Computational strategies for 3D computation of the electric field in a vibratory tribocharger for mixed granular solids

J-C Laurentie, Ph Traoré, J Wu and L Dascalescu

PPRIME Institute, UPR 3346 CNRS – University of Poitiers – ENSMA, France

E-mail: jean.charles.laurentie@univ-poitiers.fr

Abstract. In a previous paper, the authors introduced an original model for the computation of the triboelectric charges due to particle-to-particle collisions in a vibrated bed. The evaluation of the electric field inside the particle bed is a prerequisite for the accurate modelling of the tribocharging process, as it determines the trajectory of the particles as well as the charge swapping during collision. Two different approaches are presented and compared in terms of accuracy and computational time consumption. One consisted of computing the electric field as the superposition of the contributions of each point charge. The other, which proved to be much more effective, implied solving the Poisson equation for the potential generated by a given spatial distribution of charge density.

1. Introduction
Electric field separation of insulating materials and charging of toner particles for photo-copiers are two electrostatic processes that make use of the triboelectric effect [1 - 3]. Tribocharging has also disastrous effects, such as explosions in flour mills, cereal silos and supertankers, due to electrical discharges occurring between charged granules [4]. Triboelectricity is also at the origin of the electrostatic adhesion forces between charged powders and transport pipes in the chemical or pharmaceutical industries, and may cause a severe reduction of the flow-rates at which such materials are processed.

Most of the models elaborated for simulating the tribocharging effect are based on the colliding surface area and surface state [5 – 8]. In a previous paper [9], the authors have proposed an original model that takes into account the various tribo-charging mechanisms, as well as the electrical and mechanical forces to which the granules are subjected. The tribo-charging model presented in that paper is mainly based on the work done by Ali et al. [5], while the granular dynamics is modelled with the Distinct Element Method (DEM) [10].

The aim of the present work is to validate a numerical method for the computation of the electric field appropriate for the simulation of tribocharging processes in vertically-vibrated granular beds in relation to possible application in the electrostatic separation of plastics in the recycling industry.

2. Mechanical and electrical models

2.1. Tribo-charging model
The particles motion is governed by Newton’s second law
\[
m_{i} \frac{d\vec{V}_{i}}{dt} = \vec{F}_{i}
\]
\[I_{i} \vec{\omega}_{i} = \vec{T}_{i}
\]

where \(m_{i}\) and \(I_{i}\) stand for mass and moment of inertia of particle \(i\) respectively, \(\vec{V}_{i}\) and \(\vec{\omega}_{i}\) are the velocity and angular velocity. \(\vec{F}_{i}\) and \(\vec{T}_{i}\) are respectively the set of forces and torque acting on the particle \(i\). In our context the force \(\vec{F}_{i}\) is only limited to the sum of the gravity force \(m_{i}g\), the contact force applied to particle \(i\): \(\vec{f}_{i}^{\text{contact}}\) obtained by the Distinct Element method [10], and the Coulomb force \(\vec{f}_{i}^{\text{coulomb}} = q_{i}\vec{E}_{i}\) where \(q_{i}\) and \(\vec{E}_{i}\) are respectively the charge of particle \(i\) and the electric field at the location of particle \(i\). The charge of particle \(i\) at time step \(n\) during its collision with \(ncol\) other particles is given by:

\[
q_{i}^{n} = q_{i}^{n-1} + \sum_{j=1}^{ncol} \delta_{ij}^{n}
\]

where \(\delta_{ij}^{n}\) is the charge exchanged per unit area during the collision between the two spherical insulating particles \(i\) and \(j\). This charge exchanged during the collision between particles \(i\) and \(j\) is computed thanks to the tribo-charging model of [5] and modified to account for the contact surface \(A_{ij}\) which appears during the impact of two particles [9] may be expressed as follows:

\[
\delta_{ij}^{n} = \frac{\varepsilon_{0}}{\delta e} (\Phi_{i} - \Phi_{j} - \vec{E}_{ij} \cdot \frac{\vec{d}_{ij}}{\|\vec{d}_{ij}\|} \delta e)
\]

where:
- \(\varepsilon_{0}\), the permittivity of free space;
- \(\delta\), the cutoff distance of the charge transfer (typically 500 nm);
- \(e\), the electron charge;
- \(\Phi\), the surface work function, representative of the energy needed to extract an electron from the surface of a particle;
- \(\vec{E}_{ij}\), the electric field at the point of impact of the two particles.

\[
\vec{d}_{ij} = \vec{X}_{i} - \vec{X}_{j}\]

is the distance vector between particle \(i\) and \(j\).

2.2. Computation of the Electric Field.

Both this tribo-charging model and the estimation of the Coulomb force involved in Newton’s second law require the effective computation of \(\vec{E}_{ij}\). Indeed both the charge exchanged between the colliding particles and the electric forces acting on them are functions of the local intensity of the electric field. In the case of an electrostatic separator of granular materials, there are two sources of electric field: the electric field due to the charge carried by the particles themselves and the external field generated by an electrode system energized from a high-voltage supply.

To compute the electric field due to the particles, the charge is assumed to be homogeneously distributed on the surface of each granule. Consequently, the total charge of a particle is supposed to be concentrated at its center. Although prima facie this seems to be a very strong hypothesis for the insulators considered in the present study, in the conditions of a very good mixing rate of the granular materials, the contact with other particles is equiprobable for each point on the surface of a granule. This authorizes the hypothesis of a homogeneous charge distribution on particle surface.

The total value of the electric field at the center of a particle may be computed with two different strategies. The first one used the principle of superposition:
where \( N \) is the total number of charged particles involved in the simulation.

The second one is based on the Poisson equation together with the definition of the electric field with regard to electrical potential:

\[
\Delta V = -\frac{\rho}{\varepsilon_0} \quad \text{on} \quad \Omega
\]

\[
V = V_0 \quad \text{on} \quad \Gamma
\]

\[
\vec{E} = -\nabla V
\]

\( \rho \) is the volume charge density, computed as the sum all the charge of each particles located in the computational cell; \( \Omega \) is the computational domain having \( \Gamma \) as boundary. This Poisson equation is discretized with a second order finite volume method [10] and the respective system of linear equations is solved with the iterative Stone method [11].

3. Numerical results

Several numerical tests have been undertaken to compare the performance of the two above-described strategies of electric field computation in terms of accuracy and CPU time consumption. The 3-D computational domain has been divided into cells each containing a charged particle. Two tests have been performed with two sets of 9260 and \( 10^6 \) particles respectively. In each node of the domain the programme computes the electric field generated by the presence of the particles located in each cell. The iso-contours of the electric potential in the \( x \) middle plane computed with the superposition law and the Poisson equation are displayed in figure 1.

![Figure 1. Isocontours of electric potential computed with: (a) superposition law; (b) Poisson equation, for uniformly charged particles (1.10^{-10} \text{ C})](image_url)

Compared to the exact solution given by the superposition law, the accuracy of the results obtained with the Poisson equation is remarkable. However, the main difficulty with solving the Poisson equation is related to the boundary conditions. With the exception of the case of metallic walls where electric potential could be set to a fixed value (zero if the wall is grounded), the specification of boundary conditions in some other cases could be very complicated. A good alternative could be to impose on the boundary nodes the values obtained by the superposition law.
\[ V_i = \sum_{i=1}^{N} \frac{1}{4\pi\varepsilon_0} \frac{q_i}{|z_i|} \]  

where \( i \) holds for a point which belongs to the boundary. The boundary values can be conveniently computed before calling the Poisson solver.

The main drawback of the superposition law is the overall computational time which could be dramatically long as it is directly linked to the number of charged particles in the domain. Table 1 indicates the CPU time consumption for the computation of the electric field by the superposition law and by the Poisson equation for different sets of particles. For less than 10000 particles the two computational times are slightly comparable. But as the number of particles increases, solving the Poisson equation becomes largely more efficient. As seen on table 1, the computation of \( 10^6 \) is definitely not feasible for a transient computation of several thousand of time steps.

Table 1. CPU time consumption for the two computational strategies and for different sets of particles on a 3 GHz workstation

|                  | \( N_1 = 9260 \) particles | \( N_2 = 10^6 \) particles |
|------------------|----------------------------|----------------------------|
| Superposition law| 1.8 s                      | 10.45 h                    |
| Poisson equation | 1.07 s                     | 34.3 s                     |

4. Conclusions

(1) Accurate computation of the electric field is a prerequisite for modelling the behaviour of granular mixtures of insulating materials in vibrated or fluidized beds. Both numerical methods of field computation analyzed in this paper ensure similar accuracy. However, the finite volume method of solving Poisson equation is characterized by a much shorter computational time (less than 1 min, for \( 10^6 \) particles) as compared to the one based on the superposition method (more than 10 h, for the same number of particles).

(2) All the computations have been performed on a single processor since the superposition law has very bad scalability, contrary to the Poisson solver which has been efficiently parallelized. This is another argument in favour of the Poisson equation approach for the computation of the electric field, as it reduces by several orders of magnitude the overall CPU time.

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