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A new contact liquid dispersion model for discrete particle simulation

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ABSTRACT

In wet granulation and particle coating, it is important to accurately predict the liquid dispersion for process optimisation and quality assurance. In this work, a new contact dispersion model is proposed by taking into account the partial wetting of particle surfaces, which is incorporated into the Discrete Element Method (DEM). In the proposed model, individual particle surfaces are sub-divided and the liquid redistribution between these sub-divided surfaces are tracked with time. The proposed model is applied to simulate a spray drum where liquid is sprayed to initially dry particles, and the liquid dispersion rate is compared with the results obtained from the Shi and McCarthy model (Shi and McCarthy, 2008), which is one of the pioneering models for contact liquid dispersion in DEM. It is found that the Shi and McCarthy model gives faster liquid dispersion when highly viscous liquid is used, whilst the results are largely comparable in the low viscosity case.

1. Introduction

In wet granulation and particle coating, liquid is often atomised into small droplets and sprayed to dry particles. In these processes, fast and homogeneous liquid distribution among a particle bed is the key to the quality assurance of the products: narrow distributions of granule size and density (Hapgood et al., 2003) and inter- and intra-coating uniformity (Toschkoff et al., 2013). The homogeneity of liquid distribution among a particle bed may be achieved by spray (droplet) control and mechanical liquid dispersion. Therefore, many studies have been reported experimentally and theoretically, for example, the effects of the spray flux (Hapgood et al., 2003; Litster et al., 2001), droplet deposition on particle surface (Bolleddula et al., 2010; de Ruijter et al., 1999) and aggitation intensity (Iveson and Litster, 1998; Rough et al., 2005).

Discrete Element Method (DEM) (Cundall and Strack, 1979) has been widely used over the past decades to simulate particulate flow. In DEM, the equation of motion for each particle is solved and it can be facilitated to collect information in individual particle level, which is extremely difficult to achieve by experiment. An increasing number of researchers are also trying to apply DEM to simulate wet particle behaviour by taking into account liquid bonding forces, namely capillary and viscous forces (Muguruma et al., 2000; Lian et al., 1998; Zhu et al., 2011; Liu et al., 2013). The results are in good agreement with the experimental observation for a homogeneously wet particle bed, i.e. all the particles in the bed are wet with the same amount of liquid (Liu et al., 2011; Radl et al., 2010). There are also several attempts to apply DEM to perform spray simulation to dry particles. For instance, Toschkoff et al. (2013) tested several spray models for drum tablet coating and Hilton et al. (2013) developed a coating model of particle surface using a spherical harmonic formulation.

On the other hand, only limited work can be found in literature to model mechanical liquid dispersion in DEM. Mechanical liquid dispersion can largely fall into two categories: (a) convective dispersion and (b) contact (conductive) dispersion (Mohan et al., 2014) as can be seen in Fig. 1. In convective dispersion, liquid is transferred with the bulk movement of wet particle mass, whilst in contact dispersion, liquid is redistributed from one particle to another by

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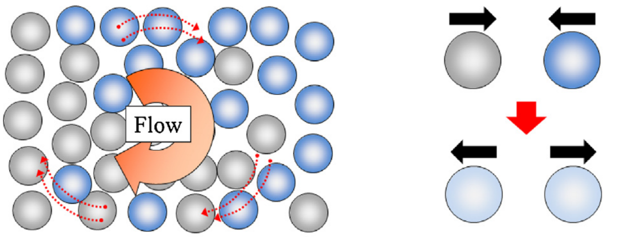

(a) Convective dispersion (b) Contact dispersion

Fig. 1 – Schematic image of liquid dispersion mechanisms.

particle–particle contacts. The convective dispersion can naturally be captured in DEM since the individual particle motion is tracked. To the best of the authors' knowledge, the first contact dispersion model used in DEM was proposed by Shi and McCarthy (2008). In the Shi and McCarthy model, as discussed in detail in Section 3.1, it is assumed that liquid is evenly (and always) coating the surface of individual particles, and the amount of liquid redistributed to the particles at the event of bridge rupture is calculated by assuming a quadratic liquid bridge profile. Mani et al. (2013) also developed a simple model to evenly redistribute liquid to particles at bridge rupture. Mohan et al. (2014) tested several contact liquid dispersion models including a model similar to heat conduction between particles and that with a finite liquid exchange rate after the contact of liquid films on particle surfaces. However, one big assumption used in these models is that the particle surface is always coated uniformly with a thin liquid layer. In other words, the liquid which is redistributed after particle contact instantaneously spreads over the entire particle surface. This assumption may be reasonable only for extremely hydrophilic particle surface with low viscous liquid (for instance, clean glass surface with distilled water). However, in many industrial applications, the particle surface can be less hydrophilic and/or liquid can be highly viscous. Hence, the currently existing models could overestimate the contact liquid dispersion.

In order to properly capture the contact dispersion in wet granulation, it is of paramount importance to take into account the partial wetting of the individual particle surface. A new model is proposed in this work: the particle surface is uniformly divided into a number of "sub-surfaces" and the liquid redistributed at particle contact is locally stored in these sub-surfaces. The proposed model is compared with the Shi and McCarthy model to investigate the difference caused by introducing the partial wetting of particle surface.

2. Theory

2.1. Governing equations

The motion of wet and spherical particle i interacting with adjacent particle j is governed by the following equations of motion for translation and rotation:

$$m_i\ddot{\boldsymbol{x}}_i = \sum_j \boldsymbol{F}_{Cij} + \sum_j \boldsymbol{F}_{Lij} + m_i\boldsymbol{g} \tag{1}$$

$$I_i\dot{\boldsymbol{\omega}}_i = \sum_j \boldsymbol{M}_{Cij} + \sum_j \boldsymbol{M}_{Lij} \tag{2}$$

where m is the particle mass, I the particle inertia moment, $\boldsymbol{x}$ the particle position, $\boldsymbol{\omega}$ the particle angular velocity and $\boldsymbol{g}$ the gravitational acceleration vector. $\boldsymbol{F}$ and $\boldsymbol{M}$ are the forces and torques due to the particle–particle and particle–wall collision (indicated by the suffix C) and the liquid bridge (indicated by the suffix L).

2.2. Contact forces

In the present work, collision forces are calculated using the well-known Hertz–Mindlin model. The detailed description of the collision force model can be found in literature (Mindlin, 1949; Mindlin and Deresiewicz, 1953; Tsuji et al., 1992).

2.3. Liquid state in particles

In wet granulation, liquid is added to dry powder and liquid may exist in different states depending on the degree of the space (pore) saturation between particles (Iveson et al., 2001) as shown in Fig. 2. When a small amount of liquid is added and distributed uniformly among powder, liquid may form a pendular bridge (Fig. 2a), i.e. one bridge formed between a pair of particles. As the amount of liquid increases, liquid may fill some of the pores among particles, which is called a funicular state (Fig. 2b). By increasing liquid amount further, the pores between particles may be completely filled and it is referred to as the capillary state (Fig. 2c). In this work, the amount of liquid added is relatively small and it is assumed that liquid exists only in the pendular state and the mass of liquid does not affect the particle movement to simplify the problem.

2.4. Liquid bridge forces

The existence of liquid causes additional bonding forces between particles. In this work, the capillary forces $\boldsymbol{F}_{cap}$, which are caused by the surface tension, and the viscous forces $\boldsymbol{F}_{vis}$, which are caused by the relative movement of particles and liquid viscosity, are taken into account:

$$\boldsymbol{F}_L = \boldsymbol{F}_{cap} + \boldsymbol{F}^n_{vis} + \boldsymbol{F}^t_{vis} \tag{3}$$

$$\boldsymbol{M}_L = \boldsymbol{r} \times \boldsymbol{F}^t_{vis} \tag{4}$$

$$\boldsymbol{r} = r\boldsymbol{n} \tag{5}$$

where the superscripts n and t indicate the normal and tangential components respectively, r is the particle radius and $\boldsymbol{n}$ is the unit normal vector running from the centre of particle i to the centre of particle j. There are several models available in literature to calculate the capillary forces for symmetric pendular bridges (Lian et al., 1998; Muguruma et al., 2000; Mikami et al., 1998; Rabinovich et al., 2005) and their results are largely comparable (Liu et al., 2011). In this work, the capillary force model proposed by Rabinovich et al. (2005) is used, which can provide reasonable results compared with experimental observations (Liu et al., 2011). The capillary forces for particle–particle and particle–wall are calculated by the following equations respectively:

$$\boldsymbol{F}^{p-p}_{cap} = \frac{4\pi\bar{r}\sigma\cos\theta}{1 + 1/\left[\sqrt{1 + \frac{V_{liq}}{\pi\bar{r}S^2}} - 1\right]}\boldsymbol{n} \tag{6}$$

$$\boldsymbol{F}^{p-w}_{cap} = \frac{4\pi r_i\sigma\cos\theta}{1 + S\sqrt{\pi r_i/V_{liq}}}\boldsymbol{n} \tag{7}$$

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