PAPER II

Towards time-averaged CFD modelling of circulating fluidized beds

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TOWARDS TIME-AVERAGED CFD MODELLING OF CIRCULATING FLUIDIZED BEDS

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Abstract - In case of large CFBs, steady state CFD simulation can be an attractive alternative for the time-consuming transient simulations. In the present paper, the features of equation closure of a steady state model are evaluated on basis of a transient 3D simulation. The computational results are analysed to determine the averaged flow properties and the main fluctuating components and their correlations. The main terms to be modelled for the steady state approach are, according to this analysis, the average gas-particle drag force and the Reynolds stresses arising from velocity fluctuations. Suggestions for approaches for steady state equation closure in case of industrial CFB applications are discussed.

INTRODUCTION

CFD modelling of circulating fluidized beds is most often done using the kinetic theory model of granular flow and a transient description. The large size of industrial CFBs makes it impossible to resolve the finest flow structures by fine meshes. The practically applicable coarse meshes necessitate development of sub-grid scale closures for the unresolved fluctuations. In transient coarse mesh simulations, the fraction of momentum transfer expressed by the subgrid-scale closures increases in comparison to the momentum transfer expressed by the average velocities and volume fractions as the mesh becomes coarser. An even larger portion of momentum transfer is expressed by closure relations in steady state models. However, there is no large conceptual difference between the steady state and the coarse mesh closure models. Since steady-state simulations should produce the average flow much faster, steady-state simulation can be an attractive alternative for large CFBs.

Several attempts to develop closure models for coarse-mesh and steady-state simulations have been presented in the literature. Closure models are usually based on transient simulations of the detailed flow structures in a fairly small scale. Agrawal et al. (2001), Andrews et al. (2005) and Igci et al. (2006) studied the average drag and stress terms through simulations in small domains with periodic boundary conditions. Zhang and VanderHeyden (2001) discussed the effects of mesh spacing on Reynolds stresses and the drag force. In Zhang & VanderHeyden (2002), they suggest an added-mass force closure for the correlation between fluctuations of the pressure gradient of the continuous phase and fluctuations of solids volume fraction. De Wilde (2007a) analysed the same term from simulations and accounted also for the drag force in the derivation of new closure models that were applied in De Wilde (2007b) for steady state simulation of a riser. Zheng et al. (2006) presented a two-scale Reynolds stress turbulence model for gas-particle flows leaving the parameters undetermined. All the correlation terms resulting from integration over a large volume and/or a long time step have been addressed in the publications listed above. Unfortunately none of these papers consider all features that would be of interest to us when studying steady state modelling of large risers. Anisotropy and the influence of the real CFB geometry are addressed in the present study.

For analysis of requirements for closure relations we have here chosen to simulate a laboratory scale process with a reasonably fine mesh. In this way we have realistic CFB conditions and at the same time we still manage to produce the main fluctuation patterns. The results are validated through comparisons with measurements, which justifies time averaging on the computational results and drawing conclusions on the significance of different terms in the equations as indications for further studies.

DESCRIPTION OF THE NUMERICAL SIMULATIONS

The case studied in Kallio (2006) and in the present paper is a cold model experiment. The particle size in the simulated case is 230 μm and the material density 1800 kg/m^3. The riser height is 7.3 m (coordinate y goes from 0 to 7.3 m) and the cross-section measures 1 m times 0.25 m (x = 0…1 m, z = 0…0.25 m). The average superficial gas velocity above the air distributor is 4 m/s. The local inlet velocities are described by means of a function based on a 2D approximation of the air distributor used in the experiment. The 3D grid of the present study consists of 102400 (40 X 160 X 16) elements and it is refined towards the walls. The time step in the simulation was 5 ms. A time period of several seconds was simulated with 2 ms time stepping, but since the fluctuation characteristics shown by the results were practically unchanged, the longer time step was chosen.

The transient simulations presented here were conducted by means of the kinetic theory model of the Fluent 6.3.26 CFD software (Fluent, 2006). The solid phase kinetic viscosity was calculated from the model by Syamlal et al. (1993). The k-ε turbulence model used in the simulations was the version modified for multiphase flows ("dispersed turbulence model", Fluent (2006)). First order discretization for time stepping and second order interpolation for spatial discretization were employed.

Since the mesh used here is too coarse to produce the smallest clusters, we have to correct the drag force. The procedure used here for gas-solid drag is the same as used in Kallio (2006). The adjustment of the drag force is based on experimental data from CFBs. Close to the minimum fluidization conditions the drag force is calculated from the Ergun (1952) equation. Elsewhere in dense conditions, an equation based on the two-phase theory of bubbling beds is applied. For more dilute suspensions the drag is calculated from an empirical correlation of an exponential form. The single particle drag law is used in extremely dilute gas-solid suspensions. The voidage function, by which the single particle drag force is multiplied in the drag model, is shown in Fig. 1.

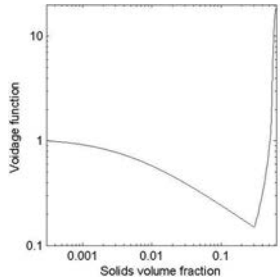


Fig. 1. The voidage function used for d_s=230 μm, ρ_s=1800 kg/m^3, and slip velocity 1 m/s.

To allow us to study the effects of wall friction on the fluctuations, one simulation was carried out using the free slip boundary condition and another one with the partial slip model of Johnson and Jackson (1987) that utilizes a specularity coefficient as a measure of the fraction of collisions which transfer momentum to the wall. To examine the maximum possible wall effects we set the specularity coefficient to one, which is certainly too high a value but useful for our purposes. Fig. 2 shows results obtained with the two models. Wall friction slows down movement of clusters at the walls and as a result the clusters grow and produce a wider wall layer. Solid concentration in the upper parts of the riser increases which is seen in Fig. 2c. No significant change in the fluctuation patterns could be observed. The rest of the analysis of this paper is based on the simulation with the free slip boundary condition, since we have more simulation data from that case. Fig. 3 shows a comparison of the measured and the simulated solid velocities and volume fractions at three different locations in the riser.

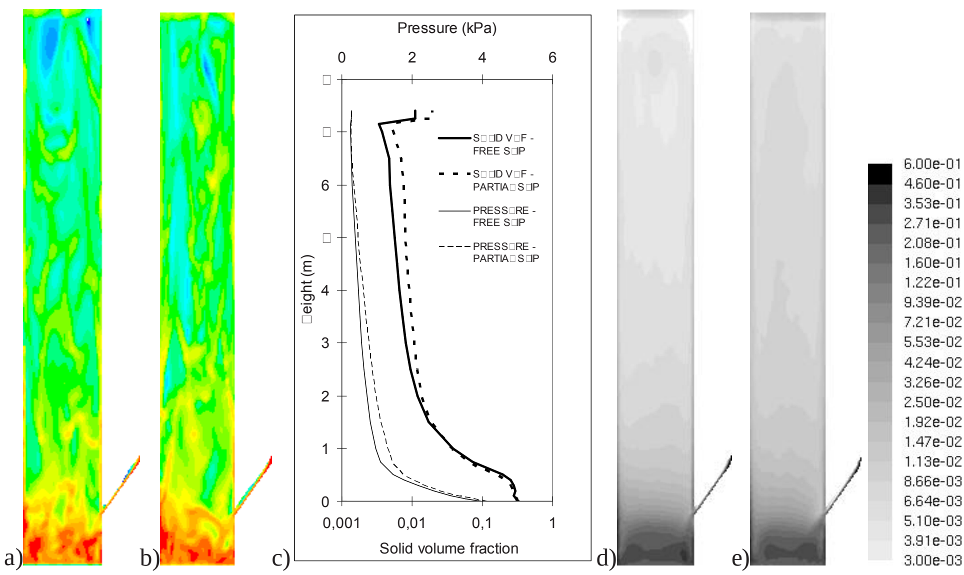


Fig. 2. Instantaneous flow patterns obtained using a) free slip and b) partial slip boundary condition. c) Vertical profiles of the average pressure and voidage distributions in the simulations with free slip and partial slip boundary conditions, respectively. Time-averaged solids volume fraction obtained with d) free slip boundary condition and e) partial slip boundary condition.

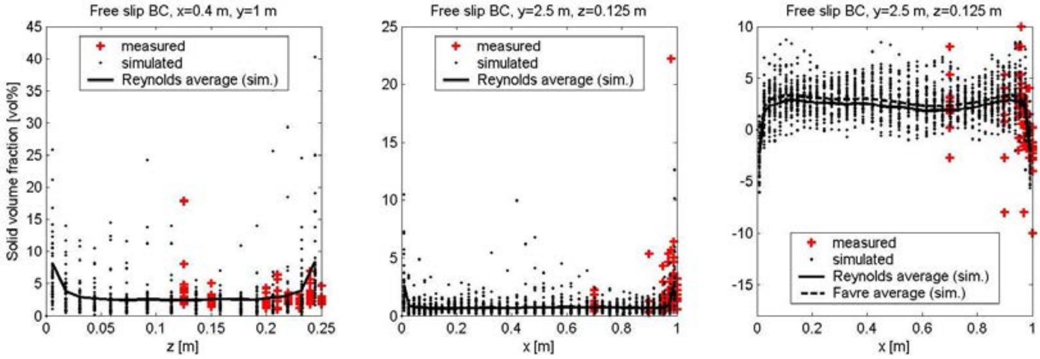


Fig. 3. Comparison between measured and simulated solid velocities and volume fractions along two cross-sectional lines. Vertical coordinate is denoted by y and the horizontal coordinates by x and z, respectively. For additional comparisons, see Kallio (2006).

ANALYSIS OF THE TERMS IN THE TIME-AVERAGED EQUATIONS

Time-averaged momentum equation

The solid phase momentum equation used in the simulations above can be written in the following form:

$$\frac{\partial}{\partial t}(\alpha_s\rho_s\mathbf{u}_s)+\nabla\cdot(\alpha_s\rho_s\mathbf{u}_s\mathbf{u}_s)=-\alpha_s\nabla p-\nabla p_s+\nabla\cdot(\alpha_s\boldsymbol{\tau}_s+\alpha_s\boldsymbol{\tau}_s^t)+\alpha_s\rho_s\mathbf{g}+K_{sf}\left(\mathbf{u}_f-\mathbf{u}_s\right) \quad (1)$$

where the stress terms are as follows:

$$\boldsymbol{\tau}_s=2\mu_s\left(\frac{1}{2}(\nabla\mathbf{u}_s+(\nabla\mathbf{u}_s)^T)\right)+(\lambda_s-\frac{2}{3}\mu_s)\nabla\cdot\mathbf{u}_s\mathbf{I} \quad (2)$$

Equation (1) will now be time-averaged. For velocities we use Favre averaging and for the rest Reynolds averaging. If a time-average is denoted by < >, we obtain the following equation:

$$\begin{aligned}\nabla\cdot\left(\langle\alpha_s\rangle\rho_s\langle\mathbf{u}_s\rangle\langle\mathbf{u}_s\rangle\right)=&-\langle\alpha_s\rangle\nabla\langle p\rangle+\nabla\cdot\left(\langle\alpha_s\tau_s\rangle+\langle\alpha_s\tau_s{}^t\rangle\right)-\langle\nabla p_s\rangle\\&+\langle\alpha_s\rangle\rho_s g+K_{sf}^*\left(\langle\mathbf{u}_f\rangle-\langle\mathbf{u}_s\rangle\right)+S_{\mathrm{Re}}+S_D+S_P\end{aligned} \quad (3)$$

where K_{sf}^* is the drag coefficient calculated from the average flow properties. The three terms resulting from correlations between fluctuations of the flow properties are

Reynolds stress term: $S_{\mathrm{Re}}=-\left[\langle\nabla\cdot(\alpha_s\rho_s\mathbf{u}_s\mathbf{u}_s)\rangle-\nabla\cdot\left(\langle\alpha_s\rangle\rho_s\langle\mathbf{u}_s\rangle\langle\mathbf{u}_s\rangle\right)\right]$ (4)

Solids volume fraction and pressure gradient correlation: $S_P=-\langle\alpha_s\nabla p\rangle+\langle\alpha_s\rangle\nabla\langle p\rangle$ (5)

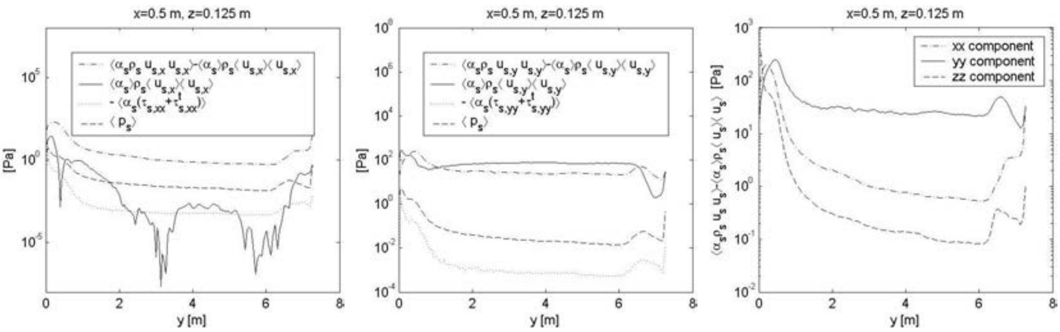
Drag correction: $S_D=\langle K_{sf}(\mathbf{u}_f-\mathbf{u}_s)\rangle-K_{sf}^*\left(\langle\mathbf{u}_f\rangle-\langle\mathbf{u}_s\rangle\right)$ (6)

In the following we analyse these terms and the averages of the local stresses from the simulation results and compare them with the other terms in the equations. From the simulation, data was collected at every 4th time step. Simulated time period was 4.5 minutes and hence we have at each studied point data from 13500 time instances.

Stress terms

Several authors (e.g. Agrawal et al. (2001)) have reported that the local stress terms arising from the particle scale phenomena and given in our work by the kinetic theory models are small compared to the stress terms produced by the fluctuating motion of clusters. The same observation was made in our work. The only term that locally has significance is the solid pressure, which in the dense conditions close to walls can be of the same order of magnitude as the leading terms in the horizontal momentum equations. Whether it, even in these situations, has any significant effect on the flow field at large is questionable. Analysis of the gas phase local turbulent stresses showed that they can locally be important in areas of very high shear rates like in the vicinity of the wall layer.

Fig. 4 shows the normal component of the local stress term in comparison with convection term and with the Reynolds stresses arising from meso-scale fluctuations. The curves are for the riser axis and there the local stresses and local solid phase pressure are negligible compared to the other terms. The Reynolds stress terms dominate solids momentum transfer in the horizontal direction throughout the riser height. In the vertical direction momentum equation, Reynolds stresses dominate in the splash zone and close to the exit of the CFB whereas in the rest of the riser convection terms are larger. Gas phase Reynolds stresses arising from meso-scale fluctuations exhibit the same pattern. However, vertical gas momentum transfer is dominated by convection also at the riser bottom. Figure 4c shows a comparison of the normal Reynolds stress components. In the bottom bed region, horizontal stresses are large, but they decrease fast above the bottom bed. Close to the exit there is again an increase in the horizontal Reynolds stress components.



a) b) c)

Fig. 4. Comparison of convection and normal stress components in the solid momentum equation on the centreline (x=0.5 m, z=0.125 m) as a function of height (u is x-direction and v y-direction velocity component, respectively).

From the data of Fig. 4c it is possible to calculate a bulk viscosity if we use an equation of the same form as equation (2) and assume that bulk viscosity alone is responsible for the normal component of the Reynolds stress. Figure 5 shows that the resulting bulk viscosities are completely different in different directions and, moreover, they change as a function of height.

Similar analysis as for the normal components was also done for the shear stress terms. Both the solid and gas phase shear stress terms are of a similar magnitude as the corresponding convection terms. Determination of the solids viscosity from the data was difficult outside the wall layer. The order of magnitude of solid viscosity was typically 1-30 kg/sm. According to our study, shear stress terms are extremely difficult to express with a single constant viscosity.

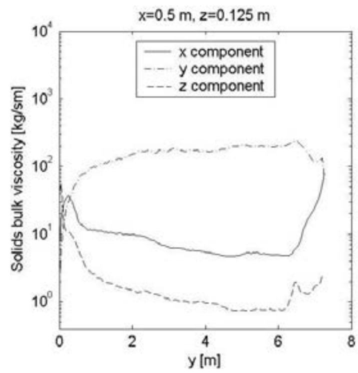


Fig. 5. Solids bulk viscosity calculated from the Reynolds stresses on the centreline (x=0.5 m, z=0.125 m) as a function of height.

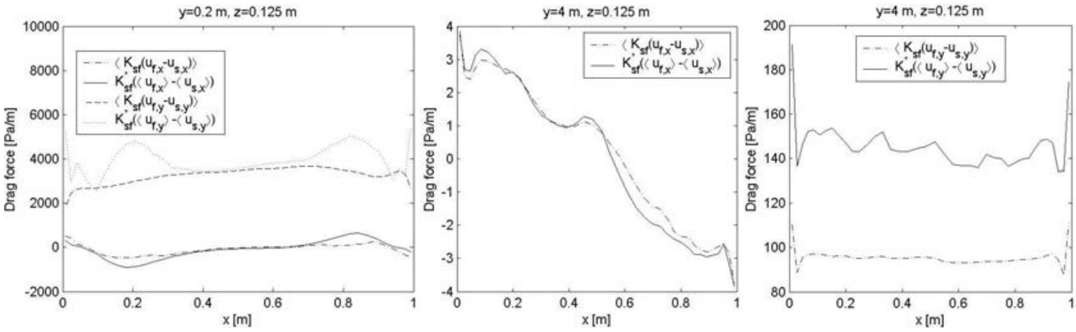
Gas-solid interaction

In the literature, the focus in coarse-mesh/steady-state modelling has often been on the terms describing gas-solids interaction, i.e. the drag term and the pressure gradient term. An effective drag coefficient for coarse-mesh/steady-state simulations has been determined by averaging the vertical drag force components from a detailed simulation (see e.g. Igci et al. (2006) and Andrews et al. (2005)). Zhang & VanderHeyden (2002) and De Wilde (2007a) found in their studies surprisingly large effect from the correlation between pressure gradient fluctuations and solids volume fraction fluctuations and derived an added mass type closure for this term. The conditions in those simulations, in which this S_P term was found to be important, were denser than in the major part of a CFB and hence we consider a further analysis necessary.

From our simulation data we have determined the three components of the drag force and S_P and compared them with the other terms in the equation. In Fig. 6 the average drag force is compared with the drag force obtained by inserting the average velocities and solids volume fraction in the same drag model that was used in the transient simulation. In Fig. 6a, the horizontal x component and the vertical y component of the obtained drag force are shown at 0.2 cm height in the riser where dense suspension conditions prevail.

Figures 6b and 6c show the x and y components of the drag force obtained at 4 m height in dilute conditions. At this height the vertical drag force component obtained from the drag law using average flow properties is systematically much higher than the actual average drag between the phases and, consequently, a correction to the drag law seems necessary. The average horizontal force component, however, is fairly well obtained from the drag model used. In the dense bottom bed conditions, the situation looks more complicated and the results do not suggest any systematic correction to the drag law.

The studies in the literature have concentrated on the vertical drag force component. Our results would indicate that the need for corrections to the drag law in the horizontal and vertical directions is not equal. This should be taken in to account in future models, since the drag force is a significant term in both gas phase and solid phase momentum equations. However, as our simulation is conducted in a fairly coarse mesh with a drag law that already includes a correction for the sub-grid scale clusters, our conclusions should be verified in simulations with fine meshes.



a) b) c)

Fig. 6. Average drag force compared with the drag that is obtained with the same model using the average velocities and voidage. a) Horizontal and vertical drag components at z=0.125 m and height y=0.2 m. b) Horizontal drag component at z=0.125 m and y=4 m. c) Vertical drag component at z=0.125 m and y=4 m.

In Fig. 7 the correction S_D to the vertical component of the drag force is compared with the Reynolds stress term S_{Re} and the term S_P (see Eqs. 4-6) at two elevations. At 0.2 m height, i.e. in the bottom bed region, the three terms are roughly of the same order of magnitude. S_P is smallest of the three terms. At 4 m height, the drag correction is the dominating term except in the wall layer, where the Reynolds stress becomes large. The term S_P that other researchers (e.g. Wilde (2007a)) have found important in dense conditions is now practically zero. Similar analysis was carried out for the horizontal terms and the horizontal Reynolds stress was found to be the dominating component throughout the riser.

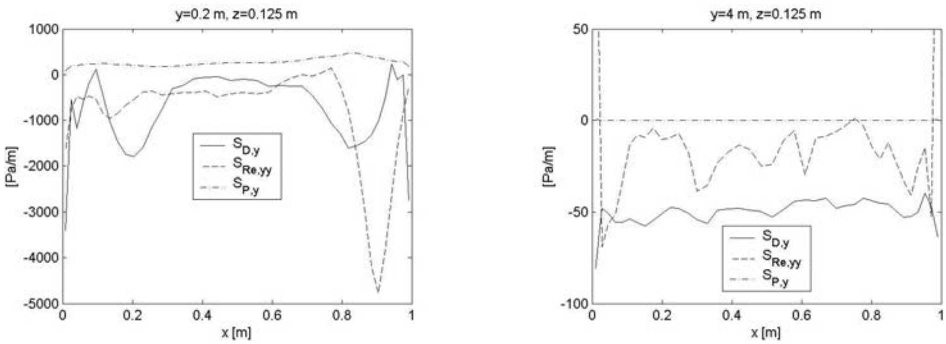


Fig. 7. The different terms in the time-averaged momentum equation. Left: at position z=0.125 m and height y=0.2 m. Right: at position z=0.125 m and height y=4 m.

Our results seem to slightly differ from the ones presented by Zhang & VanderHeyden (2002) and De Wilde (2007a). They found S_P important while we didn't find any region where it would have a dominating effect. One reason for the discrepancy is the lower suspension density of our study. Furthermore, the size of the domain studied was larger in our simulation: it is less likely to find a correlation between the local pressure and local solids content in a large riser where the pressure is determined by flow patterns in the whole riser.

CONCLUSIONS

In case of large CFBs, a steady state CFD simulation can be an attractive alternative for the time-consuming transient simulations. In the present paper, the requirements for equation closure of steady state models were evaluated on basis of a transient 3D simulation. The results were analysed to obtain averaged flow properties and the main fluctuating components and their correlations. The main terms to be modelled for the steady state approach are, according to this analysis, the average gas-particle drag force and the Reynolds stresses arising from velocity fluctuations. According to our analysis of the transient simulation results, the correction for time-averaged gas-particle interaction force should not be isotropic. The normal Reynolds stresses dominate momentum transfer in the horizontal direction and in the bottom bed also in the vertical direction. The shear Reynolds stresses are significant. On basis of the analysis, modelling of the complicated behaviour of the Reynolds stresses by means of constant viscosities seems uncertain and hence alternative approaches such as transfer equations for determining the Reynolds stresses should be considered.

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NOTATION

d	diameter [m]
$\mathbf{g}$	gravitational acceleration [m/s^2]
p	pressure [N/m^2]
u,$\mathbf{u}$	velocity [m/s]
K_{sf}	momentum exchange coefficient [kg/sm^3]
S_D	drag correction term (Eq. 6) [kg/m^2·s^2]
S_P	correlation of α_s and ∇p (Eq. 5) [kg/m^2·s^2]
S_{Re}	Reynolds stress term (Eq. 4) [kg/m^2·s^2]
α	volume fraction [-]
λ	second (bulk) viscosity [kg/m·s]
μ	dynamic viscosity [kg/m·s]
ρ	material density [kg/m^3]
$\boldsymbol{\tau}$	stress tensor [N/m^2]

Subscripts

s	solid phase
x,y,z	rectangular coordinates

Superscripts

t	turbulent

Other symbols and operators

∇	gradient operator
$\langle a \rangle$	time average of the variable a

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