Flow of particle dispersions in coating-die geometries

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Introduction

Coating of particle-fluid dispersions is very common in the manufacturing of functional materials, whose quality depends on the uniform distribution of the suspended functional particles. In practice, though, the suspended particles tend to agglomerate, marring the performance of the final product. It has been observed that the agglomeration takes place as the dispersion flows inside the coating die and can be prevented by altering the flow conditions and/or the composition of the dispersion. To investigate this agglomeration process, theoretical modeling of the dispersion flow inside the coating die is undertaken. The used method is a combination of the Finite Element Method (FEM) for the motion of the liquid phase and the Discrete Element Method (DEM) for the flow of the suspension.

Theoretical Aspects

The DEM is based on the ideas of Molecular Dynamics simulations and was first applied to the modeling of granular flows by Cundall and Strack (1979). Ever since, it has been applied to modeling flow inside fluidized beds (Hoomans et al., 2000), discharge of granular material from hopers (Langston et al., 2004), and break-up of agglomerates (Higashitani et al., 2001) among others. It is a deterministic method based on Newton's second law of motion: at each instance in time the linear and angular acceleration of each particle in the suspension is determined by the forces and torques acting on it. For the i-particle it is

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$$m_i \frac{\partial \mathbf{v}_i}{\partial t} = \sum \mathbf{F}_i \qquad \text{and} \qquad I_i \frac{\partial \boldsymbol{\omega}_i}{\partial t} = \sum \mathbf{T}_i \tag{1}$$

where m_i, I_i, $\mathbf{v}_i$, and $\boldsymbol{\omega}_i$ are the mass, moment of inertia, velocity, and angular velocity respectively of the i-particle, $\mathbf{F}_i$ refers to forces acting on the i-particle, and $\mathbf{T}_i$ are the resulting torques. The forces accounted for fall into four categories:

- Body forces: Gravity and buoyancy.
- Particle-particle interactions: Collision forces based on *soft sphere* models, electrostatic and van der Waals colloidal forces, and thin-film lubrication forces.
- Particle-wall interactions: Collision forces based on *soft sphere* models, van der Waals forces, and thin-film lubrications forces.
- Particle-fluid interactions: Drag force from the fluid flow, based on Stokes approximation.

The torques acting on a particle are readily evaluated from the corresponding forces.

The motion of each particle in the dispersion is calculated by integrating equation (1) in time using a forward Euler scheme:

$$\mathbf{v}_i(t+\Delta t) = \mathbf{v}_i(t) + \frac{\Delta t}{m_i}\sum \mathbf{F}_i(t) \qquad \text{and} \qquad \boldsymbol{\omega}_i(t+\Delta t) = \boldsymbol{\omega}_i(t) + \frac{\Delta t}{I_i}\sum \mathbf{T}_i(t) \tag{2}$$

$$\mathbf{x}_i(t+\Delta t) = \mathbf{x}_i(t) + \Delta t\, \mathbf{v}_i(t+\Delta t) \tag{3}$$

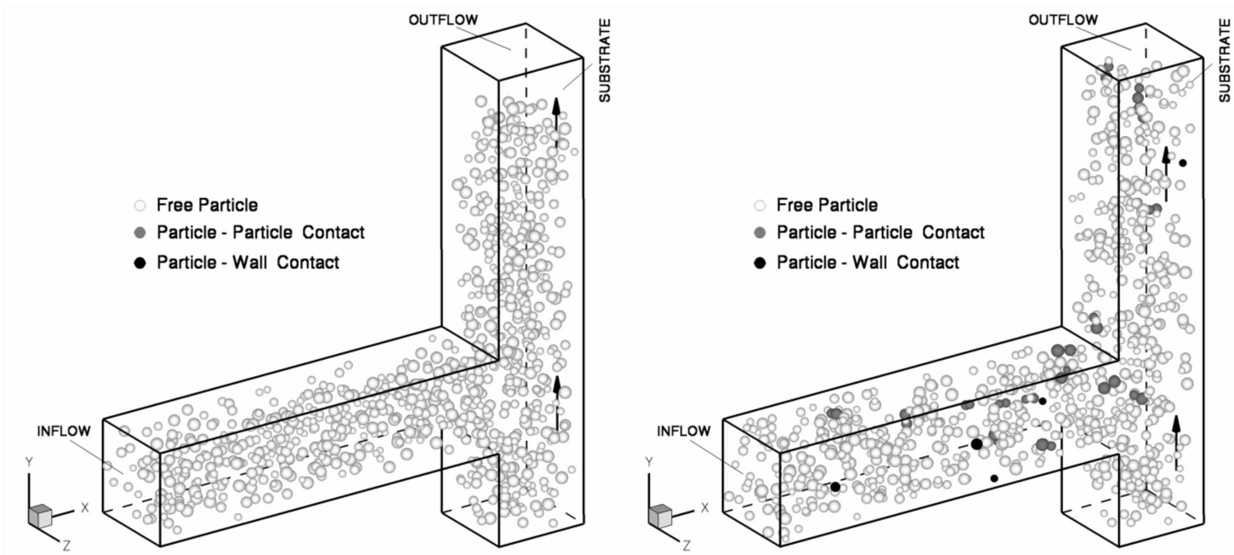
where Δt is the time increment. Once the configuration of the particles at time t is know, all the forces and torques acting on each particle are evaluated, the new linear and angular velocities are calculated using equation (2), and the position of the particles is updated using equation (3). Then, in order to march in time, the new forces are calculated and the time integration algorithm is repeated. One drawback of the method is that because of the used *soft sphere* collision model, the time increment (Δt) has to be very small, in the order of 10^{-10} seconds, which implies that a large number of timesteps must be taken to calculate for a set time. However, the choice of *soft-sphere* collisions, as opposed to *hard-sphere* models, is crucial because it allows lengthy multi-particle contacts so that agglomerates can be formed. A consequence of the small time increment, combined with the large number of suspended particles, is that the computational load is huge; hence, parallelization of the algorithm is necessary.

The motion of the fluid, considered Newtonian and incompressible, is calculated using the Navier-Stokes system of mass and momentum conservation. To simplify the calculations, it is assumed that the particles do not alter the motion of the fluid; an assumption that is valid at low particle loads. Then, provided that the configuration of the domain and the boundary conditions do not change, the fluid flows steadily filling the whole flow domain. Under these conditions, the fluid flow is solved using the commercial package FIDAP which employs an FEM approach. The velocity distribution from the FEM calculations is used in the DEM calculations for evaluating the drag force on a particle. In essence, a one-way coupling between the particle and the fluid motion is enforced: the fluid affects the flow of the particles, but the particles do not alter the fluid motion.

Results

It is of primer interest to examine the behaviour of the suspension as it exits the feed slot of a slot coater and meets the substrate. To avoid the complication arising from the presence of the menisci of the coating bead —the treatment of suspension flows with free surfaces is extremely difficult— a geometry with solid boundaries is used. This flow domain is initially filled with a suspension of sub-micro sized spherical particles with an average diameter of 0.3 μm dispersed in water at a solids load of 5% by volume. This initial configuration is shown in Figure 1a. The evolution of the particles as time progresses is followed, focusing on events of collisions between particles. Figure 1b shows the particle distribution after 0.11 ms; limited agglomeration between particles is observed.

The results indicate the importance of the forces acting on each particle on the rate and degree of agglomeration. Based on these, guidelines for preventing agglomeration through modification of the suspension chemistry and the flow geometry are obtained. Clearly, the Discrete Element Method is an important and useful tool in predicting the fate of suspensions in coating applications.



(a) Initial configuration.

(b) Particle distribution at time 0.11 ms.

Figure 1. Snapshots of suspension flow through the slot coating geometry. **(a)** Initial configuration of particles; by construction, no contact between particles or particles and wall exist. **(b)** Suspension distribution at time 0.11 ms. Particles in contact with other particles are coloured grey; particles in contact with the wall are coloured black.

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