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

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Abstract. We use the Direct Simulation Monte Carlo (DSMC) method to simulate 3D motion of the particulate phase in dilute gas-solid flows and investigate the influence of the Saffman lift force and the influence of the collision model for the particle-particle interactions on the flow structure. DSMC and the Smoluchowski formula for collisions in laminar shear flow are used as collision models and are compared. Vertical upward flow of gas-solid suspension in an entrance part of a tube is simulated and used as a test-case. Both the application of the Saffman force and the choice of collision model are proved to have considerable influence on the flow structure.
Key words: suspension flow, entrance flow in a tube, numerical simulation, discrete particle modelling, DSMC method.

1. Introduction

The DSMC method was originally developed for simulation of rarefied gas flows [1]. The DSMC method was applied following the similarities of the motion of molecules in fluid flows and particles in suspension flows, like other molecular methods (e.g. molecular dynamics), to model the motion of particles in multiphase and granular flows [2], [3], [4]. Various modifications, concerning the differences in the behaviour of macro-particles and molecules, were applied in order to make the method suitable for macro-particle modelling [2], [4].

DSMC is a stochastic discrete particle modelling method in multiphase modelling. It possesses the following advantages as a discrete particle modelling method, where individual particles are tracked – relatively simple description of the particle motion and boundary conditions for the particles, possibility

to model wide range of solid concentrations and especially low ones, possibility to consider the physical properties of the particles in the collision models, and many others [5]. They are combined with the computational efficiency of Monte Carlo methods for modelling of particle systems – statistical method for inter-particle interactions and representation of the system by a smaller number of model particles. These features of the DSMC method help to overcome the main disadvantage of the discrete particle modelling methods, namely computationally expensive tracking of large number of particles.

The DSMC is a method for numerical simulation based on the Boltzman equation [1]. The evolution of the particle system is divided in two parts within one time step – collisionless motion and inter-particle interactions. They are performed consecutively. First, the whole particle assembly moves and then collisions are performed within the cells of a computational mesh, which is generated especially for that purpose. Particles move independently of each other during their free flight to their new positions according to the Boltzman equation, without checking the new positions for overlaps, and without taking into account the interactions (collisions) between them. Inter-particle collisions are performed, between particles inhabiting the same computational cell regardless of their positions and whether they overlap.

The splitting of particle free motion and inter-particle collisions, the independent free motion of each particle and the performance of collisions in each computational cell independently from the others, are specific for the method and allow easy programming and 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. The method is employed for modelling 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 a number of models for the details – mainly approximations of forces, acting on the particles during their free flight, and collision models for inter-particle interactions, for which different implementations are possible depending on their suitability for the given application. In this study, we will explore the influence of some of these models and how the choice of one or another affects the simulation results – and precisely the influence of the collision model and the Saffman force on the motion and spatial distribution of the particle assembly.

The modelling of the radial migration of particles by the Saffman force results in more intensive radial migration than the one observed in experiments,

according to a research on a single particle moving in a Poiseuille flow [6]. Here, we will try to estimate how it influences an assembly of interacting particles, moving in a developing Poiseuille flow in a tube.

We compare the effect on the flow in two cases, with respect to the collision model – when the number of collisions is calculated using the Smoluchowski formula for collisions in laminar shear flow of suspension, and using the NTC method of the 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 influence the collision density distribution in the Smoluchowski collision model, and the presence of radial velocity of the carrier flow interacts with both collision models and affects the particle distribution in the tube volume.

2. Numerical Method

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

2.1. Fluid flow

The fluid flow is a laminar one and is developing from uniform velocity at the inlet to Poiseuille velocity profile at the outlet of the entrance part of the tube. It is modelled by Navier-Stokes equations for an axisymmetrical incompressible flow, solved by finite-difference scheme. The length of the entrance part is determined according to Schiller formula [8] (table1). One-way coupling is applied since the simulated suspensions are dilute [5], particles move in pre-calculated fluid flow field.

2.2. Particle flow

Particle motion is simulated by the DSMC method. 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 computational mesh cells according to statistical considerations, not to tracking of real encounters between particles; model particles represent a number of real particles.

Particles are considered spherical. Their interactions with surrounding medium are determined using point-particle approximation. Other approximations with regard to particles are that they collide with the other particles and with walls elastically, in order to prevent mixing the effects of non-elastic

collisions with those caused by the collision model. Also, hydrodynamic interactions accompanying inter-particle and particle-wall collisions are neglected. An investigation on particle-wall interactions [9] shows that when particles are moving with Stokes number St_v (eq.(2.3)) greater than 70, their velocity does not change while they are approaching the wall. We assume that hydrodynamic interactions during collisions are negligible, since the St_v in the simulated cases are of the order of hundreds. The model for realization of particle – particle and particle – wall encounters is based on the hard sphere approach.

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

2.2.1. Particle Free Flight

The particles are moving through the flow field under the influence of drag, weight, buoyancy and lift force from the fluid shear – eq. (2.1) [5] (see Table 1 for the notations). Only particle translation is considered.

$$m\dot{\mathbf{v}} = 3\pi\mu D f(\mathbf{u}-\mathbf{v}) + m\mathbf{g}\left(1-\frac{\rho_c}{\rho_d}\right) + \mathbf{F}_L = W(\mathbf{v}), \tag{2.1}$$

$$f = (1 + 0.15Re_p^{0.687}), \tag{2.2}$$

$$Re_p = \frac{\rho_c D\,|\mathbf{u}-\mathbf{v}|}{\mu}, \quad Re_G = \frac{\rho_c D^2}{\mu}\frac{du}{dy}, \quad St_v = \frac{1}{9}Re_p\frac{\rho_d}{\rho_c}. \tag{2.3}$$

The drag force is corrected with Schiller and Naumann correlation f (eq. (2.2)) for particle Reynolds number Re_p (eq. (2.3)) higher than in Stokes regime. The lift force $\mathbf{F}_L$ is approximated with the Saffman force eq. (2.4), corrected for larger slip velocity (Re_p) and smaller fluid shear (Re_G eq. (2.3)) with Mei's correction when necessary [5].

$$\mathbf{F}_L = 1.61D^2(\mu\rho_c)^{\frac{1}{2}}\,|\boldsymbol{\omega}_c|^{-\frac{1}{2}}\,[(\mathbf{u}-\mathbf{v})\times\boldsymbol{\omega}_c], \quad \boldsymbol{\omega}_c = \nabla\times\mathbf{u}. \tag{2.4}$$

The new particle velocity and position are calculated using implicit scheme:

$$\mathbf{v}_{n+1} = \mathbf{v}_n + \frac{\Delta t}{m}W(\mathbf{v}_{n+1}), \quad \mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{v}_{n+1}\Delta t. \tag{2.5}$$

The particles bounce off the tube wall (velocity is reflected when the particle hits the wall) and are deleted after crossing the inlet or outlet cross-sections of the tube.

2.2.2. Inter-Particle Collisions

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 during one time step is calculated using two different models:

– the Smoluchowski formula for the collision rate in laminar shear flow of mono-dispersed suspension [10]:

$$N_C = \frac{1}{2}N(N-1)N_R\frac{4}{3}\Gamma(2R)^3\Delta t V_c^{-1}. \tag{2.6}$$

Here, N is the number of particles in the cell, N_R is the number of real particles represented by one model particle, R is the particle radius, Γ is the shear rate of the flow, Δt is the time step and V_c is the cell volume. The number of possible collision pairs in the Smoluchowski formula is corrected from N^2 to $N(N-1)/2$, according to the analysis in [11].

– the DSMC "No Time Counter" (NTC) method [1], where a maximum number of collisions is calculated with an initially stated maximum value of the relative velocity c_r between the particles in the cell eq. (2.7), 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. (2.8).

$$N_{C_{\max}} = \frac{1}{2}N(N-1)N_R\pi(2R)^2 c_{r_{\max}}\Delta t V_c^{-1}. \tag{2.7}$$

$$\frac{c_r}{c_{r_{\max}}} > Rand[0,1). \tag{2.8}$$

The NTC method can be highly computationally efficient, depending on the appropriate choice of $c_{r_{\max}}$, because it avoids the extensive computations of the average relative velocity of the particles in the cell, which would be necessary for calculation of the real collision rate instead of the approximate maximum rate from eq. (2.7).

Particles post-collision velocities are calculated using hard sphere model [1].

3. Results and discussion

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

Table 1. Flow parameters and phase properties

fluid		particles	
entrance part length $l = 0.115.Re.r$ (Schiller)	0.56 m	computational mesh dimensions (r, Θ, z)	(1 mm, $\pi/10$, 2 mm)
		real/model particles N_R	5
tube radius r	0.01 m	diameter D	100 μm
material density ρ_c	1.205 kg/m^3	material density ρ_d	2500 kg/m^3
kinematics viscosity ν	15.06 e-6 m^2/s	time step Δt	0.002 s
initial velocity u_0	0.730 m/s	velocity relaxation time $\tau = \rho_d D^2/18\mu$	0.07644 s
$Re = r.u/\nu$	486		

The computational domain is divided into cells, in which the collisions are performed and the parameters of the flow are taken. The cells and the time step sizes are chosen according to the condition that a particle should not pass through a whole cell and should pass from about one third to a half of the free flight distance for one time step [1]. The time step has to be smaller than the velocity relaxation time of the particle [5]. The parameters of the particle flow, obtained from the simulation, are averaged for the cells and then a time average is taken for several moments after a stationary state is reached. The results are averaged also around the tube axis since no factor breaks the axial symmetry of the flow.

First, the influence of the Saffman force on the particle distribution and motion is considered. The Saffman force, when included in the model of particle free motion, together with the radial component of the fluid velocity near the inlet, is constantly pushing the particles toward the centre line of the tube (Fig. 1b). Collisions are dispersing the particles but not enough to occupy the whole volume of the tube – in Fig. 1d, representing the axial velocity of the phases, it is seen that at the end of the tube the particles are unrealistically contracted in a very narrow core. Particles are dispersed in the whole tube volume, when the Saffman force is excluded, although the fluid radial velocity, which is present in the first half of the tube, is maintaining higher concentration in the core (Fig. 1a). Particles are falling down near the walls in the periphery of the tube (Fig. 1c). The investigation of the Saffman force influence is performed using the Smoluchowski formula as a collision model. When collisions between particles are not performed the effect of the Saffman force is stronger (no figure is presented).

The modelling of the transverse force from the fluid shear by the Saffman force, according to a research on the motion of a single sphere in

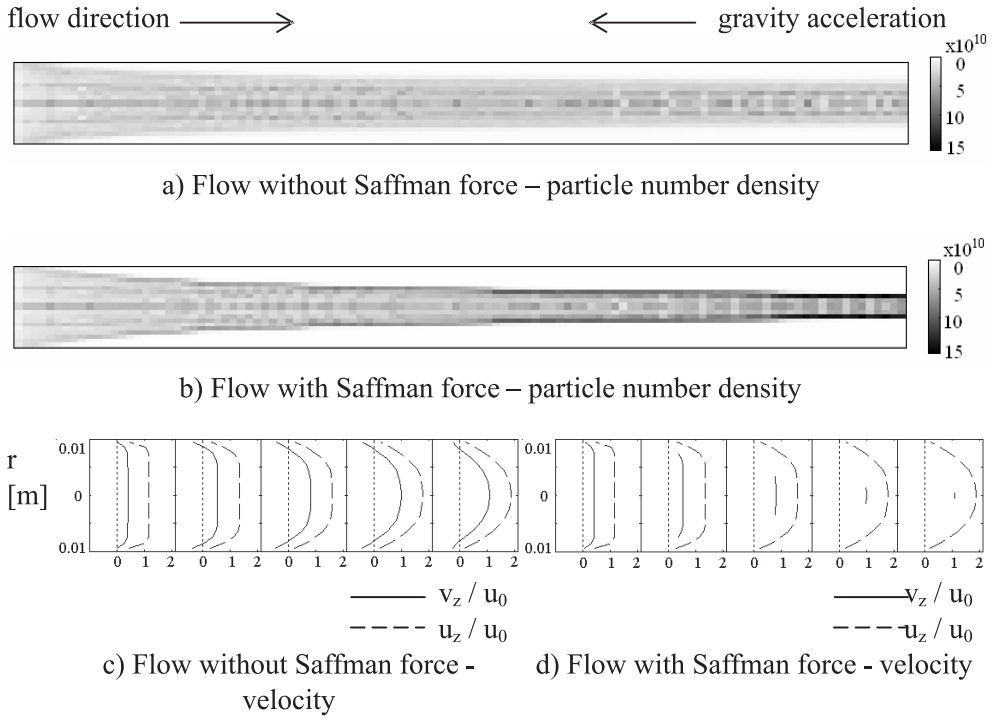


Fig. 1. Influence of the Saffman force on the flow pattern. a) and b) particle number density (particles/m^3) in the first 0.224m (40%) of the entrance part of the tube; c) and d) axial velocity of particles – v_z and fluid – u_z to the fluid initial velocity u_0 in cross-sections at 0.012, 0.06, 0.36, 0.52 m from the tube inlet

Poiseuille flow [6], causes more intensive radial migration than the migration observed in the experiments. Here, we receive a similar result for many particles – even when the Saffman force is corrected to account for the deviations (smaller fluid shear and larger slip velocity $(\mathbf{u} - \mathbf{v})$) from the conditions it is derived for, it possesses unrealistically strong influence on the radial motion of the particles and heavily suppresses the diffusion caused by collisions.

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 distinct.

Two clear differences in the results are evident between the two collision models. First, this is the distribution of the collision density. The collision density (Fig. 2a) depends on the shear rate of the flow in the case where Smoluchowski formula is used, which is larger in the periphery near the tube

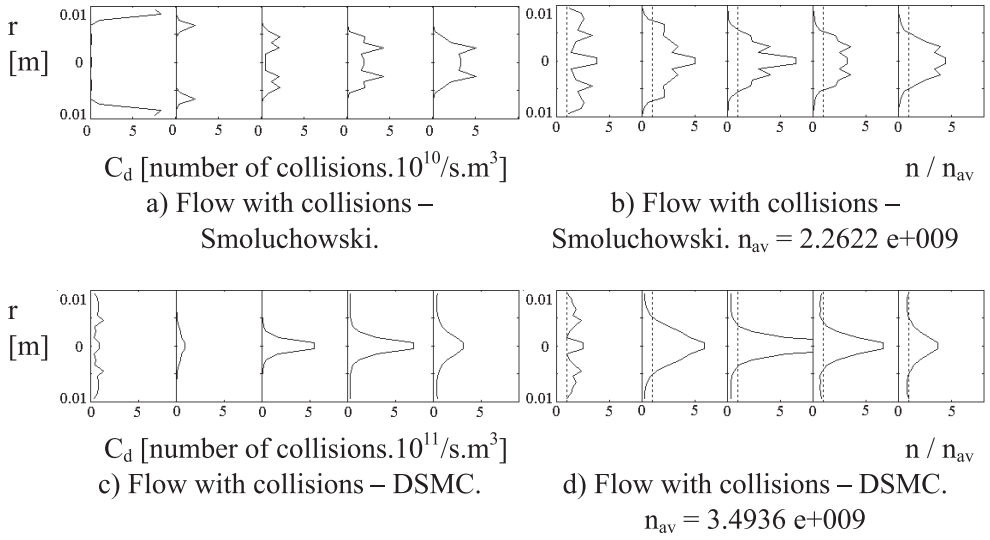


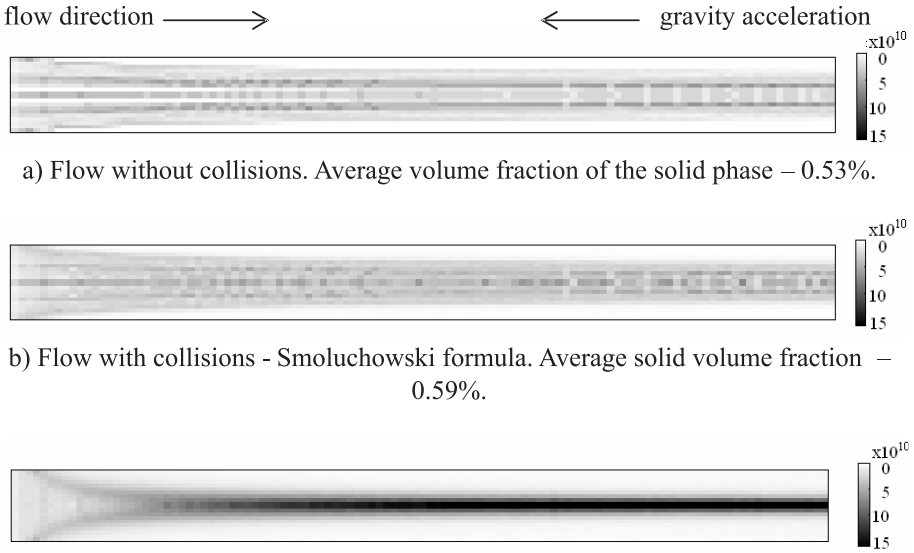
Fig. 2. Influence of the collision model. Radial distribution of the collision density C_d and normalized number density to the average number density n/n_{av} in cross-sections at 0.012, 0.06, 0.36, 0.52 m from the tube inlet

inlet in the developing Poiseuille flow (see fluid velocity in Fig. 1c). The collision density distribution in the case with DSMC collisions (Fig. 2c) is very similar to the number density distribution of the particles (Fig. 2d).

The other difference is that in DSMC case the number of collisions is about one order of magnitude larger than in Smoluchowski case.

The large number of collisions influences the structure of the flow – in the case of (Fig. 3b) the flow pattern is similar to the case without collisions (Fig. 3a), but 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 particles generation).

The radial velocity of the fluid is pushing the particles to the centre line of the tube in the first half of the tube length in the DSMC case. The concentration of the particles in the tube core increases (Figs 2d and 3c) and a large number of collisions occur there (Fig. 2c). The particles start to disperse under their influence (last two cross-sections of Fig. 2d). The particles near the centre line are confined by a neighbouring zone of high particle concentration and though, the number of collisions in the tube core is high, the diffusion to the wall is slow. For comparison, in the Smoluchowski case the space distribution



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

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 number density distribution is different (Figs 3b and 3c).

4. Conclusions

The simulated flows show that the two parts of the investigated model, namely the presence of the Saffman force in the equation of motion, and the collision model have a significant influence on the structure of the simulated flows and their application has to be carefully considered.

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