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Numerical modelling of suction filling using DEM/CFD

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ABSTRACT

Suction filling is widely employed in powder compaction processes in pharmaceutical, ceramics and powder metallurgy industries, especially for cohesive powders. However, scientific understanding of suction filling is still very much in its infancy. In this study, the fundamental mechanisms of suction filling (in the presence of air) are explored using a coupled Discrete Element Method and Computational Fluid Dynamics (DEM/CFD). The effect of suction on powder flow behaviour is examined by comparing suction filling with gravity filling. It is shown that the numerical simulations can well reproduce the experimental observations obtained by Jackson et al. (2007). Moreover, from the numerical simulations, detailed information on powder flow behaviour during suction filling, such as air pressure distribution and powder flow rate, which is difficult to be obtained in the physical experiments, is easily accessible, providing deep insights to enhance our understanding of suction filling processes. According to the simulation results, It is found that the downward motion of the punch in suction filling creates a pressure gradient across the powder bed, which augments the flow of powder into a die. As a result, the mass flow rate and critical shoe velocity are significantly increased, implying that suction filling can be employed to improve the process efficiency of die filling.

1. Introduction

Powder compaction is a process widely used to manufacture tablets and pellets in the chemical, pharmaceutical and detergent industries, and engineering components in ceramics and powder metallurgy. It generally involves several distinctive stages, such as die filling, compaction, ejection and/or sintering. Among these, die filling (i.e. delivering the powder into the die) has been recognised as the critical stage controlling the product quality (Coube et al., 2005; Mendez et al., 2010; Wu et al., 2003a; 2003b; Zhao et al., 2011). In general, a fast and consistent die filling is required to achieve high productivity with low product variability. In industrial applications, two types of die filling are generally employed: gravity filling and suction filling. Gravity filling is referred to as the die filling process in which powders are deposited into a die driven by the gravitational force as the powder mass translates over the die opening, while suction filling is a process in which a movable punch that initially occupies the die cavity moves downwards, when the powder mass completely covers the die opening, and draws ('sucks') powders into the die.

Although gravity filling has been investigated extensively, in particular over the last decade (Zahrah et al., 2001; Bierwisch et al., 2009a; 2009b; Guo et al., 2009; 2010a; 2011a; 2011b; Schneider et al., 2005; 2007; Sinka et al., 2004, Sinka and Cocks, 2009; Wu, 2008; Wu and Cocks, 2004; 2006), scientific investigation on suction filling is still very scarce. To the authors' knowledge, only two papers (Jackson et al., 2007; Guo et al., 2010b) concerning suction filling were published so far. Jackson et al. (2007) developed a model suction filling system and investigated the effect of suction on the flow behaviour of pharmaceutical powders during die filling. They found at the same shoe speed, a much higher fill ratio was obtained during suction filling compared to gravity filling. They anticipated that the creation of vacuum in the die and the consequent expansion of the air in the voids of the powder bed aided the flow of powders during suction filling so that more powders were fed into the die, compared to the gravity filling. Guo et al. (2010b) modelled suction filling from a stationary shoe using DEM/CFD and explored the effect of suction on powder flow behaviour. The numerical analysis revealed that a pressure gradient was induced as a lower air pressure environment was developed in the die when the punch moves downwards. The numerical results were consistent with the experimental observations of Jackson et al. (2007); and demonstrated that the coupled DEM/CFD method was a robust tool for analysing suction filling. Thus, it was further employed in the present study and a more comprehensive investigation was performed in order to explore fundamental mechanisms and enhance our understanding of suction filling.

This paper is organised as follows: a brief introduction of the DEM/CFD method used in this study is presented in next section

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for completeness although readers are directed to Kafui et al. (2002) for more details of the DEM/CFD method. The DEM/CFD models for simulating suction filling are given in Section 3. The powder flow behaviour during suction filling with a stationary shoe and a moving shoe are discussed in Sections 4 and 5, respectively.

2. DEM/CFD

In our in-house DEM/CFD code, the dynamics of solid particles is modelled using DEM, in which the translational and rotational motions of each particle are determined using Newton's equations of motion. For spherical elastic particles considered in this study, the particle interactions are modelled using classical contact mechanics (Thornton and Yin, 1991), for which the theory of Hertz is used to determine the normal force and the theory of Mindlin and Deresiewicz is used for the tangential force. The air-particle interaction force (i.e. the force acting on particle due to the presence of air) is determined using

$$\mathbf{f}_{api} = -\upsilon_{pi}\nabla p + \upsilon_{pi}\nabla \boldsymbol{\tau} + \varepsilon \mathbf{f}_{di} \quad (1)$$

where υ_{pi} is the volume of particle i, and p, $\boldsymbol{\tau}$, ε and $\mathbf{f}_{di}$ are the local air pressure, viscous stress tensor, void fraction and drag force, respectively.

The air is modelled as a continuum using CFD (Kafui et al., 2002), in which the continuity and momentum equations

$$\frac{\partial(\varepsilon\rho_a)}{\partial t} + \nabla(\varepsilon\rho_a \mathbf{u}) = 0 \quad (2)$$

$$\frac{\partial(\varepsilon\rho_a \mathbf{u})}{\partial t} + \nabla(\varepsilon\rho_a \mathbf{uu}) = -\nabla p + \nabla\boldsymbol{\tau} - \mathbf{F}_{ap} + \varepsilon\rho_a \mathbf{g} \quad (3)$$

are solved to obtain the air density ρ_a and air velocity $\mathbf{u}$. In Eq. (3), ∇p is a function of the void fraction ε, particle density and fluid density. The fluid-particle interaction force per unit volume, $\mathbf{F}_{ap}$, is obtained by summing up the fluid-particle interaction forces $\mathbf{f}_{api}$ acting on all the particles in a fluid cell, n_c, and dividing by the volume of the fluid cell ΔV_c, i.e.

$$\mathbf{F}_{ap} = \left(\sum_{i=1}^{n_c} \mathbf{f}_{api}\right) \bigg/ \Delta V_c \quad (4)$$

In such a way, a two way coupling between gas and solid (particle) phases is then achieved. A detailed description of this coupled DEM/CFD approach can be found in Kafui et al. (2002). It has been demonstrated that the DEM/CFD is a robust numerical method and can be used to model gravity filling in air (Guo et al., 2009; 2010a; 2011a; 2011b; Wu and Guo, 2010) and suction filling (Guo et al., 2010b).

3. Suction filling models

A 2D numerical model of suction filling with a moving shoe is shown in Fig. 1. The top of the punch, which is modelled using a physical wall of the same properties as the walls of the shoe and die, is initially located at the level of the die opening. When the powder mass in the shoe translates across the die opening, a constant downward velocity (υ_p) is specified to move the punch downwards. Two punch velocities υ_p of 100 and 276 mm/s are chosen to examine the effect of suction on the powder flow behaviour during die filling with a stationary shoe and a moving shoe. In this study, the die is of dimensions 2×4 mm and the shoe is 5 mm wide. The powder representing a typical pharmaceutical excipient, microcrystalline cellulose (grade Avicel PH101, FMC biopolymer, Philadelphia, USA) is modelled as a monodisperse system consisting of 5,000 spherical particles with a diameter of 50 μm and a particle density of 1500 kg/m^3. The particles are assumed to be elastic with Young's modulus of 8.7 GPa and Poisson's ratio of 0.3. The physical walls are also assumed to be elastic with Young's modulus of 210 GPa and Poisson's ratio of 0.3, representing typical stainless steels. Both interparticle and particle-wall friction coefficients are set to 0.3. The powder bed is colour-banded according to the initial particle position in order to visualise the macroscopic flow patterns.

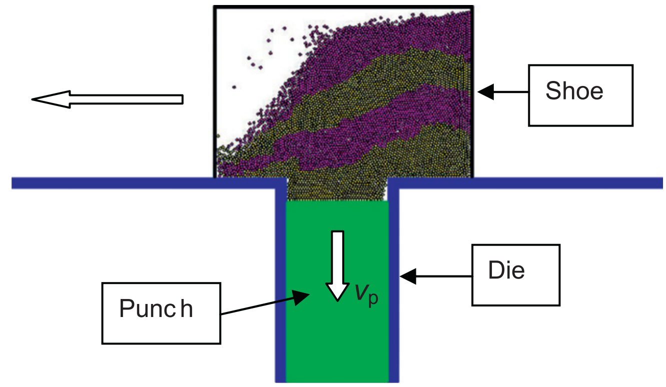

Fig. 1. Numerical model for suction filling with a moving shoe.

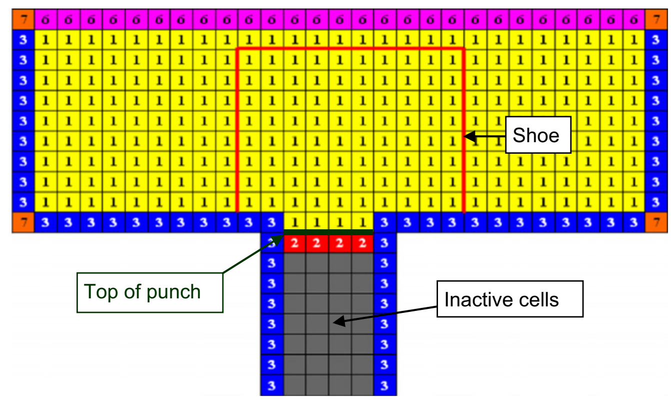

Fig. 2. Schematic diagram of the computational mesh of fluid field and surrounding boundary conditions. [1: interior fluid cell; 2: impermeable moving wall cell, no-slip boundary; 3: impermeable static wall cell, no-slip boundary; 6: continuous air flow cell; 7: corner cell.].

Fig. 2 shows the corresponding schematic diagram of computational mesh of the fluid field and the boundary conditions for incorporating CFD scheme to consider the effect of suction due to the presence of air. The field is partitioned uniformly using the identical cells. The ratio of the fluide cell size to the particle diameter is 3.8, which is in the range of 3–5 recommended for DEM/CFD modelling of gas–solid two-phase flows (Guo et al. 2009). The die walls are treated as the impermeable static no-slip wall boundaries (3), for which both normal and tangential components of air velocity should be equal to zero. The top of the system is open to the atmosphere, so that continuous air flow boundary (6) is assigned, indicating there are no gradient in air velocity and pressure at this boundary. During the suction filling process, the air flows into the die with the downward movement of the punch but it cannot penetrate the top of punch. Hence, the cells, which are just located below the top of punch, are assigned as the impermeable moving wall boundary cells (2). On this boundary, the normal component of the air velocity is set to the same value as the punch velocity (υ_p) and the tangential component of the air velocity is zero (no-slip boundary). The cells below the moving wall boundary in the die are temporarily inactive, and they will be activated sequentially as the punch moves downwards.