Modeling of Suspension Flows in Coating Dies

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1. Introduction

Coating of dispersions or suspensions of particles in a fluid is very common in the manufacturing of functional materials. Commonly, a uniform distribution of the suspended phase is required, but, in practice, agglomerates of the suspended particles appear in the final product. It has been shown experimentally that agglomeration takes place as the dispersion flows inside the coating die, before being deposited on the substrate, and that altering the composition of the dispersion and/or the flow conditions can prevent agglomeration. Experimental observations are often limited by the small size of the process and the particles, so theoretical modeling is essential in understanding the agglomeration mechanisms and finding ways of avoiding agglomeration. In this work, theoretical modeling of the flow of the suspension is undertaken by the Discrete Element Method (DEM).

2. Modeling

The DEM was first introduced to the modeling of granular flows by Cundall and Strack (1979). Ever since, it has been used successfully in modeling a wide range of process: flow in fluidized beds (e.g. Tsuji et al., 1993), the discharge of granular flows from hoppers (e.g. Langston et al., 1995), the break-up rate of agglomerates through impact (e.g. Thornton et al., 1996) or flow (e.g. Higashitani et al., 2001), and the mixing of granular materials (Bertrand et al., 2005). It is a deterministic method based on Newton's laws of motion. At any instance in time the linear and rotational acceleration of each particle are calculated by accounting for the forces and torques acting on it. For the linear acceleration it is

$$m_i \frac{\partial \boldsymbol{v}_i}{\partial t} = \mathbf{F}_{B,i} + \sum_{j}^{N_i} \mathbf{F}_{P,ij} + \mathbf{F}_{W,i} + \mathbf{F}_{F,i} \tag{1}$$

Here, $\mathbf{F}_{B,i}$ is the total body force acting on the i-particle; $\mathbf{F}_{P,ij}$ is the force acting on the i-particle by its interaction with the neighboring j-particle, where N_i is the total number of neighboring particles; $\mathbf{F}_{W,i}$ is the force acting on the i-particle by the interaction with the boundaries (walls) of the flow domain; and $\mathbf{F}_{F,i}$ is the force acting on the i-particle due to the interaction with the fluid.

Similarly, the law of conservation of angular momentum provides a relation between the rotational acceleration of the i-particle and the torques acting on it.

$$I_i \frac{\partial \boldsymbol{\omega}_i}{\partial t} = \sum_{j}^{N_i} \mathbf{T}_{P,ij} + \mathbf{T}_{W,i} + \mathbf{T}_{F,i} \tag{2}$$

Here, I_i is the moment of inertia of the i-particle and ω_i is its rotational velocity. T is the torque acting on the i-particle and the indices i, ij, P, W, and F have the same meaning as for equation (1). An account of the forces acting on each particle follows.

Body Forces

The only body forces taken into account in the model are gravitational and buoyancy.

Particle-Particle Interaction

Each particle interacts with the other particles through colloidal forces when the two particle are within a set separation. The colloidal contributions considered in this work are long-range electrostatic forces and short-range London-Van der Waals interaction. As two particles come closer and move relative to each other with only a thin film of liquid medium separating them, hydrodynamic forces, often referred to as *lubrication forces*, arise because of the motion of the interstitial liquid; the normal component of the hydrodynamic interaction is considered. Finally, when the two particles come in contact, collision forces appear. "Soft sphere" collisions are implemented with the normal and tangential components given by Walton and Braun's (1986) "elastic loading and unloading with different stiffness coefficients" model and "incremental slipping" model, respectively.

Particle-Wall Interaction

The interaction of a particle with the solid boundaries of the domain, i.e. the coating die or the substrate, include van der Walls forces, lubrication forces, and contact forces — no electrostatic forces appear because the die and the substrate are assumed grounded. The models used are similar to those for the interaction between two particles, with the tangential component of the collision force given by the model proposed by Di Renzo and Di Maio (2005).

Particle-Fluid Interaction

Because coating flows are laminar, the suspended particles are often sub-micron sized, and the particle load is low, Stokes' law for the drag on a sphere is used for the interaction between the moving fluid and each particle.

Fluid flow

The fluid is assumed Newtonian and incompressible. Its motion inside the flow domain is evaluated in three dimensions using the commercial finite element software FIDAP. In these calculations it is assumed that the particles do not affect the motion of the fluid — the fluid moves as if the particles are not present, occupying all the flow domain; hence, the motion of the fluid is steady as long as the flow conditions do not change. The results of the finite element computations are used in the DEM method for evaluating the Stokes drag on each particle. In essence, a "one-way coupling" between the fluid and the particles is imposed: the particles do not affect the flow of the fluid, but the fluid alters the motion of the particles.

3. Computer Implementation

The implementation of the Discrete Element Method in a computer code is straightforward. Prior to the DEM calculations, the steady-state solution for the liquid flow is obtained

through FIDAP. Following, the particles are randomly positioned inside the flow domain until the required solids volume fraction is reached. Once the positions of the particles are known, all the forces and torques that act on every particle are evaluated. Then, equations (1) and (2) are applied to evaluate the new velocity of the particles and the new positions, using a forward Euler scheme for integrating in time. When the particle positions are updated, the new forces acting on each particle are evaluated and the time integration algorithm is repeated. The value of the time increment of the time integration method is critical in the computations. A large time increment reduces the computational need for simulating a set time, but on the other hand its value has to be small to ensure that there is limited overlap between particles during contact, that the collisions span several timesteps, and that the *soft* collision models produce reasonable results.

Because the subject of this work is to examine the effect of the flow geometry or a specific flow characteristic on the agglomeration rate a certain region of the flow domain is examine to establish what is the fate of the particles that pass through it. During the calculations, particles are allowed to exit the domain through the outflow plane, while new particles enter the domain (join the calculation) from the inflow plane. Particles are removed from the calculations when they cross the outflow plane.

Since the ratio of particle-size to the size of the flow domain is often high, a large number of particles is included in the calculations. As the number of the particles increases, the computational demands rise, so parallelization of the code is required to efficiently handle the calculations. Parallelization is performed, using MPI for message passing, following the ideas of parallelizing molecular dynamics codes as outlined in Plimpton (1995). Computations on two, four and eight processors have been performed with exceptional speed-up results.

4. Results

The DEM is applied to modeling flow of suspensions through a coating die. The chosen geometry is one that resembles the action zone of a slot coater, one of the widely used methods for coating low to medium viscosity liquids or suspensions. Figure 1 shows the pressure contours and representative streamlines of liquid flow through the geometry. The suspension enters through the inflow plane, flows through the coating-die geometry and exits through the outflow plane dragged by the moving substrate.

Figure 2(a) shows the initial configuration of the suspension inside the coating die geometry, generated by randomly positioning the particles inside the domain. To indicate how the suspension behaves with time, one snapshot of the particle locations after $60\,\mu s$ is given in Figure 2(b). It is clear that a very limited number of contacts between particles take place as the flow progresses. In addition, by investigating the transient behavior of the particles it becomes clear that contacts are primarily binary and last for short time periods. This behavior is determined by the interplay of forces present in the system. Additional results indicate the role of the forces acting on the particles and conditions under which high degrees of agglomeration occur; obviously such conditions have to be avoided.

5. Conclusion

The presented preliminary results indicate that the Discrete Element Method can be successfully applied to the simulation of flowing coating suspensions. The proposed model, despite

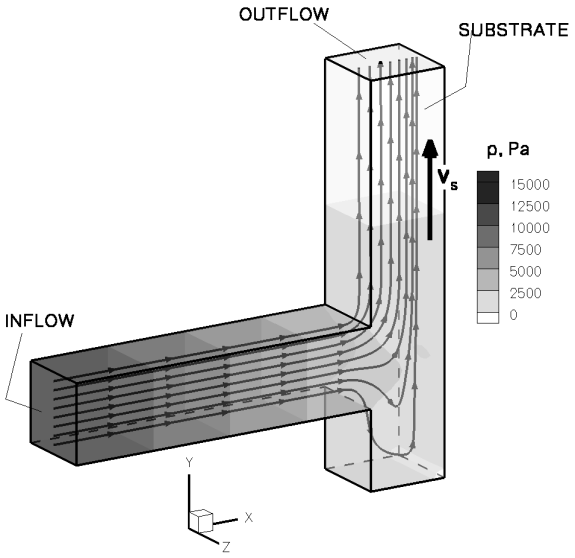
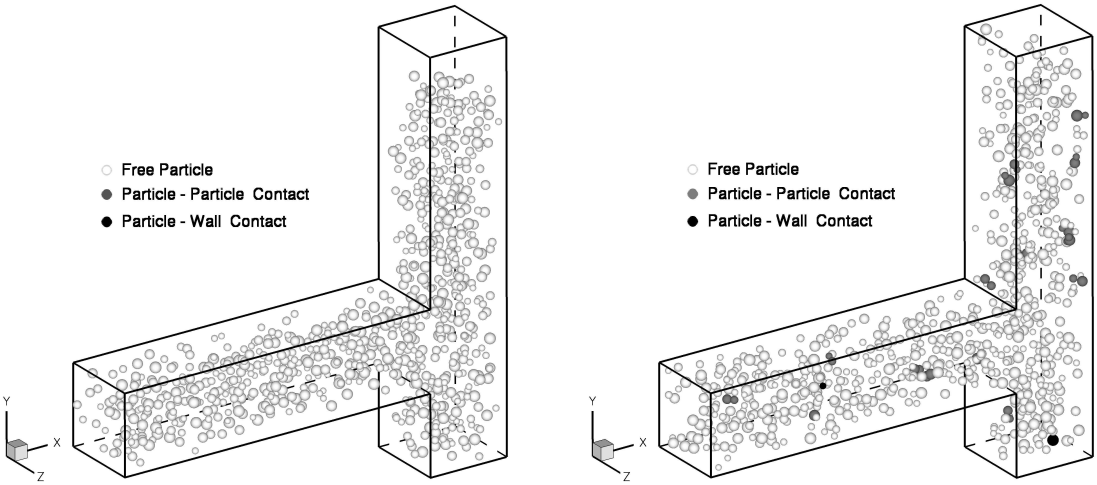


Figure 1. Pressure contours and representative streamlines of the flow inside the standard coating-like geometry.



(a) Initial Configuration. **(b)** No lubrication.

Figure 2. Snapshots of particles positions inside the coating die (a) Initial particle positions; no contact between particles. (b) Particle distribution at time 60 μs; limited particle contacts are observed. Particles in contact with other particles are colored grey, particles in contact with the wall are colored black.

its shortcomings, readily captures the basic behavior of the system; it predicts the movement of the particles with the flow, reveals the role of the individual forces, and indicates agglomeration between particles.

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