Simulating Motion of Toner Using the Discrete Element Method

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Abstract

The Discrete Element Method (DEM) is one of the most popular and powerful tools for simulating the motion of granular materials. However, the traditional DEM focuses only on cohesionless granular materials; that is, materials whose motion is dominated by extra forces without significant influence of particle to particle attractive forces. For this reason the DEM approach has seen limited application in the study of toner. This study, however, proposes a numerical DEM model that incorporates cohesive forces, namely Van der Waals' and electrostatic forces, in the study of toner movement. Van der Waals' forces are those which exist due to the polarization of molecules in the toner particles into dipoles of positive and negative charge. Electrostatic forces exist between charged particles such as toner and are directly proportional to the magnitudes of the charges and inversely proportional to the square of the distance between them. The DEM model was decomposed into three sub-models, and these decomposed sub-models were validated separately by comparing the simulation results with experimental results. Finally, the model was used to simulate the motion of toner in the developer nip of an electrophotographic imaging process. The simulation results were compared with experimental results, and the simulation results fit very well with experimental results. This work shows that it is possible to achieve quantitative agreement between DEM simulations using cohesive forces and experimental results.

Introduction to Toner

Granular materials are everywhere and are used in many engineering applications. The flow of a granular material plays a very important role in many industrial processes, such as mixing, crunching, separation, and suspension.

Toner, one of the granular materials, plays a very important role in electrophotographic (EP) printing. The two most common types of toner being used nowadays in EP printing are conventional pulverized toner as shown in Figure 1 and chemically grown toner as shown in Figure 2.

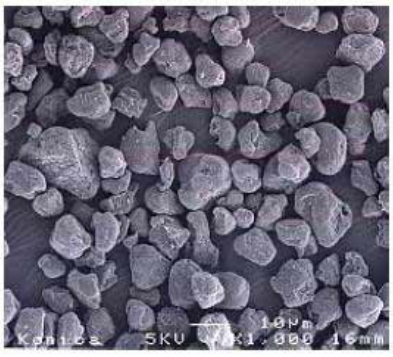


Figure 1. *Pulverized Toner*

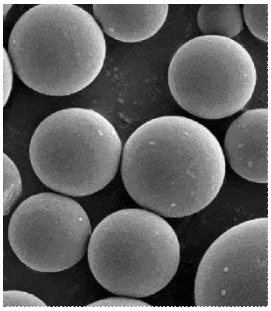


Figure 2. *Chemically Grown Toner*

Compared with pulverized toner, the chemically grown toner has a smaller particle size and a narrower particle size distribution. The shape of the chemically grown toner is more homogeneously close to a sphere. Having these characteristics, the chemically grown toner develops the latent image more precisely and at higher transfer efficiencies than pulverized toner. This type of toner is the focus of this work.

There are many ways to study the flow of granular materials. Among all approaches that have been adopted by researchers, Discrete Element Method (DEM) is one of the most powerful tools for simulating the motion of granular materials.

Introduction to DEM

The DEM was first introduced by Cundall and Strack in 1971 to analyze rock-mechanics problems [1]. Since then, DEM has been applied to study behaviors of granular materials such as mixing [2], packing [3], segregation [4], and hopper discharge [5]. DEM uses a time-stepping algorithm. It consists of repeated applications of the law of motion to each particle, the force-displacement law to each contact, and the constant updating of surface and particle positions, as shown in Figure 3. Contacts between particles, and/or contacts between particles and surfaces, are formed and broken automatically during the simulation.

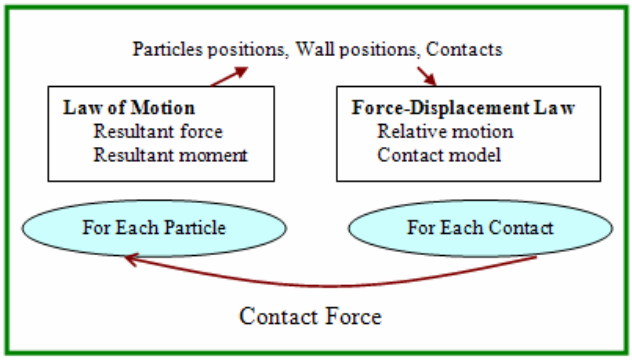


Figure 3. *DEM Calculation Cycle*

However, most of current DEM efforts only involve simulating the flow of cohesionless granular materials, which needs to be modified to use for toner application because of Van der Waals forces due to toner's fine particle sizes and electrostatic forces due to the tribocharging properties.

Thus the Model development has been divided into following steps:

- Develop a basic cohesionless DEM model without any cohesive forces,
- Develop a DEM model incorporated with Van der Waals forces,
- Develop a DEM model incorporated with electrostatic forces,
- Develop a DEM model with both Van der Waals forces and electrostatic forces.

Every sub-model developed is validated by comparing simulation results with experimental results.

Model Development & Validation

Cohesionless DEM Model – Basic Model

A basic DEM model with only contact forces and gravitational forces is developed to study angle of repose, one of the most important characteristics of granular materials. Angle of repose is defined as the maximum angle at which a material remains stable.

Y. C. Zhou et al. [6] did experiments to study angle of repose. As shown in Figure 4, a rectangular container with a fixed middle plate and two side outlets was build by Y. C. Zhou, et al. Once particles fill into the container above the middle plate and a stable state is achieved, then the two outlets will be open simultaneously. Thus, a pile of particles will be formed on the middle plate, and angle of repose can be measured from the pile.

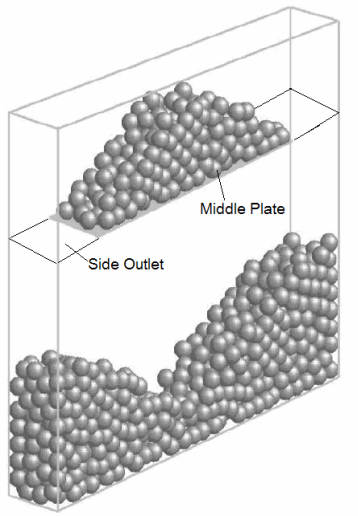


Figure 4. *Y. C. Zhou's Angle of Repose Experiments*

This experimental setup is simulated using the basic cohesionless DEM model. The pile formed on the middle plate via simulation (yellow pile) is compared with Y. C. Zhou's experimental results (black pile), and they are placed overlapped with each other, as shown in Figure 5.

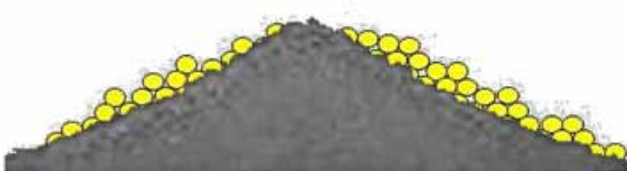


Figure 5. *Cohesionless DEM Model Validation*

It can be measured from Figure 5 that the angle of repose in simulation (yellow pile) is 29^0, and the angle of repose in Y. C. Zhou's experiment (black pile) is 28^0, the difference between experimental results and simulation results is 1^0, which is very small. Thus, it can be say that the cohesionless DEM model fit very well with experimental results.

Basic DEM Model incorporated with Van der Waals forces

The Van der Waals force is a class of intermolecular forces, and it was named after Johannes Van der Waals, a Dutch physicist and chemist. He is the first person who documented three different types of intermolecular forces which were later referred to Van der Waals forces [7].

Van der Waals forces may arise from three sources [8]: permanent electric dipoles, weak dipoles induced by polarization developed through interactions, and low temperature molecular attraction forces.

Based on the theory proposed by Lifshitz [9], equations were developed to calculate Van der Waals forces under three different cases [10], which are shown in Fig 6.

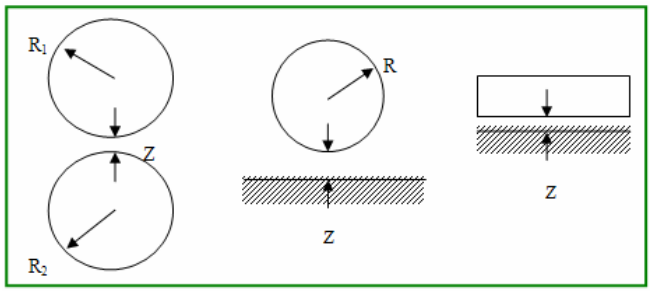


Figure 6. *Idealized Cases for Van der Waals Calculation*

For case 1, two spheres of radius R_1 and R_2, the Van der Waals force can be rewritten as:

$$F_{VDW} = \frac{hR}{16\pi Z^2} \tag{1}$$

For case 2: a sphere of radius R and a plane surface, the Van der Waals force is rewritten as:

$$F_{VDW} = \frac{hR}{8\pi Z^2} \tag{2}$$

For case 3: two parallel plane surfaces, the Van der Waals force per unit area of contact is given by:

$$p_{VDW} = \frac{\partial F_{VDW}}{\partial A} = \frac{h}{8\pi^2 Z^3} \tag{3}$$

where h is Planck's constant, Z is the separation distance between two spheres, R is the reduced radius, and is given by the following equation:

$$R = \frac{2R_1R_2}{R_1 + R_2} \tag{4}$$

In order to incorporate Van der Waals forces into the basic DEM model, at the start of each calculation cycle, position of particles and walls passed from previous cycle are used to determine the magnitude of Van der Waals forces. The updated force information is submitted to next step to calculate the motion of particles.

To validate the DEM model incorporated with Van der Waals forces, the model is used to simulate the motion of particles within a cylinder with a stirrer agitating, as shown in Figure 7.

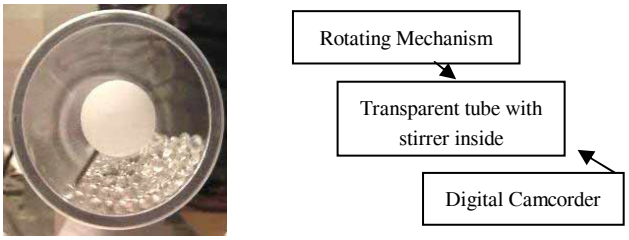
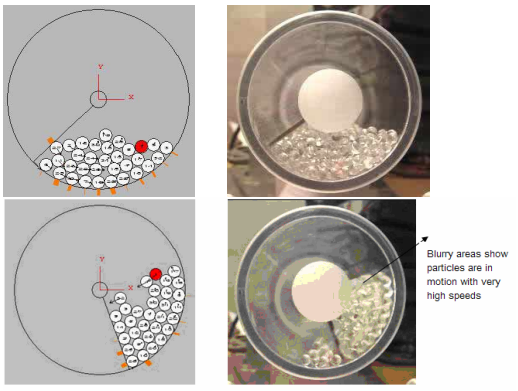


Figure 7. *Experimental Setup*

As shown in Figure 7, a transparent tube with a stirrer inside is fixed on a test bed. The stirrer is rotated via a rotating mechanism. A digital camcorder is adjusted at a height where the center of the lens falls into the same line with the center of the tube. The videos of particle motion are taken and they are used to compare with simulation results.

Particles used in experiments are chosen in such a way that Van der Waals forces can not be ignored due to the small sizes.

The simulation starts with the generation of the cylindrical wall, followed by the random generation of particles inside the cylindrical wall. Then let these particles settle down under the gravity force for several minutes until an initial balanced status is achieved. Finally, the stirrer and the stirrer rod are generated. The initialization of the model is completed, and then the stirrer rotates anticlockwise. The simulated particle motions are documented and then compared with the experimental results, as shown in Figure 8.



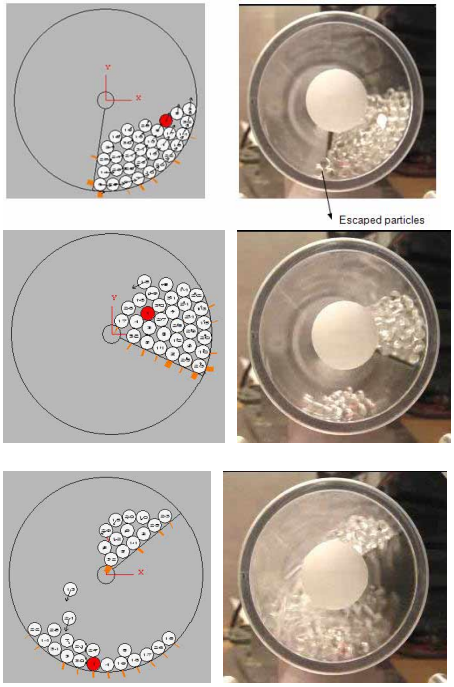


Figure 8. *DEM model with Van der Waals Forces Validation*

It can be seen from Figure 8 that the simulation results fit very well with experimental results. The DEM model incorporated with Van der Waals forces can give very good prediction on cohesive granular flow caused by Van der Waals forces.

To see the effect of Van der Waals forces, the same simulation is executed except that Van der Waals forces are ignored this time. The angle at which particles start falling off from the stirrer is shown in Figure 9 (a), and the situation without Van der Waals forces at the same angle is shown in Figure 9 (b).

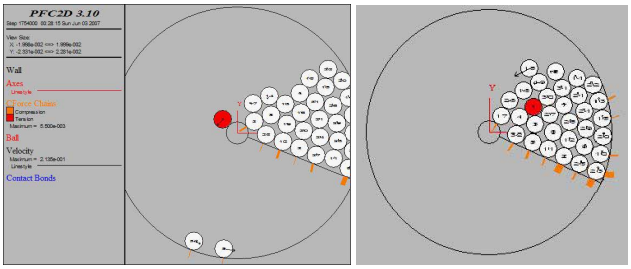


Figure 9(a). *without VDW Forces* ***Figure 9(b).*** *with VDW Forces*

As shown in Figure 9 (a), where there are no Van der Waals forces present, the angle at which particles start falling off from the stirrer is 65 degrees. At the same angle, when there are Van der Waals forces present, as shown in Figure 9 (b), particles are still holding together by Van der Waals forces. And as we can see from Figure 3-16, when there are Van der Waals forces present, particles start to fall off from the stirrer almost when the stirrer at the horizontal position, which is very different from when there are Van der Waals forces present.

Basic Model incorporated with Electrostatic Forces

The electrostatic force between two charged particles can be quantitatively calculated through Coulomb's law, as shown in Equation 5.

$$F = -\frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2} \tag{5}$$

To implement the electrostatic forces into the basic cohesionless DEM model is very similar to the implementation of Van der Waals forces. At the beginning of each DEM calculation cycle, electrostatic forces are calculated based on particle position and charge assigned to particles. The updated force information are then submitted to law of motion to calculate particle motion.

To validate the model, the same experimental setup, as shown in Figure 7, is used here also. Particles made from polystyrene are put into the tube and agitated by the stirrer for a certain amount of time. Then, tribo charges introduced on particles are measured with charge measurement equipment. The measured charge used as an input parameter to the simulation model.

The simulation results are compared with experimental results, as shown in Figure 10.

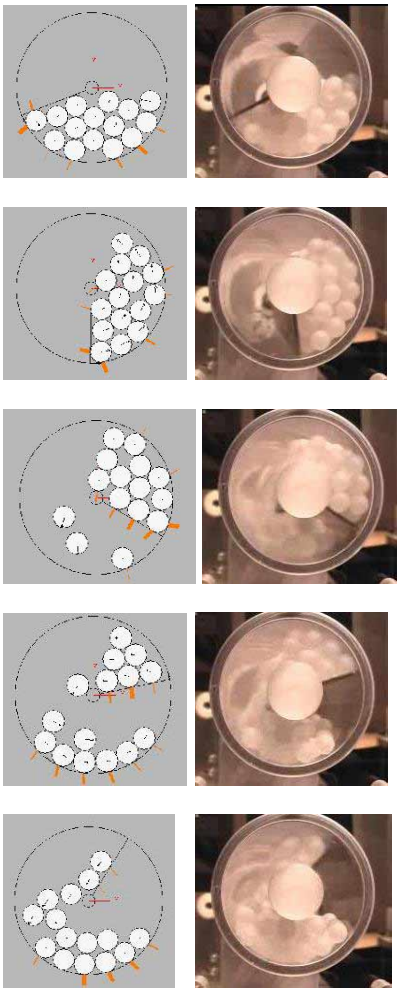
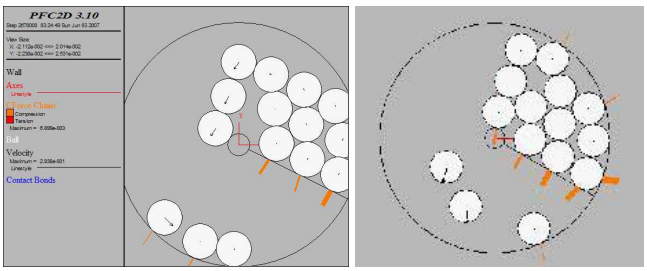


Figure 10. *DEM model with Electrostatic Forces Validation*

It can be seen from Figure 10, the simulation results match well with experimental results. Therefore, the DEM model incorporated with electrostatic forces provides a very good prediction on cohesive flow caused by electrostatic forces.

To see the effect of electrostatic forces, the same simulation is executed except that electrostatic forces are ignored this time. The profiles of particle for the situation of with / without electrostatic forces at the same stirrer angle are compared, as shown in Figure 11 (a) where electrostatic forces are present and in Figure 11 (b) where electrostatic forces are ignored.



(a) without Electrostatic Forces *(b) with Electrostatic Forces*

Figure 11. *Falling Angles with/without Electrostatic Forces*

As shown in Figure 11, when the stirrer angle is about 60 degrees, there are more particles start to fall off from the stirrer when electrostatic forces are present between particles because of the repulsive action caused by electrostatic forces between particles.

Final Model

In this section, Van der Waals forces and electrostatic forces are incorporated into the cohesionless DEM model at the same time. Thus, the model has the ability to simulate cohesive granular flow where the Van der Waals forces and electrostatic forces are major forces of cohesion, such as toner application. This modified model is used to simulate toner mass transfer, one of the most important processes in the electrophotographic process.

Hoffmann [11] observed how toner is transferred from the surface of one roller to the surface of another roller when these two rollers are connected to a DC voltage, as shown in Figure 12.

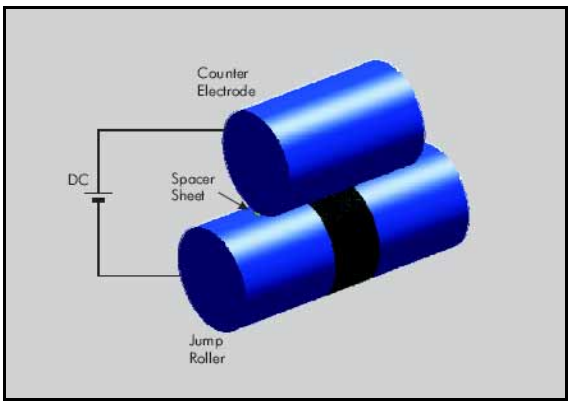


Figure 12. *Hoffmann's Toner Jump Experiments*

In Hoffmann's experiments, a printer is used to apply a uniformed layer of toner on the surface of a developer roller. Then, the printer is stopped and the developer roller is taken out of the printer. Toner is removed from the surface of the developer except for a small strip along its circumference. A second roller is placed axially to the first roller. The distance between these two rollers is carefully adjusted via a space sheet. Last, a DC voltage was then applied to two rollers. Thus, an electric field is formed in the gap between the two rollers, and toner gets transferred from one roller to another.

Several important effects have been observed from this experiment:

- Some toner gets transferred from the first roller to the second roller, but the toner only forms a diffused strip, and it can not be distinguished clearly.
- Only a very small percentage of the toner amount gets transferred; therefore, the toner strip on the first roller remains almost the same, making it hard to perceive the difference before and after.
- The width of the strip on the second roller is about the same as the width of the strip on the first roller.

To quantify the amount of toner being transferred to the second roller, Hoffmann used a white-light interference phenomenon to measure the height of the toner layer on the surface of the two rollers. Figure 13 shows the results.

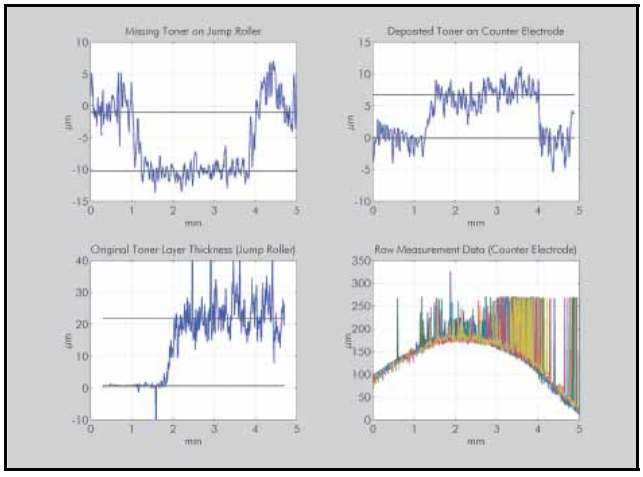


Figure 13. *Toner Height in Hoffmann's Experiments*

The two upper graphs in Figure 13 show the thickness of the missing toner. The upper left graph shows the missing toner on the first roller, and the right one shows the deposited toner on the second roller. The height of missing toner is about 8 microns in both graphs, which is about one toner layer.

The two bottom graphs show the thickness of the toner on the first roller before the experiment. The height of the toner layer on the first roller before transfer is between 20 microns and 30 microns.

Considering that the average toner particle size is between 6 microns to 10 microns, these graphs show that there are about three layers of toner deposited on the surface of the first roller, and only a single layer of toner gets transferred to the second roller. Not only particles attached to the surface of the first roller not get directly transferred, but also particles that sit on top of them do not get transferred.

The experiment described above was simulated using the DEM model developed in this work. The simulation results are shown in Figure 14.

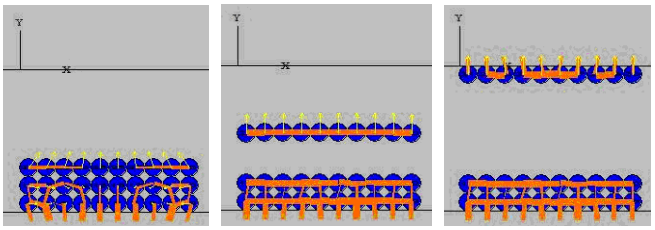


Figure 14. *Toner Mass Transfer Simulation Results*

It can be seen from Figure 14 that:

- For three layers of toner that have been packed on the surface of the first roller, only the first layer of toner particles gets transferred to the second roller.
- The layer of toner that adheres to the surface of the first roller, and the layer of toner that sits on this layer does not get transferred to the second roller.

This simulation results fit very well with findings in Hoffmann's experiments.

Summary

A DEM model is developed to describe cohesive granular flow, especially toner flow. To validate the model, the overall DEM model is decomposed into three parts: cohesionless DEM model, cohesionless DEM model incorporated with Van der Waals forces, and cohesionless DEM Model incorporated with electrostatic forces. These decomposed sub-models are validated by comparing with experimental results.

The overall model is used to simulate toner mass transfer, one of the most important processes of EP process. The simulation results are compared with Hoffmann's experimental results, and they fit each other very well.

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Hong Ren: She received her MS degree in Mechanical Engineering from Southwest Jiaotong University (1999), and will receive her PhD degree in Mechanical Engineering this coming Aug from University of Idaho. She is currently working at Hewlett-Packard Company as a hardware development engineer.

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Santiago Rodriguez: He has worked at HP for 20 years in many different areas of product generation such as manufacturing of circuit boards, development of “Surface Mount processes”, design of circuit boards, ASIC packaging design, LaserJet product development management. The last seven years he has worked as an Electro photographic engineer responsible for Laser Jet development of monochrome and color consumables. He received his M.S. in 1987 from SDSU, and B.S. from the University of Puerto Rico.