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Computer Simulation of Tablet Motion in Coating Drum

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Purpose. The purpose is to develop a new method of finding optimal conditions in tablet coating operations with the use of computer simulation. ***Methods.*** DEM(Discrete Element Method), which calculates trajectories of individual tablets by numerically integrating Newton's equations of motion, was used in this simulation. ***Results.*** The effects of tablet size, tablet loading, rotation speed on mean surface time, circulation time, and surface time deviation agree qualitatively with experimental results by other workers. ***Conclusions.*** It is found that DEM is a useful method of predicting tablet motion in a coating drum.

KEY WORDS: coating drum; tablet motion; computer simulation; surface time; circulation time.

INTRODUCTION

Rotating drums are widely used for coating tablets (1). In the drum, a spray of coating solution is ejected from a nozzle onto a moving bed of tablets and the solvent is dried by heated air. This operation is repeated until the tablets are sufficiently coated. To coat all the tablets uniformly, the tablets should be exposed the coating area at the same rate. However, in practice, the tablets are not always evenly coated. To improve coating performance, it is important to know tablet motion in the drum in detail. A few researchers have tried to study such motion experimentally. For example, Bauer (2) observed tablet motion in a transparent drum and Leaver *et al.* (3) measured the surface time of tablets by an optical method. The surface time is defined as the time that a tablet spends on the surface per mass. As far as the present authors know, no attempt has yet been made to obtain the motion of individual tablets in the drum by computer simulation. As computer power increases, it becomes possible to deal with this kind of problem by such techniques. Among various methods, a method called the "Discrete Element Method" (DEM), originally developed in the field of soil mechanics (4), has attracted attention in many fields where particle motion is concerned. In DEM, trajectories of individual particles are calculated by the Newton's equation of motion, with due account for contact forces with neighboring particles. The present authors have made an attempt to apply the DEM to the tablet motion in the coating drum. For simplicity, the tablet shape was assumed to be spherical. In this paper, the calculation is described first and then results are shown about the relation between the surface time and various factors such as tablet size, tablet loading, and drum rotation speed.

MATERIALS AND METHODS

Equations of Particle Motion

Individual particles have two types of motions, translational and rotational. Equations of translational and rotational motions are, respectively,

$$\ddot{\vec{r}} = \frac{\vec{f}_c}{m} + \vec{g} \tag{1}$$

$$\dot{\vec{\omega}} = \frac{\vec{T}_c}{I} \tag{2}$$

where $\vec{r}$ = position vector of the particle center; m = particle mass, $\vec{f}_c$ = sum of contact forces; $\vec{g}$ = gravity acceleration vector; $\vec{\omega}$ = angular velocity vector; $\vec{T}_c$ = sum of torque caused by contact forces; I = inertial moment of the particle ($I = (2/5)mr^2$); $(\dot{\cdot})$ = time derivative.

In the above, fluid forces are neglected. The new velocity and position after the time step Δt is calculated numerically by

$$\vec{v}_s = \vec{v}_{s0} + \ddot{\vec{r}}_0 \cdot \Delta t \tag{3}$$

$$\vec{r} = \vec{r}_0 + \vec{v}_{s0} \cdot \Delta t \tag{4}$$

$$\vec{\omega} = \vec{\omega}_0 + \dot{\vec{\omega}}_0 \cdot \Delta t \tag{5}$$

where suffix 0 denotes values from the preceding time step.

Contact Forces

In the coating drum, almost all particles are in contact with neighboring ones. Regarding the modeling of the contact forces, the readers can refer to reference (5) but the method is briefly described here as a minimum guide. When two particles touch each other, they deform to some degree, however small. In the DEM, such deformation is modeled only indirectly, through an imaginary overlap δ between particle surfaces as shown in Figure 1(a). The larger the overlap, the larger the repulsion force. Additionally, in the process of particle-particle interaction like this, particles lose some parts of kinetic energy. When two particles slide in the presence of a normal force, a tangential friction force occurs. Considering these forces, the contact force is modeled by mechanical elements such as springs, dash-pots and a friction slider as shown in Figure 1(b) and (c). This model of contact forces was given by Cundall & Stack (4). The spring expresses the effect of elastic repulsion and the dash-pot expresses the damping effect. Since the two particles are

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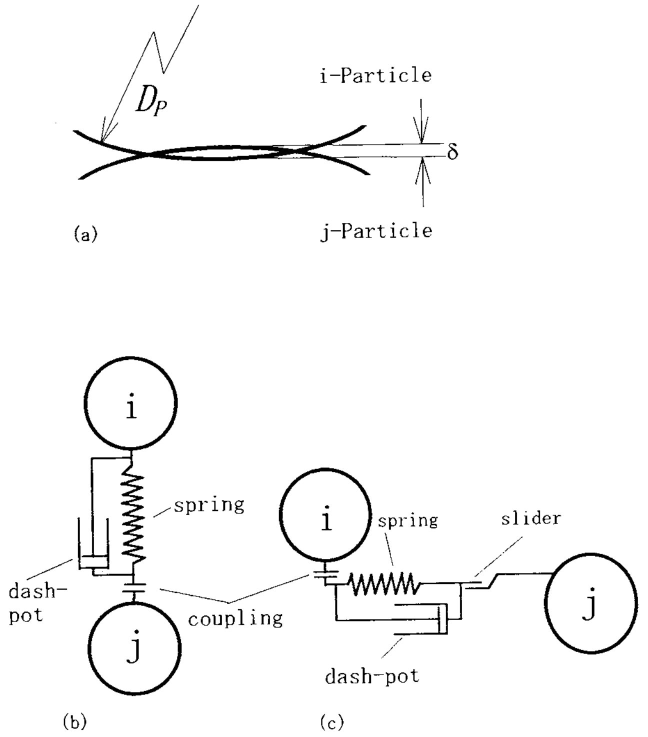

Fig. 1. Model of contact forces, (a) displacement of particles in contact, (b) normal force, (c) tangential force.

allowed to separate due to the repulsion force, a coupling should exist between the particles. If the diameter of one particle is set to be infinite, the model corresponds to the particle-wall contact. Effects of these mechanical elements on particle motion appear though the following parameters: k, stiffness; η, damping coefficient; μ_f, friction coefficient; when two particles denoted by i and j are in contact, the normal component of the contact force, $\vec{f}_{cnij}$, acting on the particle i is given by the sum of the forces due to the spring and the dash-pot,

$$\vec{f}_{cnij} = (-k_n\delta_{nij}^{3/2} - \eta_n\vec{v}_{rij}\cdot\vec{n}_{ij})\vec{n}_{ij} \tag{6}$$

where δ_{nij}: displacement of particle caused by the normal force, $\vec{v}_{rij}$: velocity vector of particle i relative to particle j and $\vec{n}_{ij}$: unit vector directed from the center of particle i to that of particle j.

The tangential component of the contact force, $\vec{f}_{ctij}$, is given by

$$\vec{f}_{ctij} = -k_t\vec{\delta}_{tij} - \eta_t\vec{v}_{sij} \tag{7}$$

where k_t and $\vec{\delta}_{tij}$ are respectively the stiffness and displacement vector in the tangential direction. In the above equations, the suffixes n and t mean the components corresponding to the normal and tangential directions, respectively. $\vec{v}_{sij}$ is the slip velocity of the contact point, which is given by

$$\vec{v}_{sij} = \vec{v}_{rij} - (\vec{v}_{rij}\cdot\vec{n})\vec{n} + r_s(\vec{\omega}_i + \vec{\omega}_j)\times\vec{n} \tag{8}$$

where r_s is the radius of the particle. If the following relation is satisfied

$$|\vec{f}_{ctij}| > \mu_f|\vec{f}_{cnij}| \tag{9}$$

particle i slides and the tangential force is given by

$$\vec{f}_{ctij} = \mu_f|\vec{f}_{cnij}|\vec{t}_{ij} \tag{10}$$

instead of eq.(6). Eq.(10) is the Coulomb-type friction law. $\vec{t}_{ij}$ in eq.(10) is the unit vector defined by

$$\vec{t}_{ij} = \frac{\vec{v}_{sij}}{|\vec{v}_{sij}|} \tag{11}$$

In general, a given particle will be in contact with several other particles. Therefore the total force and torque acting on a particle is obtained by taking the sum of forces due to all contacts with surrounding particles.

The next step after modeling the contact forces is to determine the values of the stiffness k, damping coefficient η and friction coefficient μ_f. Among these parameters, the friction coefficient μ_f is measurable and regarded as a parameter which can be given empirically. The damping coefficient η can be calculated by Hertzian contact theory when the Young's modulus and Poisson ratio are known. The relations between the stiffness and such physical properties are shown in reference (5).

Calculation Conditions

The coating drum simulation here was a miniature version of the commercial machine because the number of tablets is limited by the capacity of the computer used. The diameter of the cylinder is 60 mm, which is one-eighth that of the laboratory machine Hi-Coater type 48 (HCT-48N) manufactured by Freund Industrial Co., Ltd. The key parameter of particle motion in the drum is the ratio of the centrifugal force to the gravitational force, that is, $r\omega^2/g$. In order to make the ratio equal between the simulation and practical machine, the value $r\omega^2$ must be the same in both cases. In the Hi-Coater type 48, the diameter of drum is 480 mm and the rotation speed in operation is usually set to be around $\omega = 18$ rpm, the corresponding rotation speed in the simulation is about $\omega = 50$. The rotation speed ω was changed from $\omega = 50$ rpm to $\omega = 150$ rpm in this work.

The characteristic properties of tablets in the present simulation are as follows. Tablets were assumed to be spheres. The density was 2690 kg/m^3. The Young modulus and Poisson ratio were 1.0×10^5 N/m^2 and 0.3, respectively. The coefficients of restitution and friction were 0.9 and 0.3, respectively. The cases of three different diameters were calculated, 2.0, 3.0, and 4.0 mm. The computer used in this work was a Hewlett Packerd 700 series Type 735.

RESULTS

At first, tablets are at rest and the surface of the tablet layer is horizontal. As the drum begins to rotate, the surface forms at the dynamic angle of repose. Three dimensional patterns of tablet motion can be viewed on the computer

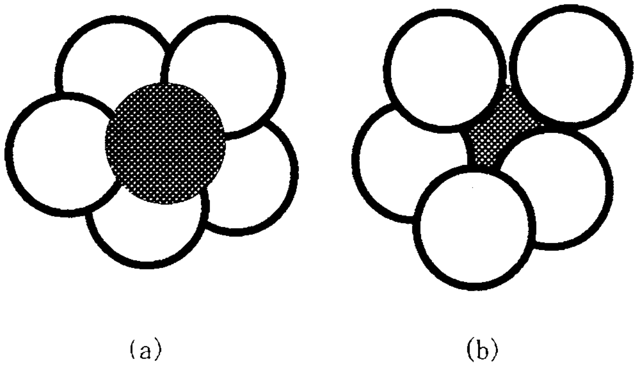
(a) (b)

Fig. 2. Tablets in the coating zone, (a) tablet on the surface, (b) tablet behind other tablets.

display, and are similar to those observed in physical experiments. When a tablet lies within the circle of the spray zone, coating of the tablet is assumed to take place. The circle was located in the central part of the surface, with a diameter assumed to be 16 mm. The present simulation enables one to trail motion of individual tablets at every moment and thus detailed information of tablet motion can be obtained.

The surface time is the most important factor for the coating process. In this simulation, the surface time was obtained by the following procedure. If a tablet is on the top of the surface and within the spray zone, it receives the spray on the whole area facing the spray as shown in Figure 2(a). However, if the tablet is near the surface but behind other tablets, the area receiving the spray decreases. The surface ratio, α, is defined by

$$\alpha = A_1/A_0 \tag{12}$$

where A_0 is the projected area of the whole tablet and A_1 is the projected area exposed to the spray as shown in Figure 2(b). The α value of the tablet on the top of the surface is 1 and α of the tablet behind other tablets is less than 1. Most of the time, α of the tablet is zero, because it is deep in the tablet layer.

Figure 3 shows the change of α of a tablet plotted over the time. The surface time T_s is defined by the following equations in this work. T_s is the averaged value of the summation of the time length in which α is larger than 0.5.

$$T_i = t_{i1} + t_{i2} + \cdots + t_{in} = \sum_{j=1}^{n} t_{ij}$$
$$T_s = \frac{T_1 + T_2 + \cdots + T_N}{N} = \frac{\sum_{i=1}^{N} T_i}{N} \tag{13}$$

where n is the total number of events for which α of a tablet is larger than 0.5 and N is the total number of tablets. Only numerical simulation makes such rigorous definition of the surface possible. In this work, the value of 0.5 is used for convenience as a representative value between 1 and 0.

It was confirmed that tablet motion is steady by observing that the dynamic angle of repose reaches a constant value. In this work, the relation between the surface time and the rotation speed ω was investigated first and it was confirmed that the qualitatively same results as shown experimentally by Leaver *et al.* (3) were obtained, *i.e.*, the surface time becomes smaller as the rotation speed ω and tablet loading increase, and the larger the tablet size, the longer the surface time.

Not only the surface time but the standard deviation of the surface time is important, which is difficult to measure in practical operations. The deviation σ is defined by

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N}(T_i - T_s)^2}{N}} \tag{14}$$

Figure 4 shows the standard deviation of the surface time in the case of T_0 = 10 s where T_0 is the time from the moment when the drum begins to rotate from the starting time. In Figure 4(a), the number of tablets N is varied and the tablet diameter D_p = 4 mm is fixed, while the diameter D_p is the variable parameter in Figure 4(b). The number of tablets is proportional to tablet loading in the operation when the diameter is fixed. In Figure 4(b), the volume of the tablet layer is fixed at 30% of the whole volume of the drum. Therefore, the number of tablets in each case of Figure 4(b) is different. Also, these results are qualitatively the same as those obtained in physical experiments (3). That is, the standard deviation becomes smaller as the rotation speed ω and tablet

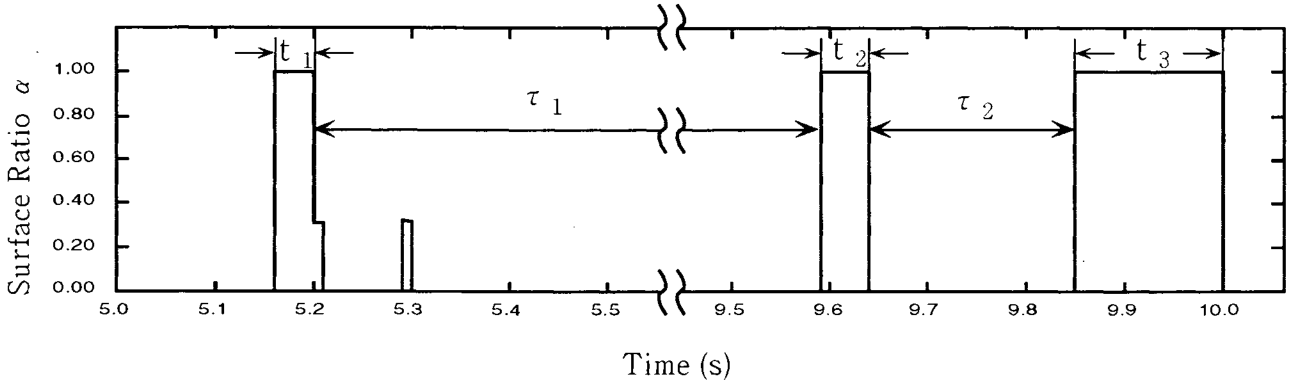

Fig. 3. Pulsating signals showing appearance of tablet on the surface.

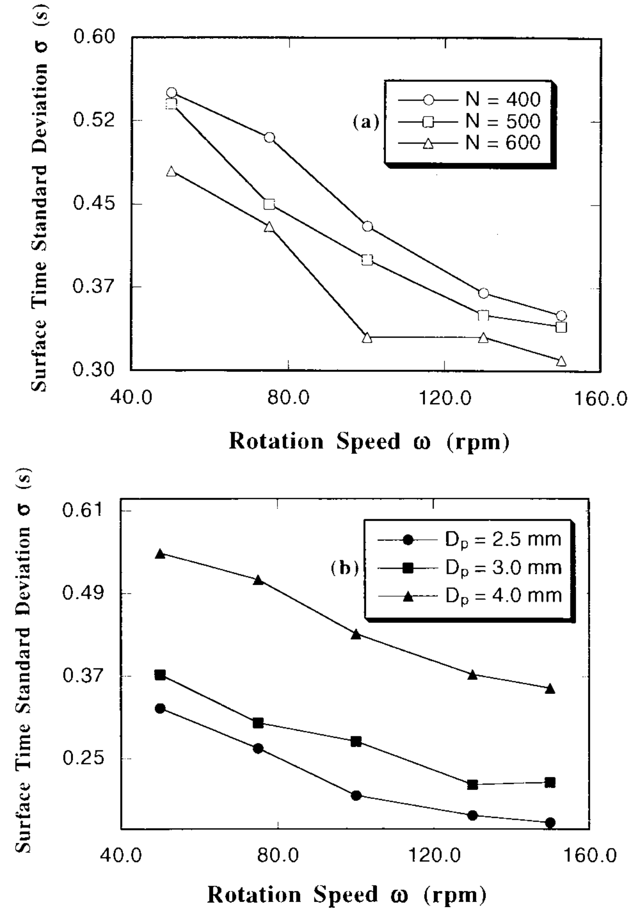

Fig. 4. Average circulation time (T_0 = 10 s), (a) effect of tablet loading (D_p = 4 mm), (b) effect of tablet size (volume ratio of tablet layer to the drum = 30%).

loading increase, and the larger the tablet size, the larger the standard deviation.

Figure 5 shows the relation between the average circulation time T_c and the rotation speed ω. These results are those obtained after 10 s from the starting time. The average circulation time T_c is defined by

$$I_i = \frac{\tau_{i1}+\tau_{i2}+\cdots+\tau_{in}}{n} = \frac{\sum_{i=1}^{n}\tau_{ij}}{n}$$

$$T_c = \frac{I_1+I_2+\cdots+I_N}{N} = \frac{\sum_{i=1}^{N} I_i}{N} \qquad (15)$$

where $\tau_1, \tau_2 \cdots \tau_n$ are intervals between events of tablet appearance on the surface as shown in Figure 3 Like Figure 4, the effects of rotation speed, tablet loading and tablet size can be seen in Figure 5(a) and 5(b). The results in Figure 5 also agree qualitatively with experimental results (3).

Though figures are omitted here, variations of the standard deviation with time were investigated in this work and

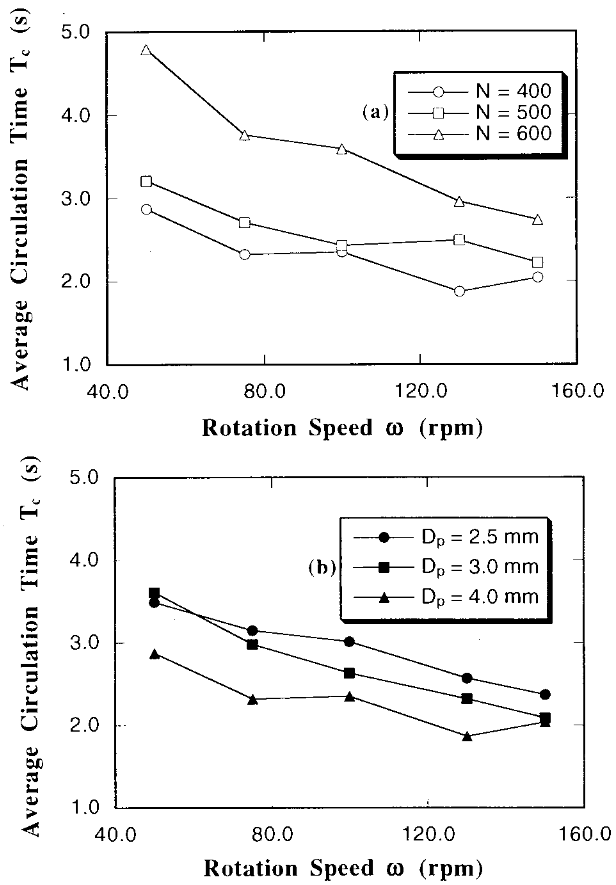

Fig. 5. Deviation of surface time (T_0 = 10 s), (a) effect of tablet loading (D_p = 4 mm), (b) effect of tablet size (volume ratio of tablet layer to the drum = 30%).

it is found that large deviation is observed at small rotation speed. This kind of information is difficult to obtain from physical experiments.

CONCLUSIONS

Numerical calculation of tablet motion in a coating drum was performed. Motion of all individual tablets was calculated by the Newton's equations of motion, taking into account contact forces between tablets. For simplicity, the tablet shape was assumed to be a sphere. The contact forces were modeled by the Discrete Element Method (DEM). The results of the surface time, circulation time, and deviation of surface time agree with experimental results qualitatively.

The present authors did not make physical experiments under the same conditions as the simulation, and thus nothing can be said regarding quantitative comparison with experiments. However, considering that the present analysis did not use any information from experiments with coating drums, the results are satisfactory. Simulations made under more realistic conditions than the present one, particularly about a drum size and tablet number, are planned in continuation of the present work.

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