Numerical simulations of granular materials with the patch model for same materials tribocharging

Nicolas Preud'homme

GRASP Laboratory, University of Liège, Belgium

mail: n.preudhomme@uliege.be

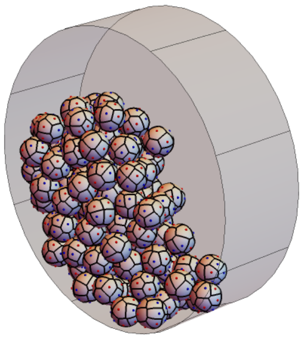
supervisors: Geoffroy Lumay and Eric Opsomer

1 Introduction

Same materials tribocharging occurs when charges are exchanged between two identical materials (*i.e.* materials with identical chemical composition) that are rubbed against each other or simply put in contact. This effect explains for instance the charging of granular materials measured in sand storms, in pharmaceutical powders [1], or in volcanic ash plumes [2]. Although it is observed in many situations, this effect still has some secrets to discover as fundamental questions like « What is the nature of the charges transferred at contact? » do not have a clear answer yet.

IN THIS WORK

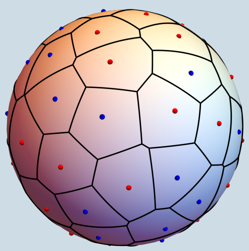
We reproduced numerically the flow of granular materials in a rotating drum and we implemented the **patch model** used for same materials tribocharging [3,4]. This model postulates the existence of charges **acceptor** and **donor sites** on the surface of the objects. We adapted the model to spherical particles and measured the charge of the system. We paid close attention to the charging of **binary mixtures**.



2 Numerical simulations

We used the Discrete Element Method (DEM) which consists in computing the various forces acting on spherical particles and integrating them (leap-frog) using a constant time step [5]. We modeled the contact charging using the patch model. The patches on the particles are defined by a **spherical Voronoi diagram**.

The patch model for spherical particles



1. Generators are placed uniformly at the surface of the particles.
2. For each generator *i*, a patch is defined by the ensemble of points which are closer to *i* than to any other generator.
3. Patches can either be donors (in red) or acceptors (in blue)

→ **donor probability** *p*.

TRANSFER OF CHARGES

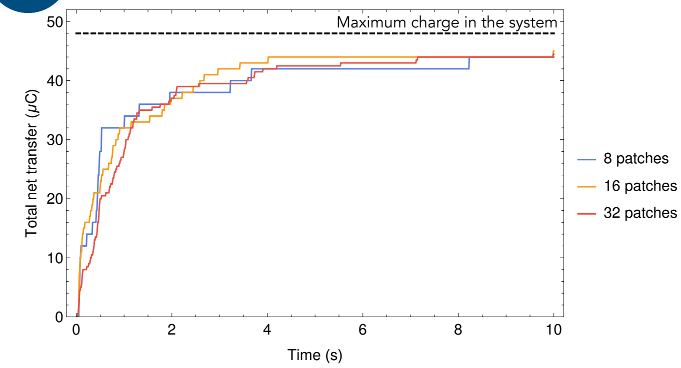
A transfer of (negative) charges must occur at contact between two particles A and B if:

1. The patch at the point of contact on A is a donor and is facing an acceptor on B or inversely.
2. The charges on both patches involved in the contact are smaller than a maximum charge per patch.

Patches can now interact due to **Coulomb interaction**:

$$\mathbf{F_A} = \frac{q_i q_j}{4\pi\epsilon_0}\frac{1}{r_{ij}^2}\hat{\mathbf{r}}_{\mathbf{ij}} = -\mathbf{F_B}$$

3 Transfer of charges

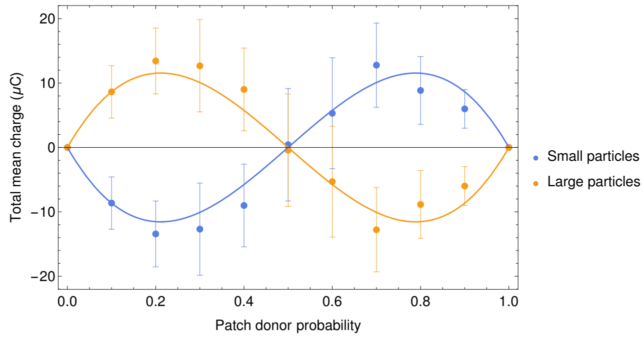


The transfer of charges rapidly increases at the onset of the simulation then reaches a **saturation** as all of the patches have been charged. The system reaches a charge which is smaller than the maximum it could attain.

4 Binary mixtures

Parameters

Size ratio = 0.5, the **patch size is kept constant** so that large particles have more patches on their surface, the total charge per size of particle is measured after 2 seconds of simulation and averaged over 10 simulations which were repeated with identical parameters.



Depending on the probability for a given patch to be a donor, the polarity of large or small particles changes. When *p<0.5*, large particles always charge positively and small particles always charge negatively. Solid line is the following analytical expression for the final saturation charge:

$$Q_s = -2 n_s n_p \Delta q \; p(p-1)(p-0.5) = -Q_L$$

CONCLUSIONS

The patch model correctly reproduces the contact charging of identical particles in granular materials. The distribution of donor patches at the surface of granular materials is sufficient to explain the charging of binary mixtures. Our results are also consistent with actual hypotheses on water patches.

[1] Rescaglio, A., De Smet, F., Aerts, L., & Lumay, G. (2019). Tribo-electrification of pharmaceutical powder blends. *Particulate Science and Technology*.
[2] Méndez Harper, J., & Dufek, J. (2016). The effects of dynamics on the triboelectrification of volcanic ash. *Journal of Geophysical Research: Atmospheres*, *121*(14), 8209-8228
[3] Grosjean, G., Wald, S., Sobarzo, J. C., & Waitukaitis, S. (2020). Quantitatively consistent scale-spanning model for same-material tribocharging. *Physical Review Materials*, *4*(8), 082602.
[4] Apodaca, M. M., Wesson, P. J., Bishop, K. J., Ratner, M. A., & Grzybowski, B. A. (2010). Contact electrification between identical materials. *Angewandte Chemie International Edition*, *49*(5), 946-949.
[5] Preud'Homme, N., Lumay, G., Vandewalle, N., & Opsomer, E. (2021). Numerical measurement of flow fluctuations to quantify cohesion in granular materials. *Physical Review E*, *104*(6), 064901.

LIÈGE université