NUMERICAL SIMULATION OF SUSPENSION FLOW USING DIRECT SIMULATION MONTE CARLO (DSMC) METHOD FOR THE PARTICULATE PHASE

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ABSTRACT. We use Direct Simulation Monte Carlo (DSMC) method to model and simulate the 3D motion of the particulate phase in dispersed solid-fluid flows through tubes and investigate the influence of some model features on the flow pattern.

The carrier laminar fluid flow is modeled by Navier-Stokes equations for an axisymmetrical incompressible flow. The dispersed phase consists of solid spherical particles on which act gravity, hydrodynamic drag force and lift (Saffman) force from the fluid shear. According to the DSMC method, particle free flight and inter-particle collisions are performed consecutively in each time step. Particle motion in the free flight is determined by the second Newton’s law. Inter-particle collisions are decided under statistical considerations according to the DSMC method.

Since one of the features of the method is the modeling of the particles as discrete objects moving under the influence of forces and impacts with obstacles, the influence of the Saffman lift force and the influence of the collision model for particle-particle interactions on the flow structure were studied. Vertical up-flow of gas-solid suspension flow in an entrance part of a tube is simulated. In all the cases Saffman force, even corrected for smaller fluid shear and larger slip (particle velocity relative to the fluid velocity), has very strong influence on the flow structure, and collects the particles in the tube core. When Saffman force is excluded from the model, particles are still pushed towards the axis near the tube entrance, where the radial fluid velocity is present, downstream particles are dispersed by the collisions. The investigation of the influence of the inter-particle collisions and the
collision model on the flow structure show non-negligible influence of the collisions between the particles on their space distribution in gas-solid flows (particles with relatively large inertia) even in the cases of relatively low volume fractions (less than 1%). The choice of collision model (DSMC and Smoluchowski formula for collisions in laminar shear flow are compared) affects the distribution and the motion of the particles.

**Key Words:** suspension flow, entrance part of a tube, numerical simulation, discrete particle modeling, DSMC method

### 1. Introduction

DSMC method was originally developed for simulation of rarefied gas flows [1]. Following the similarities of the motion of the molecules in the fluid flows and the particles in suspension flows, DSMC method was applied, like other molecular methods, to model the motion of the particles in multiphase and granular flows. Various modifications, concerning the differences in the behavior of macro-particles and molecules, were later made in order to make the method suitable for macro-particle modeling [2, 3, 4].

In multiphase modeling DSMC is a stochastic discrete particle modeling method. It combines the advantages of the discrete particle modeling methods – relatively simple description of the particle motion and boundary conditions for the particles; with the computational efficiency of Monte Carlo methods for modeling of particle systems, statistical method for inter-particle interactions derived from Boltzman equation and representation of the system by a smaller number of model particles. The splitting of particle free motion and inter-particle collisions and the performance of collisions in the computational mesh cells are specific for the method and allow easy parallelization of the calculations. These features make the DSMC method very efficient and applicable to systems containing relatively large number of particles with large inertia. Due to its advantages the method is employed for modeling of particle systems in industrial processes and applications of great economical importance, like fluidized beds [2], chemical reactors [3], granular flows [4] and others, and is continually developing and improving to be more suitable for this purpose.

The method combines number of models for the details – approximations of forces, acting on the particles, collision models for the inter-particle interactions, for which different implementations are possible depending on the researchers’ decision on their applicability. In this study we will explore the influence of some of this models and how the choice of one or another affects the results of the simulation – and precisely the influence of Saffman force on the motion and spatial distribution of the particle ensemble and the influence of the collision model on the flow pattern.

According to the research for a single particle moving in Poiseuille flow [5] the modeling of the radial migration of particles with Saffman force, corrected if
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necessary [6], results in more intensive radial migration than observed in experiments.

With respect to the collision model we compare the effect on the flow when the number of collisions is determined using Smoluchowski formula for the number of collisions in laminar shear flow of suspension with NTC method of DSMC model.

We perform the investigation on a dilute gas-solid suspension flow in an entrance part of a tube. We choose the entrance part because it is less explored and often encountered. The developing zones of large shear also show interesting effects on the collision density distribution in Smoluchowski collision model.

2. Numerical Method

The numerical model is briefly presented. More details are available in [7].

The fluid flow is laminar and developing from uniform velocity at the inlet to Poiseuille velocity profile at the outlet of the tube. Since the suspension is dilute, one-way coupling is applied, particles move in pre-calculated flow field.

Particle motion is simulated by DSMC method. Only particle translation is considered. The main features of the method are: operator splitting – free particle motion and collisions between particles are separated and performed consecutively in each time step; inter-particle collisions are binary and spatial independent – colliding pairs of particles are decided within the mesh cell according to statistical considerations, not to tracking of real encounters between particles; model particles represent a number of real particles.

The particle motion algorithm consists of following steps for each time step: generation of particles; free flight with particle-wall interactions; inter-particle collisions.

Particles are moving through the flow field under the influence of the drag, weight, buoyancy and lift force from the fluid shear - eq. (2.1) [6].

\[
\begin{align*}
3 \pi \mu D f (u - v) + mg \left( 1 - \frac{\rho_c}{\rho_d} \right) + \mathbf{F}_L &= W(v), \\
f &= (1 + 0.15 Re_p^{0.687}), \quad Re_p = \frac{\rho_c D |u - v|}{\mu}, \quad Re_c = \frac{\rho_c D^2}{\mu} \frac{du}{dy}.
\end{align*}
\]

The drag force is Stokes drag corrected with Schiller and Naumann correlation for higher Reynolds number Re_p of the particles. The lift force is approximated with Saffman force eq. (2.2), corrected for larger slip velocity (Re_p) and smaller fluid shear (Re_c) with Mei’s correction when necessary [6].

\[
\begin{align*}
\mathbf{F}_L &= 1.61 D z (\mu \rho_c)^{\frac{1}{2}} |\mathbf{v}| \left( \mathbf{u} - \mathbf{v} \right) \times \mathbf{e}_c, \quad \mathbf{e}_c = \nabla \times \mathbf{u}.
\end{align*}
\]

Particle new velocity and position are calculated using implicit scheme:

\[
\begin{align*}
\mathbf{v}_{n+1} &= \mathbf{v}_n + \frac{\Delta t}{m} W(\mathbf{v}_{n+1}), \quad \mathbf{x}_{n+1} &= \mathbf{x}_n + \mathbf{v}_{n+1} \Delta t.
\end{align*}
\]
Collisions are performed within the cells of a uniform cylindrical mesh generated in the computational volume. First the number of collisions $N_C$ to be performed in each cell for the time step is calculated using two different models:

- Smoluchowski formula for the collision rate in laminar shear flow of mono-dispersed suspension:

$$N_C = \frac{1}{2} N (N - 1) N_R \frac{4}{3} \Gamma (2R)^3 \Delta t V_c^{-1}. \tag{2.4}$$

Here $N$ is the number of the particles in the cell, $N_R$ is the number of the real particles represented by one model particle, $R$ is the particle radius, $\Gamma$ is the shear rate of the flow, $\Delta t$ is time step and $V_c$ is the cell volume.

- DSMC – Null Time Counter (NTC) method [1], where the maximum number of collisions is calculated with initially stated maximum value of the relative velocity $c_r$ between the particles in the cell eq.(2.5) and then candidates for collision pairs are randomly chosen among the particles in the cell and accepted for collision according to the rule from eq. (2.6).

$$N_{C_{\text{max}}} = \frac{1}{2} N (N - 1) N_R \pi (2R)^2 c_{r_{\text{max}}} \Delta t V_c^{-1} \tag{2.5}$$

$$\frac{c_r}{c_{r_{\text{max}}}} > \text{Rand}(0,1) \tag{2.6}$$

Particles post-collision velocities are calculated using hard sphere model.

3. Results and discussion

A simulation of a vertical up-flow of a gas-solid suspension in an entrance part of a tube is performed employing the two collision models described above and two models of the particle free flight - with and without Saffman force. The parameters of the flow are listed in Table 1.

<table>
<thead>
<tr>
<th>Table 1. Flow parameters and phase properties</th>
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<tbody>
<tr>
<td>fluid flow</td>
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<tr>
<td>entrance part length $l = 0.115 Re \cdot r$ (Schiller)</td>
</tr>
<tr>
<td>computational mesh dimensions $(r, \Theta, z)$</td>
</tr>
<tr>
<td>tube radius $r$</td>
</tr>
<tr>
<td>diameter $D$</td>
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<tr>
<td>material density $\rho_c$</td>
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<tr>
<td>material density $\rho_d$</td>
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<tr>
<td>kinematic viscosity $\nu$</td>
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<tr>
<td>time step $\Delta t$</td>
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<tr>
<td>Initial velocity $u_0$</td>
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<tr>
<td>velocity relaxation time $\tau = \rho_d D^2 / 18 \mu$</td>
</tr>
</tbody>
</table>

$Re = r \cdot u / \nu$ 486

The computational domain is divided into cells in which collisions are performed and the parameters of the flow are taken. The parameters for the particle flow obtained through the simulation are averaged for the cells and then time average
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flow direction \[\rightarrow\] \[\leftarrow\] gravity acceleration

a) Flow without Saffman force

b) Flow with Saffman force

c) Flow without Saffman force
d) Flow with Saffman force

Fig. 1. Influence of the Saffman force on the flow pattern. a) and b) particle number density (particles/m³) in the first 0.224m (40%) of the entrance part of the tube; c) and d) axial velocity of particles – \(v_z\) and fluid – \(u_z\) to the fluid initial velocity \(u_0\) in cross-sections at 0.012, 0.06, 0.36, 0.52m from the tube inlet.

is taken for several moments after a stationary state is reached. Since no factor breaks the axial symmetry of the flow, the results are averaged also around the tube axis.

First the influence of the Saffman force on the particle distribution and motion is considered. When included in the model of particle free motion, Saffman force, together with the radial component of the fluid velocity near the inlet, is constantly pushing the particles toward the centerline of the tube (fig.1 b)). Collisions are dispersing the particles but not enough to occupy the whole volume of the tube – in fig. 1 d), representing the axial velocity of the phases, is seen that at the end of the tube the particles are unrealistically contracted in a very narrow core. Without the action of the Saffman force particles are dispersed in the whole tube volume, although the fluid radial velocity, which is present in the first half of the tube, is maintaining higher concentration in the core. In the periphery of the tube particles are falling down near the walls (fig.1 c)).

According to a research on a single sphere in Poiseuille flow [5] the modeling of the transverse forces acting on the sphere in a shear flow by Saffman force causes more intensive radial migration than that observed in experiments. Here we receive a similar result for many particles.
a) Flow without collisions. Average volume fraction of the solid phase – 0.53%.

b) Flow with collisions - Smoluchowski formula. Average solid volume fraction – 0.59%.

c) Flow with collisions - DSMC method. Average solid volume fraction– 0.91%.

Fig. 2. Influence of the collision model. Particle number density (particles/m$^3$) in the first 0.224m (40%) of the entrance part of the tube.

Next the influence of the collision model on the flow pattern is investigated. Saffman force is not included in the particle motion equation and the influence of the collisions is more pronounced.

Two clear differences are evident between the two collision models. First is the distribution of the collision density. In the case where Smoluchowski formula is used it depends on the shear rate of the flow (fig.3 a)), which is larger in the periphery near the tube inlet in the developing Poiseuille flow (see fluid velocity in fig.1 c)). In the case with DSMC collisions (fig.3 c)) the collision density distribution is very similar to the number density distribution of the particles (fig.3 d)). The other difference is that in DSMC case the number of the collisions is about 10 times more than the other case.

The large number of collisions influences the structure of the flow – in the case of fig.2 b) the flow pattern is similar to the case without collisions (fig.2 a)), but the particles are more dispersed. Collisions cause a decrease of the average particle velocity and respectively an increase of the volume fraction of the particles (all cases are calculated with equal rate of generation of the particles).

In the DSMC case, near the tube inlet, the radial velocity of the fluid is pushing the particles to the centerline of the tube in the first half of the tube length. The concentration of the particles in the tube core increases (fig.3 d)) and a large
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Fig. 3. Influence of the collision model. Radial distribution of the collision density $C_d$ and normalized number density to the average number density $n / n_{av}$ in cross-sections at 0.012, 0.06, 0.36, 0.52 m from the tube inlet.

number of collisions occur there (fig.3 c)). Under their influence the particles start to disperse (fig.3 d) last 3 cross-sections). But near the centerline particles are confined by the neighboring zone of relatively high particle concentration and though the number of the collisions there is very high, the diffusion to the wall is slow. For comparison, in the Smoluchowski case the space distribution of the collisions is preventing the formation of highly concentrated core zone in the first half of the tube and the pattern of the particle distribution is very different (fig.2 b) and 2 c)). We can conclude that the choice of collision model influences the flow structure and has to be considered.

REFERENCES


R. Shtinkova, E. Toshev

