Direct numerical simulation of viscous incompressible flow with spherical particles in the flat channel

D V Esipov, V N Lapin, D S Kuranakov and D V Chirkov
Institute of Computational Technologies SB RAS, Novosibirsk, 630090, Russia
E-mail: esipov@ict.sbras.ru

Abstract. The paper deals with numerical simulation of 3D fluid flow with relatively large spherical particles in the flat channel. The simulation is performed using the previously developed SIMPLE based immersed boundary method. The collision model, describing particle-particle and particle-wall collisions, complements the numerical method. This model prevents particle overlapping and takes into account the complicated fluid flow in the space between the particles. The computed flow rates decrease significantly with increasing the particle concentration. It is shown that the value of the particle diameter has a small influence on the flow rate. The flow rate can be approximated using the value of effective viscosity computed by Maron – Peirce formula with the use of extremely high packing concentration. Particles are moving faster than the mixture, and the difference increases with increasing concentration.

1. Introduction
Flows of mixtures of viscous fluid with spherical particles often arise in technological processes. If the particle diameter is small relative to the channel width \(d \ll W\), there are several appropriate approaches, in which the mixture is represented as a homogeneous fluid with effective viscosity dependent on the particles volume concentration. Specific expressions for the effective viscosity can be obtained by averaging the influence of particles and using some phenomenological assumptions [1,2,3]. Large particles significantly affect the flow field and these approaches are no longer suitable. Nevertheless, it is desirable to find an expression for effective viscosity even in this case.

In the present work, such particle-laden flows in a flat channel are computed using the direct numerical simulation approach. The mathematical model consists of the Navier – Stokes equations for a viscous incompressible fluid and the set of equations of motion and rotation for each particle. An immersed boundary method (IBM) similar to [4] is used. The fluid is considered to occupy the entire domain of the channel including the space inside the particles. The presence of particles at a given point is taken into account in the Navier – Stokes equations by adding a special force term. This force is calculated such that the no-slip condition on the immersed boundary be approximately satisfied.

2. Problem statement
The flow of a viscous, incompressible fluid in a channel with rigid particles of diameter \(d\) placed within is considered, as shown in figure 1. The fluid flow is governed by the following equations

\[
\begin{align*}
\rho \frac{du}{dt} &= \mu \nabla u - \nabla p + f, \\
\nabla \cdot u &= 0,
\end{align*}
\]

(1)
where \( \mathbf{u} \) is the velocity vector, \( p \) is the pressure, \( \mu \) and \( \rho \) are the fluid dynamic viscosity and density respectively. Because IBM is used for the numerical solution, \( f \) indicates the fictitious body force that affects the fluid flow near the surface of the immersed body. The specific value for \( f \) is chosen in such a way that the no-slip condition on the immersed boundary is satisfied. Here, \( \frac{d\mathbf{u}}{dt} \) is the total (substantial) derivative

\[
\frac{d\mathbf{u}}{dt} = \frac{\partial \mathbf{u}}{\partial t} + \nabla (\mathbf{u} \otimes \mathbf{u}).
\]

It is assumed that gravity does not affect the fluid or particles. In a certain sense, it can be considered as a zero buoyancy case.

Let us derive equations of the particle movement. The velocity of each point of an absolutely rigid particle \( \mathbf{u}_p \) can be decomposed into a translational part and a rotational part according to

\[
\mathbf{u}_p = \mathbf{u}_c + \mathbf{\omega} \times \mathbf{r},
\]

where \( \mathbf{u}_c \) is the translational velocity of the particle centroid, \( \mathbf{\omega} \) is the angular velocity of the particle, and \( \mathbf{r} \) is a radius vector from the centroid to the point of the particle. The motion of one immersed particle is described by the Newton–Euler motion equations for \( \mathbf{u}_c \) and \( \mathbf{\omega} \)

\[
\rho_p V_p \frac{d\mathbf{u}_c}{dt} = \int_{\Gamma_p} (\mathbf{\sigma} \cdot \mathbf{n}) d\Gamma + \mathbf{F}_n,
\]

\[
\rho_p V_p \frac{d^2\mathbf{\omega}}{dt^2} = \int_{\Gamma_p} [\mathbf{r} \times (\mathbf{\sigma} \cdot \mathbf{n})] d\Gamma + \mathbf{r} \times \mathbf{F}_t.
\]

Here, \( \rho_p \) is the density of the particle, \( V_p \) is the volume of the particle with the surface \( \Gamma_p = \partial V_p \), \( \mathbf{n} \) is the outward-pointing unit normal to \( \Gamma_p \), and \( \mathbf{\sigma} \) is the viscous stress tensor. In the right-hand side of equations (4) the first term stands for the force acting on the particle from the fluid flow, and the second term is the force and the moment of particles interaction with each other or with the wall when the collision occurs. The normal component \( \mathbf{F}_n \) and the tangent component \( \mathbf{F}_t \) of the force are not equal to zero only for small periods of time when the particles are in contact. The particle is assumed to be homogeneous and continuous (without cavities). The viscous stress tensor is calculated for a Newtonian fluid as follows
\[ \sigma = -I p + \mu(\nabla \bf{u} + \nabla \bf{u}^T), \]  

where \( I \) is a unit tensor. Evaluating \( \sigma \cdot \bf{n} \) from equations (1) one can rewrite (4) as

\[ \rho_p V_p \frac{d\bf{u}_p}{dt} = \rho \frac{d}{dt} \int_{\Omega_p} \bf{u} dV - \int_{\Omega_p} \bf{f} dV + \bf{F}_n, \]

\[ \rho_p \frac{d^2}{dt^2} \frac{d\bf{u}_p}{dt} = \rho \frac{d}{dt} \int_{\Omega_p} (\bf{r} \times \bf{u}) dV - \int_{\Omega_p} (\bf{r} \times \bf{f}) dV + \bf{r} \times \bf{F}_r. \]

As proposed in [4] we assume that the velocity of the fluid “inside” the solid particle satisfies the rigid body motion (3). Substituting (3) into (6), the following motion equation can be obtained

\[ (\rho_p - \rho)V_p \frac{d\bf{u}_p}{dt} = -\int_{\Omega_p} \bf{f} dV + \bf{F}_n, \]

and the following rotation equation can be obtained

\[ (\rho_p - \rho) \frac{d^2}{dt^2} \frac{d\bf{u}_p}{dt} = -\int_{\Omega_p} (\bf{r} \times \bf{f}) dV + \bf{r} \times \bf{F}_r. \]

For each particle equations (7) and (8) are valid. In order to close this system of equations it is necessary to use collision model and derive expressions for \( \bf{F}_n \) and \( \bf{F}_r \), which will be discussed later.

At the inflow \( \Gamma_{\text{in}} \) and outflow \( \Gamma_{\text{out}} \) boundaries, the periodic boundary conditions are stated for the velocity vector \( \bf{u} \). It is assumed that the fluid flow is driven by the constant pressure drop between the inlet and outlet cross sections. For the case of a pure Poiseuille flow the pressure is a linear function of the channel length, \( p = p_s(x) \), and

\[ \frac{\partial p}{\partial x} = -\frac{16}{Re}. \]

Here, \( Re = \frac{2 \rho U_{\text{max}} W}{\mu} \) is the Reynolds number of the fluid flow in the flat channel unperturbed by the particles. The pressure can be split into two parts, namely, \( p(x, y, z) = p_s(x) + p_v(x, y, z) \). First part \( p_s \) is responsible for the pure Poiseuille flow through the channel, and the second one \( p_v \) is responsible for fluctuations caused by the movement of the particles. Periodic boundary conditions are used for \( p_v \). When a particle reaches the outflow boundary, the particle segment that goes beyond the boundary is instantly translated to the inflow with conservation of its velocity and rotation. The initial condition for fluid field is taken from the undisturbed Poiseuille flow. The initial conditions for the particles are also taken from the same flow for an arbitrary position of the particle measured by the distance from the boundary \( h_0 \). At the initial time the particles are placed randomly in the channel.

The considered particle-laden flows are characterized by four main parameters: the Reynolds number \( Re \), the relative diameter of the particles \( d/W \), their buoyancy or the ratio of particle density to fluid density \( \rho_p/\rho \) and the volume concentration of particles \( c \). Equations (1) are solved by the SIMPLE method on the uniform staggered grid. Equations (7) and (8) are integrated over time by the Euler method. The forces of interaction \( \bf{F}_n \) and \( \bf{F}_r \) are determined by the collision model.

3. Collision model
The simulation of the motion of many particles needs particle-particle and particle-wall collision model to overcome the overlapping of particles, as well as penetration through the channel walls \( \Gamma_w \). Particle velocities can be different at the contact time, and elastic interaction should be taken into account. The elastic interaction is described by the model of soft sphere similar to the one used in [8] and taken into account by the term \( \mathbf{F}_e \) in (7). We neglect the friction force \( \mathbf{F}_f \) in (8) arising from different rotation velocities of the particles.

The modeling of interaction through a thin layer of fluid is very difficult due to the following. Let us consider a case when the rigid spherical particle moves to the wall along the perpendicular line, as shown in figure 2. As the particle approaches the wall, the cross-flow ahead occurs in the thin space between them. The velocity of this flow is higher, the closer the particle is to the wall. Consequently, the fluid pressure increases when the particle moves towards the wall. Moreover, when the particle reaches the wall at the contact point \( A \), according to the Navier – Stokes equations, the cross-flow velocity should become infinite. Therefore, the fluid pressure becomes infinite too. A similar behavior, but with the opposite sign, should also occur when the particle moves outward from the wall.

Taking into account the use of coarse computational meshes and large time steps, together with the above-described singularity in interaction, direct numerical simulation of the collisions is unsuitable. We propose to describe the interaction through a thin layer of fluid, also using the force \( \mathbf{F}_n \).

The normal component of particle’s approaching velocity in the fluid is small relative to the velocity of the entire flow. In this case, the force acting on the particle far away from the obstacle can be evaluated using Stokes formula \( F = 3\pi \mu d v_p \), where \( v_p \) is particle’s velocity. Near the wall or particle, a change in the value of the force acting on the particle can be represented using a correction factor \( \lambda(\varepsilon) \) depending on the dimensionless distance \( \varepsilon = 2l / d \):

\[
F = 3\pi \mu d v_p \lambda(\varepsilon).
\]  

The hydrodynamics problem with collision can be solved analytically in the Stokes stationary approximation. In this approximation, the correction factor \( \lambda(\varepsilon) \) can be found as the sum of a series of exponential functions [5]. In [6] the approximations of this series are given. In the case of the particle-particle collision, its approximation is equal to

\[
\lambda(\varepsilon) = \frac{1}{2\varepsilon} - \frac{9}{20} \ln \varepsilon - \frac{3}{56} \varepsilon \ln \varepsilon + 1.346,
\]

and in the case of the particle-wall collision, its approximation is equal to

\[
\lambda(\varepsilon) = \frac{1}{\varepsilon} - \frac{1}{21} \ln \varepsilon + 0.9713.
\]

Despite the expression on the force (10) with (11) and (12) contain non-integrable terms with \( 1 / \varepsilon \), it is widely used in modeling of particle-laden flows [7,8,9]. On the other hand, formulae (11) and (12) are valid only for \( \varepsilon < 3 \). Solving model problems of particle collisions in fluids, it was found that the developed numerical method predicts correct force value only for \( \varepsilon > 0.2 \). Thus, the interaction for large distances \( \varepsilon > 0.2 \) is described by the developed numerical method, while for small distances \( \varepsilon < 0.2 \) the interaction is described using (11) for \( \mathbf{F}_n \) in (7).

The collision model was validated on experimental data from [10]. Good agreement on the energy dissipation is obtained. For considered in the paper Stokes numbers Sk < 10, after the collision, approximately 3% of the kinetic energy of the particle is retained.

4. Results

A flat channel of length \( L = 5 \), width \( W = 1 \) and depth \( D = 2 \) is considered (figure 1). In \( z \) direction the boundary conditions of symmetry are set. The flow of the mixture along the \( x \) axis is enforced by
the pressure gradient (9). Calculations were carried out using the uniform Cartesian Euler grid with 250×50×100 cells. The time step was taken $\tau = 0.001$. Each calculation was unsteady. Time interval $t \in [0,15]$ proved to be enough for reaching the quasi-steady state, meaning that the average characteristics of the flow are settled. Subsequent time interval $t \in [15,30]$ was computed to accurately calculate the averaged flow characteristics. Velocities were averaged over each horizontal section $y = \text{const}$ and over time.

Figure 3 shows the averaged longitudinal velocity for various particle concentrations and diameters. The velocity profile looks like the Poiseuille profile, while the mixture velocity is higher near the channel walls and lower in its center. The velocity decreases significantly with increasing the concentration of particles $c$. The increase of concentration leads to a formation of an almost rigid core in the center of the channel (close to the plateau in the velocity profile in figure 3 c).

![Figure 3](image)

**Figure 3.** Distributions of the average longitudinal velocity of a mixture $\langle u \rangle(y)$ of neutrally buoyant particles for $Re = 100$, various concentrations: a – $c = 0.14$, b – $c = 0.21$, c – $c = 0.28$, and various diameters: $\phi - d/W = 0.3$, $\Delta - d/W = 0.38$. The dashed line shows the Poiseuille velocity profile with the effective viscosity calculated by the formula (13).

In the field of hydraulic fracturing simulation, where similar flows arise [11,12], the Maron–Peirce formula for effective viscosity obtained experimentally in [13] and derived theoretically with some phenomenological assumptions in [3] is often used:

$$\mu_{\text{eff}} = \mu \left( 1 - \frac{c}{c^*} \right)^2,$$

where $c^*$ is the packing concentration. For comparison the Poiseuille velocity profile with effective viscosity (13) is shown in figure 3. Here, the concentration of dense packing is taken equal to $c^* = \pi / \sqrt{18} \approx 0.74$ (the hexagonal dense packing of spheres). Nevertheless, for the diameters under consideration ($d/W = 0.3; 0.38$), such a dense packing in the flat channel is not achievable due to the presence of flat walls.

The average flow rate is obtained by integrating the average velocity over the channel width:

$$\langle q \rangle = \int_0^W \langle u \rangle \, dy.$$  

Table 1 shows the flow rates obtained in the simulations and using formula (13). The flow rate is significantly affected by the particle concentration, while the influence of particle diameter is weaker. The flow rates obtained by the formula (13) with extremely high packing concentration are close to the ones obtained by direct numerical simulation.
Table 1. Average mixture flow rate \( <q> \) for various particle concentrations and diameters.

| \( d/W = 0.3 \) | \( d/W = 0.38 \) |
|----------------|----------------|
| \( c = 0.14 \) | 0.43552 | 0.45482 | 0.43827 |
| \( c = 0.21 \) | 0.32222 | 0.34952 | 0.34197 |
| \( c = 0.28 \) | 0.24310 | 0.25463 | 0.25760 |

Table 2. Average velocity of particles \( <u_p> \) for various particle concentrations and diameters.

| \( d/W = 0.3 \) | \( d/W = 0.38 \) |
|----------------|----------------|
| \( c = 0.14 \) | 0.47655 | 0.48612 |
| \( c = 0.21 \) | 0.36923 | 0.38346 |
| \( c = 0.28 \) | 0.26870 | 0.28725 |

Table 2 shows the average longitudinal particle velocities obtained by direct numerical simulation. Accounting \( W = 1 \), the average flow rate of the mixture \( <q> \) equals the average velocity of the mixture. Comparing the values in tables 1 and 2, one can conclude that particles move faster about 8–12% than the mixture, and this difference increases with increasing concentration \( c \).

5. Conclusion
Averaged velocity profiles of the fluid-particles mixture across the channel are computed by direct numerical simulation. The velocity profiles are close to the Poiseuille profile but have a more convex shape. The flow rates decrease significantly with increasing the particle concentration. The value of the particle diameter has a small influence on the flow rate. The flow rate can be approximated using the value of effective viscosity computed by Maron – Peirce formula with the use of extremely high packing concentration. In many papers devoted to the simulation of the hydraulic fracturing (e.g. [10]), the Maron – Peirce formula is used but with smaller packing concentration, which can lead to the unreliable results. Particles are moving faster than the mixture, and the difference increases with increasing concentration. The continuation of the present work would be driven by varying the value of the Reynolds number.

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