**Tribocharging Simulations: A Sensitivity Study of the Charge Distribution by Grain Size** L.S. Morrissey[1,2], D. Carter[3] , C. M. Hartzell[3], ([1]Catholic University/CRESST II, *20064, Washington, DC, United States,* [2] NASA Goddard Space Flight Center *Greenbelt, Maryland, 20771, United States*, [3] Department of Aerospace Engineering, *University of Maryland, College Park, Maryland, 20740, United States*)

**Introduction:** Large electric potential differences can be generated in granular mixtures, even between chemically identical grains [1]. This process, known as tribocharging, has been the focus of intense analytical and experimental study due the potentially dangerous electrical discharges that can occur in both natural and man-made environments. This is particularly relevant for dusty extra-terrestrial bodies such as the Moon and Mars where colliding grains can potentially produce highly charged environments [2]. Recent research efforts have focused on predicting the charge distribution of chemically identical, tribocharged grains as a function of the grain sizes within a particular mixture. For example, Carter et al. [3] developed an experimental methodology for measuring in-vacuum granular tribocharging due to particle-to-particle triboelectric charge exchange. By conducting these experiments in a vacuum, the authors were able to reduce the effects of the atmosphere and adsorbed water on the charging process. Experimental results showed that large grains charged negatively, while small grains were charged positively [1]. These findings were a reversal from the size dependence trends observed in commonly referenced previous experiments [4]. Carter et al. [1, 3] concluded that this polarity reversal was due to the experiment removing atmospheric contaminants but noted that additional investigation was necessary to develop a predictive model of tribocharging between dielectric grains of the same material.

The applicability of existing analytical tribocharging models is limited as the sensitivity of the resulting charge distribution to various key parameters remains unknown. We have performed tribocharging simulations to investigate the sensitivity of the resulting charge distribution to several key input parameters including the material's charge, mobile carrier density, and charge transfer probability.

**Methods:** First, a granular LIGGGHTS (LAMMPS improved for general and granular heat transfer simulations) simulation was conducted, resulting in a list of grain states and collisions [5]. LIGGGHTS is an open-sourced discrete element method particle simulation software that extends the commonly used molecular dynamics software, LAMMPS. LIGGGHTS simulations output the state of each grain at specific intervals, along with the collisions created between grain pairs at each time step. However, LIGGHTS does not consider the charge transfer potentially occurring between grains during each collision. As a result, a series of MatLab scripts were developed to post-process these output files to calculate the resulting charge distribution as a function of grain size. The charge was transferred between the two particles in collision based on the model presented in Carter et al. [1]. At each diameter, a weight was assigned to each data point using a normal distribution with standard deviation. The mean charge was found by taking the weighted average of all points. The variance was then found as the weighted root-mean-square sum of the difference between the charge and the mean, using the same weights.

When calculating the charge distribution, the material parameters are supplied by the user within the post-processing MatLab file. In this study we considered a grain comprised of silica/zirconium [4], with a modulus of $7.3\times10^{7}$ Pa, a Poisson's ratio of 0.17, a density of 3800 kg/m$^3$ and a grain size diameter distributed between 110-280 μm. We then simulated a range of mobile carrier charges ($-3.2\times10^{-19}$, $-1.6\times10^{-19}$, $1.6\times10^{-19}$, $3.2\times10^{-19}$ C) and mobile carrier densities (hereto referred as sigma) values (10, 50, 100, 250 electrons/μm$^2$) to determine their effect on the resulting charge distribution with grain size. When simulating the effect of charge a sigma of 50 electrons/μm$^2$ was used, whereas a charge of $-1.62\times10^{-19}$ C was used when simulating the effect of sigma.

**Results:** Figure 1 and 2 show the charge distribution as a function of diameter for a range of different mobile carrier densities and charges, respectively. For all cases the general shape and behavior of the distribution is consistent. The charge to mass ratio (CMR) crosses the x-axis at grain diameters of approximately 128 μm and 195 μm (i.e., these grains are, on average, neutral). Similarly, peaks in the magnitude of the CMR (i.e., the most highly charged grains) also occurred at diameters of approximately 180 μm and 210 μm. With increasing sigma, the distribution had a larger peak magnitude in the mean (Fig 1.). For example, at a sigma of 10 electrons/μm$^2$ the mean peaks occurred at a CMR of $-6.4\times10^{-9}$ and $7.3\times10^{-9}$ C/kg. At a sigma of 250 electrons/μm$^2$, these peaks in the mean were increased to $-1.6\times10^{-7}$ and

$1.84 \times 10^{-7}$ C/kg. For these peaks there is a linear dependence on sigma.

Similarly, with increasing transferred charge magnitude there was an increase in the magnitudes in the mean. Furthermore, the CMR sign was dependent on the sign of the transferred charge, with the magnitude staying the same. Figure 3B shows the peaks in mean as a function of the charge. Again, for both peaks there is a linear dependence on the charge.

We observed a strong polarity dependence on the magnitude and polarity of the charge transferred. As existing models of tribocharging do not match experimental results, it has been suggested that a charge carrier other than electrons may be causing the observed charge build-up. These results indicate that, for this charge transfer model, increasing the charge and polarity of the transferred species strongly influences the final charge distribution of grains. This investigation informs the sensitivity of the final charge distribution to the charge density and transferred charge polarity and magnitude. Understanding these sensitivities, and comparing with experimental results, is important for developing a predictive model of triboelectric charging of regolith.

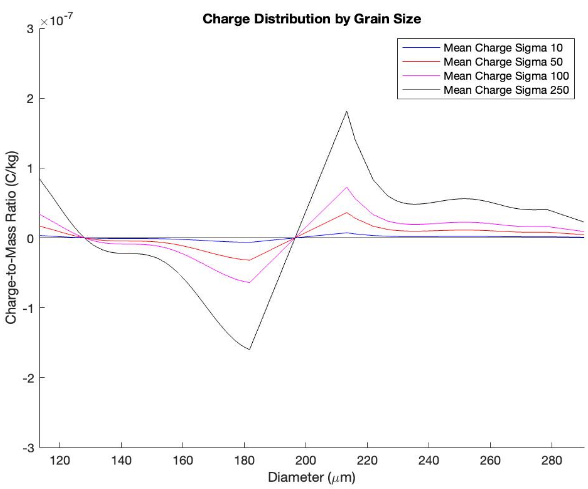


Fig 1: Mean (A) and variance (B) of the charge distribution as a function of grain size for a range of sigma values (in units electrons/$\mu m^2$)

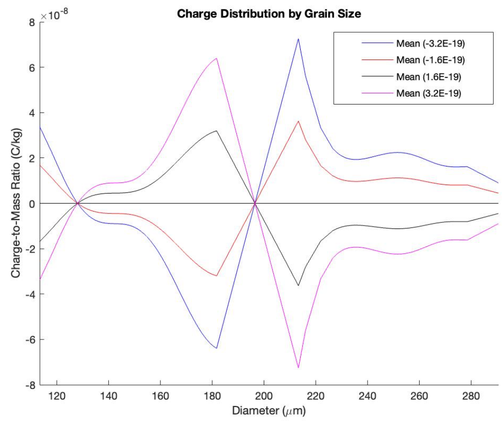


Figure 2: Mean of the charge distribution as a function of grain size for a range of transferred charge magnitudes and polarities (in units C).

**References:**

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