Determining Trajectory of Triboelectrically Charged Particles, Using Discrete Element Modeling

Contamination Control

The Kennedy Space Center (KSC) Electrostatics and Surface Physics Laboratory is participating in an Innovative Partnership Program (IPP) project with an industry partner to modify a commercial off-the-shelf simulation software product to treat the electrodynamics of particulate systems. The industry partner, DEM Solutions, Inc., has developed EDEM, a program that can calculate the dynamics of particles. Discrete element modeling (DEM) is a numerical technique that can track the dynamics of particle systems. This technique, which was introduced in 1979 for analysis of rock mechanics, was recently refined to include the contact force interaction of particles with arbitrary surfaces and moving machinery. In our work, we endeavor to incorporate electrostatic forces into the DEM calculations to enhance the fidelity of the software and its applicability to (1) particle processes, such as electrophotography, that are greatly affected by electrostatic forces, (2) grain and dust transport, and (3) the study of lunar and Martian regoliths [1].

After contact force is calculated, additional body forces acting on each particle are calculated. In this step, any desired force can be added to the simulation. After the forces on each particle are calculated, the linear and angular accelerations of each particle are updated according to Newton's second law. Then the positions and orientations of each particle are updated with an explicit time-marching algorithm.

The introduction of electrostatic forces into the current EDEM configuration requires the addition of a long-range model that works in conjunction with the existing dynamic calculations. This long-range force model is based on a version of Coulomb's law [2] that takes into account the electrostatic screening of adjacent particles. The electrostatic force, F, is given by

$$F = -\frac{dU_e}{dr} = \frac{q_1 q_2}{4\pi\varepsilon_0}\left[\frac{\kappa}{r} + \frac{1}{r^2}\right] \tag{1}$$

where q_1 and q_2 are the charges of two particles, r is the distance between their centers, ε_0 is the permittivity of free space (8.854×10^{-12} F/m), U_e is the electrostatic potential, and κ is the inverse of the Debye length, λ_D, and is based on the local charge concentration.

For charge generation, we modify a charge generation equation [3] to model many particles.

$$Q(t) = Nq_s\left(1 - e^{-\alpha t}\right) \tag{2}$$

where N is the number of particles, $Q(t)$ is the total charge on the particles, q_s is the saturation charge, and α is the charge generation constant.

We developed a simple inclined-plane apparatus to compare theoretical results with experimental data (Figure 1). The inclined plane allowed 500 2.0-mm-diameter glass spheres to roll down over various polymer and metal surfaces and into a Faraday cup, where total charge on the spheres was measured. By timing the roll of the spheres down the plane and knowing the total charge, $Q(t)$, we were able to calculate the charge generation constant for the materials under test. The inclined-plane materials tested were low-density polyethylene (LDPE), polyvinyl chloride (PVC), nylon 6/6, polytetrafluoroethylene (PTFE), aluminum, and copper.

Initial results of the EDEM model of the inclined plane show good comparison to values of $Q(t)$ and α calculated from experimental data. Figure 2 compares the EDEM simulation output and example $Q(t)$ data.

The EDEM modeling tool can be applied to systems of charged particles that are of interest to NASA, for example, charged lunar and Martian regoliths. Proposed future work includes the addition of dilectrophoretic force and Van der Waals forces, electrodynamic forces from charged surfaces, and the modeling of nonspherical particles.

Figure 1. EDEM simulation of spheres rolling down the inclined plane.

References:
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[2] F.J. Bueche, *Introduction to Physics for Scientists and Engineers*, 3rd ed., McGraw-Hill, Inc., 1980, p. 343.
[3] W.D. Greason, "Investigation of a test methodology for triboelectrification," *Journal of Electrostatics*, Vol. 49, Issue 3–4, August 2000, pp. 245–256.
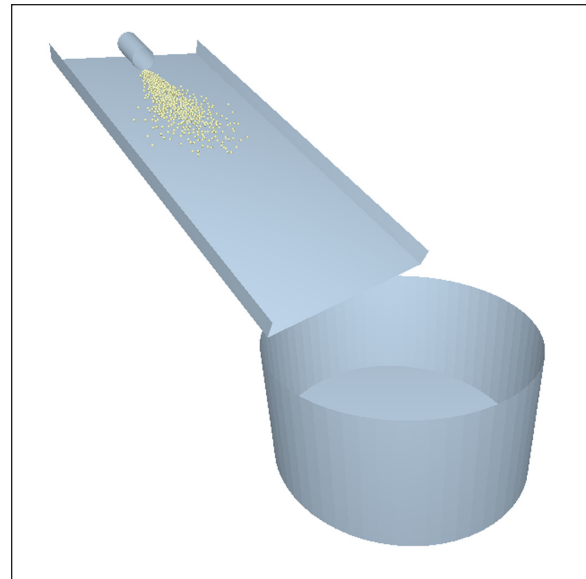
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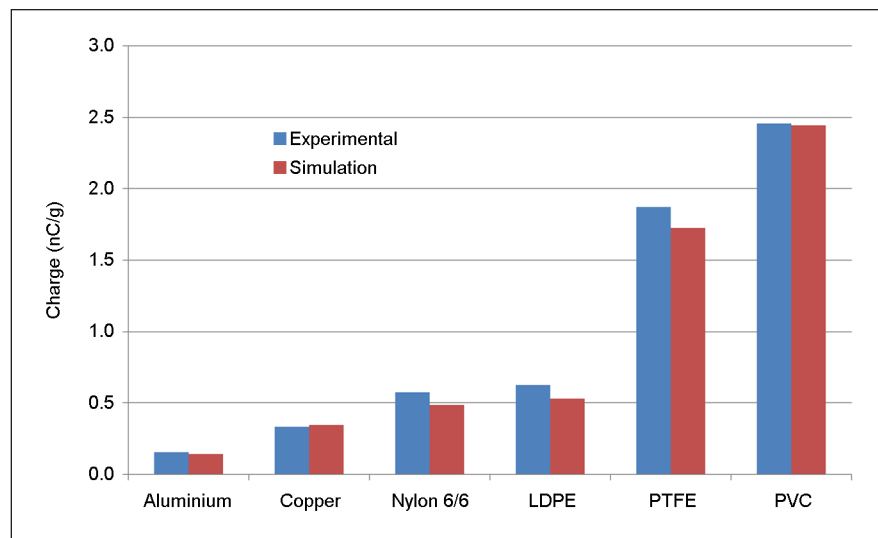
Figure 2. Charge-to-mass ratio for 15-degree experiment compared with simulation results for the six plane materials.