3D MATHEMATICAL MODELING OF GAS-SOLID FLUIDDYNAMICS IN FLUIDIZED BED

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Abstract. *Processes using fluidized bed reactors are well known since 1920, although in some processes like combustion, this equipment only started to be used in the 80's and 90's with special application to installations for electric generation. Fluidized bed process make possible the use of raw materials with quality lower than the materials normally used in similar processes. The fluidized bed technics are not spread out in Brazil yet, where the problems with energetic matrix open the options to use new processes to electric generation. Thermal generation is one of this options, which can use fluidized bed reactor to burn materials like coals and biomasses. The brazilian coals presents high ash and sulfur content fact that disable the direct use in conventional thermoelectric facilities. Therefore, the use of fluidized bed to produce hot gas for power generation is a promissing technique to overcome the use of impure raw materials with high combustion efficiency and energy savings. Mathematical models have proved their efficiency to investigate optimum operational conditions and reproduce virtually the industrial processes. The objective of this work is to develop a computational model that simulate the fluidized bed phenomena considering two phases. The model uses the multiphase concept to simulate the flow in a 3D fluidized bed reactor. Transport equations of mass, momentum and energy are solved by the finite volume method for non-orthogonal system implemented in a complex computational code written in Fortran 90/95. The phases are modeled using continuum mechanics principles where collection of particles is considered identical having a representative diameter and density. This model has been an innovation of fluidized bed study by considering 3D transient features. The results shown good agreements with experimental and computational results previously investigated.*

Keywords*: Multiphase flow; Mathematical modeling; Three dimensional; computational simulation.*

1. INTRODUCTION

Reactional processes using fluidized bed are not new; this technique is well known since 1920 and became widely use since 1970 in many processes of chemical and oil industry "Bittanti *et al*. (2000)". The fluidized bed, however, earned popularity in the 80's and 90's with increase of the demand for installations of energy generation, due to the flexibility of fuels and positive environmental influences obtained with this process. The operation of fluidized bed is simple, consists basically in to pass an air flux through fixed particles bed and the fuels used in the process can present quality lower than those normally used in factories, which can be low rank coals, mine residues, trash and several types of biomasses "Bittanti *et al*. (2000)". The models of fluidized bed combustors are scarce yet owing to the complex mathematical modeling and numerical instability of numerous equations that must be solved to represent the process "Zhou *et al*. (2004)". The fluidized bed technique is not spread out in Brazil yet, but needs of energetic matrix diversification have opened the opportunity to use new processes for electric generation. Thermal generation is one of these options that can use fluidized bed reactor to flame coals and biomasses and some residues from industrial and agricultural segments. The Brazilian coals are characterized by their high ash and sulfur content fact that make impossible to use them directly in conventional thermoelectric facilities. Therefore, the use of fluidized bed to produce hot gas for power generation is a promissing technique to overcome the use of impure raw materials with high combustion efficiency and energy savings. Modeling the motion of gas-solid fluidized bed within the interior of reactors is a complex task, because the interface is unknown, transient and the interactions are understood only for a limited range of conditions "Taghipour *et al*. (2005)". Two methods have been used for modeling gas-solid fluidized bed: first one use the discrete method based on molecular dynamics (Lagrangian model); second one uses a continuum approach based on continuum mechanics treating the two phases as interpenetrating continua (multifluid or Eulerian-Eulerian model) "Taghipour *et al.* (2005)". The Lagrangian models simulate individual particles, thus limiting the simulation in a small number of particles. However, in industrial scale the particle number necessary to represent the process is huge and has limited the application of such as approach. On the other hand, successfully efforts have been made in order to develop continua models able to reproduce average industrial scale behavior with reasonable computational work.

Mathematical models have proved their efficiency to investigate optimum operational conditions and reproduce virtually the industrial processes. The objective of this work is developing a computational model that simulates the fluidized bed phenomena considering two phases. The model uses the multiphase concept to simulate the flow in a 3D experimental fluidized bed reactor. Transport equations of mass, momentum and energy are solved using the finite volume method for non-orthogonal system implemented in a complex computational code written in Fortran 90/95. The phases in this model are modeled using continuum mechanics principles where collection of particles is considered identical having a representative diameter and density. The solid phase momentum equation is modified by an additional term to account for momentum exchange due to particle-particle collisions based on kinetic theory model (Gidaspow, 1994). The granular temperature, Θ, is defined to represent the specific kinetic energy of velocity fluctuations or the translational fluctuation energy resulting from the particle velocity fluctuations "Taghipour *et al.* (2005)". In granular flow, particle velocity fluctuations about the mean are assumed to result in collisions between particles being carried by the mean flow. The granular particle temperature equation can be expressed in terms of production of fluctuations by shear, dissipation by kinetic and collisional heat flow, dissipation proper to inelastic collisions, production by fluid turbulence or collisions with molecules, and dissipation owing to interaction with the fluid (Gidaspow, 1994). Several studies have shown the capability of the kinetic theory for modeling fluidized beds e.g. (Ding and Gidaspow, 1990), "Pain *et al.* (2001)". Despite of the development of models to simulate fluidized beds achieved maturity validation with experimental measurements must be carried out, mainly because some correlations used in the models are empirical or semi-empirical. This work considers a 3D transient model to analyze the motion and volume fractions of gas-solid phases in a column of an experimental scale fluidized bed reactor. This column was used to develop and validate the model by comparison with literature results for the behavior of solid particles in same conditions.

2. MATHEMATICAL MODELING

2.1. Transport equation

The present model consists of describing the phenomena that occurs in the interior of a rectangular column where a system with two phases is considered. The mathematical formulation assumes the continuous media hypothesis expressed by transport equations of mass, momentum and energy. The phenomena of mass, momentum and energy transfer inside column are represented by the general transport equation (equation 1). Where the index i represent the phases gas and solid. The effective diffusion coefficient (Γ_ϕ) describes different meanings depending upon equation to be solved, for example, if the momentum equation will be solved the effective diffusion coefficient assigns the dynamic viscosity. The source term (S_ϕ) represents generation or consumption of mass, momentum and energy. In the source term are considered for example the phenomena of interaction among phases, mechanics interactions resulting in the coupling between the equations of conservation of mass, momentum and energy. The models of momentum and energy were obtained from literature and were detailed in previous studies like fluidized bed and blast furnace "Taghipour *et al.* (2005)" and (Castro, 2000). In addition, this formulation was applied the kinetic theory of granular flow to account for the conservation of solid fluctuation energy and determining the solid stress terms of the momentum equations "Taghipour *et al.* (2005)".

$$\frac{\partial\left(\varepsilon_i\rho_i\phi_i\right)}{\partial t} + div\left(\varepsilon_i U_i\phi_i\right) = div\left(\varepsilon_i\Gamma_{\phi_i}\, grad\ \phi_i\right) + S_{\phi_i} \qquad (1)$$

The equation to consider the fluctuations energy of solid particles was introduced in the model and can be described by equation 2, "Taghipour *et al.* (2005)". This equation is solved and is used to determine the source of momentum in equation 1, in addition to the apparent viscosity term.

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\Theta_s\right) + grad\left(\varepsilon_s\rho_s\Theta_s\vec{v}_s\right)\right] = \left(-p_s\bar{I} + \bar{\tau}_s\right) : grad\,\vec{v}_s + grad\left(k_{\Theta_s}\cdot grad\,\Theta_s\right) - \gamma_{\Theta_s} \qquad (2)$$

Where, (Θ_s) is the granular temperature, (I) is the admensional stress tensor, ($\bar{\tau}_s$) is the stress tensor calculated by equation $\tau_s = \varepsilon_s\mu_s\left(\nabla\vec{v}_s + \nabla\vec{v}_s^T\right) + \varepsilon_s\left(\lambda_s - \frac{2}{3}\mu_s\right)\nabla\cdot\vec{v}_s I$, where λ_s is the bulk viscosity, p_s is the solid pressure, (γ_{Θ_s}) is the collision energy dissipation.

2.2. Boundary and initial conditions

To the set of differential equations represented by equation 1 must be imposed initial and boundaries conditions representing conditions of the process. Following the nomenclature presented in figure 1, the applied boundary conditions at the inlet is of prescribed value type. Wall type boundary conditions assume zero fluxes and tangential velocities and the particles can slip by the wall. The pressure reference is set at the inlet position while at outlet is assumed fully developed flow and symmetry is considered for all variables. The prescribed values and model parameters applied to simulate the fluidized bed are summarized in table 1, this parameters was obtained from literature and was used to validate the model with results obtained by others researchers. The initial conditions were assumed zero velocity, inlet pressure was 4400Pa and granular temperature (Θ_s) of 100m^2/s^2.

Table 1. Simulation model Parameters

Description	Value	Comment
Particle density, ρ_p	2500 kg/m^3	Glass beads
Gas density, ρ_g	1.225kg/m^3	Air
Mean particle diameter, d_p	275μm	Uniform distribution
Restitution coefficient, e_{ss}	0.90	Literature value
Initial solids packing, ε_{s0}	0.60	Fixed value
Superficial gas velocity, U	0.38m/s	~6*U_{mf}
Bed width	0.28m	Fixed value
Bed thickness	0.025m	Fixed value
Bed height	1.00m	Fixed value
Static bed height	0.40m	Fixed value
Inlet boundary condition	Velocity	Superficial gas velocity
Outlet boundary condition	Outflow	Fully developed flow
Time steps	0.001s	Specified
Convergence criteria	10^{-6}	Specified

2.3. Source terms

The gas and solid phases interacts exchanging momentum and energy. The momentum exchange is modeled by equation 3, with drag coefficient expressed by equation 4. This study uses the modified Richardson and Zaki drag function equation in order to represent the conditions of fluidized bed.

$$F_m = -C_{d_{g-s}}\left[\frac{3\varepsilon_s\rho_s}{4d_s\varphi_s}\right]\left[\vec{U}_g - \vec{U}_s\right]\left(\vec{U}_g - \vec{U}_s\right) \tag{3}$$

$$C_{d_{g-s}} = \left[\frac{24}{\mathrm{Re}_{g-s}}\left(1 + a\,\mathrm{Re}_{g-s}^{\,b}\right) + \frac{c}{1 + \dfrac{d}{\mathrm{Re}_{g-s}}}\right]\left(\frac{\varepsilon_g}{\varepsilon_g - \varepsilon_s}\right)^{-4,65} \tag{4}$$

Where the terms a, b, c and d are functions of shape factor of solid (φ) (Castro, 2000). Observing the drag function equation (equation 4) is perceivable that even so the volumetric fraction of the solid phase can be zero, the Reynolds number will not be, therefore the condition of similarity for the momentum equation will not be reached, because always will exist particles' drag.

2.4. Numerical features

The set of non linear partial differential equations with corresponding boundary and initial conditions was solved numerically applying the finite volume method. The discretization equations are obtained in an irregular and structured mesh with non-orthogonal system located in the bottom corner, where each control volume has a local system of coordinate related to a global one. The discretized set of algebraic equations is solved by iterative line by line method (ADI) using the algorithm for solution of a tri-diagonal matrix. The coupling pressure-velocity for the gas phase is treated using the SIMPLE algorithm with staggered grid. The solid phase uses the continuity equation to calculate its volumetric fraction. The mesh used in this study is show in figure 1 with 6x30x102 divisions defining a total of 11200. These dimensions where selected aiming to minimize numerical errors and the time step selected 1×10^{-06} showed good numerical stability.

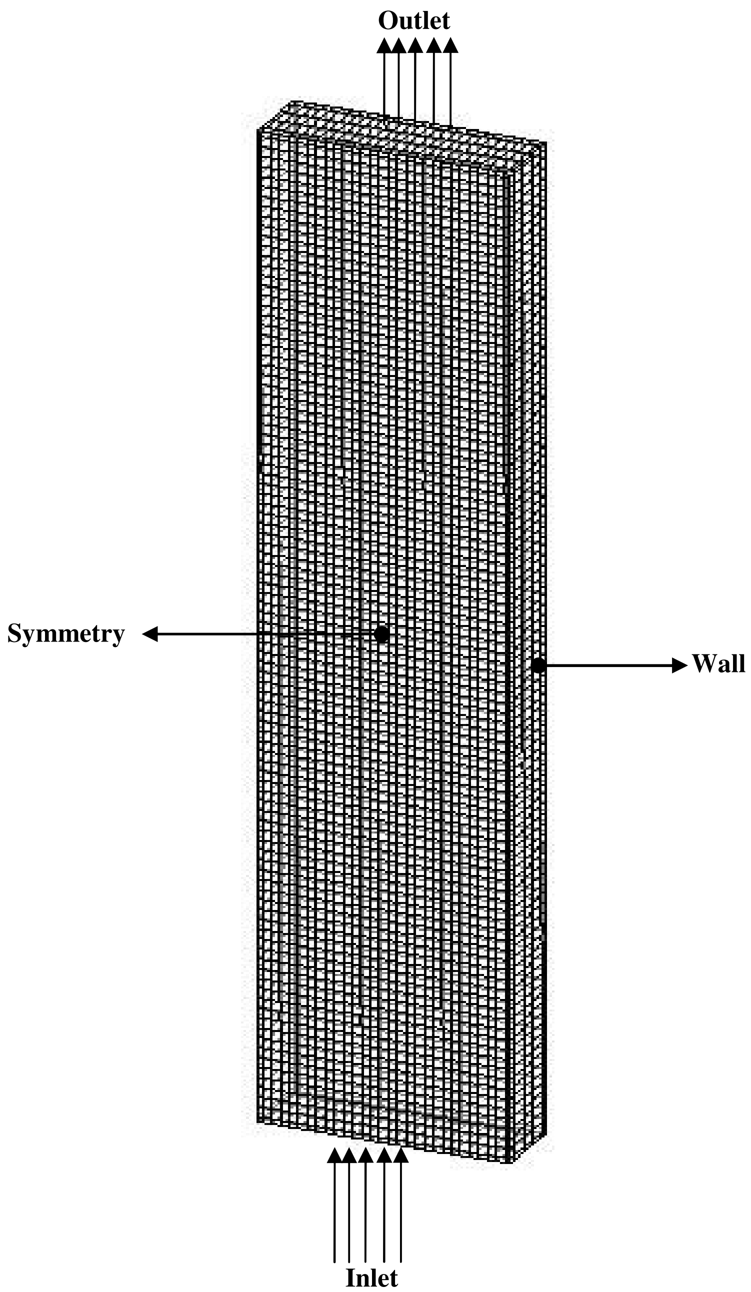


Figure 1. 3D image showing the finite volume mesh and boundary conditions types used for model predictions

3. RESULTS AND DISCUSSION

The results presented in this section were calculated using experimental physical model with similarity to industrial scale of fluidized bed reactor used to gasification of coal and biomasses. The mass flow rates values and boundary conditions were used directly in the model. The computed results are compared with previous work selected from literature. The minimum fluidization velocity a key parameter for fluidized bed processes was assumed (U_{mf} = 0.065 m/s) and the gas velocity used for fluidization was approximately $6U_{mf}$ (U= 0.38 m/s).

The figure 2 shows 2D images representing time evolution of fluidization phenomena for a total simulation time of 3s. It is observed a continuum bed height evolution until stabilization occurs for a time of 2.5s and then, only recirculation of the particles is observed. At early stages bubbles formation is observed and bed expansion is very fast. After 2.5s only fluctuation of particle and bubbles formation is observed with a fluidization pattern. Despite the bubbles formation is evidenced this bubbles are explosives and are formed near the gas inlet, but few centimeters of elevation the bubbles transforms into a slug, these characteristics are in accordance with experimental results as narrated by "Hoomans *et al*.(1996)". In the following times is observed a disorganized movement of particles within the bed which characterize that fluidization was developed with chaotic transient bubble generation and particle movement as described by "taghipour *et al*. (2005)".

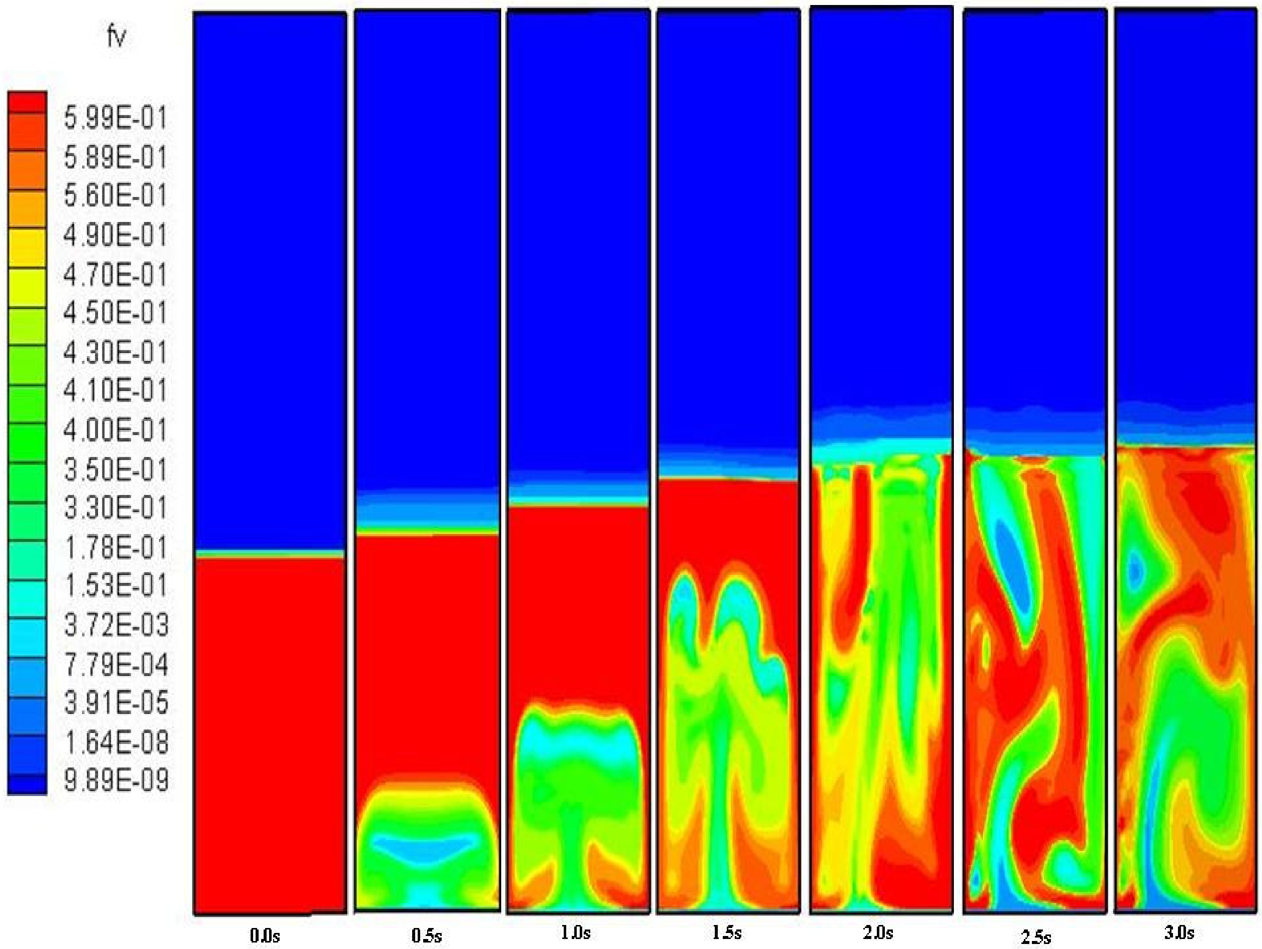
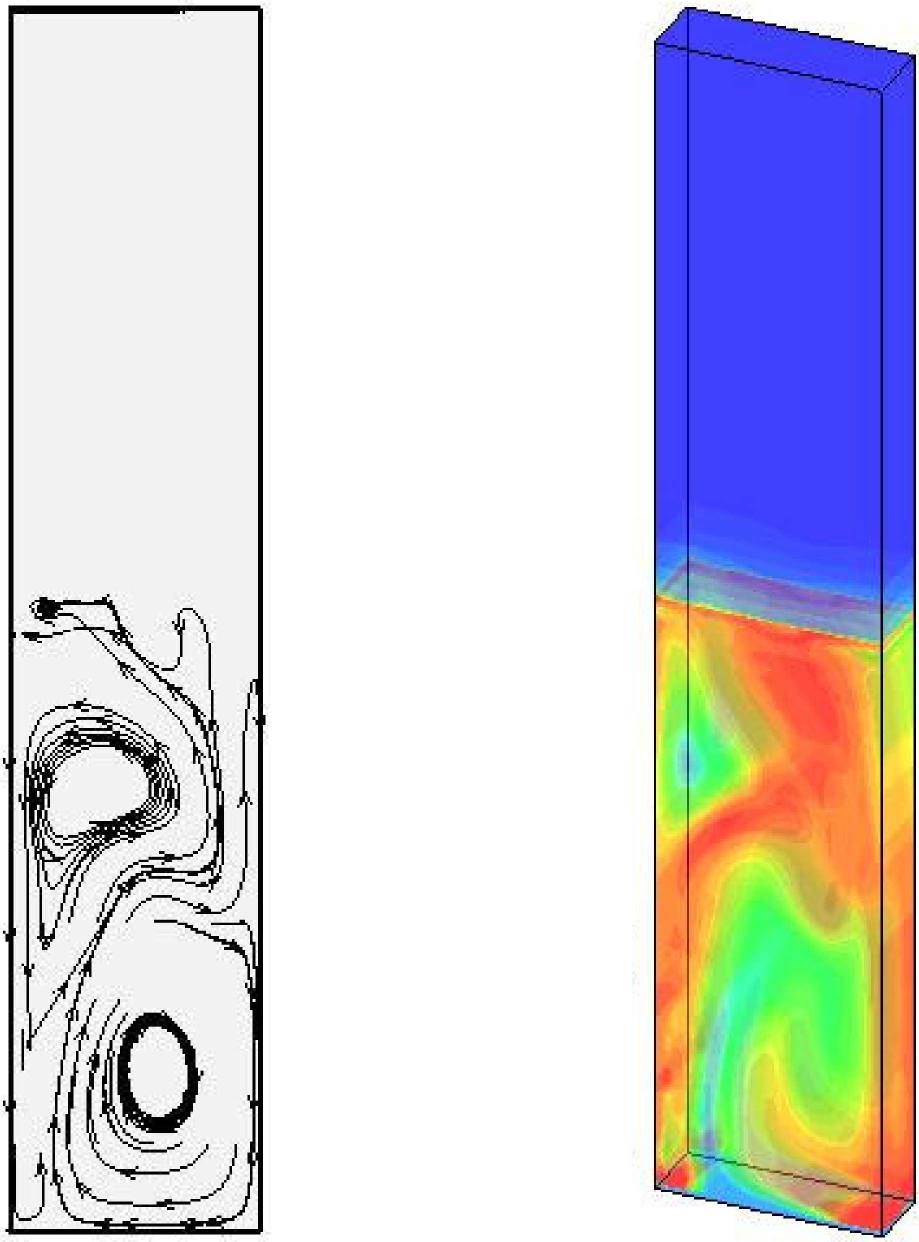


Figure 2. Model predictions of fluidized bed height evolution in a vertical plane (t =0s-3s), with time step of $1x10^{-06}$ s

Figure 3 (a) shows the stream traces for solid particles in the bed at time (t = 3s). In this figure can be seen that the particles in the inferior part of the bed, where the particles movement characterizes the fluidization phenomena, are continuously rising up and falling down in the bed. The recirculation of particles is evidenced showing that the fluidization is developed and the particles residence time in the recirculation region increases which is important for fluidized bed reactor efficiency. As pointed out in previous work, the solid particles in the lower region start to circulate as the gas velocity increase beyond U_{mf} "Kawaguchi *et al.* (1998)". The extent of circulation is a function of gas velocity U, and increases with gas velocity until the maximum value. When the gas velocity becomes higher than the maximum value the solid particles are carried from the bed and unstable operational conditions is observed characterizing slugging transport. In figure 3(b) the 3D image showing fluidized volumetric fraction of solid particles is presented for t=3s. Fluidized bed expansion is evident and a pattern of large particle cluster is observed.



(a) (b)

Figure 3. Stream lines showing the motion of solid particles in the fluidized bed (a) and 3D image showing contour plot of volumetric fraction of solid particles in fluidized bed column in (b), after (t = 3s).

In order to verify the influence of gas velocity on fluidization pattern some cases were investigated. In figure 4, two selected cases are shown with U= 0.12m/s and U=0.72m/s. Figure 4(a) shows the fluidized bed pattern for lower velocity. In this case fluidization pattern was observed, however, bed expansion was not evidenced and also bubbles formation was insignificant. In this case the gas motion was predominantly vertical and fluctuation of solid volume fraction was negligible. On the other hand, for high velocity conditions, $U \geq 0{,}38$m/s, the bubbles formation is significant and the bed expansion reaches larger values together with higher fluctuation of the solid volume fraction. In figure 4(b) the gas velocity is very high compared with the minimum fluidization, U=0.72 m/s, in this condition the bed expansion is very fast and reached high values (H/H_0 = 0.35), particles are moved to upper part of the bed and some particles starts to be carried toward the outlet of the reactor, indicating undesirable operational condition. From these simulations, is possible to recommend operational flow rates which leads to velocities in the range of 0.4 m/s to 0.6 m/s as safety conditions in order to guaranty stable and efficient operation.

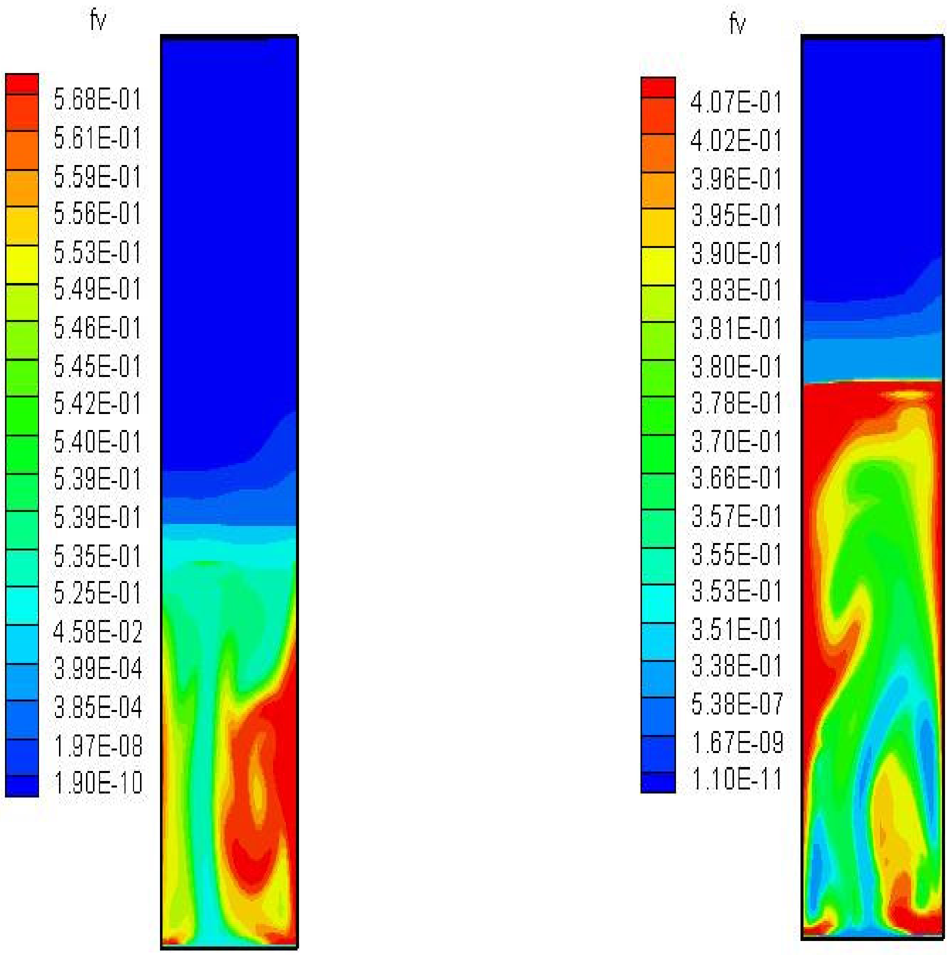


Figure 4. The contour plot of volumetric fraction of solid particles using differents gas velocities, (a) U= 0.12m/s, (b) U= 0.72m/s.

Some parameters are normally monitored during fluidization process, among them one of the most important is the pressure drop, ΔP. This parameter is important because the volume fraction of gas-phase across the bed can be estimated from ΔP (Kunii and Levenspiel, 1991). The pressure drop predicted by this model is compared with other models in figure 5, "Taghipour *et al.* (2005)". In this figure presents results of ΔP obtained using Syamlal, O'Brien and Gidaspow models, usually implemented in commercial software, favorably compared with this model. At the beginning of the simulation the model predicted slightly higher pressure drop and then become stable around the averaged value. The discrepancy observed at the beginning compared with other models could be attributed to the methodology for calculating the solid volume fraction which in this model is based on direct solution of the continuity equation, instead of empirical correlations based on pressure drop as implemented in previous work. Other way to justify the discrepancy could be attributed to the convergence criteria used in this work which was 1.10^{-06} while in previous work was 1.10^{-03} this difference meaning great stability in the calculus presented in this work. The pressure drop instability reflects the total fluctuation and formation of bubbles and clusters, which in turn after stabilization indicates suitable fluidization conditions for operation. Another important parameter in fluidized bed is the expansion rate, because this parameter shows the displacement of particle column of fluidized bed. This parameter can be seen in the figure 6, where the rate obtained in this work with simulated velocities (U=0.12, 0.38, 0.72m/s) are compared with experimental and same previous models results. As observed, the model presents expansion rates values closer to previous models following same pattern when compared with experimental data. The explanation for such behavior is owing to the drag coefficient functions used in all models can not cover all the fluidization ranges observed locally within the reactor, however all models presented similar trends compared with experimental results.

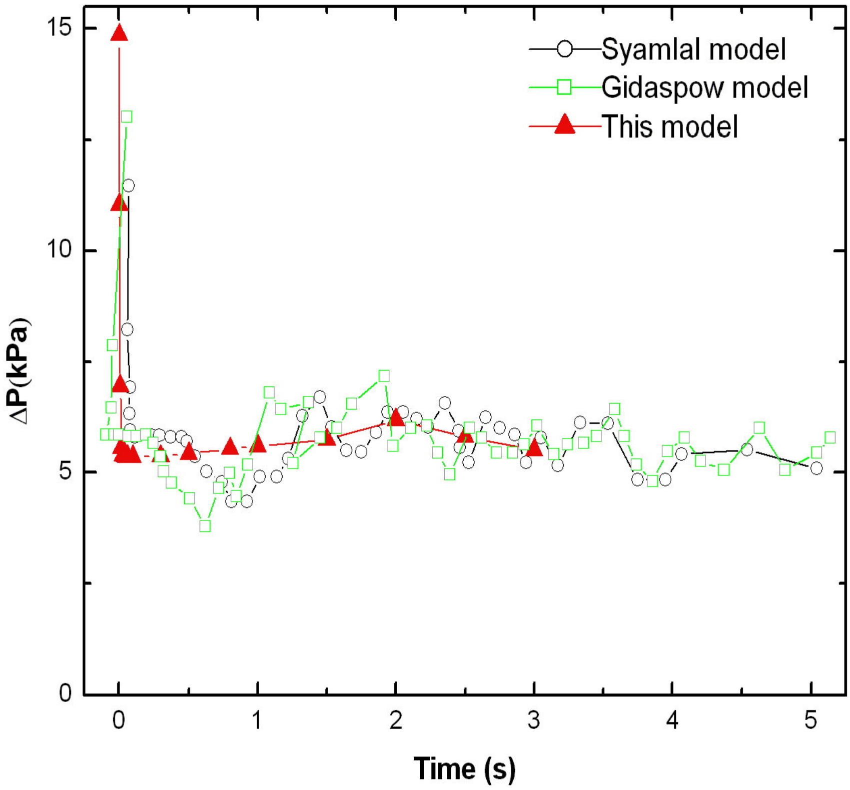


Figure 5. Pressure drop (ΔP) obtained by this model and after “taghipour *et al*. (2005)” using differents drag coefficient functions.

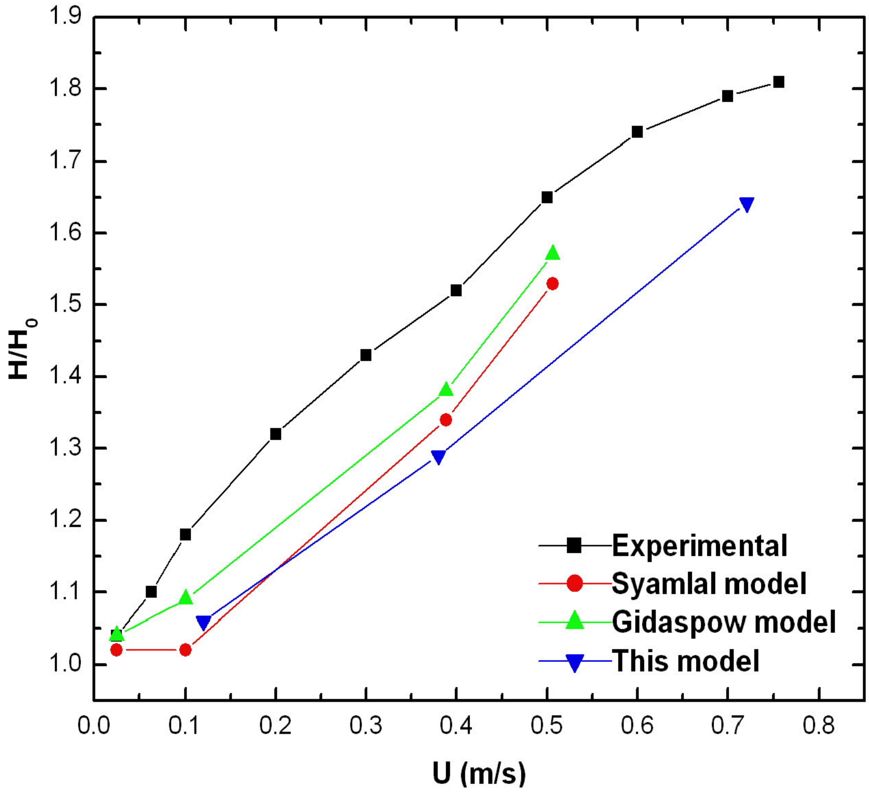


Figure 6. Comparison of experimental and simulated expansion rate of fluidized bed H/H_0 presented by “taghipour *et al*. (2005)”and this model to gas velocity of (U= 0.12, 0.38, 0.72m/s), respectively.

4. CONCLUSIONS

A computer code based on transport equations discretized on the basis of finite volume method has been developed to simulate the fluidized bed reactors considering gas-solid systems. The model has been compared with literature results and showed close agreement for conditions of similarity with experimental scale. Results in two and three dimensions were presented and discussed aiming to elucidate the behavior of solid particles into the fluidized bed column. Parameters such as ΔP and the bed expansion rate showed good agreements with experimental and previous results obtained from literature using different drag functions than the used in this model development. The bed expansion rate in this model showed almost linear behavior. The volumetric fraction contour lines for all cases analyzed presented similar pattern when compared with previous work. The bubble formation is seen in the beginning of process, but these are formed on gas inlet, therefore, some centimeters of gas inlet it explodes and the slug is characterized in the process. This fact could be explained not only by distance between bubbles not be favorable to the growing, but also the diameter and density of particles inhibit the bubbles formation beyond particles tend to float at the bed surface "Zhou *et al*. (2004)".

5. ACKNOWLEDGEMENTS

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