DEM Modeling and Simulation of Axial Vibration Microfeeding System

Ning Ma¹, Xiaopeng Sun¹ and Song Chen¹*, Xiaopeng Wang²

¹State Key Laboratory of Fluorine & Nitrogen Chemicals Xi’an Modern Chemistry Research Institute Xi’an, China
²School of Mechanical Engineering and State Key Laboratory for Strength and Vibration of Mechanical Structures Xi’an Jiaotong University Xi’an, China

¹xpwang@xjtu.edu.cn
*Corresponding author’s e-mail: marknumber1@sina.com

Abstract—The conical head axial vibration microfeeding method was proposed for quantitative filling drug powder into the miniature multi-tank of a controlled-release drug delivery system. The discrete element method (DEM) model of the axial vibration microfeeding system was established by the commercial software PFC3D. Simulation research of the microscopic flow mechanism of powder in conical head under the axial harmonic excitation was carried out, and the effects of the conic angle of conical head, vibration amplitude on the flow rate were also studied. Results showed that powder in a conical tube under the axial harmonic excitation fell from the bottom to the top layer by layer, the powder also vibrated slightly in the falling process, and the friction between powders particles decreased because of the slight vibration. When the powder began to flow, the gap was significantly greater than the initial gap of the powder, and the gap fluctuated with the vibration excitation. The greater the angle of conical head, the more difficult the powder flowed out, and the flow rate was reduced. When the vibration frequency was a constant, the flow rate of the powder was decreased with the increase of the vibration amplitude. These results provide a reference for the design of axial vibration microfeeding system.

1. INTRODUCTION

Using traditional drug delivery methods, the drug concentration is difficult to control, which can lead to side effects and low bioavailability. Implantable controlled-release drug delivery system is an outstanding new drug delivery system, which can make up the shortage of traditional drug delivery methods [1], thus it has a good prospect of application. The preparation of implantable controlled-release drug delivery system is composed of the pressing of the carrier, powder filling, bonding and detection. In powder filling process, a small quantitative drug powder is required to put into a small cavity (about 75μl) of the carrier, and the requirements are different when filling different powder materials. Therefore, a new dispensing method is necessary to meet the demands of various drug powders filling.

Numerous studies on the small quantitative filling of metallic powders have been done in some literatures. The pneumatic method was a common method, such as the aspirating-dispensing head designed by A.R. Gupte et al., the powder was dosed by aspiration of a pre-selected volume and
dispensed by injection intermittently. It was able to deposit powder in a single dose with the mass from 0.5 to 10mg. There were several configurations for the volumetric methods. Arrays of vertically disposed tubes with openings at their bottoms and sliding pistons mounted in were lowered into a continuous layer of powder, and the pistons were raised to fill the chamber of each tube. Then the device was moved to target position and the pistons were pushed to empty the chamber and deposit powder [2]. The electrostatic image method put forward by Ashok can position particles in a single layer. The pre-selected area on photoconductive platform was charged and then the particles were oppositely charged, which lead to the particles attach to the charged region. The single layer can reach to 5–10 μm when the fine powder was used. The powder can flow freely because the powder cluster was scattered by vibration excitation when the vibratory method was used. The special capillary glass hopper was used as the dispensing head by Hou Yali et al., and the vibration excitation was caused by a small DC motor or piezoelectric ceramic actuator. According to the relationship between the directions of powder flow and vibration excitation, vibratory methods can be divided into the lateral style and axial style[3-5]. The powder in the special capillary glass hopper was dosed by the instantaneous inertial force caused by the piezoelectric ceramic actuator, and the single dose of this method can reach microgram level. With ultrasonic methods, the powder in special capillary glass hopper was dosed by ultrasonic excitation, which was available for controlling the flowing of fine powder [6]. While with ultrasonic traveling wave method, the attenuating traveling wave on the wall of tube caused by ultrasonic vibration was used to push the powder to move, and this method was well suitable for accurate powder dosing of small quantitative powder [7].

Much work of the microfeeding of small quantitative powder is mainly on metal powders and other good fluidity powders. For the relevant studies at the initial stage, the cost of these methods is pretty high and their application conditions are complex. So far, there are few studies on microfeeding of small quantitative drug powder. Because the powder filling method based on vibration can conquer the adhesive attraction among powder and between the powder and the wall of carrier, the stability of the powder flow can be reached. In addition, the experimental system of the vibration powder filling method is simple, and the cost of which is low [8]. Therefore, a new method for microfeeding of small quantities of medicinal powder, conical head axial vibration microfeeding method, was proposed in this work. Moreover, the feasibility of this method is verified by the previous tests.

Currently, the research methods of particles flow mainly are experimentation and computer simulation based on mathematic or mechanical models. The experimental method costs too much and is quite occasional and empirical. The simulation of particles’ behaviors in certain conditions avoids the high cost of experimental method and makes some research possible. It also has great reference value for practical application. The computer simulation mainly consists of continuum mechanics method and the discrete method (DEM). DEM is based on the natural traits of discrete objects, and the simulation based on DEM can describe the state of the particle flow accurately and intuitively. Therefore, DEM has been widely used as a tool to study the properties of granular materials [8-10], and DEM is more suitable for the particle flow research of microfeeding. Persson established a 3D DEM model of the pharmaceutical granule flow, the rolling friction, sliding friction and cohesion were studied by the model. The results were consistent with the experimental results [11]. Material flow patterns in three different hoppers were observed and compared by DEM simulation, and the results also proved that DEM can be used to study the complex particle flow [12]. 2D and 3D DEM simulations of cohesive spherical particles were applied to assess the benefit of point source vibration inducing flow in wedge-shaped hoppers, and the effects of exciting point, vibration amplitude and frequency on powder flow were obtained [13].

The DEM model for axial vibration microfeeding system was built by PFC3D in this paper. Moreover, simulation research on the microscopic flow mechanism of the powder in conical head under the axial harmonic excitation was performed, and the effects of conic angle of conical head, vibration amplitude on the flow rate were also studied.
2. THE DISCRETE ELEMENT METHOD
DEM was first proposed by Cundall and Strack in 1979 based on molecular dynamics theory [14], which was originally used to analyze the problems of rock mechanics. Using DEM, the parameters and properties of particle materials, not only single particle, but also overall particles could be studied in depth. It offers the potential for a deeper understanding of the particle materials. The target analyzed is regarded as a collection of discrete rigid units in DEM, and then the whole movement state of the target can be obtained through iterative operation. This method allows relative movements between the units without meeting the displacement continuous condition and deformable coordination condition. Therefore, DEM is very suitable for solving nonlinear problems and large displacement because of its fast calculating speed and lower memory space.

The discrete body is regarded as a collection of particles with certain shape and quality in DEM, each particle is a unit. In order to facilitate analysis, the following assumptions are made in this work:

- The particles are treated as rigid bodies, and the whole behavior of such a system is described in terms of the movement of each particle.
- The contacts occur over a vanishingly small area.
- Behavior at the contacts uses a soft-contact approach where the rigid particles are allowed to overlap one another at contact points.
- The magnitude of the overlap is related to the contact force via the force-displacement law, and all overlaps are small in relation to particle sizes.
- Bonds can exist at contacts between particles.

2.1. Contact models
The process of movement spreading among particles can be simulated by DEM, and the movements inevitably cause collisions between the particles, a force will be generated between the contact particles. Contact model is the foundation of DEM. There are various fundamental contact models in DEM, such as Hertz-Mindlin no sliding contact model, Hertz-mindlin bond contact model, Linear bond contact model, motion surface contact model and linear elastic contact model. However, the various calculations of the contact forces have the same computational principle. Different contact models should be selected for different simulation objects. In this work, the linear elastic contact model was used to study the dispensing mechanism of the conical head axial vibration microfeeding method.

Force-displacement law reflects the relationship of the relative displacement and contact force between two contact units. For both ball-ball and ball-wall contacts, contact force is caused by the deformation of the units at the contact point. The contact force vector \( \mathbf{F} \) can be resolved into shear component \( \mathbf{F}_s \) and normal component \( \mathbf{F}_n \). The shear contact force is determined by the shear relative displacement and the shear stiffness, and the normal contact force is determined by the normal relative displacement and the normal stiffness.

For ball-ball contact, the relevant equations are presented for the case of two spherical particles, labeled A and B in Fig.1.
\[ \mathbf{s}_A, \mathbf{s}_B, \text{and } \mathbf{s}_C \] are the position vectors of the centers of balls A, B and the contact point. \( R_A \) and \( R_B \) are the radius of balls A and B. \( d \) is the distance between the ball centers. \( U^+ \) denotes the overlap in the normal direction, \( \hat{n} \) is the unit normal of the contact plane.

For ball-wall contact, the relevant equations are presented for the case of a spherical particle and a wall, labelled b and w, respectively, in Fig.2. The definition of relevant variables is the same as that in ball-ball model. \( \hat{n} \) is the unit normal to the corresponding wall segment. \( d \) is the shortest distance between ball and wall.

![Figure 2. Notation used to describe ball-wall contact.](image)

The normal and the shear contact force vectors are calculated by (1) and (2).

\[ F_n^i = K^n U_n^i \hat{n} \]
\[ \Delta F_s^i = -k_s \Delta U_s^i \]
\[ F_s^i = \left[ F_s^i \right]_{\Delta t,2} + \Delta F_s^i \]

where \( K^n \) is the normal stiffness [force/displacement] at the contact. \( k_s \) is the shear stiffness at the contact. \( \Delta U_s^i \) is the shear component of the contact displacement-increment vector. \( |F|_{\Delta t} \) is the shear force vector after two time steps at the initial conditions.

### 2.2. Law of motion

The motion of a single rigid particle is determined by the resultant force and moment vectors acting upon it, and can be described in terms of the translational motion of a point in the particle and the rotational motion of the particle. The translational motion of the center of mass is described in terms of its position \( \mathbf{x}_i \), velocity \( \dot{\mathbf{x}}_i \), and acceleration \( \ddot{\mathbf{x}}_i \); the rotational motion of the particle is described in terms of its angular velocity \( \dot{\omega}_i \) and angular acceleration \( \ddot{\omega}_i \). The equations of motion can be expressed as two vector equations: one relates the resultant force to the translational motion; and the other relates the resultant moment to the rotational motion. The equation for translational motion and rotational motion can be written in the vector form by (3) and (4).

\[ \mathbf{F}_i = m_i \left( \ddot{\mathbf{x}}_i - \mathbf{g} \right) \]
\[ M_i = \frac{2}{5} m_i R_i^2 \dot{\omega}_i \]

where \( \mathbf{F}_i \) is the resultant force vector, the sum of all externally applied forces acting on the particle; \( m_i \) is the mass of \( i \)th particle; and \( \mathbf{g} \) is the gravity acceleration vector, \( \ddot{\mathbf{x}}_i \) is the resultant moment acting on the particle, and \( R_i \) is the radius of the particle.

The following expressions describe the translational and rotational accelerations at time \( t \) in terms of the velocity values at mid-intervals. The accelerations are calculated as:
where $\Delta t$ is the time step. Inserting these expressions into (3) and (4), and solving for the velocities at time $t+\Delta t/2$, result in:

$$
\begin{align*}
\dot{x}_i^{(t+\Delta t/2)} &= \dot{x}_i^{(t-\Delta t/2)} + \left( \frac{F_i}{m_i} + \gamma \right) \Delta t \\
\omega_i^{(t+\Delta t/2)} &= \omega_i^{(t-\Delta t/2)} + \left( \frac{5M_i}{2m_i R_i^2} \right) \Delta t
\end{align*}
$$

Finally, the velocities in (7) are used to update the position of the particle center as

$$
\dot{x}_i^{(t+\Delta t)} = \dot{x}_i^{(t)} + \dot{x}_i^{(t+\Delta t/2)} \Delta t
$$

The calculation cycle for the law of motion can be summarized as follows. Given the values of $\dot{x}_i^{(t-\Delta t/2)}$, $\omega_i^{(t-\Delta t/2)}$, $F_i^{(t)}$, and $M_i^{(t)}$, (7) is used to obtain $\dot{x}_i^{(t+\Delta t/2)}$ and $\omega_i^{(t+\Delta t/2)}$. Then (9) is used to obtain $\dot{x}_i^{(t+\Delta t)}$. The values of $F_i^{(t+\Delta t)}$ and $M_i^{(t+\Delta t)}$, to be used in the next cycle, are obtained by application of the force-displacement law.

3. DEM MODEL OF THE CONICAL HEAD AXIAL VIBRATION MICROFEEDING SYSTEM

The schematic of the conical head axial vibration microfeeding system is shown Fig.3.

The microfeeding of small quantities of medicinal powder was realized by conical head which driven by vibration exciter, and the vibration exciter was controlled by the m+p system in the laboratory. The simulation model of the conical head axial vibration microfeeding method was established based on the software, PFC3D. The height of the conical head was 3 cm. The cone-apex angle was taken as 5° based on the actual shape parameters of the conical head. The diameter ranges of the particles used in this model was from 50μm to 75μm, which followed a uniform probability distribution, and the initial porosity was set to be 0.4. The physical model is shown in Fig.4.
Fig. 4 (a) is the initial model, where wall 3 is the model of the conical head; wall 1, 2 and 6 are the auxiliary walls for generating particles; wall 4 and 5 are the container holding the falling particles. Because the particles are generated by the expansion coefficient method in certain area, the particles will push each other. Therefore, the stress among particles produced by squeezing can be released after wall 2 is taken away, and the particles will rise and fall when hitting wall 6, then the system reaches the equilibrium state. Finally, wall 1 and 6 are taken away. In order to describe the flow of particles clearly, the particles are hierarchically stained. The final model is shown in Fig. 4(b). The sinusoidal vibration excitation is applied to the DEM model, and this process is realized by setting the velocity of wall 3 in PFC3D.

There are three kinds of contact models in PFC3D: stiffness model (linear spring and simplified Hertz-mindlin), slip model (frictional slip) and bonding models (contact bond and parallel bond). In this work, the linear-spring model was used and the slips between particles, or between particle and wall, were prescribed in terms of a friction coefficient. We mainly analyzed the microscopic flow of particles in the conical head excited by vibration, and the bonds between particles were ignored to simple the parameter selection and calculation of the model.

The 5-fluorouracil was taken as the researching object, and its density is 700g/ml. According to the relevant empirical data, the main parameters of the powder are shown in Table 1.

| Parameter          | Ball-Ball | Ball-Wall | Unit |
|--------------------|-----------|-----------|------|
| Stiffness          | $5 \times 10^4$ | $5 \times 10^6$ | N/m  |
| Friction coefficient| 1.5       | 0.8       | -    |
| Damping ratio      | 0.5       | 0.5       | -    |

To verify the DEM model, the experimental and simulation results of the powder flow rate under the harmonic excitation were compared, the vibration frequency was 50Hz and the vibration amplitude was 250 μm. The experimental result of the average powder flow rate is 0.643 mg/s, and simulation result is 0.667 mg/s, the error is 3.7%. Therefore, the simulation and the experiment are in good agreement. The performance and mechanism of the conical head axial vibration microfeeding system can be investigated by the simulation model.

4. RESULTS AND ANALYSIS

4.1. Microscopic analysis of the conical head axial vibration microfeeding method

The flow of particles under vibration excitation was analyzed based on the DEM model established in Section 3, the vibration frequency was 50Hz and the vibration amplitude was 150μm. The calculation
time step was set to be 2.0e-7 s\(^{-1}\). The realistic time was 0.5s for 2,500,000 steps. As shown in Fig. 5, the time-dependent state figures of particles flow were captured per 0.05s during the whole simulation.

![Figure 5](image)

Figure 5. The state figures of particles flow under axial vibration excitation.

As shown in Fig.5, there isn’t an obvious mixing between different powder layers due to vibration. All the powder layers ran off the conical head in sequence in the vertical direction.

In order to analyze the particles microscopically, ten particles were selected separately on the axis and the edge of the conical head from top to bottom. The falling balls' trajectories were monitored and the z axis displacement-time curves of these balls are shown in Fig.6. The upward direction of the Z-axis is positive, and zero point is at the outlet section of the powder. From Fig.6, we can see that the entire z axis displacement-time curves decline with fluctuation (fluctuation amplitudes are about a few microns) above zero point, and the space between each series curve remained stable. It can be inferred in a sinusoidal vibration excitation, all particles in the conical head fall with micro vibration. At the same time, the powder fall layer-by-layer. The micro vibration transforms the static friction between particles at the static state into the kinetic friction. The micro vibration between particles also makes powder arch difficult to form, which ensures that vibration excitation is able to start and maintain the flow of powder. At the same time, the micro vibration also improves the anti-blocking property of the microfeeding method.

![Figure 6](image)

Figure 6. The z axis displacement-time curve of relevant balls.

(upp_edge: uppermost edges of the particles; up_edge: upper edge of the particles; mid_edge: edge of the intermediate portion of the particles; bot_edge: lower edge of the particle; bott_edge: lower most edge of the particles; upp_cen: center of the uppermost particles; up_cen: upper center of the particles;
mid_cen: center of the middle portion of the particles; bot_cen: the lower center of the particles; bott_cen: lowest part of the particles at the center.)

The measurement sphere command in PFC3D was adopted. The measurement spheres with the radius of 0.2mm were separately placed at 0.5mm, 0.15mm and 0.25mm above the bottom of the conical head. The curves of the powder porosities at upper, middle and lower parts of the conical head that vary with time measured by the three measurement spheres are shown in Fig.7. As shown in Fig.7, powder porosity in every part of the conical head is around 0.5 in the initial equilibrium state. The porosities of powder at upper, middle and lower parts of conical head fluctuate with time by the vibration excitation. The porosity of powder at lower part increases obviously compared with that in the initial equilibrium state. The porosities of powder at upper and middle parts fluctuate at the state of stability. It shows that powder at lower part becomes loose because of vibration excitation and then the powder fall down. The fluctuation of powder porosity turns the powder into liquid-like phase. This ensures that the microfeeding is stable and reliable and also improves the anti-blocking properties of the microfeeding method.

Figure 7. The powder porosity-time curve of relevant balls.

4.2. Effect of cone-apex angle on microfeeding

The conical head is the main part of the axial vibration microfeeding method for quantitative dispensing. The effect of cone-apex angle on microfeeding is studied by simulation. The conical heads with different cone-apex angles 5°, 15°, 25°, 35° and 45° are simulated. The diameter of the small end of the conical head is 450μm. The modeling and the selection of relevant parameters accord with those of the microscopic analysis of the conical head axial vibration microfeeding method. The powder flow rate-time curves of axial vibration microfeeding method with different cone-apex angles were shown in Fig.8. Through Fig.8, it can be found that the quantitative dispensing process of axial vibration microfeeding is stable. The flow rate of powder becomes smaller and the powder becomes more difficult to escape from the conical head as the cone-apex angle of conical head becomes bigger.

Figure 8. The powder flow rate-time curves under different cone-apex angles.
4.3. Effect of vibration amplitude on microfeeding

The quantitative dispensing of the conical head axial vibration microfeeding method is realized by controlling vibration frequency and amplitude. Vibration frequency is usually kept as a constant, and the quantitative dispensing is achieved by vibration amplitude adjustment. In order to study the effect of vibration amplitude on microfeeding, different vibration amplitudes of 50μm, 100μm, 150μm, 200μm and 250μm are simulated, respectively. The cone angle of cone head is 5° and the excitation frequency is 80Hz. The other parameters are the same as those of the microscopic analysis of the conical head axial vibration microfeeding method. The powder flow rate-time curves in different vibration amplitudes are shown in Fig.9. Clearly when the powder in the conical head flows steadily with a fixed vibration frequency, the powder flow rate decreases with the increase of the vibration amplitude.

![Figure 9. The powder flow rate-time curves under different vibration amplitude.](image)

4.4. Conclusions

The DEM model of axial vibration microfeeding system was established by PFC3D. Simulation research of microscopic flow behavior of the powder in conical head under the axial harmonic excitation was performed. The results reveal the dispensing mechanism of this microfeeding method.

Under the axis vibration excitation, all particles in the conical head fall with micro sinusoidal vibration, which makes the forces between particles decrease. The porosity of powder at lower part of the conical head increases obviously compared with that in the initial equilibrium state. So the powder at lower part becomes loose because of vibration excitation and then falls down.

The effects of cone-apex angle and vibration amplitude on microfeeding are studied by simulation. Results show that the conical head with small cone-apex angle is more appropriate to this microfeeding method, and the dispensing flow rate of the microfeeding method worked in a fixed vibration frequency can be controlled by adjusting vibration amplitude.

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