

Title: **Modeling and simulation of the effects of
mesoscale structures in circulating fluidized beds**

Author(s): Duan Z. Zhang and W. B. Vanderheyden

Submitted to:

<http://lib-www.lanl.gov/la-pubs/00796388.pdf>

Modeling and simulation of the effects of mesoscale structures in circulating fluidized beds

D.Z. Zhang and W.B. VanderHeyden
Theoretical Division, Fluid Dynamics Group
T-3, B216
Los Alamos National Laboratory
Los Alamos, NM 87545

Abstract

Mesoscale structures such as particle clusters have been observed both experimentally and in numerical computer simulations of circulating fluidized beds. In numerical simulations, these structures result from nonlinearities present in even the simplest of two-fluid models based on closure models that account only for phase interactions at the scale of the particles. Simple particle-fluid drag closure models are one example. In many cases, the mesoscale structures have been demonstrated to have predominant effects on the macroscopic behavior of fluidized beds. As a result, some two-phase flows can be computed using very simple two-phase flow averaged conservation equations as long as enough resolution is used. Such an approach, however, is impractical for engineering simulations of fluidized beds due to excessive computational costs. To predict the macroscopic behavior of a fluidized bed with reasonable computation cost, averaged equations must be developed with more sophisticated closure relations that model the mesoscale structures. To obtain such closure models, we perform a second average over the simple averaged equations for two-phase flows and develop insight into closure models using data from high-resolution computer simulations. From these data we examine the characteristics of the basic physics involved in these terms. We suggest some tentative closure models.

1 Introduction

It has been found both experimentally and numerically, that mesoscale structures, such as, bubbles, particle clusters and streamers exist in gas-solid two phase flows. These mesoscale structures significantly affect the dynamics of fluidized beds. Recently, Agrawal *et al.* (2000) performed two-dimensional simulations using a set of two-phase flow equations and kinetic theory to

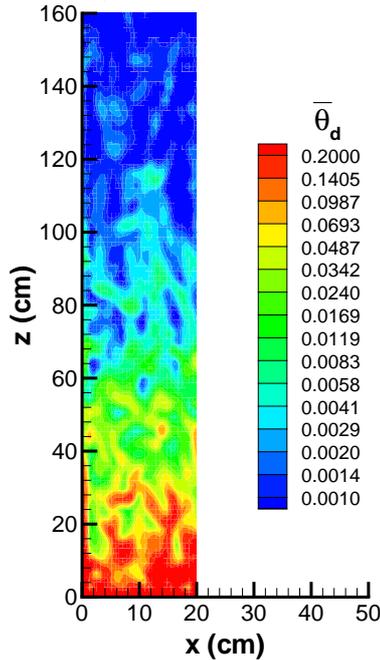


Figure 1: A snapshot of particle volume fraction contour on a mid-plane of the experimental device used by Van den Moortel *et al.*(1998). The experimental section of the device is a square duct with 20cm side, and 200cm in height. The overall volume fraction in the device is 3%. The particle material density is 2.4 g/cm^3 , and mean diameter is $120\mu\text{m}$ with $20\mu\text{m}$ of standard deviation. The fluid is gas at room temperature.

model effects of particle-particle interactions. They found that the averaged terminal velocity of the particle phase does not converge until very fine grids are used. They also found that Reynolds stresses in the particle phase result mainly from the mesoscale interactions and the contribution from the kinetic theory of granular materials is negligible. Furthermore, Zhang and VanderHeyden (2000) used a set of highly simplified equations for two-phase flow, and neglected all particle-particle interactions at the particle scale, to simulate an experiment performed by Van den Moortel *et al.* (1998). When high grid resolution was used, a mesoscale structure was observed as shown in Figure 1, and good quantitative agreement between numerical results and experiment were found. For instance, the comparison of the calculated mass fluxes are compared to experimental values in Figure 2. This agreement with data is further evidence that the macroscopic behavior of a gas-solid fluidized bed is dominated by mesoscale interactions.

Although, these mesoscale scale structures can be captured with the fine grid resolution used in our simulation, direct application of the equations used to engineering practice is not realistic. To simulate 21 seconds of real time in the small fluidized bed of Van den Moortel *et al.*, we used an SGI Origin 200 machine with two processors in parallel. It took us 51 days of wall-clock time or about 100 CPU days. For engineering applications, we seek to derive a set of macroscopic equations that accounts for the effects of

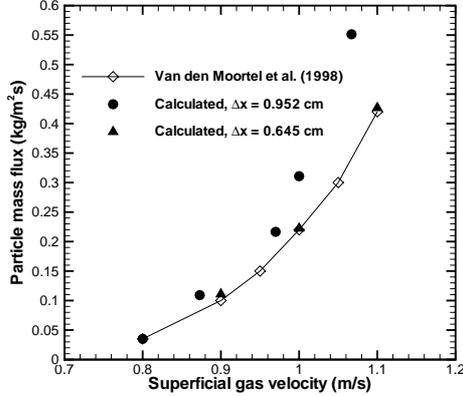


Figure 2: Comparison of calculated mass fluxes with the experimental values.

mesoscale interactions.

2 Phase interaction forces at difference scale

By performing an ensemble phase average of momentum equations Zhang and VanderHeyden (2001b), found that the macroscopically averaged equations for both phases can be written as

$$\rho_d \left[\frac{\partial \theta_d \mathbf{u}_d}{\partial t} + \nabla \cdot (\theta_d \mathbf{u}_d \mathbf{u}_d) \right] = \theta_d \nabla \cdot \boldsymbol{\sigma} + \nabla \cdot (\theta_d \mathbf{R}_d) + \theta_d (\mathbf{f}_d + \mathbf{f}_m) + \theta_d \rho_d \mathbf{g}, \quad (1)$$

$$\rho_c \left[\frac{\partial \theta_c \mathbf{u}_c}{\partial t} + \nabla \cdot (\theta_c \mathbf{u}_c \mathbf{u}_c) \right] = \theta_c \nabla \cdot \boldsymbol{\sigma} + \nabla \cdot (\theta_c \mathbf{R}_c) - \theta_d (\mathbf{f}_d + \mathbf{f}_m) + \theta_c \rho_c \mathbf{g}, \quad (2)$$

where ρ is density, θ is volume fraction, \mathbf{u} is the averaged velocity, \mathbf{R} is the Reynolds stress, \mathbf{f}_d is average drag acting on each of the particles in the flow, \mathbf{f}_m is the averaged mesoscale force, and $\boldsymbol{\sigma}$ is the averaged continuous stress. Subscript d in the above quantities stands for the disperse (particle) phase and subscript c stands for the continuous phase. The mesoscale force \mathbf{f}_m is defined as

$$\theta_d \mathbf{f}_m = \overline{\theta'_d \nabla \cdot \boldsymbol{\sigma}'_c}, \quad \boldsymbol{\sigma}'_c = \boldsymbol{\sigma}_c - \boldsymbol{\sigma}, \quad (3)$$

where $\boldsymbol{\sigma}_c$ is the stress of the continuous phase averaged on the particle scale level. The prime denotes the fluctuation of the quantity. It is seen that the force \mathbf{f}_m results from the correlation of fluctuations in volume fraction and fluctuations in stress divergence. It vanishes in a homogeneous flow. To further understand the physical meaning of this force, let us consider a particle cluster with a constant volume fraction fluctuation θ'_d . Let V be the volume of the cluster, then the integral

$$\int \theta'_d \nabla \cdot \boldsymbol{\sigma}'_c dV = \theta'_d \int_{\partial V} \boldsymbol{\sigma}'_c dS, \quad (4)$$

represents the interfacial force on the cluster surface. This force represents the interaction of the cluster and the surrounding medium. In the case of non-constant θ'_d , the force \mathbf{f}_m can be viewed as the averaged interfacial force acting on the fuzzy surface of clusters. Interactions between the mesoscale structures and the surrounding medium can be divided into a drag and an added mass force similar to the case for a particle in a fluid. Typically, in a gas-solid flow, gas inertia is negligible. For the case of mesoscale structures, the surrounding medium is not pure gas but the mixture of solid and gas, which has a much larger density than the gas. Therefore the mesoscale added-mass force between the two phases is important. In Figure 3, based on our high resolution simulation (Zhang and VanderHeyden, 2001a), the force \mathbf{f}_m is shown as a function of height in the fluidized bed.

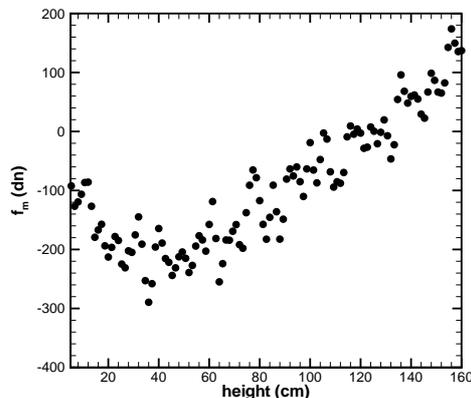


Figure 3: Mesoscale force \mathbf{f}_m as a function of height. The superficial gas velocity is $1.1m/s$.

The mesoscale force \mathbf{f}_m is negative, resisting upward motion of the particle phase, in the lower half of the fluidized bed. It is positive, pushing the particle phase upward, in the upper half of the fluidized bed. The positive part of the force is due to the average cluster drag as a result of relative motion between the particle clusters and surrounding medium. The negative part of the force cannot be explained by the alone. It can only be explained by an added mass force since at the lower portion of the fluidized bed the relative acceleration between the two phases is large compared to the upper half. In this region the relative acceleration between the particle phase and the gas phase is in the upward direction while the added-mass force acting on the particle phase is downward and the mesoscale force becomes negative. In the case of a fluidized bed, the added mass part of the mesoscale force is more important since it is difficult to distinguish cluster drag from the ordinary drag resulting from the particle scale interactions.

The effect of the mesoscale is not only restricted to the mesoscale force. Within a particle cluster the particle phase falls in the wake generated by the

leading part of the cluster and the relative velocity is significantly less than the averaged the relative velocity. Therefore the drag, \mathbf{f}_d , is significantly reduced as shown in Figure 4. If we used the averaged relative velocity experienced by the particles to calculate the drag force, close agreement with the numerical results are found as shown in Figure 4.

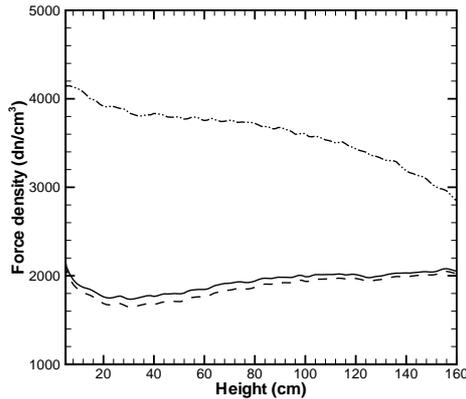


Figure 4: Averaged particle drag force as a function of height. The solid line is results from numerical simulation and the dashed line is calculated using the averaged gas velocity experienced by particles v defined in eq. (7). The dot and dash line is calculated using averaged relative velocity $\mathbf{u}_d - \mathbf{u}_c$. The superficial gas velocity is $1.1m/s$.

Both the mesoscale added mass and the reduction of drag contribute significantly to the macroscopic behavior of a fluidized bed. For the mesoscale added mass force we propose

$$\theta_d \mathbf{f}_m = -C_a \rho_m \left(\frac{\partial \mathbf{u}_d}{\partial t} + \mathbf{u}_d \cdot \nabla \mathbf{u}_d - \frac{\partial \mathbf{u}_c}{\partial t} - \mathbf{u}_c \cdot \nabla \mathbf{u}_c \right). \quad (5)$$

where $\rho_m = \theta_d \rho_d + \theta_c \rho_c$ is the density of the mixture, and C_a is the added mass coefficient. The added mass coefficient is apparently dependent on the shape and the flow condition of the mesoscale structures.

For the drag term, we propose (White, 1974)

$$\mathbf{f}_d = -\frac{3}{4d} \theta_c C_d \rho_g |v| v, \quad (6)$$

where v is the relative velocity in the vertical direction.

$$v = (1 - C_r)(u_{dz} - u_{cz}), \quad (7)$$

and C_r is relative velocity reduction coefficient.

Figures 5 and 6 illustrate the effects of the added mass coefficient C_a and coefficient of relative velocity reduction C_r in a one-dimensional vertical

fluidized bed simulation. Note that these forces modifications significantly affect the pressure gradient and volume fraction profiles.

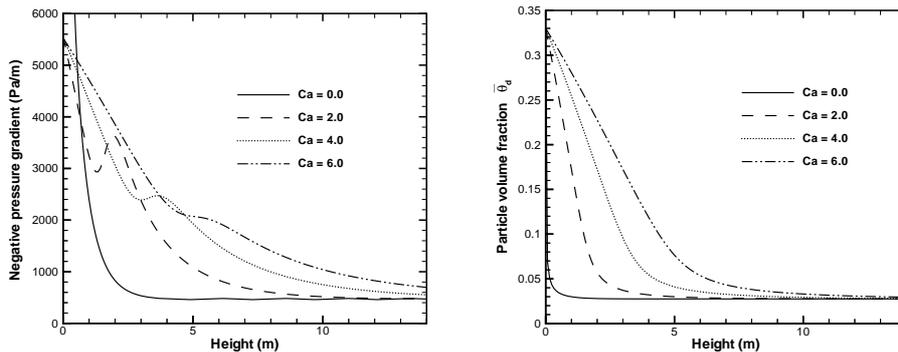


Figure 5: Vertical distribution of pressure gradient and averaged particle volume fraction calculated using different added mass coefficients C_a . The relative velocity reduction coefficient C_r is fixed at 0.9 in all the calculations.

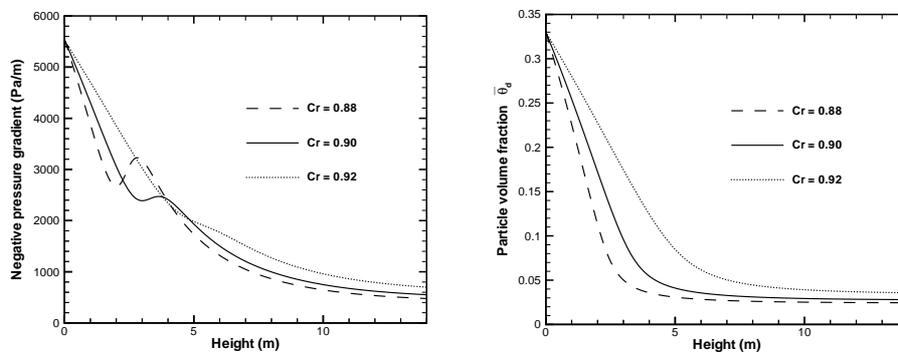


Figure 6: Vertical distribution of pressure gradient and averaged particle volume fraction calculated using different relative velocity reduction coefficient C_r . The added mass coefficient C_a is fixed at 4.0 in all the calculations

3 Conclusions

Both numerical simulation and experimental observation suggests that mesoscale structures exist in gas-solid two-phase flow. In many cases, mesoscale interactions have dominating effects on macroscopic behavior of two-phase flows. Except for the drag term, the interactions at the particle scale do not have a significant affect on the macroscopic flows although they control the way

energy is dissipated at the particle scale. This is similar to the role of molecular viscosity in a turbulent flow. It does not affect the large scale motion directly, although it determines the Kolmogorov eddy scale.

A set of macroscopic equations accounting for the mesoscale interactions is derived. It is found that the most important effects of mesoscale structures are drag reduction and mesoscale added-mass. Simple models for these effects are proposed. Effects of these models on industrial sized fluidized beds are investigated.

References

Agrawal, K., Loezos, P.N., Syamlal, M., and Sundaresan, S., 2000, The role of mesoscale structure in gas-particle flows. *J. Fluid Mech.*(submitted).

Van den Moortel, T., Azario, E. Santini, R., and Tadriss, L., 1998, Experimental analysis of the gas-particle flow in a circulating fluidized bed using a phase Doppler particle analyzer. *Chem. Eng. Sci.* **53**, No. 10, 1883-1899.

White, F.M., 1974, *Viscous fluid flow*, McGraw-Hill, New York.

Zhang, D.Z. and VanderHeyden, W. B., 2001a, High-resolution three-dimensional numerical simulation of a circulating fluidized bed. *Powder Technology*. (in press).

Zhang, D.Z. and VanderHeyden, W. B., 2001b, The effects of mesoscale structures on interfacial forces in two-phase flows and macroscopic equations. *Int. J. multiphase flow*. (submitted).