminary study was performed, extending the simulation up to 30 s. In the simulations, there is initiation process of the fluidized bed that consists on the adaptation of the bed to the air inlet forced. The bed of particles, resting at the initial concentration, starts to rise, most like a plugged flow. After this effect, the bed begins to exhibit recurrent behavior on its flow, bubble formation and particle displacement. Then, an evaluation is done to determine the point where values will start to be taken. This study was done by analyzing the moving average pressure drop between gas inlet and outlet, and the behavior of this parameter compared to the average of drop pressure fluctuations. The calculated average and standard deviation are, respectively, 2002.92 Pa and 38.88 Pa (1.94%). So, it is possible to observe that, after 5 s of simulation, the values of moving average are inside standard deviation boundaries, as shown in figure 4.2, indicating a stability in bed pressure fluctuations.

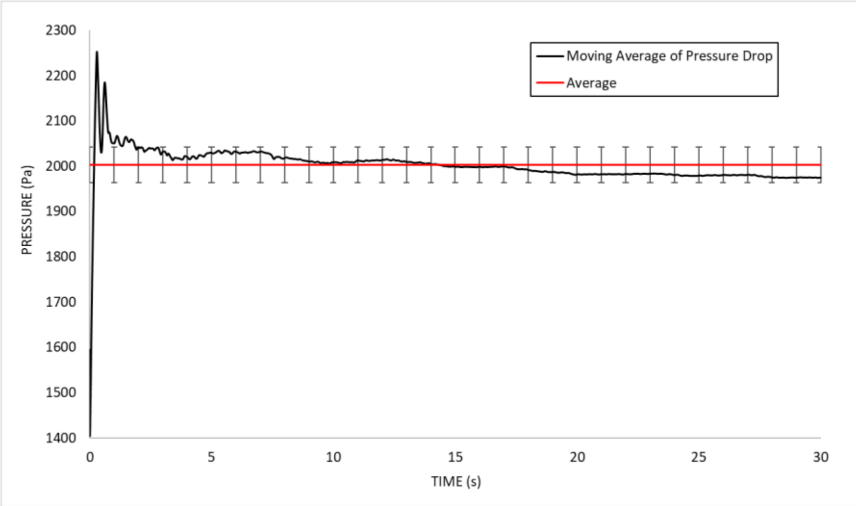

Figure 4.2. Analysis of the moving average of the pressure drop in fluidized bed and bed pressure stability.

Identified the initial time to start to take the result values, the next step was to determine the interval to calculate the time-average for the results. A study evaluating the volumetric fraction of the particles in a horizontal line at the height of 140 mm from the bottom (gas inlet) for time interval from 5 to 10 s, 5 to 15 s, 5 to 20 s, 5 to 25 s, and 5 to 30 s, as can be seen in Figure 4.3. The purpose of this evaluation is to determine the minimum necessary simulation time to obtain values that represent the bed behavior without unnecessarily extending the computation time. In this work, with the hardware utilized, the time required to obtain 1 second is approximately 80 minutes. Then, the evaluation and quantification of the time required to obtain convergent results tends to drastically reduce the total time required for the computation. For two-dimensional simulations with relatively small meshes, this influence represents a few hours, but for meshes of larger geometries, or even 3D, this determination can save days of numerical simulation.

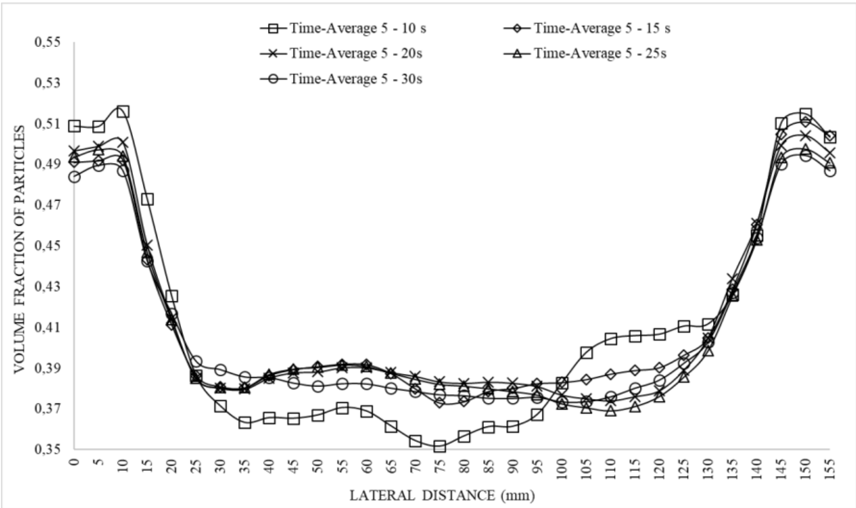

Figure 4.3. Time-average volume fraction of particles at 140 mm above inlet surface study to time determination

After performing this preliminary study to determine the simulation time, it is possible to observe that the result from the time-average between 5 and 20 s presents the maximum deviation of 0.71% compared to the values obtained in the 5 to 25 s and 5 to 30 s. Thus, the results to be presented will be determined for average values taken in time between 5 and 20 s of simulation.

The last validation test performed in the present study, was to define the drag coefficient. An evaluation of the Arastoopour, Gidaspow, and Syamlal models is done. Arastoopour's drag coefficient is not in Loha's proposal, but previous works in literature have indicated this coefficient for fluidized beds with Geldart group B particles. Then, the bed, the geometry and mesh parameters were maintained, as well as the boundary conditions, by just modifying the drag coefficients model. The three models (Gidaspow, Syamlal and Arastoopour) are compared with the experiment results proposed by Jung et al. (2005).

5. RESULTS AND DISCUSSION

In order to make the validation study of a Star CCM+ mathematical model, a comparison between the results of this work and from Loha et al. (2012), is done and showed in Figure 5.1. It is notorious that some discrepancies are present in the results when compared to each other. Analyzing the data from Loha et al., the bed is less compacted in the bottom, close to the air inlet, and it tends to go higher than the fluidizing bed proposed by this work. As the parameters were based on the previous study, with the same geometry and mesh size, some proposals for these discrepancies can be assumed. Parameters as the air properties and the restitution coefficient for particle-wall contact are not determined in paper from Loha et al. (2012), and these probably differences in fluid and solid properties can affect the results of volume fraction and velocities.

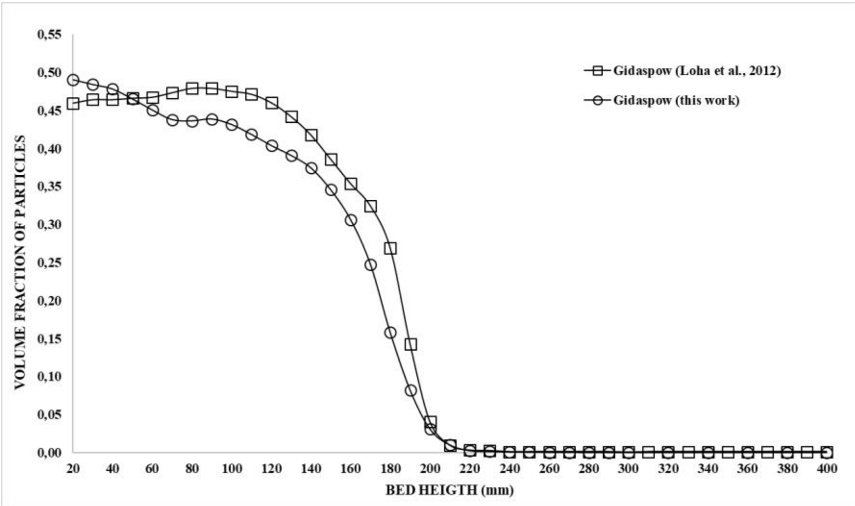

Figure 5.1. Comparison of central axis volume fraction of particles, between this work and Loha et al. (2012).

When the analysis is done comparing the simulation using different drag coefficients, it is possible to observe, as shown in Figure 5.2, that the numerical simulation with Gidaspow and Arastoopour models present results that converge to the experimental results from Jung et al. (2005). The results represented by the simulation using Syamlal-O'Brien drag model are not close to the experimental data.

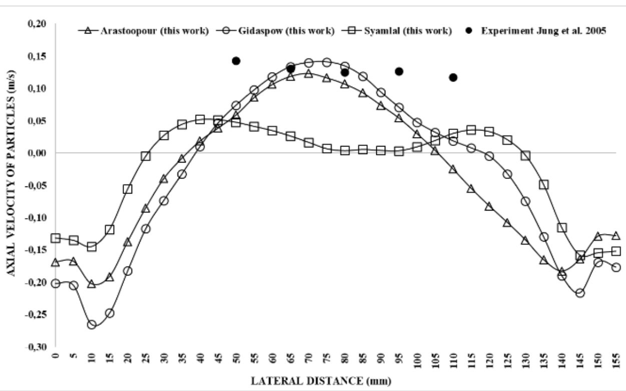

Figure 5.2. Time-average axial velocity of particles at 140 mm above inlet surface.

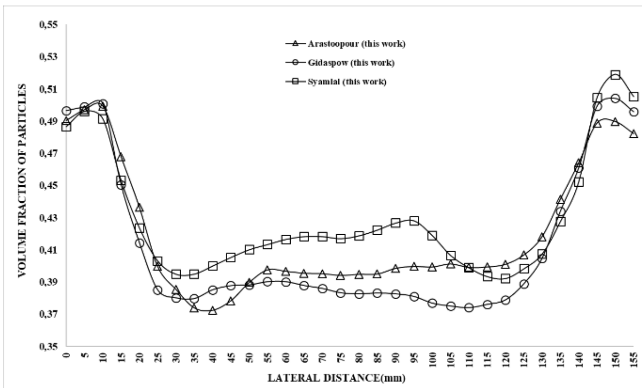

Figure 5.3. Time-average axial volume fraction of particles at 140 mm above inlet surface.

The same comparison can be done when analyzed the results of volume fraction of particles, in the bed height of 140 mm above the inlet surface, as shown in Figure 5.3. The time-average data obtained by this evaluation shows that the results from the study using Gidaspow and the onde using Arastoopour present, in average, 3.1% discrepancy, with a peak value of 6.9%. Then, this analysis shows that both the drag coefficient models proposed by Gidaspow and Arastoopour area acceptable to be used when doing a numerical study of particle B of Geldart fluidized bed.

6. CONCLUSION

In this study of a 2D fluidized bed, with Geldart B particles, the results have shown that a mesh cell size larger 10 times the particle diameter fits very well the mesh independence. Even if there is no refinement in edges, it is understood that the flow behavior is well descripted comparing to finer and coarser grid, because it must compute the continua of two particles, at least, inside the cell, in order to calculate parameter of particle-particle chocks in fluid media. Also, the time simulation of 20 s was evaluated to be enough to converge the parameter results analyzing a time-average study in the fluidized bed. Removing the first 5 s of output data to calculate the time-average parameter, can avoid the fluctuations of the bed response when it is going to star to fluidize. Furthermore, it is possible to observe that both Gidaspow and Arastoopour drag models provide results very close to those which are presented by an experimental study. In other hand, using the Syamlal-O'Brien drag model on computation, the results are not convergent with Jung et al. (2005), data. For further studies, it becomes necessary to evaluate all the unknown parameter of particles, fluid media and boundary condition, or even the mathematical model utilized, in order to determine the reasons for those divergence in behavior on different commercial software responses.

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