

The Influence of a Particle Size Distribution on the Granular Dynamics of Dense Gas-Fluidized Beds: A Computer Simulation Study

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A hard-sphere discrete particle model of a gas-fluidized bed was extended in order to allow for a continuous particle size distribution to be taken into account. For each solid particle the Newtonian equations of motion are solved taking into account the inter-particle and particle-wall collisions. The gas-phase hydrodynamics is described by the spatially averaged Navier-Stokes equations for two-phase flow. Pressure peaks inside a slugging fluidized bed decreased with increasing geometric standard deviation of the log-normal size distribution. This could be observed during the initial stages of a simulation with 2400 particles starting from minimum fluidization conditions. In a bubble formation simulation using 40,000 particles of uniform size, small 'satellite' bubbles appeared above and alongside the main bubble. This could neither be observed in the simulation with polydispersed particles nor in the experiment duplicating the simulation which indicates the importance of taking a particle size distribution into account, especially when locally very close packing can prevail.

Due to increasing computer power granular dynamics simulations have become a very useful and versatile research tool to study the hydrodynamics of gas-fluidized beds. In these simulations the Newtonian equations of motion for each individual particle in the system are solved. Particle-particle and particle-wall interactions are taken into account directly which is a clear advantage over two-fluid models which require closure relations for the solids-phase stress tensor (Gidaspow (1), Sinclair and Jackson (2) and Kuipers *et al.* (3) among others). Tsuji *et al.* (4) developed a soft-sphere discrete particle model based on the work of Cundall and Strack (5). In their approach the particles are allowed to overlap slightly and from this overlap the contact forces are calculated subsequently. Hoomans *et al.* (6) used a hard-sphere approach in their discrete particle model which implies that the particles interact through binary, quasi-instantaneous, inelastic collisions with friction. An important advantage of a discrete particle model is given by the fact that a particle size distribution can easily be taken into account which is far more complex, if not impossible, in case a continuum modelling approach is adopted. Furthermore when simulating the particle dynamics directly with a uniform particle size the local particle configuration can approach a closest packing which leads to very low void fractions which in turn can influence the bed dynamics significantly. In this work the influence of a particle size distribution on the granular dynamics of dense gas-fluidized beds will be studied.

PARTICLE DYNAMICS

Since most details of the model are presented in a previous paper (Hoomans *et al.* (6)), the key features will be summarized briefly here. The collision model as originally developed by Wang and Mason (7) is used to describe a binary, instantaneous, inelastic collision with friction. The key parameters of the model are the coefficient of restitution ($0 \leq e \leq 1$) and the coefficient of friction ($\mu \geq 0$). In our hard-sphere approach a sequence of binary collisions is processed one collision at a time. This implies that a collision list is compiled in which for each particle a collision partner and a corresponding collision time is stored. A constant time step is used to take the external forces into account and *within* this time step the prevailing collisions are processed sequentially. In order to reduce the required CPU time neighborlists are used in order to decrease the number of particles to be checked for possible collisions. Efficient algorithms obtained from the field of Molecular Dynamics (MD) are employed to achieve very efficient computational procedures.

External Forces

The incorporation of external forces differs somewhat from the approach followed in our previous paper (Hoomans *et al.* (6)). In this work we use the external forces analogous to those implemented in the two-fluid

model described by Kuipers *et al.* (3) where, of course, the forces now act on a single particle:

$$m_p \frac{d\mathbf{v}_p}{dt} = m_p \mathbf{g} + \frac{V_p \beta}{(1-\varepsilon)} (\mathbf{u} - \mathbf{v}_p) - V_p \nabla p \quad (1)$$

where m_p represents the mass of a particle, \mathbf{v}_p its velocity, \mathbf{u} the local gas velocity and V_p the volume of a particle. In Equation (1) the first term is due to gravity and the third term is the force due to the pressure gradient. The second term is due to the drag force where β represents an interphase momentum exchange coefficient as it usually appears in two-fluid models. For low void fractions ($\varepsilon < 0.80$) β is obtained from the well-known Ergun equation:

$$\beta = 150 \frac{(1-\varepsilon)^2}{\varepsilon} \frac{\mu_g}{d_p^2} + 1.75(1-\varepsilon) \frac{\rho_g}{d_p} |\mathbf{u} - \mathbf{v}_p| \quad (2)$$

where d_p represents the particle diameter, μ_g the viscosity of the gas and ρ_g the density of the gas. For high void fractions ($\varepsilon \geq 0.80$) the following expression for the interphase momentum transfer coefficient has been used:

$$\beta = \frac{3}{4} C_d \frac{\varepsilon(1-\varepsilon)}{d_p} \rho_g |\mathbf{u} - \mathbf{v}_p| \varepsilon^{-2.65} \quad (3)$$

The drag coefficient C_d is a function of the particle Reynolds number:

$$C_d = \begin{cases} \frac{24}{\text{Re}_p} (1 + 0.15 \text{Re}_p^{0.687}) & \text{Re}_p < 1000 \\ 0.44 & \text{Re}_p \geq 1000 \end{cases} \quad (4)$$

where the particle Reynolds number in this case is defined as follows:

$$\text{Re}_p = \frac{\varepsilon \rho_g |\mathbf{u} - \mathbf{v}_p| d_p}{\mu_g} \quad (5)$$

For the integration of Equation (1) a simple explicit first order scheme was used to update the velocities and positions of the particles.

PARTICLE SIZE DISTRIBUTION

Hardly any distribution of particle size encountered in fluidization studies is symmetrical, most of them are skewed to larger diameters (Seville *et al.* (8)). A

symmetrical size distribution like a normal or a Gaussian distribution is therefore not representative for particles used in laboratory or industrial practice. In this work the particle diameters are obtained from a log-normal distribution which is asymmetrical and can be represented in mathematical terms as follows:

$$df = \frac{1}{\sqrt{2\pi} d_p \ln \sigma_g} \exp \left[-\frac{(\ln d_p - \ln d_{p,CMD})^2}{2(\ln \sigma_g)^2} \right] dd_p, \quad (6)$$

where df is the fraction of particles having diameters whose logarithms lie between $\ln d_p$ and $\ln d_p + d(\ln d_p)$. In Equation (6) $d_{p,CMD}$ is the count median diameter and σ_g is the geometric standard deviation. When creating the particle size distribution all the diameters which are smaller than $d_{p,CMD} - \sigma_g$ or larger than $d_{p,CMD} + \sigma_g$ are rejected which mimics the effects of sieving. An example of a particle size distribution generated with this method is represented in a (discrete) frequency histogram in Figure 1.

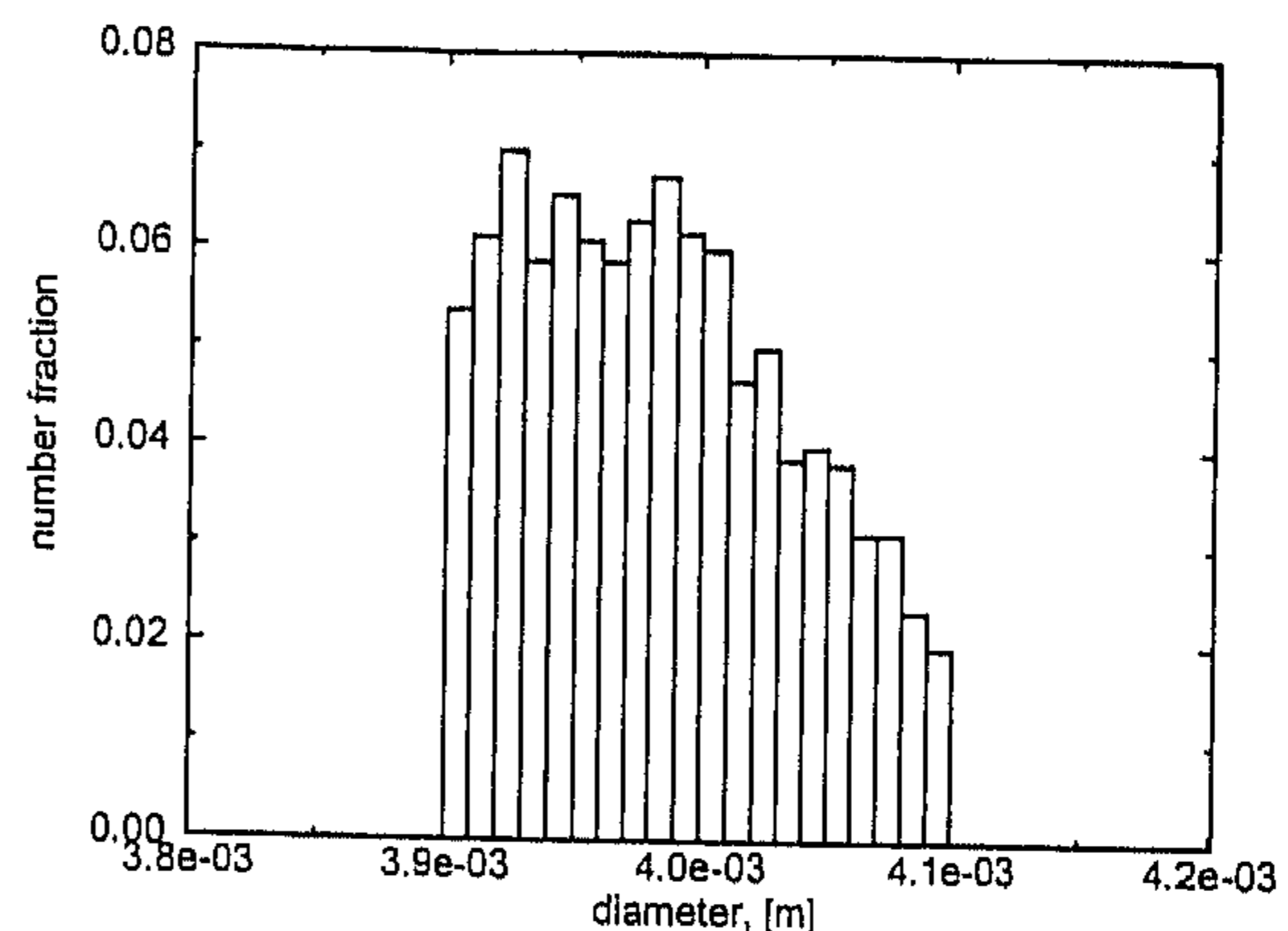


Figure 1, Frequency histogram of a log-normal particle size distribution with a count median diameter of 4.0 [mm] and a σ_g of 0.1 [mm].

GAS PHASE HYDRODYNAMICS

The motion of the gas-phase is calculated from the following set of equations which can be seen as a generalised form of the spatially averaged Navier-Stokes equations for a two-phase gas-solid mixture (Kuipers *et al.* (3)).

Continuity equation gas phase:

$$\frac{d(\varepsilon \rho_g)}{dt} + (\nabla \cdot \varepsilon \rho_g \mathbf{u}) = 0. \quad (7)$$

Momentum equation gas phase:

$$\frac{d(\varepsilon \rho_g \mathbf{u})}{dt} + (\nabla \cdot \varepsilon \rho_g \mathbf{u} \mathbf{u}) = -\varepsilon \nabla p - \mathbf{S}_p - (\nabla \cdot \varepsilon \boldsymbol{\tau}_g) + \varepsilon \rho_g \mathbf{g} \quad (8)$$

In this work transient, two-dimensional, isothermal ($T = 293 \text{ K}$) flow of air at atmospheric conditions is considered. The constitutive equations and the boundary conditions used can be found in Hoomans *et al.* (6). The void fraction (ε) is calculated from the particle positions in the bed. There is one important modification with respect to our previous model and that deals with the way in which the two-way coupling between the gas-phase and the particle motion is established. In the present model the reaction force to the drag force exerted on a particle per unit of volume is fed back to the gas-phase through the source term \mathbf{S}_p [Nm^{-3}]. A more detailed discussion on this approach can be found in Delnoij *et al.* (9).

RESULTS

Influence of Distribution Width

At first the influence of the distribution width was studied. Simulations were performed using 2400 particles with a count median average diameter of 4.0 [mm] and a density of 2700 kg/m^3 ($u_{mf} = 1.78 \text{ [m/s]}$) contained in a system of 0.15 [m] width and 0.5 [m] height. A discretization of 15 cells horizontally and 25 cells vertically was applied. A time step of 10^{-4} [s] was used and all simulations were run for 10 [s] real time. The coefficient of restitution (e) was set equal to 0.9 and the coefficient of friction (μ) was set equal to 0.3 for both particle-particle and particle-wall collisions. The initial configurations were obtained by placing the particles in the system and allowing them to fall under the influence of gravity while the gas inflow was set equal to u_{mf} . Simulations were performed for a system consisting of particles of uniform size and systems consisting of particles with a log-normal size distribution with a geometric standard deviation $\sigma_g = 0.1, 0.5$ and 1.0 [mm] respectively. A homogeneous gas inflow at $1.5 u_{mf}$ was specified at the bottom of the system.

In Figure 2 the pressure fluctuations inside the bed at 0.2 [m] above the centre of the bottom plate are

presented for all the four cases. It can be observed that the pressure peaks decrease with increasing geometric standard deviation of the size distribution. This can be explained by the lower void fraction in the uniform case due to the closer packing which results in a higher force acting on the particles which in turn causes the higher pressure peaks. After the first 1.5 [s] the differences become far less pronounced which indicates that especially in situations where close packing can occur such as at minimum fluidization conditions it is important to take polydispersity into account.

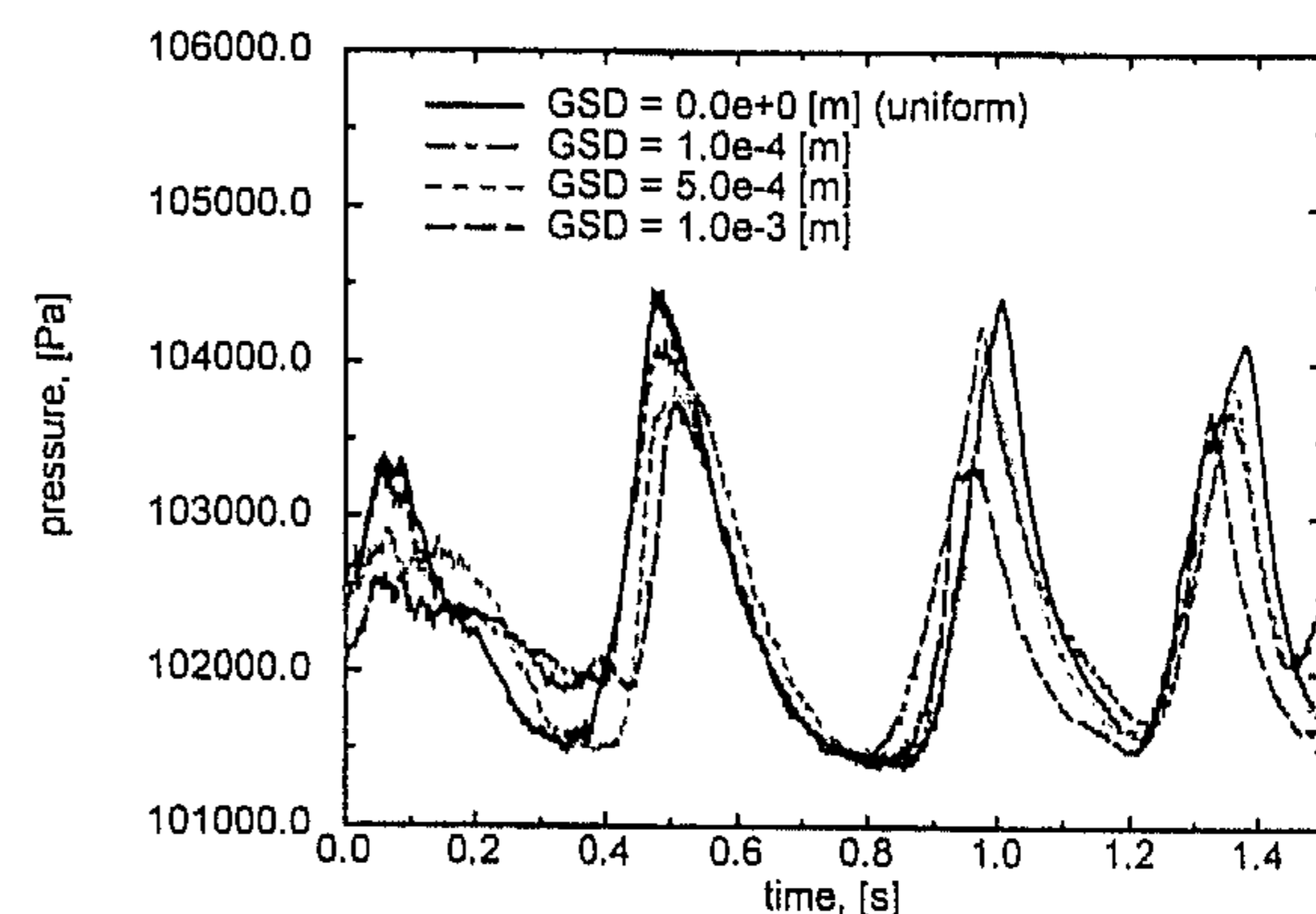
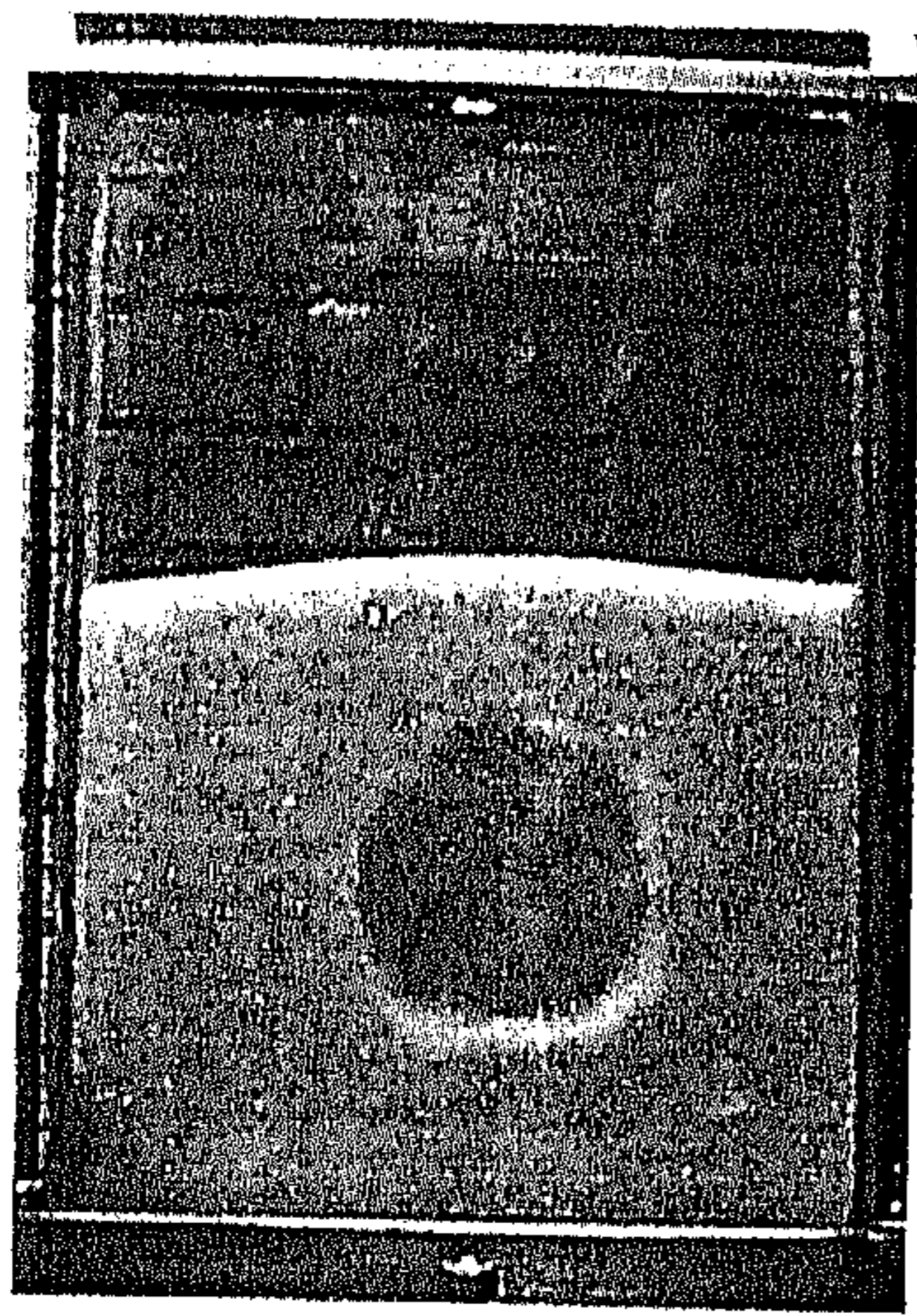


Figure 2, Pressure fluctuations 0.2 [m] above the centre of the bottom plate as a function of time for the four cases, GSD = geometric standard deviation (σ_g).

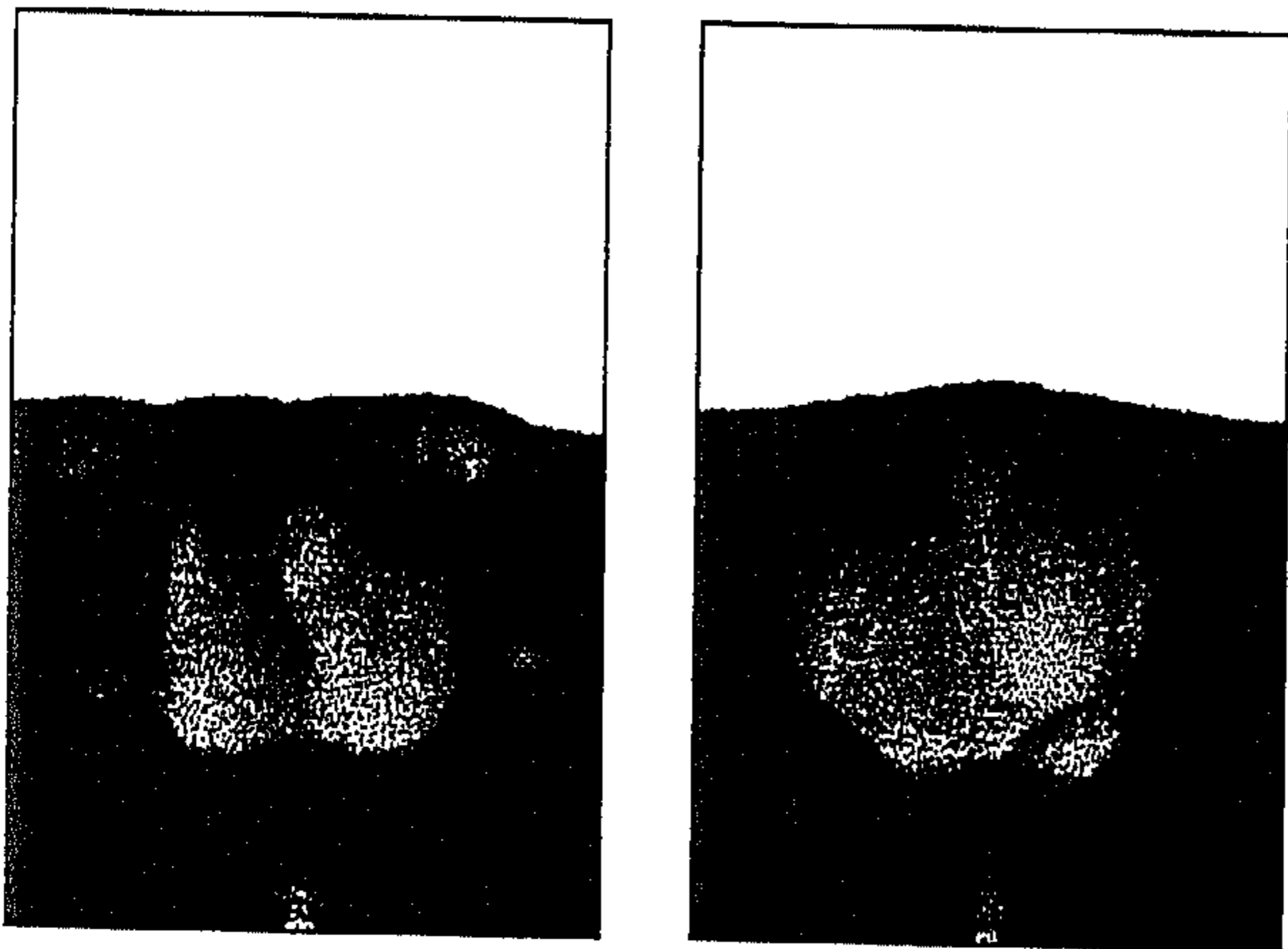
Experimental Validation

In order to test whether the simulation results were improved by taking the particle size distribution into account a comparison with experiment was performed. The main features of the experimental set-up were reported earlier (Hoomans *et al.* (6)). A sieve fraction of glass ballotini particles between 800 and 900 [μm] with a density of 2930 [kg/m^3] ($u_{mf} = 0.5 \text{ [m/s]}$) was used. The bed (width 0.2 [m] and height 0.3 [m]) was equipped with a porous bottom plate which featured a central nozzle (15 [mm]) through which excess gas could be injected into the bed. The background fluidization velocity was kept equal to u_{mf} whereas during the first 0.2 [s] excess gas was injected through the nozzle at $5 u_{mf}$. The simulations were performed using 40,000 particles. The coefficient of restitution was 0.96 for particle-particle collisions and 0.86 for particle-wall collisions and the coefficients of friction were 0.15 in both cases. A discretization of 39 by 60

cells was used together with a time step of 10^{-4} [s]. A simulation was performed where the particle diameters were obtained from a log-normal distribution with a count median average of 850 [μm] and a geometric standard deviation of 50 [μm] as well as a reference simulation with particles of uniform diameter (850 [μm]). Snapshots at $t = 0.2$ [s] of both simulations and the experiment are presented in Figure 3.



a)



b)

c)

It can be observed that in the case of the uniform particle assembly small 'satellite' bubbles appear above and alongside the main bubble. This is neither observed in the experiment nor in the simulation with the polydisperse particle assembly. These 'satellite' bubbles are probably due to low local void fraction due to close packing. The size of the main bubble agrees rather well with the experiment for both simulations which is rather encouraging especially since all model parameters were obtained on beforehand and independently. Further improvement can be achieved by extending the model to three dimensions because although the experimental bed was quasi two-dimensional it was still 16 [mm] deep.

CONCLUSIONS

Granular dynamics simulations have been performed with particles which diameters have been obtained from a log-normal distribution. The main influence of the polydispersity could be observed when the particles were in a rather close packing. Pressure peaks inside a slugging fluidized bed decreased with increasing geometric standard deviation of the log-normal size distribution during the initial stages of a simulation starting from minimum fluidization conditions. In a bubble formation simulation with particles of uniform size small 'satellite' bubbles appeared above and alongside the main bubble. This could neither be observed in the experiment nor in the simulation with the polydisperse particles. This indicates that it is especially important to take a particle size distribution into account in systems where locally very dense particle configurations can occur.

Due to the fact that a particle size distribution can be dealt with in a natural and fundamental manner (i.e. without invoking difficulties in formulating closure laws for particle stress) it is anticipated that the effect of fines on fluidization behaviour, which is well known to the experimentalist but which is unfortunately poorly understood, can now be studied in detail.

Figure 3, Snapshots at $t = 0.2$ [s] of: a) experiment, b) simulation with uniform particles, c) simulation with log-normal particle size distribution.

NOTATION

C_d	drag coefficient, [-]
e	coefficient of restitution, [-]
d_p	particle diameter, [m]
g	gravitational acceleration, [m/s ²]
m_p	particle mass, [kg]
p	pressure, [Pa]
\mathbf{r}	position vector, [m]
S_p	momentum source term Eq. (8), [N/m ³]
t	time, [s]
\mathbf{u}	gas velocity vector, [m/s]
\mathbf{v}_p	particle velocity vector, [m/s]
V_p	particle volume, [m ³]

Greek symbols

β	defined in Eqs (2) and (3), [kg/m ³ s]
ε	void fraction, [-]
μ	coefficient of friction, [-]
μ_g	gas viscosity, [kg/ms]
τ	gas-phase stress tensor, [kg/ms ²]
ρ_g	gas density, [kg/m ³]
σ_g	geometric standard deviation (GSD), [m]

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