CHEMICAL ENGINEERING TRANSACTIONS
VOL. 32, 2013
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet
Chief Editors: Sauro Pierucci, Jiří J. Klemeš

ISBN 978-88-95608-23-5; **ISSN** 1974-9791
DOI: 10.3303/CET1332360

Estimation of charge distribution of polymer particles based on new contact charging model

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A new method for simulating the charging behavior of polymer particles was proposed as part of the fundamental investigation of the charging behavior of toner particles in an electrophotographic system. In this system, which is representative of systems using small charged particles, the design of the charge characteristics of the toner particles is required for miniaturization and high image quality. Toner particles, which are derived from insulating polymers, are charged by contact with metals or other charged toner particles during operation of the system. The surfaces of the model polymer particles used in the simulation were divided into many small regions, as we can assume that the particles have numerous charging sites on their surfaces. While a given polymer particle is flowing, each of its charging sites is charged by contact with metals or the charging site of another particle. The amount of charge on a polymer particle can be represented by the summation of charge at all surface sites.

The measurement system for the contact charge on polymer particles under precisely controlled contact conditions was developed to measure the metal-polymer or polymer-polymer charge transfer in the model. Small amounts of metal-polymer and polymer-polymer charge transfer were measured precisely.

The charging experiment was carried out using flowing spherical particles of polystyrene in a vibrating box. The charging behavior of these particles was simulated using the discrete element method (DEM) and the application of model charging particles. The simulated charge distribution of the particles agreed well with those determined experimentally, meaning that the proposed simulation method will be useful in designing the charging characteristics of toner particles.

1.Introduction

Technologies using charged particles have been widely developed, including electrophotography, dry powder coating, and electrostatic separation. In particular, electrophotography systems that electrify functional toner particles and form images by electrostatic force have played a key role in the transfer of information. Electrophotography used in photocopying machines and printers such as laser printers has the advantage that it can print on any paper at high speed with highly fidelity; however, it has significant cost, the image quality is inferior, and the equipment is bulky compared with other types of printers such as Ink Jet printers. Accordingly, electrophotographic instruments must provide higher performance, such as high-speed printing, high resolution, and miniaturization in order to compete. To meet these demands, the toner characteristics must be selected carefully. In particular, the design of toner particles with appropriate charges is very important.

The simulation of developer behaviors in electrophotographic systems using the distinct element method (DEM) has been developed to aid in the design of the device and the running conditions and has yielded much useful information (2006-Mio, et al., 2009, Seko et al., 2002). However, the simulations of toner behavior reported up to now have not considered any changes in the degree of electrification, nor have they incorporated the simple electrification model based on the number of toner rotations. Therefore, prediction of the exact distribution of toner electrification was impossible using simulations. In order to thoroughly evaluate electrophotographic systems and design toner particles, it is necessary to have a model simulating the behavior of toner particles that incorporates a charging model which takes into account the contact/friction phenomena of charged toner particles. However, because toner particles are

Please cite this article as: Satake M., Shimosaka A., Shirakawa Y., Hidaka J., 2013, Estimation of charge distribution of polymer particles based on new contact charging model, Chemical Engineering Transactions, 32, 2155-2160 DOI: 10.3303/CET1332360

composite materials consisting of polymers, pigments, waxes, CCA, and combinations thereof, the mechanisms of charge transfer are influenced by many factors thus are quite complicated. The charging mechanism of toners has not been fully elucidated, meaning that it is necessary to empirically evaluate the contact/friction charge transfer between particles and a substrate in order to build a model.

In this study, we derived the relationships among the charge transfer, metal-polymer contact, and polymer-polymer contact through electrification/charging experiments using our new measuring system that enables precise control of the contact/frictional conditions (Higashiura, et al., 2012). In addition, we propose the DEM simulation of charging and flow behavior of particles that incorporates a particle model that divides each particle surface into multiple charging sites and can account for charge transfer between contact sites to obtain the charge transfer relationships. We validated the model by comparing the simulation of the electrification of polymer particles in vibration fields with experimental results.

2. Experimental procedure

2.1Contact and tribo-electrification/charging experiments

Figure 1a shows a schematic of the contact electrification or charge measuring system, which consists of a pedestal control, a target plate, and a unit for measuring electrification. The column stage for holding sample pellets was installed perpendicular to the stepping motor using an automatic Z axis crossed roller guide stage (SURUGA SEIKI Co., Ltd, KS303-100). This stage can be driven in micrometer units toward the target plate at speeds of 0.005–0.012 m/s using the computer-integrated controller (SURUGA SEIKI Co., Ltd, D212). The experiments were conducted at a constant speed of 0.01 m/s. The surface potential before and after contact between the pellet placed on the stage and the target plate was accurately measured using a non-contact electrostatic voltmeter (Trek, MODEL347). Moreover, the amount of charge on each pellet was measured using a portable faraday cage connected to an electrometer (KEITHLEY, Model6514A).

In addition, the proposed system was also applicable to tribo-electrification measurements by installing the stage horizontally to the stepping motor using the automatic Z axis, as shown in **Figure 1b**.

Figures 2 and **3** show an image and a number-based size distribution of binder resin particles (Mitsui Chemicals, Inc., CPR600B) used as a pellet material. The binder resin pellets were formed into a circular pellet 20 mm in diameter and about 2 mm thick by compression molding with a maximum pressure of 30 kN and retention time of 120 s using a universal testing machine (SHIMADZU, AG-1). In order to handle allogeneic charge transfer, either an aluminum plate or a second pellet was used as the target plate.

First, the initial surface potential was measured using an electrostatic voltmeter after producing an initial uniform charge on the surface of pellet. Then, contact was made between the pellet and the target plate via the motor-driven stage. The transferred potential □V, transferred from the target plate to the pellet, was calculated from the difference between the initial and final contact surface potential of the pellet. In cases where a second pellet was used as the target plate, the potentials of the surfaces of both the sample and the target pellet were measured.

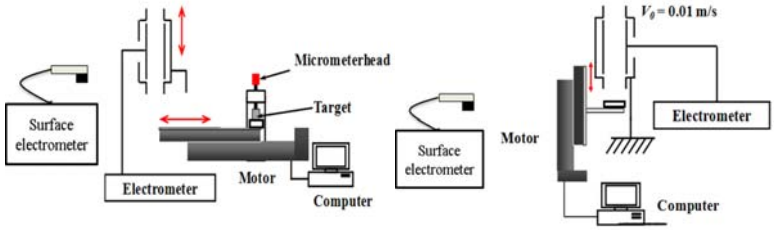

Figure 1: Electrification or charge measuring system:a) Contact-electrification mesurements. b) Tribo electrification mesurements

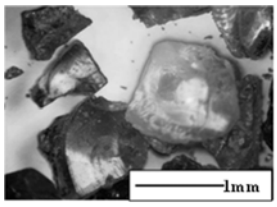

Figure 2: Photomicrograph of binder resins

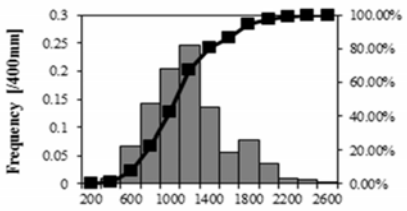

Figure 3: Particle size distribution of binder resins

In the tribo-electrification experiment, the pellet and the target plate were slid against each other at various friction distances. This operation was carried out 50 times for each pellet. Because the transferred potential was influenced by the initial surface potential, the metal target plate was grounded at the time of each measurement and the pellets were wiped with alcohol to ground them before receiving an initial charge. This experiment was

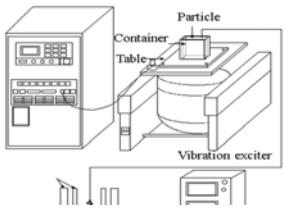

Figure 4: Vibration experimental apparatus

performed at various initial potentials under controlled conditions (relative humidity 30 5 % and air temperature 30 5°C).

2.2Particle charging experiments in vibration field

Figure 4 shows a schematic view of the apparatus used for the particle charging experiment. A sine wave was generated using a function generator (LGF-1310, Leader Electronics) through an amplifier (VA-600-100, IMV) to a vibration apparatus (VA-600-100, IMV), and was ultimately delivered to a cubic vessel fixed on a vibration table. The cubic vessel was made of Al with dimensions of 100 × 100 × 100 mm. After removing the residual charge from polymer particles (diameter 3.175 mm) formed by binder resin particles, they were transferred into the vessel. The time dependence of the charge of each particle was measured using a faraday cage connected to an electrometer.

3. DEM simulation of particle charging and flow behavior

DEM (Cundall and Strack, 1979) is one of the most famous and reliable simulation methods for the analysis of particles in which equations of motion are solved for each particle and the behavior of all particles is analyzed by solving those equations.

As shown in **Figure 5**, a model which divides a particle into multiple charging sites and considers the location and the degree of electrification was used to estimate the electrostatic charge distribution (Yoshida et al., 2003). It was assumed that a given site had no influence on other sites. Thus, this model was able to capture the characteristics of polymer insulators as well as both positively and negatively charged particles, as particle charge polarity depended on the sum of charges at all sites. However, increasing subdivision led to greater computation time. In order to correctly express the degree of particle electrification, it was not clear how far the particle surface should be subdivided.

In the present study, we propose a simulation method for the electrostatic charge distribution of particles using a new site model that does not consider the location of the charge. That is, the particle contact site is determined at random, and charge is transferred according to the potential between the determined sites. By adopting this method, the calculation load decreased sharply and the size of a site could be determined according to the smallest material unit. The charge transfer between contact sites was calculated based on the equations of transferred potential obtained through electrification experiments.

The simulation of charging and flow behavior of particles in a vessel was carried out under the same conditions as the charging experiments in a vibration field. The simulation conditions and physical properties are listed in Table 1.

4. Experimental results

4.1 Contact electrification experiment (metal plate–polymer pellet)

Figure 6 shows the relationship between the initial potential of a binder resin pellet and the transferred potential after contact with the Al plate, confirming that the relationship was linear. It is known that the transferred potential is proportional to the initial potential, supporting that the experiment was performed properly. The obtained slope of linear relationship was negative, indicating that electrons were transferred to the equilibrium potential because contact was made with the pellet after removing the charge from the target plate. On the basis of this result, the transferred potential of the binder resin pellet upon contact with the Al plate is given as a function of the initial potential of the pellet as follows:

$$y = -0.2285x - 16.183 \quad (1)$$

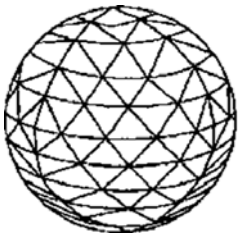

Figure 5: Charging site models of the particle

Table1: Simulation condition

Total time	140	[s]
Time step	4.0×10^{-7}	[s]
Particle diameter	6.35×10^{-3}	[m]
Density	1350	[kg/m^3]
Number of particle	1,10	[-]
Number of site	500	[-]
Amplitude	9.3×10^{-4}	[m]
Vibration frequency	40	[Hz]

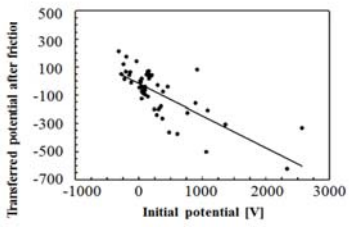

Figure 6: Relationship between initial potential and transferred potential of pellet

4.2 Contact electrification experiment (pellet–pellet)

The results of the pellet-pellet contact electrification experiment are shown in **Figure 7**. The x, y, and z axes represent the initial potential of sample pellet, the initial potential of the target pellet, and the transferred potential of the sample pellet after contact, respectively. The hexagonal plane in the figure shows an approximate plane; the approximation formula of this plane was obtained as z=-38.6-0.218x+0.13y with a decision coefficient of R2=0.57. This result confirmed the correlation among these three variables and that the transferred potential upon pellet-pellet contact was given as a function of the initial potential of both pellets.

4. 3 Tribo-electrification experiment (metal plate–polymer pellet)

Because the tribo-electrification experiment was conducted after the pellet made contact with the target plate, the potential transferred by slide friction was calculated using the initial potential of the pellet minus the potential transferred by contact as described in section 4.1. **Figures 8, 9**, and **10** show the relationship between the initial potential and the transferred potential of the pellet calculated through the tribo-electrification experiment at 2, 4, and 6 mm of friction distance, respectively. The transferred potentials for all three distances were larger than the values obtained in the contact electrification experiment and increased with increasing friction distance. It was determined that the slope of the equation of the transferred potential as a function of initial potential increased dramatically, as shown in Figures 8-10.

4. 4 Tribo-electrification experiment (pellet–pellet)

In order to ensure that the sample pellet was always slid on a new surface, the tribo-electrification pellet-pellet experiment was performed using an enlarged target pellet at 2, 4, 6, 8, and 10 mm of friction distance. This procedure was carried out 20 times for each pellet after removing the charge of both pellets to ensure that the initial potentials were the same. The average calculated transferred potential is shown in **Figure 11**. The transferred potential increased with increasing friction distance, and saturation was not confirmed. The equation for transferred potential as a function of friction distance was obtained as follows:

$$y = 0.2083x^3 - 3.0357x^2 + 18.095x - 4 \quad (2)$$

4. 5 Particle charging simulation and vibration field experiments

The simulation of the electrification behavior of polymer particles incorporating the equations of transferred potential obtained by the previous experiments was carried out using a vibrational frequency of 30 Hz at an amplitude of 4.38 mm. Here, the amount of charge and the potential of the polymer surface were in good proportionality, as shown in **Figure 12**. The simulated potential values

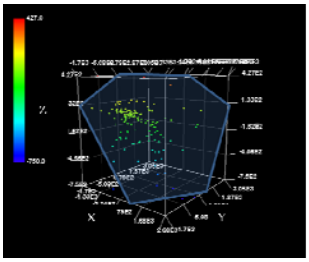

Figure 7: Relationship among initial potential of sample and target pellet, and transferred potential

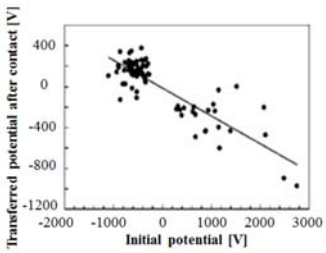

Figure 8: friction length 2mm

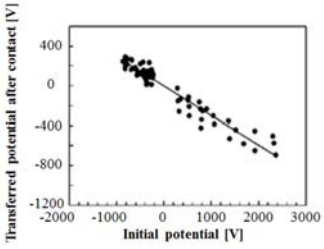

Figure 9: friction length 4mm

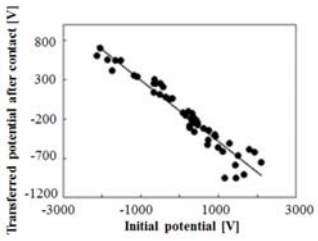

Figure 10: friction length 6mm

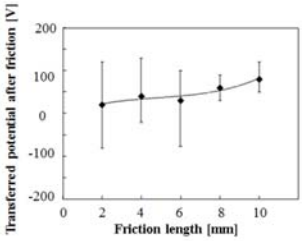

Figure 11 Relationship between frictional length and transferred potential

were converted into the charge using this relationship, and the results were compared with those obtained experimentally. **Figure 13** shows both the simulated and the experimentally determined temporal variation of the total charge of the particles. **Figure 13a** and **b** show the results for one particle and ten particles, respectively. Both the experimental and simulated results confirmed that the polymer particle gained negative charge over time, finally saturating the total charge. The calculated value was within ~0.2 nC of the value obtained experimentally, suggesting that the charge transfer between the particle and the vessel wall as well as between two particles was calculated correctly, and that the proposed method provided a good representation of the actual particle charging and behavior in a vibrational field.

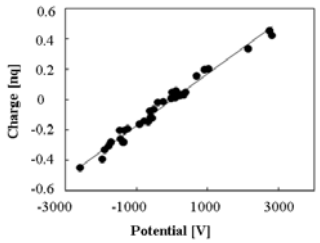

Figure 12: Relationship potential [V] and charge [nq]

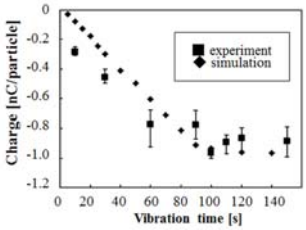

Figure 13a: Compare experimen value and simulation value (1 particle)

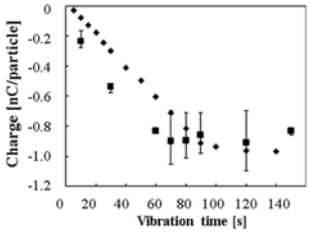

Figure 13b: Compare experimental value and simulation value (10 particles)

5. Conclusion

The transferred potential of the binder resin through contact between the polymer pellet and the Al plate as well as between two polymer pellets was measured using a new measuring system with precise control of the contact and frictional conditions. All the results obtained showed a correlation between the initial potential and the transferred potential of the polymer pellet. The potential transferred by frictional electrification was larger than that transferred by contact electrification and increased with increasing friction distance.

The equations of transferred potential obtained through these experiments are summarized as follows:

Contact electrification
Pellet - Al: $y = -0.2285x - 16.183$ (where x is the initial potential of pellet)
Pellet - Pellet: $z = -38.6 - 0.218x + 0.13y$
(where x is the initial potential of sample pellet and y is the initial potential of target pellet)

Frictional electrification
Pellet - Al: $y = -0.2736x - 12.243$ (2 mm, where x is the initial potential of pellet)
$y = -0.2950x - 2.257$ (4 mm)
$y = -0.3906x - 98.664$ (6 mm)

Pellet - Pellet: $y = 0.2083x^3 - 3.0357x^2 + 18.095x - 4$ (where x is frictional distance)

The simulation of polymer particle charging behavior by incorporating the equations of transferred potential obtained as well as the new charging site model was accomplished. The temporal variation of the total charge of the particles obtained by simulation was in good agreement with the experimentally determined values, validating the proposed simulation method.

Thus, because the simulation of particle charging and flow behavior based on precision measurements of electrical charge is also applicable to particles mixed with an electrification control agent such carbon black and silica particles, which constitute toner with binder resin, we expect this method to aid in the design of toner particles.

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