CHARACTERIZATION AND QUANTIFICATION OF COHERENT STRUCTURES IN A GAS-SOLID FLOW: INFLUENCE OF THE DISCRETIZATION SCHEME FOR THE ADVECTIVE TERM

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Abstract. *The effects of the order of the discretization schemes in the results of numerical simulation for single phase flows are widely argued in the literature. However, due to the complexity of the equations system involved and of the numerical solution methods, suches studies become of difficult interpretation for several phase flows. In this work it applies an methodology for the identification and characterization of coherent structures in well-known as clusters in the results of numerical simulation for the gas-solid flow in the ascending tube of a circulating fluidized bed (CFB) and they evaluate the effects of the order of the discretization schemes of convective term on the quantification and characterization of the same. It develops numeric simulation using two models to the knowledge: the traditional model of two fluid calculating the viscosity and pressure of the solid phase through empiric correlations and the model based in the kinetic theory of the granular flows (KTGF) with a partial differential equation for compute of the granular temperature. In the simulations it uses the code MFIX developed in NETL (National Energy Technology Laboratory). The introduced results comprehend graphs of the clusters properties according to the introduced methodology. They consider the upwind discretization scheme of first order and Superbee scheme of second order. At work was going used a computational mesh in cartesian coordinates 2D. The results show that the order of the discretization schemes exercises a considerable influence in the quantification and characterization of the coherent structures – clusters. Comparisons considering three-dimensional simulation must clear even the differences here pointed.*

Keywords: *Numerical simulation, numerical diffusion, discretization schemes, circulating fluidized bed, clusters.*

1. INTRODUCTION

In this paper a methodology of identification and characterization of coherent structures mostly known as clusters is applied to hydrodynamic results of numerical simulation generated for the riser of a circulating fluidized bed (CFB). After a cluster is identified, its four basic characteristics, as defined by Tuzla *et al.* (1998) and Sharma *et al.* (2000), can be calculated. These characteristics are average duration time, average solid volumetric fraction, fraction of existence time and frequency of occurrence. The identification of clusters is performed by applying a criterion related to the time average value of the volumetric solid fraction. A qualitative rather than quantitative analysis is performed mainly owing to the unavailability of operational data used in the considered experiments. It intends to evaluate the qualitative influence in the performance of CFB considering the characterization and quantification of the clusters, when it varies the order of the convectives schemes for discretization of the respective terms present in the conservation equations. Concerning qualitative analysis, the simulation results are in good agreement with literature.

2. MATHEMATICAL FORMULATION

The numerical simulation is performed using the MFIX (Multiphase Flow with Interphase eXchanges) code developed in NETL (National Energy Technology Laboratory) (SYAMLAL *et al.* (1993)), which includes the two-fluids IIT's hydrodynamic model B. It develops numeric simulation using two models to the knowledge: the traditional model of two fluid calculating the viscosity and pressure of the solid phase through empiric correlations, the traditional procedure was going applied by Tsuo and Gidaspow (1990), Sun and Gidaspow (1999), Huilin and Gidaspow (2003), and Cabezas-Gómez and Milioli (2003, 2004, 2005a,b), among others, and the model based in the kinetic theory of the granular flows (KTGF) with a partial differential equation for compute of the granular temperature (Tab. 1.). The model presented in the Tab. 1 is identical to model presented by Agrawal's *et al.* (2001), with the next modifications: the correlation for the radial distribution function g_0 is due Carnahan and Starling (1969) and option standard in the code MFIX. Other consideration refers to the momentum equations for both the phases where considers the model B and a last difference is due to the model of drag considered.

Table 1. Hydrodynamic Model B using the KTGF procedure for the computation of the solids phase constitutive relations.

1. Continuity equation, phase k (k = g, s)

$$\frac{\partial(\rho_k\alpha_k)}{\partial t}+\nabla\cdot(\rho_k\alpha_k \mathrm{v}_k)=0\ .$$

2. Momentum equation

Gas phase:

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g\vec{v}_g\right)+\nabla\cdot\left(\alpha_g\rho_g\vec{v}_g\vec{v}_g\right)=-\vec{\nabla}P+\rho_g\vec{g}+\alpha_g\nabla\cdot\tau_g-\vec{f}$$

Solid phase:

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s\vec{v}_s\right)+\nabla\cdot\left(\alpha_s\rho_s\vec{v}_s\vec{v}_s\right)=\alpha_s\left(\rho_s-\rho_g\right)\vec{g}+\alpha_s\nabla\cdot\tau_s-\nabla\cdot P_s+\vec{f}$$

3. Conservation of Granular Energy:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\alpha_s\rho_s\theta\right)+\vec{\nabla}\cdot\left(\alpha_s\rho_s\vec{v}_s\theta\right)\right]=-\vec{\nabla}\cdot\vec{q}-\tau_s:\nabla\vec{v}_s+\Gamma_{desl}-J_{col}-J_{vis}\ ,$$

where:

$\Gamma_{desl}=\dfrac{81\alpha_s\mu_g^2\left|\vec{v}_g-\vec{v}_s\right|}{g_0 d_p^3\rho_s\sqrt{\pi\theta}}$: Rate of granular energy production due to the sliding gas-particle;

$J_{col}=\dfrac{48}{\sqrt{\pi}}\eta(1-\eta)\dfrac{\rho_s\alpha_s^2}{d_p}g_0\theta^{3/2}$: Rate of granular energy dissipation due to inelastic collisions;

$J_{vis}=3\beta\theta$: Rate of granular energy dissipation due viscous deadening.

Constitutive relations and of closing:

4. Gas phase stress tensor

$$\tau_g=-\mu_g\left[\nabla\vec{v}_g+\left(\nabla\vec{v}_g\right)^T-\tfrac{2}{3}\nabla\cdot\vec{v}_g I\right]$$

5. Drag between solid and gas phases:

$\vec{f}=\beta\left(\vec{v}_g-\vec{v}_s\right)$ and β given by:

Interface drag function , β, Model B,

Ergun (1952) for $\alpha_s \geq 0{,}2$:

$$\beta=150\frac{\alpha_s^2\mu_g}{\alpha_g^2(d_p\phi_s)^2}+1.75\frac{\rho_g\alpha_s\left|\mathrm{v}_g-\mathrm{v}_s\right|}{(\alpha_g d_p\phi_s)}\ .$$

Wen and Yu (1966) for $\alpha_s < 0{,}2$:

$$\beta=\frac{3}{4}C_{Ds}\frac{\rho_g\alpha_s\alpha_g\left|\mathrm{v}_g-\mathrm{v}_s\right|}{(\alpha_g d_p\phi_s)}\alpha_g^{-2.65}$$

Where

$$C_{Ds}=\begin{cases}\dfrac{24}{Re_s}(1+0.15\cdot Re_s^{0.687})\ Re_s<1000\\ 0.44 \qquad\qquad Re_s\geq 1000\end{cases}$$

and $$Re_s=\frac{\alpha_g\rho_g\left|\mathrm{v}_g-\mathrm{v}_s\right|d_p\phi_s}{\mu_g}$$

6. Solid phase stress tensor:

$$\tau_s=\left[\alpha_s\rho_s\left(1+4\eta\alpha_s g_0\right)\theta-\eta\mu_b(\nabla\cdot\vec{v}_s)\right]I-\left(\frac{2+\alpha}{3}\right)\left\{\frac{2\mu^*}{g_0\eta(2-\eta)}\left(1+\tfrac{8}{5}\alpha_s g_0\right)\left(1+\tfrac{8}{5}\eta(3\eta-2)\alpha_s g_0\right)+\tfrac{6}{5}\eta\mu_b\right\}S$$

with:

$$S=\tfrac{1}{2}\left(\nabla\vec{v}_s+(\nabla\vec{v}_s)^T\right)-\tfrac{1}{3}\left(\nabla\cdot\vec{v}_s\right)\bar{\bar{I}}\ ,$$

$$g_0=\frac{\left(2-\alpha_s\right)}{2\left(1-\alpha_s\right)^3}\ ,\qquad \mu^*=\frac{\mu}{1+\dfrac{2\beta\mu}{(\rho_s\alpha_s)^2g_0\theta}}\ ,$$

$$\mu=\frac{5\rho_s d_p\sqrt{\pi\theta}}{96},\quad \mu_b=\frac{256\mu\alpha_s^2 g_0}{5\pi},\quad \eta=\frac{(1+e)}{2}\ .$$

7. Solid phase pressure:

$$P_s=\rho_s\alpha_s\theta\left[1+2\left(1+e\right)g_0\alpha_s\right].$$

8. Granular energy diffusive flux:

$$\vec{q}=-\frac{\lambda^*}{g_0}\left\{\left(1+\tfrac{12}{5}\eta\alpha_s g_0\right)\left(1+\tfrac{12}{5}\eta^2(4\eta-3)\alpha_s g_0\right)+\frac{64}{25\pi}\left(41-33\eta\right)\eta^2\alpha_s^2 g_0^2\right\}\nabla\theta$$

and $$\lambda^*=\frac{\lambda}{1+\dfrac{6\beta\lambda}{5(\rho_s\alpha_s)^2g_0\theta}}\ ,\quad \lambda=\frac{75\rho_s d_p\sqrt{\pi\theta}}{48\eta\left(41-33\eta\right)}\ .$$

9. Solid phase Boundary condition (Johnson & Jackson (1987))

$$\vec{n}\cdot\tau_s\cdot t+\frac{\pi}{2\sqrt{3}\alpha_{s\,max}}\phi'\rho_s\alpha_s g_o\theta^{1/2}v_{sl}=0,$$

$$\vec{n}\cdot\vec{q}=\frac{\pi\sqrt{3}}{6\alpha_{s\,max}}\phi'\rho_s\alpha_s g_0\theta^{1/2}\left|v_{sl}\right|-\frac{\pi\sqrt{3}}{4\alpha_{s\,max}}\left(1-e_w^2\right)\rho_s\alpha_s g_0\theta^{3/2}$$

$$v_{sl}=v-v_w$$

3. IDENTIFICATION AND CHARACTERIZATION OF THE CLUSTER

Soong *et al.* apud Sharma *et al.* (2000) had been based on the following lines of direction to define clusters:

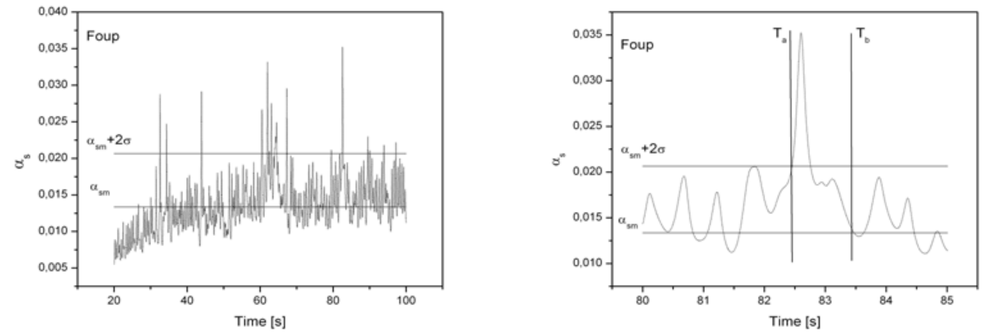
- The concentration of solids in the cluster must be significantly higher than the local time-averaged solid concentration at a given local position for a particular set of operational conditions.
- A perturbation in the concentration of solids due to clusters must be higher than the random ground fluctuations of the solid fraction.
- This concentration perturbation should be measured in a sample volume with characteristic length one or two orders of magnitude longer than the particle diameter.

Considering the above, Soong *et al.* (2000) proposed the following criterion: the value of the local instantaneous solid volumetric fraction for a cluster should be higher than its time-averaged value by two times the standard deviation (2σ). This way the clusters can be identified and considered as such when an instantaneous solid fraction exceeds that limit. This criterion was used by Tuzla *et al.* (1998) to detect clusters in a downer fluidized bed. Sharma *et al.* (2000) slightly changed the above criterion on the basis of experimental evidence. In addition to the Soong *et al.* (2000) developments, Sharma *et al.* (2000) proposed the following criteria for life-time of a cluster:

- The cluster is detected when the instantaneous solid fraction becomes larger than the time-averaged solid fraction plus two times the standard deviation (2σ).
- The starting time of a cluster corresponds to the last time at which the instantaneous solid fraction exceeds the time-averaged solid fraction before satisfying the 2σ criterion.
- The end time of a cluster corresponds to the first time at which the instantaneous solid fraction falls below the time-averaged solid fraction after falling below the 2σ criterion.

The proposition of Sharma *et al.* (2000), denominated as the average-referenced criterion, renders a cluster duration longer than that provided by the 2σ criterion of Soong *et al.* (2000).

The proposed procedure by Sharma *et al.* (2000) adopted in this work is illustrated in the Fig. 1. Figure 1(a) illustrates a temporal signal of the local solid volumetric fraction resultant of the numeric simulation. Be indicated the solid average concentration in time $\overline{\alpha}_s$ and the threshold $\overline{\alpha}_s + 2\sigma$. In the Fig. 1(b) presents an enlargement of this signal between 80 and 85 seconds, where observes the existence of "cluster" in the interval T_a and T_b. Once "clusters" are identified by the reference average criterion, the four basic characteristics of the clusters can be calculated, that are, the average duration time, the occurrence frequency, the existence time fraction and the average solid concentration.



(a) (b)

Figure 1. Temporal variation of typical local volumetric fraction of solid resultant of the simulation and application of Sharma *et al* (2000) proposition for quantification life time of cluster.

4. METHODOLOGY FOR IDENTIFICATION AND CHARACTERIZATION OF THE CLUSTERS

Average duration time (τ_c): the average time of duration of all clusters in a sample volume. (In Sharma *et al.* (2000) the relevant volume is the volume of the used capacitance probe; when results of simulation are used the relevant volume is that of one computational cell.) Assuming τ_i is the duration time of a single cluster, τ_c results: $\tau_c = \frac{\sum_1^n \tau_i}{n}$ where n is the total number of clusters detected in the observation period.

Frequency of occurrence (N_c): the frequency at which the clusters are observed in the sample volume. It is calculated as the average number of clusters per second that are observed during the entire observation period.

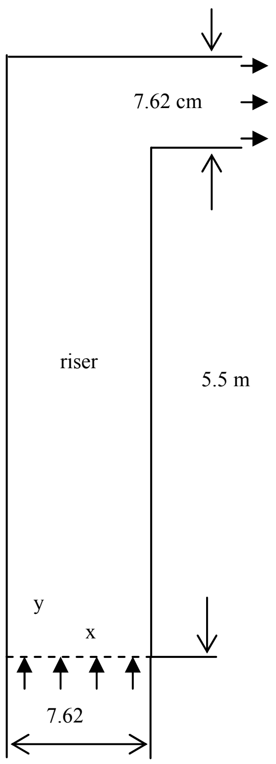
Existence time fraction (F_c): the fraction of the observation period in which there are clusters in the sample volume: $F_c = \frac{\sum_1^n \tau_i}{\tau}$.

Average solid concentration (α_{sc}): the sum of the time-averaged solid fractions for all the clusters over the total number of clusters detected (n) in the observation period, i.e., $\alpha_{sc} = \frac{\sum_1^n \overline{\alpha}_{s,i}}{n}$.

The above characteristics can also be calculated for cross-sectional average values, i.e., $\langle f \rangle = \frac{1}{2R}\int_0^{2R} f(x)dx$ where x is the horizontal coordinate direction and $2R$ is the cross-sectional length.

This section was based in Cabezas-Gómez (2003) e Cabezas-Gómez *et al.* (2008).

5. COMPUTATIONAL DOMAIN AND INITIAL AND BOUNDARY CONDITIONS



Simulation data:

Solids particle diameter: d_p = 520 μm
Solids particle density: ρ_s = 2620kg/m^3
Solids recirculation rate: G_s = 24.9 kg/(m^{2}s)
Gas phase dynamic viscosity: $\mu_g = 1.8\times10^{-5}$ Pa s

Initial conditions:

Empty riser
P = 101.325 kPa
T = 300 K

Inlet boundary conditions:

v_s = 0.386 m/s
v_g = 4.979 m/s
α_s = 0.0246
P = 120.6639 kPa
T = 300 K

Outlet boundary conditions:

Continuity condition: $\frac{\partial f}{\partial n} = 0$
where f is either α_g, u_g, or u_s.
Gas phase pressure: P = 117.2049 kPa

Wall boundary conditions:

Gas phase: no-slip
Solids phase: partial slip $\vec{v}_{s,w} = -\frac{d_p}{\alpha_s^{1/3}}\frac{\partial \vec{v}_s}{\partial n}$
Solids fraction and pressure: null normal gradient

Computational conditions:

Numerical mesh:
Mesh: (20×146) 2920 knots: δx = 0.381 cm, δy = 3.81 cm
Simulation time: t = 100 s

Figure 2. Geometry and initial and boundary conditions used in the simulations assuming Cartesian coordinates. (In accordance with Luo, (1987)).

Figure 2 shows the computational domain used in the developed simulations. It considers Cartesian system of coordinates. The geometric dimensions and initial, boundary, inlet and outlet conditions are specified in the figure for both phases. In the case of the gas phase it considers the condition of no slip. For the simulations using the traditional model in the solid phase it uses the partial slip condition in the tangential direction to the wall according with Ding and Gidaspow (1990) (this partial slip condition for the solid phase was implemented in MFIX for the development of this work). In the normal direction it considered null speed for both the phases. For the pressure and the fraction of solid in the walls it considered free slip, or be, null gradient in the normal direction to the wall.

6. NUMERICAL RESULTS

In the present work comparisons among clusters properties obtained from results of simulation with the schemes Foup and "Superbee" and the physical models considered in three sections different from the bed are presented. These sections characterize regions which vary of the dense to the dispersed according with the Fig. 3. It owes note that although reference average criterion detect "clusters" in the region inferior of the bed, this was not considered for ends of analysis of the properties of "clusters", because the same is a region characterized by the high concentration of solid and your performance it resembles to the of a bubbling bed (Johnsson *et al.*, 2000) and thus "clusters" can't exist in fact. For bigger details to consult Cabezas-Gómez (2003).

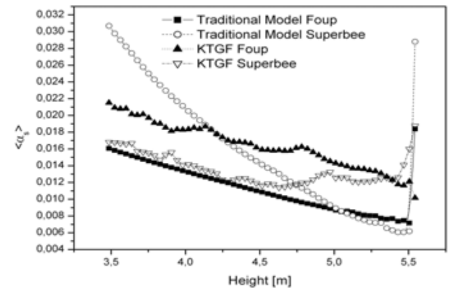


Figure 3. Average volumetric fraction of solid in the section in function of the bed height for the considered models and Foup and Superbee schemes

In the densest and more dispersed regions of the bed it verifies the existence of a quantitative difference in the compute of the volumetric fraction of solid by the different discretization schemes and considered physical models (Fig. 3). This difference influences compute of clusters properties as it can be observed in the Fig. 5 – 7.

As much in the densest region represented by the Fig. 5 as in the more dispersed region represented in the Fig. 7 it observes significant differences for average frequency of occurrence of clusters, $\langle N_c \rangle$ and for the time fraction of average existence of clusters, $\langle F_c \rangle$ when considered KTGF's model regarding the traditional model. For this ones properties it evidences an inversion in the order of the values, that is, in the larger part of transversal section of the densest region so much $\langle N_c \rangle$ as $\langle F_c \rangle$ computed from results of simulation obtained with KTGF present smaller values in comparison to the traditional model while in the more dispersed region occurs the opposite, agreeing with the quantitative behavior of the average volumetric fraction of solid in this regions and represented in the Fig. 3. For average duration time $\langle \tau_c \rangle$ and for average solid fraction $\langle \alpha_{sc} \rangle$ of clusters the biggest differences meet in the regions next to the wall.

When the discretization schemes for the advective terms are considered, the dispersed region is that one which supplies the most interesting data. The Fig. 3 evidences that for the KTGF model the results of simulation with the Superbee scheme characterize throughout the bed a more dispersed region than the obtained when it uses the Foup scheme. And even so, the clusters observed in this region present larger concentration of solid and consequently smaller time of duration (Figs. 5, 6), thus the wavering of the solid phase volumetric fraction (α_s) are more intense and better captured with the high order schemes. This phenomenon evidences the high degree of the numeric viscosity present in the Foup scheme carrying thus the gradient smoothing of α_s, as shown in the Fig. 4.

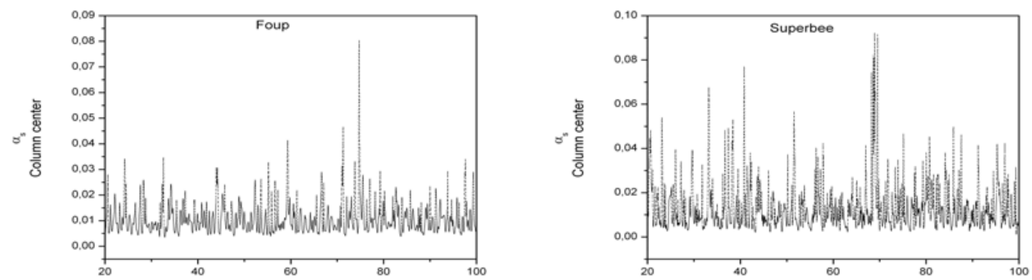


Figure 4. Temporal variation of volumetric fraction of solid obtained to 5.5 m of the bed entrance from simulation results with the KTGF model

This must be one of the aspects to be considered when if objective to investigate the influence of the numeric diffusion in the results of simulation of a circulating fluidized bed.

In the intermediary region represented in the Fig. 6 the calculated properties from the results of simulation with both models don't present significant differences except for $\langle \tau_c \rangle$ and of $\langle \alpha_{sc} \rangle$ in the regions next to the bed walls.

It verifies in the dispersed region (Fig. 7) that all of the models captured the bed geometry influence (lateral exit to the right), introducing clusters with larger density and larger time of duration in the left wall, region characterized by recirculation and accumulation of solid.

Section 3.5 meters

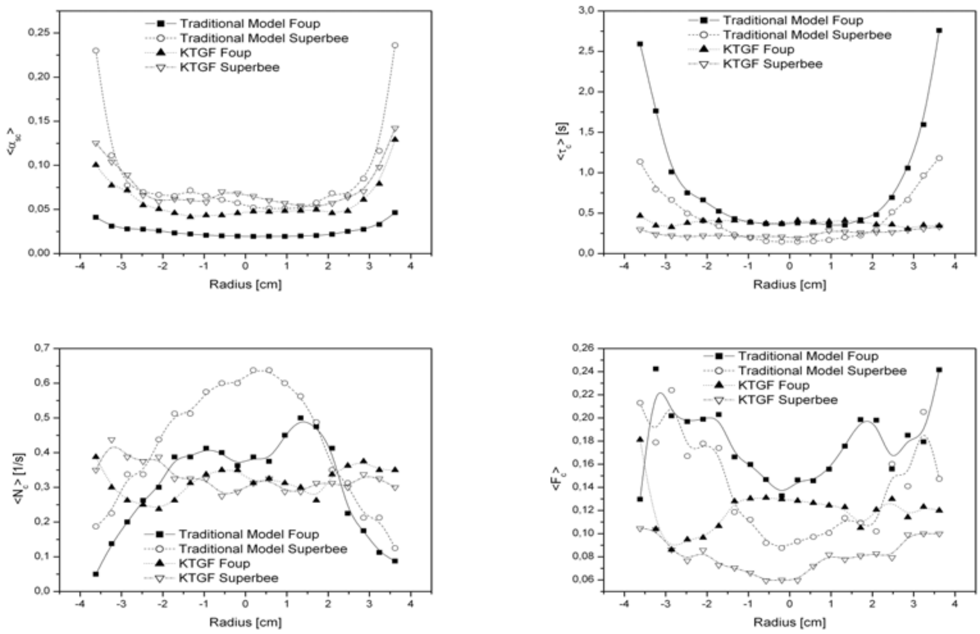


Figure 5. Average properties of clusters in the section 3.5 meters above of the bed entrance obtained with the traditional and KTGF models

Section 4.5 meters

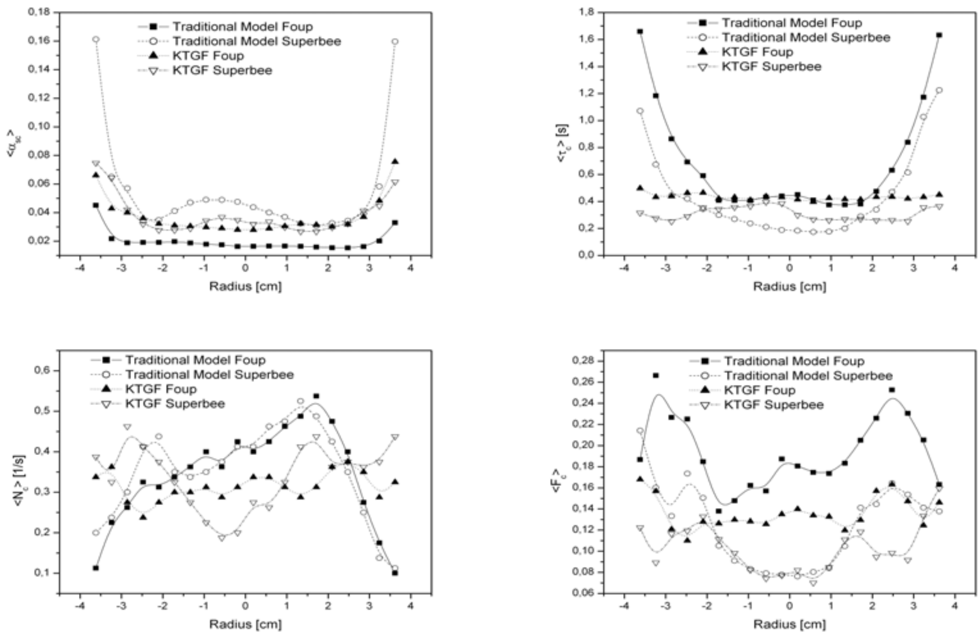


Figure 6. Average properties of clusters in the section 4.5 meters above of the bed entrance obtained with the traditional and KTGF models

Section 5.5 meters

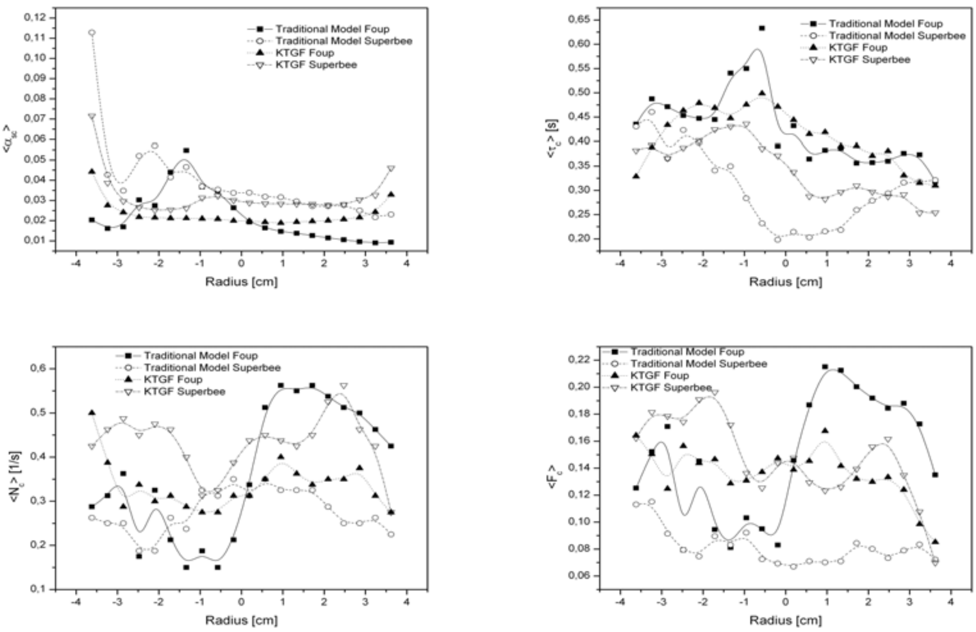


Figure 7. Average properties of clusters in the section 5.5 meters above of the bed entrance obtained with the traditional and KTGF models

7. CONCLUSIONS

With base in the Fig. 5 to 7 and in the definitions of the clusters properties (section 4) can establish the next relationships when it considers the order of the discretization schemes for the advective terms:

i) The order high schemes provide capture of the clusters with larger density and with smaller time of duration along the column;

ii) By they present smaller time of duration, these clusters present an minor time frequency of existence, $\langle F_c \rangle$, compared with the captured when it uses the first order scheme;

iii) The frequency of occurrence of clusters, $\langle N_c \rangle$, seems to be directly related with the concentration of volumetric fraction of solid, α_s, in the observed region. And thus presents values larger in the dense and intermediary region with the different models for the results obtained with the high order scheme and in the dispersed region the biggest values are obtained with the first order scheme, Foup, like shown in the Fig. 8;

iv) An immediate consequence of the situation presented in the item iii) is just that clusters number observed along the column presents the same behavior, as it can be evidenced in the Fig. 9.

The relationships iii) and iv) are assertions based in the results of simulation obtained, being necessary a more careful investigation, mostly about the influence of the refine of mesh in the two-dimensional results presented here.

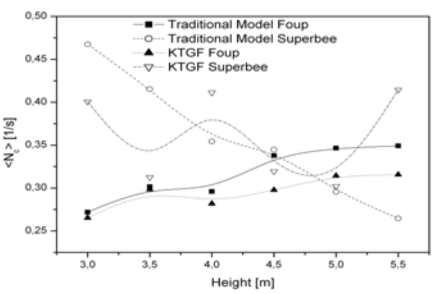


Figure 8. Average occurrence frequency of clusters along the column with the different models and Foup and Superbee schemes

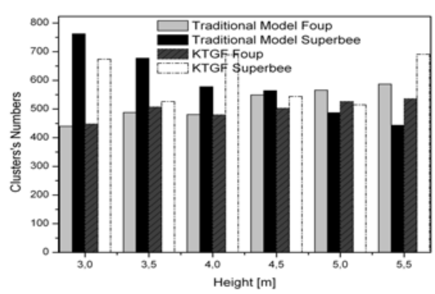


Figure 9. Clusters Number observed along the column with the different models and Foup and Superbee schemes

8. ACKNOWLEDGEMENTS

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