FLUID-PARTICLE INTERACTION FORCE FOR POLYDISPERSE SYSTEMS FROM LATTICE BOLTZMANN SIMULATIONS

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ABSTRACT

Gas-solid fluidized beds are almost always polydisperse in industrial application. However, to describe the fluid-particle interaction force in models for large-scale gas-solid flow, relations are used which have been derived for monodisperse system, for which ad-hoc modifications are made to account for polydispersity. Recently it was shown, on the basis of detailed lattice Boltzmann simulations, that for bidisperse systems these modifications predict a drag force which can be factors different from the true drag force. In this work fluid-particle interaction forces for polydisperse system are studied by means of lattice Boltzmann simulation, using a grid that is typically an order of magnitude smaller than the sphere diameter. Two different lognormal size distributions are considered for this study. The systems consist of polydisperse random arrays of spheres in the diameter range of 8-24 grid spacing and 8-40 grid spacing, a solid volume fraction of 0.5 and 0.3 and Reynolds number 0.1 to 500. The data confirms the observations made for bidisperse systems, namely that an extra correction factor for the drag force is required to adequately capture the effect of polydispersity. It was found that the correction factor derived by van der Hoef et al (J. Fluid Mech. 528 (2005) 233) on the basis of bidisperse simulation data, applies also to general polydisperse systems.

Keywords: Polydispersity, Fluid-particle interaction force, Lattice Boltzmann simulation

INTRODUCTION

Packed bed or fluidized bed reactors are widely used in the chemical, metallurgical and petrochemical industries, where in most cases the beds are polydisperse in nature. One of the weakest links in the modeling of gas-fluidized beds is our limited understanding of the resistance behaviour of an assembly of particles to fluid flow, judging from the many different drag force relations available in the literature, even for monodisperse systems. The most widely used correlation for the gas-particle interaction force as a function of the solid volume fraction ϕ and particle Reynolds number Re is Ergun's relation (Ergun (1952)), which for a static bed reads:

$$F_{\text{mono}}^{\text{tot}} = \frac{150}{18}\frac{\phi}{(1-\phi)^3} + \frac{1.75}{18}\frac{\text{Re}}{(1-\phi)^3} \qquad (1)$$

where $F_{\text{mono}}^{\text{tot}}$ is the total gas-particle interaction force normalized by the Stokes-Einstein force $3\pi\mu dU$, and Re $= \rho d|U|/\mu$, in which U, μ, and ρ are superficial velocity, viscosity, and density of the gas-phase, respectively, and d the diameter of a particle. Ergun's relation is derived from the pressure drop data over beds of spheres, sand and pulverized coke and is applicable to dense systems like packed beds, but not to dilute systems (solids fraction < 0.2), for which the Wen and Yu (1966) relation is used.

$$F_{\text{mono}}^{\text{tot}} = \left[1 + 0.15\,\text{Re}^{0.687}\right]\varepsilon^{-4.65} \qquad (2)$$

Recently, on the basis DNS type simulations data for flow past monodisperse and bidisperse arrays of spheres, Beetstra et al. (2007) showed that the linear scaling of dimensionless drag force with the Reynolds number (as is the case in the Ergun correlation, and many others), is an over simplification. Similarly, in the Wen and Yu relation, the dependence of drag force on void fraction ε^{-n} is an oversimplification of the contribution of neighbouring particles to the drag force. On the basis of the DNS data, an new relation for monodisperse systems has been suggested by Beetstra et al. (2007).

Another difficulty with the current class of drag force relations is that they are not well defined with respect to homogeneity, sphericity and monodispersity. With respect to the latter, the degree of polydispersity is not explicitely included into the drag force correlations. That is, the gas-solid force on a single particle is calculated from the particle's slip velocity and diameter, and local void fraction, without taking into consideration the (variation in) diameters of the particles in the immediate neighbourhood. In other words, the same drag force correlations (monodisperse) are used for polydisperse systems, where the diameter that appears in the monodisperse drag relation (such as the Ergun equation) is simply replaced by the individual diameter of a particle. In two earlier publications (van der Hoef et al. (2005); Beetstra et al. (2007)) it was shown that an extra correction factor - which depends on the local degree of polydispersity in the neighbourhood of the particle for which the drag is to be evaluated - is required to get good agreement with the data from DNS simulations for binary system. In this work, we have extended the DNS simulations to general polydisperse systems which have a lognormal size distribution, to test whether this correction factor also applies to such systems. Two different range of diameters are chosen: 8-24 grid spacing and 8-40 grid spacing, for two average porosities packing fraction (0.5 and 0.3), and Reynolds numbers ranging from 0.1 to 500. Simulation data are compared with the prediction from the relation by van der Hoef et al. (2005).

DRAG RELATION FOR POLYDISPERSE SYSTEM

We consider a fluid (liquid or solid), with superficial velocity U is flowing past a static array of polydisperse spheres, in which there are N_i spheres with diameter $d_i, i = 1,2,3,...,m$ (where m represents different "Components" (diameter in this case) of particles). For convenience we consider only flow in one direction, which allows us to use scalar notation (instead of a vector notation) for the forces and velocities. Assuming all the particles with same diameter experience the same fluid to particle force, we write the total fluid-particle interaction force $F_{g\rightarrow s,i}$ on a particle of type i as the sum of the drag force ($F_{d,i}$), which exists if there is relative velocity between fluid and particles, and buoyancy force which appears due to the static pressure gradient (∇P):

$$F_{g\rightarrow s,i} = F_{d,i} - V_i \nabla P \tag{3}$$

with V_i is the volume of the particle of type i. Note that in literature often both $F_{g\rightarrow s}$ and F_d are defined as drag force, which is a matter of taste (for monodisperse systems one can show that $F_{g\rightarrow s} = F_d/(1-\varepsilon)$. In this paper, we will consider the total interaction force rather than drag force. It is convenient to consider this force in its dimensioneless form by normalizing it by the Stokes-Einstein drag force $3\pi\mu d_i \mathbf{U}$:

$$F_i^{tot} = F_{g\rightarrow s,i}/3\pi\mu d_i U \tag{4}$$

where μ is the viscosity.

In two recent publications (van der Hoef et al. (2005), Beetstra et al. (2007)), it is shown that for bidisperse systems a correction factor (f_i) should be applied to the monodisperse drag force correlation F_{mono}^{tot} to describe the fluid-particle interaction force i.e.

$$F_i^{tot} = f_i \, F_{\text{mono}}^{tot}(\langle \text{Re} \rangle, \varepsilon) \tag{5}$$

$$f_i = \varepsilon \frac{d_i}{\langle d \rangle} + (1-\varepsilon)\frac{d_i^2}{\langle d \rangle^2} + 0.064\varepsilon \frac{d_i^3}{\langle d \rangle^3} \tag{6}$$

where $\langle \text{d} \rangle$ is the Sauter mean diameter defined as

$$\langle \text{d} \rangle = \frac{\sum_i N_i d_i^3}{\sum_i N_i d_i^2}$$

In principle the correction factor is not coupled to a particular F_{mono}^{tot}, that is, one could take any correlation for a monodisperse system which one expects to be the most accurate for the system at hand. For comparison with the polydisperse DNS data it is logical to use a correlation for F_{mono}^{tot} that is derived from DNS data of similar (but monodisperse) systems, as given by Beetstra et al. (2007):

$$F_{mono}^{tot} = \frac{10\phi}{(1-\phi)^3} + (1-\phi)(1+1.5\phi^{\frac{1}{2}})$$
$$+ \frac{0.413\text{Re}}{24(1-\phi)^3}\left\{\frac{(1-\phi)^{-1} + 3\phi(1-\phi) + 8.4\text{Re}^{-0.343}}{1+10^{3\phi}\text{Re}^{-\frac{(1+4\phi)}{2}}}\right\} \tag{7}$$

with $\phi = 1-\varepsilon$ the solids volume fraction, and $\langle \text{Re} \rangle$ defined as

$$\langle \text{Re} \rangle = \frac{\rho U \langle d \rangle}{\mu} \tag{8}$$

It was shown that this equation differs significantly from the well-used Ergun and Wen & Yu correlations given in section 1. In this work, our aim is to test whether expression (5) is also valid for general polydisperse systems and for this reason we have performed number of DNS simulations of fluid flow past random arrays of spheres with ten different diameters.

It should be stressed that the correction factor f_i as given above is valid for the *total* gas-solid force. For the normalized *drag* force $F_{d,i}/3\pi\mu d_i U$, the correction factor is $f_i = \varepsilon d_i/\langle d \rangle + (1-\varepsilon)d_i^2/\langle d \rangle^2 + 0.064\varepsilon d_i^3/\langle d \rangle^3$, where it is understood that in the contribution to the gas-solid force from the pressure gradient $V_i \nabla P$ the individual diameter of the particle is taken. In our earlier publications (van der Hoef et al. (2005); Beetstra et al. (2007)) we wrongly assumed that both forces had the same correction factor; this was derived from our assumption that $F_{g\rightarrow s,i} = F_{d,i}/\varepsilon$, which is, however, only true for monondisperse systems (for polydisperse systems, the individual forces $F_{g\rightarrow s,i}$ and $F_{d,i}$ cannot be related by a simple single relation).

SIMULATION RESULTS

The DNS simulations were performed using the lattice Boltzmann method to resolve the fluid flow between the spheres, under the condition of no-slip boundary conditions at the surface of the sphere. For details on the simulation method we refer to the paper by Ladd (1994a). The simulation procedure to measure the drag force is similar to what we used for binary systems, the details of which are described in van der Hoef et al. (2005); we just briefly summarize the method below. A static (random) array of spheres is set to move with a constant velocity through the LB fluid. The change in fluid momentum resulting from setting the local fluid velocity equal to the surface velocity of a particle "*a*" is equal (when taken per unit time), to the total force that the particle *a* exerts on the fluid; the inverse of this force is then the instantaneous gas-solid interaction force $\bar{F}_{g\rightarrow s,a}$ on particle *a*, which is monitored in time for each particle. Averaging over time (when steady state is reached) and over all particles *a* of the same type *i* yields the average gas-solid interaction force $F_{g\rightarrow s,i}$. To improve accuracy, additional averaging over different (typically 5) initial configurations is done. Note that a uniform force density is applied to the fluid which counteract the solid-to-fluid force, otherwise the system would continue to accelerate.

The random arrays of spheres are created by starting with a regular array (typically BCC), which is subsequently randomized by a Monte Carlo procedure as described in Beetstra et al. (2007). At the domain boundary periodic boundary condition are employed. The configurations we studied contain 512 and 1000 spheres in total of ten different diameters both with a log-normal and a Gaussian size distribution. The results for the Gaussian distributions will be published elsewhere (Sarkar et al. (2008)). In this paper, we will show results from the the log-normal distributions, for spheres in the range of 8-24 and 8-40 lattice spacings (see Figure 1 for the precise number of particles present for each particular diameter).

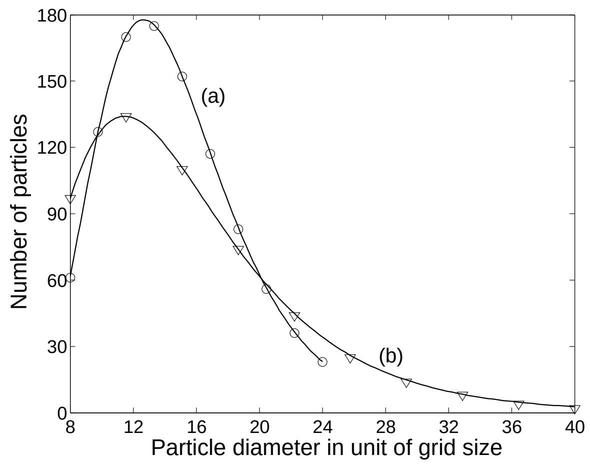

Figure 1: Two different size distribution of particles. log-normal: (a) diameter range of 8-24 for 1000 particles in total and (b) diameter range of 8-40 for 512 particles.

In Figure 2 to 5 simulation data are compared with the prediction (5) using the monodisperse relation (7) of Beetstra et al. (2007) at packing fraction 0.3 and 0.5 and Reynolds number 0.1, 10.0, 100.0, 500.0. It can be seen that excellent agreement is found for all the Reynolds numbers and packing fractions.

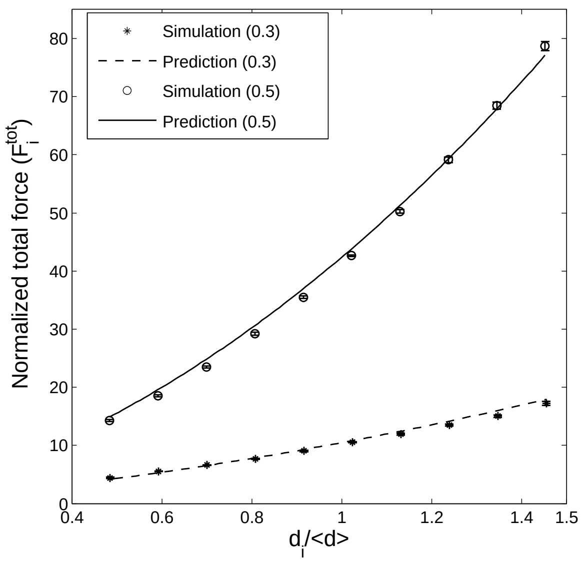

Figure 2: Comparison of simulated individual normalized total force with the prediction (5) as a function of individual diameter over the average diameter ($d_i/<d>$) for a lognormal particle size distribution (type (a)) with a diameter range of 8 to 24 grid spacings, at Reynolds number(i) $<$ Re $>$=0.1.

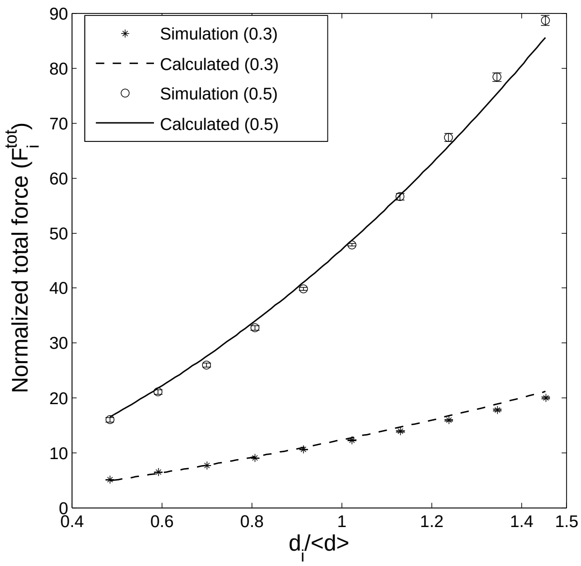

Figure 3: As figure 2, but now for Reynolds number $<$ Re $>$ = 10.

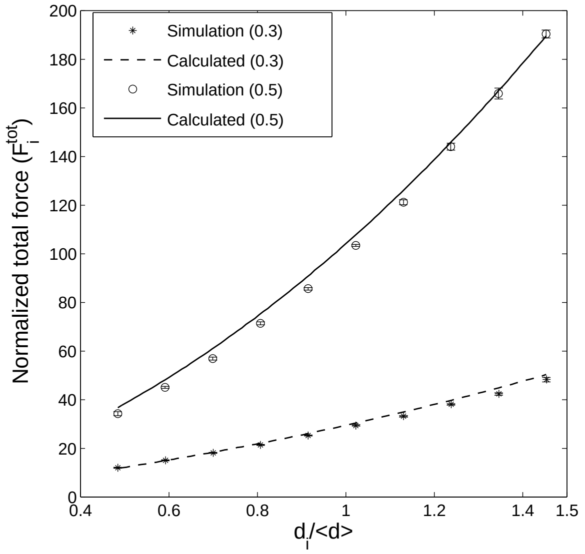

Figure 4: As figure 2, but now for Reynolds number $< Re >$ = 100.

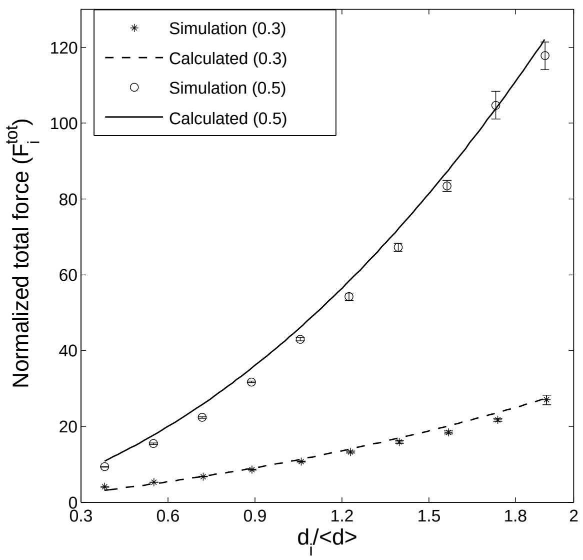

Figure 6: As figure 2, but now for for a lognormal size distribution (type (b)) with a diameter range of 8 to 40 grid spacings and Reynolds number $< Re >$=0.1.

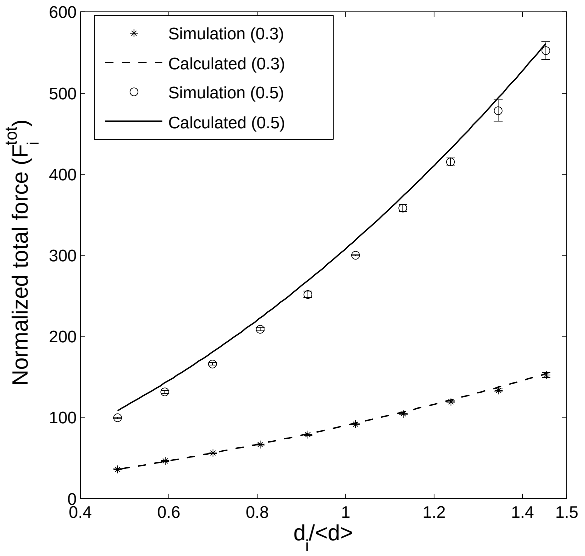

Figure 5: As figure 2, but now for Reynolds number $< Re >$ = 500.

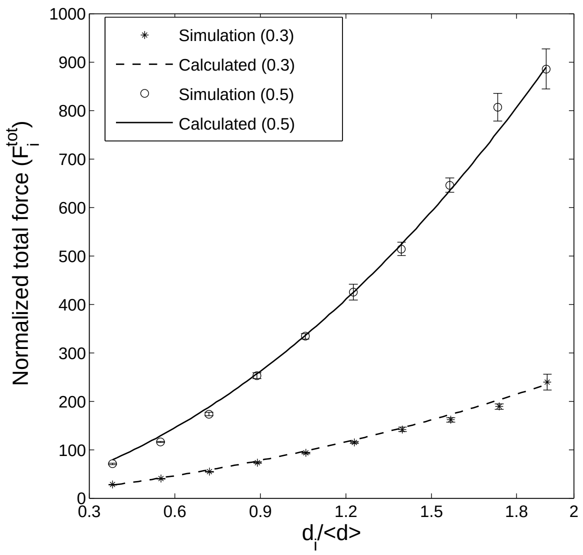

Figure 7: As figure 6, but now for Reynoldsnumber $< Re >$ = 500.

Simulated data are compared for larger range of diameter in Figures 6 and 7 at packing fraction 0.3 and 0.5 and Reynolds number 0.1 and 500. Again a very good agreement is observed between the simulated data and the prediction.

CONCLUSIONS

In this paper we have presented the results of the gas-particle interaction force from DNS simulations of fluid flow past static arrays of polydisperse spheres. We considered two different size ranges with a log-normal distribution. We found that the individual drag force is predicted very well by expression (5), in combination with the monodisperse relation (7) of Beetstra et al. (2007). Note that when the correlation by Ergun is used, with the diameter replaced by the individual diameter of the particle species, the disagreement with the simulation data can amount to up to 200 %. In a more extended future publication (Sarkar et al. (2008)) we will present results for a Gaussian distribution, as well as a detailed comparison with predictions using various other monodisperse relations.

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REFERENCES

Beetstra R., van der Hoef M.A., and Kuipers J.A.M., 2007. Drag force of intermediate Reynolds number flow past mono- and bidisperse arrays of spheres *AICHE Journal*, **53**: 489.

Beetstra R., van der Hoef M.A., and Kuipers J.A.M., in Press. Erratum to "Drag force of intermediate Reynolds number flow past mono- and bidisperse arrays of spheres"[AICHE Journal 53 (2007) 489-501] *AICHE Journal*.

Ergun S., 1952. Fluid flow through packed columns. *Chem. Engng. Progs.*, **48**: 89.

Ladd A. J. C., 1994(a). Numerical simulations of particulate suspensions via a discretized Boltzmann equation Part I. Theoretical foundation *J. Fluid Mech.*, **271**: 285.

Sarkar S., van der Hoef M.A., and Kuipers J.A.M., 2008. Drag force from lattice Boltzmann simulations for flow through polydisperse random arrays of spheres *submitted to Chemical Engineering Science.*

van der Hoef M.A., Beetstra R., and Kuipers J.A.M., 2005. Lattice Boltzmann simulations of low Reynolds number flow past mono- and bidisperse arrays of spheres: results for the permeability and drag force. *J. Fluid Mech.*, **528**: 233.

Wen C.Y., and Yu Y.H., 1966. Mechanics of fluidization. *Chem. Engng. Prog. Symp. Ser.*, **62**: 100.