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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

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

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

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

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

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.

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

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

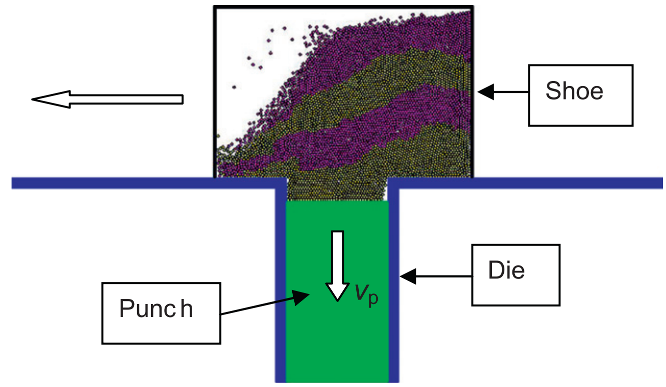

Fig. 1. Numerical model for suction filling with a moving shoe.

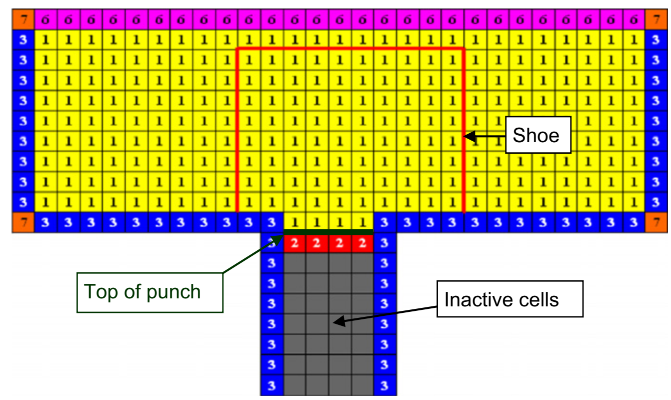

Fig. 2. Schematic diagram of the computational mesh of fluid field and surrounding boundary conditions. [1: interior fluid cell; 2: impermeable moving wall cell, no-slip boundary; 3: impermeable static wall cell, no-slip boundary; 6: continuous air flow cell; 7: corner cell.].

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. 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.

Fig. 3 illustrates the procedure to update the fluid cells in the die region during suction filling. As the top of punch moves down from the current layer to the layer below, the newly approached cells are activated as the interior fluid cells (1). Meanwhile, the cells immediately below the interior fluid cells are set to the impermeable moving wall cells (2). This procedure proceeds until the top of the punch reaches the bottom of the die region, and then the punch stops and the cells at the bottom layer are set to the impermeable static wall cells (3).

4. Suction filling with a stationary shoe

Fig. 4 shows a comparison of the typical powder flow patterns during gravity filling in a vacuum, gravity filling in air and suction filling with a punch velocity of 100 mm/s. During gravity filling in a vacuum, the powder flows into the die smoothly as a continuous column (Fig.4(a)). However, during the filling process two narrow empty regions close to die walls are formed due to the ‘empty annulus’ effect (Seville et al., 1997). During gravity filling in air (Fig. 4(b)), the air is entrapped inside the die and the build-up of air pressure hinders the flow of powder into the die. Two air bubbles are initially formed close to the die walls, resulting in a much thinner powder flowing stream (Fig. 4(b)) at the centre compared to the gravity filling in a vacuum (Fig. 4(a)). The air bubbles rise up and finally burst out on the top surface of the powder mass. After gravity filling in air, the interfaces between different coloured layers appear obscurer than those in a vacuum, due to the chaotic powder flow in the presence of air. During suction filling with a punch velocity of 100 mm/s (Fig.4(c)), a continuous column of a powder is drawn into the die as a plug with the downward movement of the punch, and the empty regions as observed in gravity filling are no longer formed. Therefore, it can be concluded that the gravity filling in air is the slowest and most chaotic filling process, while suction filling is the fastest and most consistent filling process among the cases considered.

The corresponding air pressure distributions at the specified time instants during suction filling with a punch velocity of 100 mm/s are shown in Fig. 5. It can be seen that in the shoe region the air pressure decreases towards the die opening and a lower air pressure environment is developed inside the die. As the punch moves downwards, a decrease in air pressure is obtained close to the top of the punch. Inside the die, the air pressure decreases from the top to the bottom, however, a uniform air pressure distribution in the horizontal direction is observed.

Fig. 6 shows the vertical profiles of air pressure difference, P–P_0, vertical air velocity, u_y, and void fraction, ε, in the central column of the system at various time instants. P_0 represents the standard atmospheric pressure (i.e., $P_0 = 1.01325 \times 10^5$ Pa). As the punch moves downwards, a negative pressure gradient is generated with a decrease in air pressure through the powder bed. Above the powder bed, it is occupied by the air, where the air remains the standard atmospheric pressure. Due to the pressure gradient, the air is driven to flow downwards dragging the particles into the die. The location and the depth of the powder bed can be clearly identified from the profiles of P–P_0 and ε, because P–$P_0 = 0$ and $\varepsilon = 1$ outside the powder bed while P–$P_0 < 0$ and $\varepsilon < 1$ in the powder bed. In the profile plot of u_y, the negative sign indicates that the direction of vertical air velocity is downward. The magnitude of the vertical velocity of interstitial air is larger than the punch velocity, even though the vertical air velocity at the top of the punch (i.e. at the air/punch interface) is specified at the same value as the punch velocity. A sudden change in the vertical air velocity is also observed at the interface between the air and the top surface of the powder bed. This is attributed to the sudden change in the void fraction. When the air flows downwards into the voids of the powder bed, the decrease in void fraction causes a sharp decrease in the cross-sectional area for the flow of air. In order to keep the conservation of mass, the air velocity has to be increased as the cross-sectional area decreases. During the suction filling process, the pressure gradient increases with the downward movement of the punch until it stops. Similar phenomena are also observed at a higher punch velocity (i.e., 273 mm/s, see Guo, 2010).

In order to quantify the powder flow during die filling, an average mass flow rate $\overline{M}$ is introduced as

$$\overline{M} = \frac{m_{total}}{\overline{T}} \quad (5)$$

in which m_{total} is the total mass of particles deposited into the die, $\overline{T}$ is the duration of die filling. A comparison of average mass flow rates under various filling conditions is shown in Fig. 7. The lowest mass flow rate is obtained for gravity filling in air, in which the entrapped air inhibits the flow of particles into the die (Fig. 4(b)). When the air is absent in gravity filling (i.e., gravity filling in a vacuum), the average mass flow rate is improved by a factor of 5. The same average mass flow rate as gravity filling in a vacuum is obtained for suction filling with a punch velocity of 100 mm/s. For suction filling at a punch velocity of 276 mm/s, the mass flow rate is more than an order of magnitude (i.e. 10 times) high than that in gravity filling in air. The increase in powder flow rate during suction filling is facilitated by the negative pressure gradient induced. It can be seen that the powder flow rate during die filling can be increased through operating in a vacuum or suction filling. However, in the engineering practice, it is usually difficult and expensive to perform die filling in a vacuum, so that suction filling could be a more promising technique in order to improve the filling efficiency.

5. Suction filling with a moving shoe

Suction filling with a moving shoe at a velocity of 140 mm/s is also investigated and the results are presented in Figs. 8–10. Fig. 8

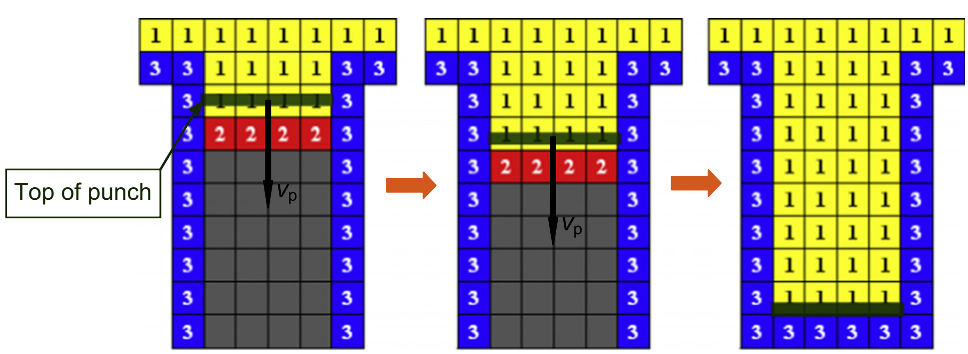

Fig. 3. Updating procedure of the fluid cells in the die region.

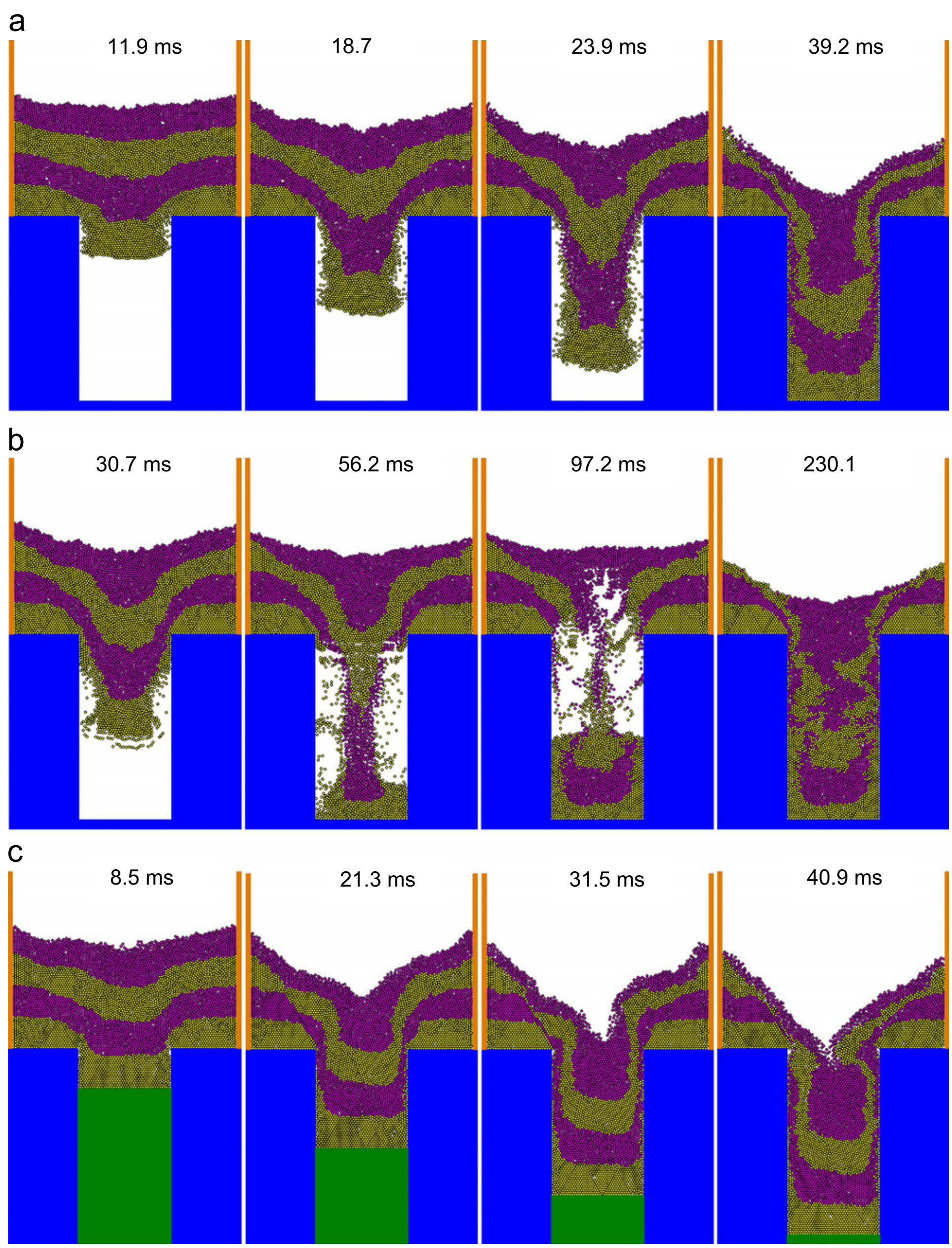

Fig. 4. Power flow patterns during (a) gravity filling in a vacuum (top row), (b) gravity filling in air (middle row) and (c) suction filling (bottom row) with a punch velocity of 100 mm/s. A stationary shoe is used. The labels indicate the elapsed time from the start of die filling.

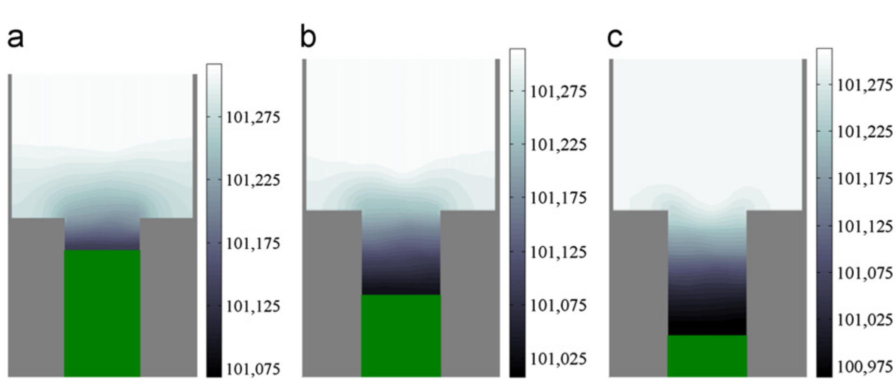

Fig. 5. Air pressure distributions at various time instants during suction filling with a punch velocity of 100 mm/s. (a) t=8.5 ms, (b) t=21.3 ms and (c) t=31.5 ms.

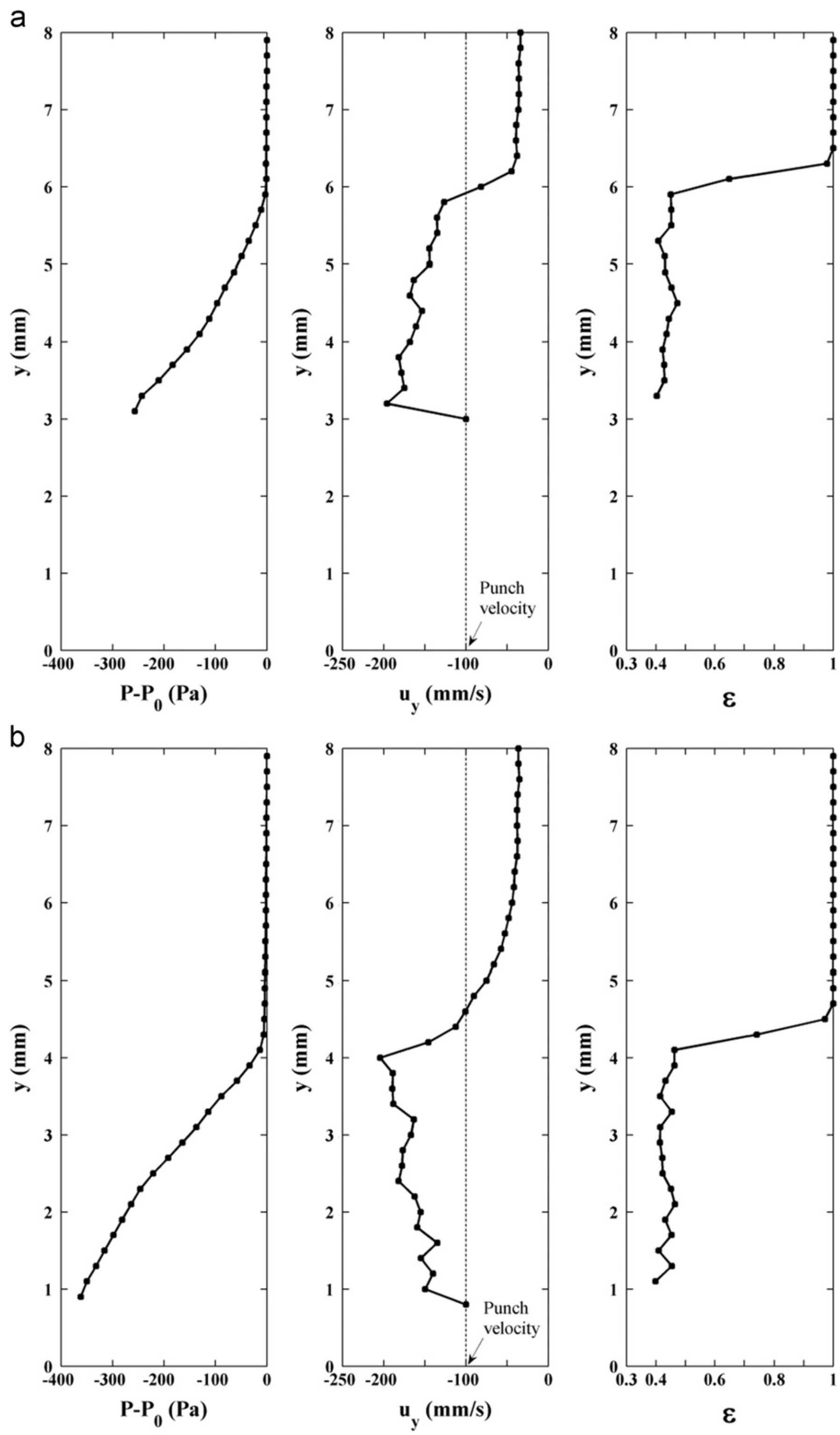

Fig. 6. Vertical profiles of air pressure difference, P–P_0, vertical air velocity, u_y, and void fraction, ε, in the central column of the system at various time instants during suction filling with a punch velocity of 100 mm/s. (a) $t=8.5$ ms and (b) $t=31.5$ ms.

shows a comparison of powder flow patterns between gravity filling and suction filling. Thinner powder flow streams are observed in gravity filling. For gravity filling in a vacuum, the bottom two layers of the powder in the shoe are delivered into the die (Fig. 8(a)). When air is present, the air can be entrapped in the die and the build-up of air pressure opposes the flow of powder. As a result, only the particles from the bottom layer flow into the die (Fig. 8(b)). During suction filling, the powder is 'sucked' into the die as a plug. This phenomenon is consistent with the experimental observations of Jackson et al. (2007) and Sinka and Cocks (2009). For suction filling with a lower punch velocity of 100 mm/s, the punch has not reached the lowest position yet when the powder mass in the shoe has moved across the die opening (Fig. 8(c)). This causes a reduction in effective filling area at the late stage of filling process and a partially filled die, implying that the shoe and punch kinematics needs to be optimised to achieve the best performance and to increase the efficiency during suction filling. Nevertheless, more particles are deposited into the die when compared to the gravity fillings (Fig. 8(a and b)). When the punch velocity is increased to 276 mm/s, the punch can reach the lowest position before the shoe moves across the die opening, and the die is completely filled (Fig. 8(d)).

Fig. 9 shows the average mass flow rates for gravity filling and suction filling at various shoe velocities. The lowest average mass

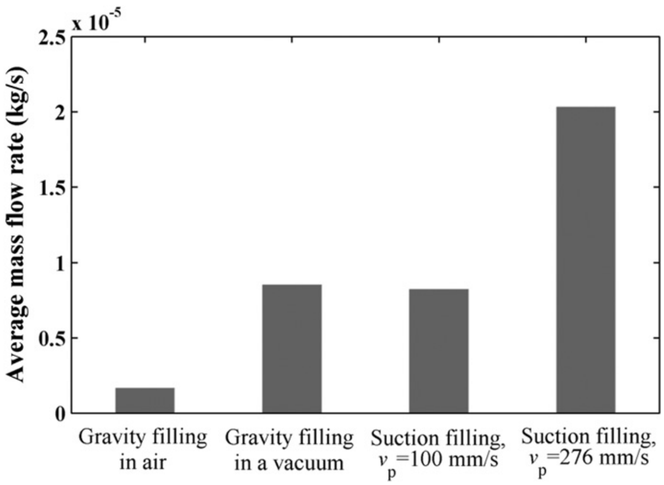

Fig. 7. Average mass flow rates under various filling conditions.

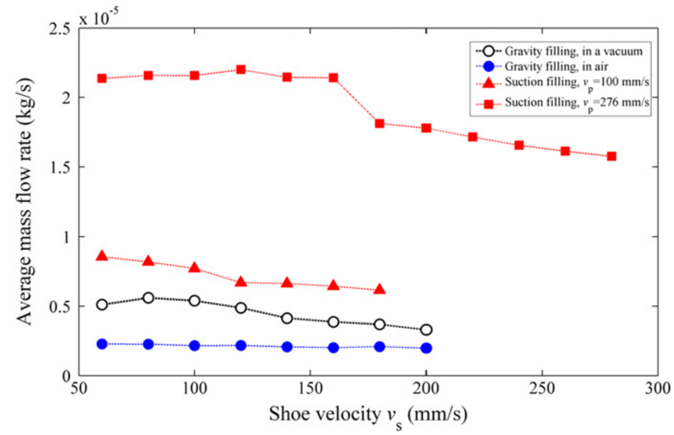

Fig. 9. Variation of average mass flow rate with shoe velocity for gravity filling and suction filling.

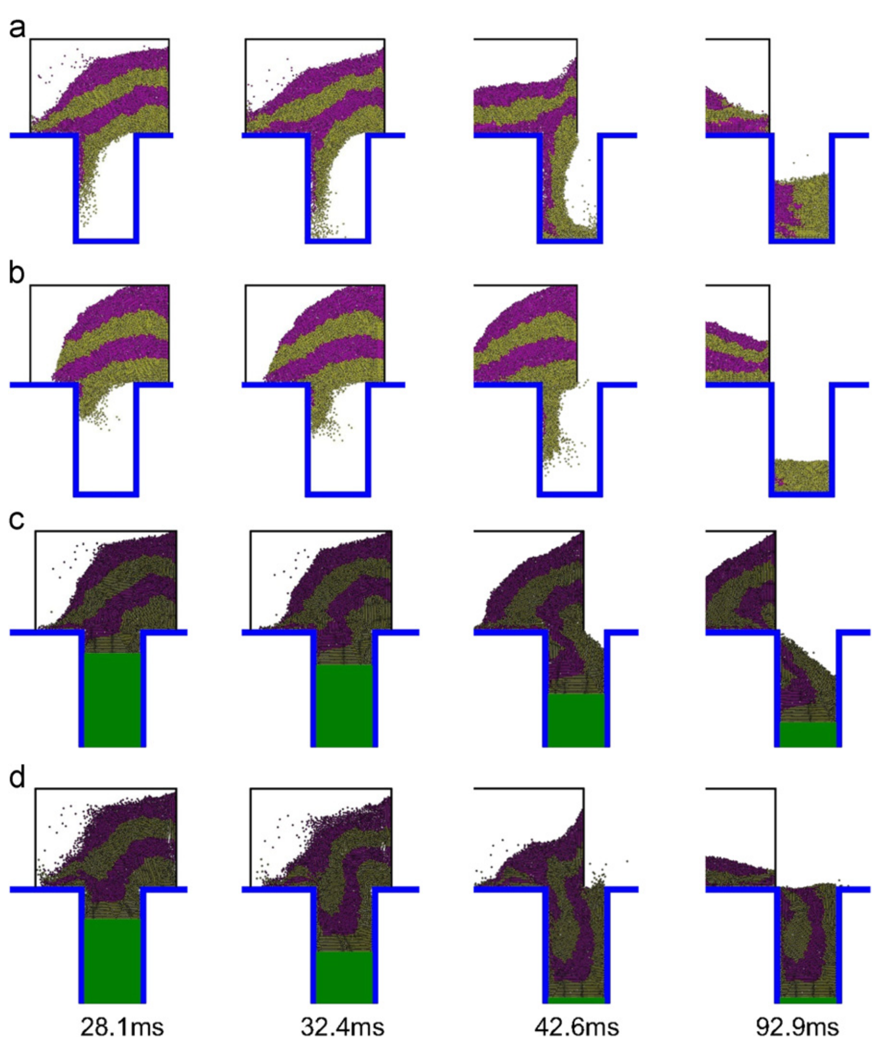

Fig. 8. Power flow patterns during (a) gravity filling in a vacuum, (b) gravity filling in air, (c) suction filling with a punch velocity of 100 mm/s and (d) suction filling with a punch velocity of 276 mm/s. The shoe velocity is set to 140 mm/s. The labels indicate the elapsed time from the start of die filling.

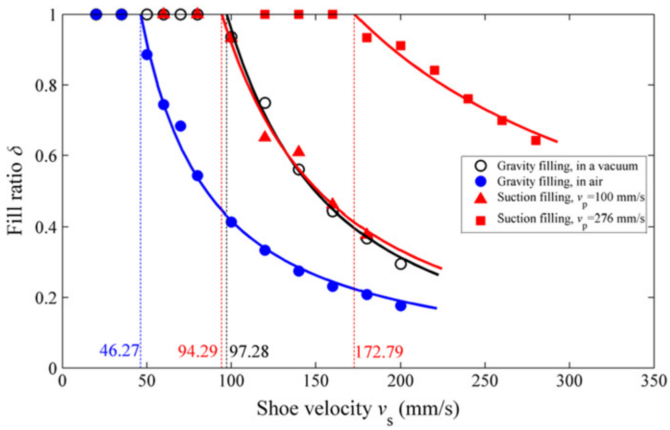

Fig. 10. Fill ratio as a function of shoe velocity for gravity filling and suction filling.

flow rates are obtained with gravity filling in air due to the effect of the entrapped air in the die. The flow rates are improved by a factor of 2 with gravity filling in a vacuum. It is evident that the mass flow rates can be significantly increased in suction filling due to the effect of air pressure gradient. The mass flow rates in suction filling with a punch velocity of 100 mm/s are more than 3 times higher than those with gravity filling in air. A higher punch velocity of 276 mm/s can lead to dramatically high mass flow rates, which are about an order of magnitude higher than those with gravity filling in air.

As shown in Fig. 9, the average mass flow rate decreases slightly with the shoe velocity for gravity filling in air and in a vacuum. The dependence of the average mass flow rate on the shoe velocity in gravity filling is primarily related to the flow patterns (i.e., bulk flow and nose flow), which have been extensively examined in the literature (Wu et al. 2003b, Sinka et al., 2004.). In suction filling with a punch velocity of 100 mm/s, the average mass flow rate decreases as shoe velocity increases. In suction filling with a punch velocity of 276 mm/s, the average mass flow rate is essentially constant when the shoe velocity is not higher than 160 mm/s and a sudden decrease occurs when the shoe velocity exceeds 160 mm/s. For suction filling with a low shoe velocity, the die is always filled by a consistent and thick powder plug, which moves at the same speed as the punch. Therefore, the mass flow rate of powder depends on the punch velocity rather than the shoe velocity. However, when a high shoe velocity (e.g. $v_s > 160$ mm/s) is employed, the punch has not reached the lowest position while the tail wall of the shoe has arrived above the die opening. Under this condition, the filling still proceeds when the tail wall of the shoe is moving across the die opening. During this period, the effective discharging area is smaller than the die opening and the powder flow stream becomes thinner. As a result, the average mass flow rate is reduced in suction filling when the shoe velocity is relatively high.

Fig. 10 shows fill ratio as a function of shoe velocity for gravity filling and suction filling. The fill ratio is defined as the ratio of the mass of the powder eventually delivered into the die to the mass of powder in a fully filled die (Wu et al., 2003b, Wu, 2008; Schneider et al., 2005, 2007; Sinka et al., 2004). In suction filling, the delivery of powder into the die starts only after the die opening is completely covered by the powder mass in the shoe. Although the filling duration is less than that in gravity filling, the mass of powder delivered into the die is significantly increased, especially with a high punch velocity, due to the high mass flow rate (see Fig. 9). Therefore, the highest fill ratios are obtained in suction filling with a punch velocity of 276 mm/s. The deposition of a powder can be restrained by the punch when the punch moves downwards at a low velocity. As a result, the fill ratios in suction filling with a punch velocity of 100 mm/s are close to those in gravity filling in a vacuum, although they are still higher than that in gravity filling in air.

Table 1
Critical shoe velocity v_c and parameter α for various cases considered.

Case	v_c (mm/s)	α
Gravity filling in a vacuum	97.28	1.61
Gravity filling in air	46.27	1.14
Suction filling (v_P=100 mm/s)	94.29	1.46
Suction filling (v_P=276 mm/s)	172.79	0.85

It is clear from Fig. 10 that the fill ratio δ is essentially equal to a value of unity at lower shoe velocities for all cases considered, implying the die is completely filled, while it is less than one and decreases with the increasing shoe velocity at higher shoe velocities as the die is just partially filled. Hence, there exists a maximum shoe velocity at which the die can be completely filled, which is referred to as critical shoe velocity (Wu et al. 2003b, Wu, 2008; Schneider et al., 2005; 2007; Sinka et al. 2004). For incomplete filling, the fill ratio can be expressed in terms of the shoe velocity as (Wu and Cocks, 2004; Sinka et al., 2004; Schneider et al., 2005, 2007)

$$\delta = \left(\frac{v_c}{v_s}\right)^{\alpha} \tag{6}$$

with the shoe velocity v_s being higher than the critical shoe velocity v_c, i.e., $v_s > v_c$. Parameter α depends on the powder properties and process conditions. The values of v_c and α for various cases considered are obtained by treating them as free-fitting parameters and fitting Eq. (6) to the data shown in Fig. 10, as given in Table 1.

It can be seen that the critical filling velocity is increased by a factor of 2 in gravity filling in a vacuum compared to in the presence of air, implying that the die can be completely filled at a much higher die filling speed in a vacuum than in air. Suction filling with a punch velocity of 100 mm/s leads to nearly the same critical filling velocity as gravity filling in a vacuum. By increasing the punch velocity to 276 mm/s, the critical filling velocity is increased dramatically due to the strong effect of suction. At shoe velocities above the critical filling velocity, the fill ratio in suction filling with a punch velocity of 276 mm/s decreases less abruptly than in other cases, indicating that relatively high fill ratios at speeds above the critical filling velocity can still be obtained using the suction filling. Similar results were ever obtained experimentally by Jackson et al. (2007). Therefore, suction filling, especially with a high punch velocity, can dramatically improve die filling efficiency.

6. Conclusions

Suction filling is numerically analysed using a coupled DEM/CFD method. The numerical results are in broad agreement with those obtained by Jackson et al. (2007). The suction filling results are compared with those obtained for gravity filling. It has been found that, in suction filling, a lower air pressure environment is created below the powder mass due to the downward motion of the punch and a thick powder plug is drawn into the die under the combined effects of gravity and air pressure gradient. As a result, the mass flow rate and critical shoe velocity are significantly increased, compared to gravity filling in which the powder is deposited into the die only by gravitational force and the build-up of air pressure in the die inhibits the powder flow. Suction filling with a relatively high punch velocity can enhance filling efficiency with increased mass flow rate and critical shoe velocity.

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