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Eulerian modeling of mono-disperse gas–particle flow with electrostatic forces

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Abstract

Due to triboelectric charging, the solid phase in gas–particle flows can become electrically charged, which induces an electrical interaction between all the particles in the system. Because this force decays very rapidly, many current models neglect the contribution of the electrostatic interaction between the particles. Nevertheless, the impact that this force can have in many industrial configurations is well documented. In this work an Eulerian–Eulerian model for gas–particle flow is proposed in order to take into consideration the electrostatic interaction between the particles. We use the kinetic theory of granular flows to derive the transport equation for the electrical charge for dense gas–particle systems. We show that the electric charge transport equation can be derived without presuming the for the particle charge distribution. In order to close the collision integrals in the Chapman–Enskog equation, we proposed a linear model for the charge-velocity correlation. The model was tested in a 3 dimensional periodic box. The results shows that the dispersion phenomenon have two contributions: a kinetic dispersion due to the random motion of particles (predominant in dilute systems) and collisional dispersion due to the electron transfer during a particle-particle collision (predominant in dense systems). Another effect that contributes to the particle transfer is the triboconductivity effect, which is the motion of electrons following the global electric potential difference. The dispersion and triboconductivity characteristic times where calculated, and the analysis shows that, in dense systems, the two effects are comparable if the dispersion characteristic length is equal to the particle diameter.

Introduction

Nowadays, gas–particle flows play an extremely important role in many industrial technologies. Fluidized beds, cyclonic separators and the transport of air pollutants are just a few examples of this type of flow. In some configurations the particles collide with other solid materials (either another particle or a solid boundary). During these interactions the particles can get electrically charged due to the triboelectrification effect (Matsusaka, S. & Masuda, H. 2003). The electrically charged particles can now interact with other charged particles via the Lorentz force. Because the particle velocity is very small compared to the speed of light, the magnetic contribution can be dropped, and only the electrostatic term is relevant.

The generation of electrical charges can be undesirable for many industrial processes. There are safety hazards such as the risk of explosions due to a spark, wall sheeting and the generation of an intense electric field. Dynamically, the presence of electrostatic forces modifies the behavior of a gas–particle flow: modifications on the minimum fluidization velocity, rise in the entrainment rate, modification on the heat transfer coefficient are just a few example of the effects of

the electrostatic force (Hendrickson, G. 2006; Miller, C. & Logwinuk, A. 1951).

All these electrostatic effects are well documented in the literature. Sowinski, A. et al. (2009, 2010) built a fluidized bed with a Faraday cup to measure the total particle charge after fluidization. Their results showed that the particles get charged and that the magnitude depends on the fluidization velocity. Moreover the entrained fines particles and the bed particles have an inverse polarity. Salama, F. et al. (2013) extended the study to the particles inside the bed. They observed that, although globally the bed is charged negatively, there are a small percentage of particle with a positive charge. This suggests the wall sheet is formed by consecutive layers of negative and positive charged particles. Zhou, Y. et al. (2013) introduced a moving probe inside a fluidized bed to map the electric potential inside the column. Their data reveal that the bed is negative charged at the bottom and positive charged at the top. Moreover, they also found a difference in the radial profile; with the wall having a stronger potential than the center of the bed. The gas-dynamics can also be impacted; Dong, K. et al. (2015) placed 4 electrostatic probes inside a fluidized bed to analyze the effect of the electrostatic force on the bubble's motion. The authors ob-

served that the bubble size decrease as the electrostatic force increases. They attributed this result to the fact that most of the particles have the same charge sign, this creates a repulsive force between them, leaving less space to the bubble to grow.

The eulerian modeling is widely used to study gas-particle flow (Hamidouche et al. 2018). The governing equation can be derived from the Boltzmann and Chapman-Enskog equations (Chapman, S. et al. 1990). In dense configuration the collision term must be closed. Jenkins, J. & Savage S. (1983) achieved a closed form of the collision integral assuming a molecular chaos and a Maxwellian velocity distribution. If the Maxwellian hypothesis is too restrictive, a non-equilibrium distribution can be obtained following the Grad's theory (Grad, H. 1949; Jenkins, J. T. & Richman, M. W. 1985) or the Richmann method (Richman, M. 1989).

Currently, some efforts have been made in order to add the electrostatic force to the Eulerian codes. Rokkam, R. G. et al. (2010) developed a model in which the electrostatic effect is added as a body force in the solid momentum equation. Later, the same authors (Rokkam, R. G. et al. 2013) tested this model in a fluidized bed reactor using Fluent. Their model was in good agreement with the experimental observation, specially concerning the radial segregation of the solid phase. In this approach, however, the electrical charge is an input parameter and remain fixed throughout the simulation.

A more complex model was proposed by Kolehmainen, J. et al. (2018); they used the kinetic theory of granular flow to derive a transport equation for the particle charge. Using an uncorrelated Maxwellian and Gaussian probability density distributions for the velocity and the particle charge, they were able to close the collision integral and to derive a collisional dispersion coefficient. However, this coefficient was not enough to account for all the particle dispersion, and therefore, they decided to add a kinetic dispersion coefficient following an analogy with the heat transfer coefficient (Hsiau, S. & Hunt, M. 1993). The results showed that this new formulation was in accordance with DEM simulations. More recently Ray, M. et al. (2019) extended that model and computed the charge-velocity correlation in order to derive the kinetic dispersion coefficient. The authors were also able to derive the charge variance equation in order to fully close the transport equation. They implemented their model using OpenFOAM and simulated a two-dimensional fluidized bed. The results showed that they were able to successfully predict the thickness of the particle layer formed at the wall of the reactor.

In our work, we propose a closure for the collisional and kinetic dispersion terms in the mean charge balance derived in the framework of the kinetic theory. In particular, we show that the closure assumption for the collisional contribution can be derived without presuming an uncorrelated Maxwellian probability distribution for the particle electrical charge. In addition, we derive a closure for the dispersion term due to transport by the random velocity from the transport equation governing the electrical charge due to the fluctuating particle velocity.

Particle dynamics

Following the approach described by Gatignol, R. (1983) and Maxey, M. & Riley J. (1983) the motion equation for a single particle follows the Newton's second law:

$$m_p \frac{du_{p,i}}{dt} = -V_p \frac{\partial P_g}{\partial x_i} + m_p g_i + F_{d,i} + q_p E_i \quad (1)$$

Hereinafter all the equation are presented in tensor notation using the Einstein summation convection over all indexes except p .

m_p is the mass of the particle, u_p the particle velocity, V_p the particle volume, P_g is the pressure of the gas-phase, g is the gravity F_d is the drag force, E in the electric field and q_p is the particle electric charge.

The right hand side of the equation represents the sum of forces acting on the particles. There we found in order: the Archimedes force, the gravity force, the drag force (see Simonin, O. et al. (2016) for a detailed description), and the last term is the electrostatic force due to the electric field generated by the presence of other charged particles.

Following the Maxwell's equation we can find the electrical field:

$$\nabla^2 \varphi = -\frac{\varrho}{\epsilon} \quad (2)$$

$$E_i = -\nabla \varphi \quad (3)$$

Where φ is the electrical potential, ϱ is the charge density and ϵ is the mixture permittivity.

Collision dynamics

One of the most important aspects of particle dynamics, are the particle-particle collisions, and the exchange of momentum and electric charge during the collision. For the sake of simplicity, we will limit our study to binary collisions of spherical particles.

Let's consider two particles p_1 and p_2 located at \vec{x}_{p1} and \vec{x}_{p2} . They have a given velocity \vec{c}_{p1} and \vec{c}_{p2} and electric charge ξ_{p1} and ξ_{p2} . We define \vec{k} as the unit vector going from the center of p_1 to the center of p_2 , we also define \vec{g} as the relative velocity of the particles $g_i = c_{p1,i} - c_{p2,i}$.

Using the momentum and kinetic energy conservation law, we can derive the particles velocity after the collision \vec{c}_{p1}^+ and \vec{c}_{p2}^+ :

$$c_{p1,i}^+ = c_{p1,i} - \frac{1}{2} (1 + e_c) (g_j k_j) k_i \quad (4)$$

$$c_{p2,i}^+ = c_{p2,i} + \frac{1}{2} (1 + e_c) (g_j k_j) k_i \quad (5)$$

To take into account the triboelectrification phenomenon, we are going to use the model developed by Kolehmainen, J. et al. (2017). They used a Hertzian collision model to calculate the overlapping area during a collision between two particles. Using the triboelectrification model proposed by Laurentie, J. et al. (2013) they were able to compute the charge transfer during the impact:

$$\xi_{p1}^+ = \xi_{p1} - \varepsilon_0 \mathcal{A}_{max}(g_m k_m) (E_l^* k_l) \quad (6)$$

$$\xi_{p2}^+ = \xi_{p2} + \varepsilon_0 \mathcal{A}_{max}(g_m k_m) (E_l^* k_l) \quad (7)$$

Where E^* is the total electric field, which has the contribution of the resolved electric field, plus the contribution of the electric field generated by the colliding particles:

$$E_i^* = E_i - \frac{\xi_{p2} - \xi_{p1}}{\pi \varepsilon_0 d_p^2} \quad (8)$$

And $\mathcal{A}_{max}(g_m k_m)$ is given by the Hertzian model:

$$\mathcal{A}_{max}(g_m k_m) = 2\pi r^* \left(\frac{15m_p^*}{32Y^* \sqrt{r^*}} \right)^{2/5} (g_m k_m)^{4/5} \quad (9)$$

Where r^* is the effective particle radius, Y^* is the effective Young's modulus and m_p^* is the effective particle mass:

$$\frac{1}{r^*} = \frac{1}{r_1} + \frac{1}{r_2} \quad (10)$$

$$\frac{1}{Y^*} = \frac{1 - \nu_1^2}{Y_1} + \frac{1 - \nu_2^2}{Y_2} \quad (11)$$

$$\frac{1}{m_p^*} = \frac{1}{m_{p1}} + \frac{1}{m_{p2}} \quad (12)$$

r is the particle radius, Y is the Young's modulus, ν is the Poisson ratio, and m_p is the particle mass.

Finally the charge transfer model by collision can be written as:

$$\xi_{p1}^+ = \xi_{p1} - \left[\beta E_i k_i + \frac{\beta}{\gamma} (\xi_{p2} - \xi_{p1}) \right] (g_m k_m)^{4/5} \quad (13)$$

$$\xi_{p2}^+ = \xi_{p2} + \left[\beta E_i k_i - \frac{\beta}{\gamma} (\xi_{p2} - \xi_{p1}) \right] (g_m k_m)^{4/5} \quad (14)$$

With:

$$\beta = \varepsilon_0 2\pi r^* \left(\frac{15m_p^*}{32Y^* \sqrt{r^*}} \right)^{2/5} \quad (15)$$

$$\gamma = \pi \varepsilon_0 d_p^2 \quad (16)$$

Eulerian modeling of the electrostatic phenomenon

In order to derive a continuum model for the solid phase, we will use the fact that the motion of particles in a rapid granular flow is very similar to the motion of molecules in a gas. This allows us to use the kinetic theory to obtain the governing equation of the solid phase. Let $f(\vec{x}, \vec{c}_p, \xi_p, t)$ be the particle number density function which gives the number of particles per unit of volume at the position \vec{x} with a velocity $\vec{u}_p = \vec{c}_p$ and a charge $q_p = \xi_p$. Using this function we have the definition for the particle number density (n_p) and the mean value for any property ϕ :

$$n_p = \int_{\mathbb{R}^3} \int_{\mathbb{R}} f d\xi_p d\vec{c}_p \quad (17)$$

$$\langle \phi \rangle = \frac{1}{n_p} \int_{\mathbb{R}^3} \int_{\mathbb{R}} \phi f d\xi_p d\vec{c}_p \quad (18)$$

This allows us to define some useful quantities such as the particle mean velocity:

$$U_{p,i} = \langle c_{p,i} \rangle = \frac{1}{n_p} \int_{\mathbb{R}^3} \int_{\mathbb{R}} c_{p,i} f d\xi_p d\vec{c}_p \quad (19)$$

The particle fluctuant velocity:

$$c'_{p,i} = c_{p,i} - U_{p,i} \quad (20)$$

The particle kinetic stress tensor:

$$R_{p,ij} = \langle c'_{p,i} c'_{p,j} \rangle = \frac{1}{n_p} \int_{\mathbb{R}^3} \int_{\mathbb{R}} c'_{p,i} c'_{p,j} f d\xi_p d\vec{c}_p \quad (21)$$

For an isotropic flow, this tensor can be reduced to:

$$q_p^2 = \frac{R_{p,ii}}{2} \quad (22)$$

When we can assume an uncorrelated motion of particles, the granular temperature can be defined as:

$$\Theta = \frac{R_{p,ii}}{3} = \frac{2}{3} q_p^2 \quad (23)$$

The particle mean electric charge:

$$Q_p = \langle \xi_p \rangle = \frac{1}{n_p} \int_{\mathbb{R}^3} \int_{\mathbb{R}} \xi_p f d\xi_p d\vec{c}_p \quad (24)$$

The fluctuant electric charge:

$$\xi'_p = \xi_p - Q_p \quad (25)$$

The electric charge variance:

$$Q = \langle \xi'_p \xi'_p \rangle = \frac{1}{n_p} \int_{\mathbb{R}^3} \int_{\mathbb{R}} \xi'_p \xi'_p f d\xi_p d\vec{c}_p \quad (26)$$

Boltzmann equation

The dynamic evolution of f is given by the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_i} [c_{pi} f] + \frac{\partial}{\partial c_{pi}} \left[\left\langle \frac{du_{pi}}{dt} \middle| \vec{x}, \vec{c}_p, \xi_p \right\rangle f \right] + \frac{\partial}{\partial \xi_p} \left[\left\langle \frac{dq_p}{dt} \middle| \vec{x}, \vec{c}_p, \xi_p \right\rangle f \right] = \left(\frac{\partial f}{\partial t} \right)_{coll} \quad (27)$$

The notation $\langle G | \vec{x}, \vec{c}_p, \xi_p \rangle$ is a short form for the conditional expectation $\langle G | \vec{x}, \vec{u}_p = \vec{c}_p, q_p = \xi_p \rangle$.

The right hand side of the Boltzmann equation accounts for the variation due to particle-particle collisions.

We will consider that the particle charge only changes due to the collisions with other particle, hence $dq/dt = 0$.

From the Boltzmann equation, we can derive a general transport equation for any property ϕ :

$$\begin{aligned} & \frac{Dn_p \langle \phi \rangle}{Dt} + n_p \langle \phi \rangle \frac{\partial U_{pi}}{\partial x_i} + \frac{\partial n_p \langle \phi c'_{pi} \rangle}{\partial x_i} - n_p \left\langle \frac{D\phi}{Dt} \right\rangle \\ & - n_p \left\langle c'_{pi} \frac{\partial \phi}{\partial x_i} \right\rangle - n_p \left\langle F_i \frac{\partial \phi}{\partial c'_{pi}} \right\rangle + n_p \frac{DU_{pi}}{Dt} \left\langle \frac{\partial \phi}{\partial c'_{pi}} \right\rangle + \\ & n_p \left\langle c'_{pj} \frac{\partial \phi}{\partial c'_{pi}} \right\rangle \frac{\partial U_{pi}}{\partial x_j} = \mathcal{C}(\phi) \quad (28) \end{aligned}$$

This is called the Chapman-Enskog equation (Chapman, S. et al. 1990)

The right hand side of the equation accounts for the mean transfer rate of the property ϕ due to collision. Following formulation proposed by Jenkins, J. & Savage S. (1983) the term can be written as the contribution of a source term and a flux term:

$$\mathcal{C}(\phi) = \chi(\phi_p) - \frac{\partial}{\partial x_i} \theta_i(\phi_p) \quad (29)$$

Where

$$\chi = \frac{d_p^2}{2} \int_{\vec{g} \cdot \vec{k} > 0} \Delta \phi(g_i k_i) f^{(2)} d\vec{k} d\xi_{p1} d\xi_{p2} d\vec{c}_{p1} \vec{c}_{p2} \quad (30)$$

$$\theta_i = -\frac{d_p^3}{2} \int_{\vec{g} \cdot \vec{k} > 0} \delta \phi(g_i k_i) f^{(2)} k_i d\vec{k} d\xi_{p1} d\xi_{p2} d\vec{c}_{p1} \vec{c}_{p2} \quad (31)$$

Where $f^{(2)} = f^{(2)}(\vec{x}_{p1}, \vec{c}_{p1}, \xi_{p1}, \vec{x}_{p1} + d_p \hat{k}, \vec{c}_{p2}, \xi_{p2}, t)$ is the particle-particle pair distribution.

$\Delta \phi$ accounts for the total variation of the property ϕ during the collision:

$$\Delta \phi = \phi_{p1}^+ - \phi_{p1} + \phi_{p2}^+ - \phi_{p2} \quad (32)$$

$\delta \phi$ is the variation of ϕ for the particle p_1 :

$$\delta \phi = \phi_{p1}^+ - \phi_{p1} \quad (33)$$

In order to close the collision integrals (equations 30 and 31), we need to give an expression for the single particle number density function f . Assuming an uncorrelated particle motion, Kolehmainen, J. et al. (2018) and Ray, M. et al. (2019) proposed the following model:

$$f^{(2)} = g_0 f(\vec{x}_{p1}, \vec{c}_{p1}, \xi_{p1}, t) f(\vec{x}_{p2}, \vec{c}_{p2}, \xi_{p2}, t) \quad (34)$$

Where g_0 is the radial distribution function. $f(\vec{x}_p, \vec{c}_p, \xi_p, t)$ is given by an uncorrelated Maxwellian and Gaussian distribution for the velocity and the charge respectively:

$$f = \frac{1}{(2\pi Q)^{1/2} (2\pi \Theta)^{3/2}} e^{-\frac{\xi_p^2}{2Q}} e^{-\frac{c_p^2}{2\Theta}} \quad (35)$$

In our study, will will not assume this form for the number density function, instead we will show that the electric

charge part does not have to be presumed a priori. Using the definition of the probability density function, we have:

$$\int_{-\infty}^{\infty} \phi_{p1} f^{(2)} d\xi_{p1} d\xi_{p2} = \langle \phi_{p1} | \vec{x}_{p1}, \vec{c}_{p1}, \vec{x}_{p2}, \vec{c}_{p2} \rangle f^{*(2)} \quad (36)$$

Now we are going to suppose that the property of the first particle is not correlated with the presence of the second colliding particle, therefore:

$$\langle \phi_{p1} | \vec{x}_{p1}, \vec{c}_{p1}, \vec{x}_{p2}, \vec{c}_{p2} \rangle = \langle \phi_{p1} | \vec{x}_{p1}, \vec{c}_{p1} \rangle \quad (37)$$

To take into consideration the correlation between the property ϕ and the particle velocity, we chose a linear model of the form:

$$\langle \phi_{p1} | \vec{x}_{p1}, \vec{c}_{p1} \rangle = \langle \phi_{p1} \rangle + B_j c'_{p,j} \quad (38)$$

Where the coefficient B_j is given, so the first two statistical moments are satisfied:

$$B_i = R_{p,i,j}^{-1} \langle \phi c'_{p,j} \rangle \quad (39)$$

Which, in a hydrodynamic isotropic model, simplifies to:

$$B_i = \frac{\langle \phi c'_{p,i} \rangle}{2/3 q_p^2} \quad (40)$$

Now, $f^{*(2)} = f^{*(2)}(\vec{x}_{p1}, \vec{c}_{p1}, \vec{x}_{p2}, \vec{c}_{p2}, t)$ is the particle-particle velocity distribution, which does not depend on the electric charge of the particles. This function can be modeled using the same methodology as the one shown above:

$$f^{(2)} = g_0 f^*(\vec{x}_{p1}, \vec{c}_{p1}, t) f^*(\vec{x}_{p2}, \vec{c}_{p2}, t) \quad (41)$$

Here, we chose to close the probability distribution using a Maxwellian distribution:

$$f^* = \frac{n_p}{(2\pi \Theta)^{3/2}} e^{-\frac{c^2}{2\Theta}} \quad (42)$$

With this model, the collisions terms can be fully solved.

Charge transport equation

If we now use $\phi = \xi_p$ in the equation 28, we find the following expression for the charge transport equation:

$$n_p \frac{\partial Q_p}{\partial t} + n_p U_{pi} \frac{\partial Q_p}{\partial x_i} + \frac{\partial n_p \langle \xi_p c'_{pi} \rangle}{\partial x_i} = \mathcal{C}(\xi_p) \quad (43)$$

From this equation, two terms need to be closed: the last term on the left hand side accounts for the correlation between the charge and the velocity and the right hand side represents the mean rate of change for the charge due to collisions.

Due to the charge conservation law, it can be shown that the source term of the collision integral vanishes:

$$\chi(\xi_p) = 0 \quad (44)$$

Using the methodology described above, the flux term can be computed:

$$\begin{aligned}
\theta_i(\xi_p) &= d_p^3 \beta E_i g_0 n_p^2 (q_p^2)^{9/10} \Upsilon^{(1.1)} \\
&\quad - d_p^4 \frac{\beta}{\gamma} \frac{\partial Q_p}{\partial x_i} g_0 n_p^2 (q_p^2)^{9/10} \Upsilon^{(2.1)} \\
&\quad + g_0 d_p^5 \frac{\partial U_t}{\partial x_j} \frac{\beta}{\gamma} \frac{\partial Q_p}{\partial x_i} (q_p^2)^{2/5} n_p^2 \Psi_{tlij}^{(2.1)} \Upsilon^{(2.2)} \\
&\quad + d_p^3 \frac{\beta}{\gamma} B_i g_0 n_p^2 (q_p^2)^{7/5} \Upsilon^{(2.3)} \\
&\quad - \Upsilon^{(2.4)} d_p^4 g_0 \frac{\partial U_t}{\partial x_j} \frac{\beta}{\gamma} B_l n_p^2 (q_p^2)^{9/10} \Psi_{ltji}^{(2.4)} \Upsilon^{(2.4)} \quad (45)
\end{aligned}$$

Where $\Upsilon^{(\cdot)}$ are constants, and $\Psi_{abcd}^{(\cdot)}$ are 4-order constant tensors.

If we insert this, into the collision term definition, and we neglect any term proportional to $\partial U / \partial x$, we get:

$$C(\xi_p) = -\frac{\partial}{\partial x_i} (\sigma_p E_i) + \frac{\partial}{\partial x_i} \left(\kappa_p^{\text{coll}} \frac{\partial Q_p}{\partial x_i} \right) \quad (46)$$

$$\kappa_p^{\text{coll}} = d_p^4 \frac{\beta}{\gamma} g_0 n_p^2 (q_p^2)^{9/10} \frac{2^{57/10} 5}{3^{19/10} 7} \Gamma\left(\frac{12}{5}\right) \Gamma\left(\frac{3}{2}\right) \quad (47)$$

$$\sigma_p = d_p^3 \beta g_0 n_p^2 (q_p^2)^{9/10} \frac{2^{57/10} 5}{3^{19/10} 7} \Gamma\left(\frac{3}{2}\right) \Gamma\left(\frac{12}{5}\right) \quad (48)$$

Where $\Gamma(\cdot)$ is the gamma function.

κ_p^{coll} is the collisional dispersion coefficient and it accounts for the particle charge dispersion due to particle-particle collisions. σ_p is the triboconductivity coefficient and it represents the charge transport generated by the electric field when two particles are in contact.

The second term in the charge transport equation (equation 43) that needs to be closed is the charge-velocity correlation $\langle c'_p \xi_p \rangle$. To accomplish this, we will write a transport equation for the correlation between the particle velocity and charge. Therefore we set $\phi = \xi_p c_{p,i}$ in the Chapman-Enskog equation (equation 28):

Charge-velocity correlation

$$\begin{aligned}
n_p \frac{D \langle \xi_p c'_{pi} \rangle}{Dt} + \frac{\partial n_p \langle \xi'_p c'_{pi} c'_{pj} \rangle}{\partial x_j} + n_p \langle c'_{pi} c'_{pj} \rangle \frac{\partial Q_p}{\partial x_j} \\
- n_p \langle F_i \xi'_p \rangle + n_p \langle c'_{pk} \xi_p \rangle \frac{\partial U_{pi}}{\partial x_k} = C(\xi_p c'_{p,i}) - Q_p C(c'_{p,i}) \quad (49)
\end{aligned}$$

In order to find a first approximation for the charge-velocity correlation, we will make a series of assumptions to simplify the equation:

1. Steady-state ($D/Dt = 0$)
2. No-velocity gradient ($\partial U / \partial x = 0$)

3. We neglect the third order momentum $\langle \xi_p c'_{p,i} c'_{p,j} \rangle$

4. Electric charge does not change during a collision

With this assumptions the charge-velocity transport equations reduces to:

$$n_p \langle c'_{pi} c'_{pj} \rangle \frac{\partial Q_p}{\partial x_j} = C(\xi_p c'_{p,i}) - Q_p C(c'_{p,i}) \quad (50)$$

Again the collision term can be fully computed:

$$\begin{aligned}
C(\xi_p c'_{p,i}) - Q_p C(c'_{p,i}) = \\
- \frac{2^{13/2} \pi^{1/2}}{3^{5/2}} d_p^2 g_0 n_p \eta (q_p^2)^{3/2} R_{p,ij}^{-1} n_p \langle c'_{pj} \xi'_p \rangle \quad (51)
\end{aligned}$$

Hence the final transport equation becomes:

$$\begin{aligned}
n_p \langle c'_{pi} c'_{pk} \rangle \frac{\partial Q_p}{\partial x_k} = \\
- \frac{2^{13/2} \pi^{1/2}}{3^{5/2}} d_p^2 g_0 n_p \eta (q_p^2)^{3/2} R_{p,ij}^{-1} n_p \langle c'_{pj} \xi'_p \rangle \quad (52)
\end{aligned}$$

If we assume a hydrodynamic isotropic flow:

$$n_p \frac{2}{3} q_p^2 \frac{\partial Q_p}{\partial x_j} = - \frac{2^{11/2} \pi^{1/2}}{3^{3/2}} d_p^2 g_0 n_p \eta (q_p^2)^{1/2} n_p \langle c'_{pj} \xi'_p \rangle \quad (53)$$

With this model, we can derive a gradient model for the charge-velocity correlation:

$$n_p \langle \xi_p c'_{p,i} \rangle = -\kappa_p^{\text{kin}} \frac{\partial Q_p}{\partial x_i} \quad (54)$$

$$\kappa_p^{\text{kin}} = \frac{3^{1/2}}{2^{9/2} \pi^{1/2} \eta d_p^2 g_0} (q_p^2)^{1/2} \quad (55)$$

Where $\eta = 1/2(1 + e_c)$

Inserting this into the charge transport equation, we obtain:

$$\begin{aligned}
n_p \frac{\partial Q_p}{\partial t} + n_p U_{pi} \frac{\partial Q_p}{\partial x_i} = \\
- \frac{\partial}{\partial x_i} (\sigma_p E_i) + \frac{\partial}{\partial x_i} \left((\kappa_p^{\text{coll}} + \kappa_p^{\text{kin}}) \frac{\partial Q_p}{\partial x_i} \right) \quad (56)
\end{aligned}$$

As we can observe, we have derive a transport equation for the electric charge. The effects of adding taking into consideration of the charge velocity correlation is much clearer now. The term κ_p^{kin} is the kinetic dispersion coefficient and it accounts for the dispersion phenomenon due to the random motion of particles. This terms is similar to the one found by Ray, M. et al. (2019). However we have shown that it can be derived using less restrictive hypothesis on the particle density distribution.

Collisional and kinetic dispersion coefficients

The kinetic theory has shown that the particle charge dispersion can be explained as the contribution of two independent phenomena. When two particles collides, there is a charge transfer that takes place. This is characterize by a collisional dispersion coefficient (κ_p^{coll}). This coefficient is proportional to the radial distribution function g_0 , which tends to infinity as the solid fraction volume ($\alpha_p = n_p V_p$) goes to the maximum compacity. This is coherent, because the more particles are in the flow, the more probable is a collision to happen, and therefore the particle charge is transported faster.

The second contribution to the dispersion coefficient is the kinetic contribution κ_p^{kin} . This can be explained as the particle charge diffusion due to random motion of particles. This coefficient is important in dilute system, because $g_0 n_p \rightarrow 0$. This is because a particle is able to travel further where there are few other particles.

Figure 1 shows the value of the two dispersion coefficient as a function of α_p , for $\Theta = 0.01 \text{ m}^2/\text{s}^2$. As we can see for dilute system the kinetic contribution is the most important, and for dense system the collisional terms is the dominant one. Also is worth noting that for an intermediate value of α_p both terms have the same order of magnitude and therefore both have to be considered.

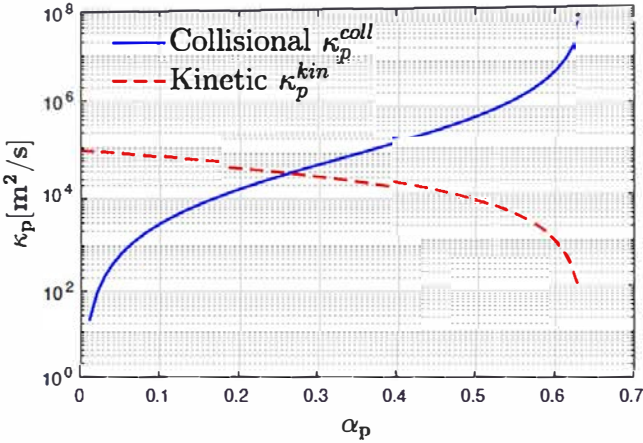


Figure 1: Collisional and kinetic dispersion coefficients as a function of the solid volume fraction for $\Theta = 0.01 \text{ m}^2/\text{s}^2$

To see the effect of these dispersion coefficients, we are going to study one of the test cases proposed by Kolehmainen, J. et al. (2018). He studied a 3D periodic box of $192d_p \times 8d_p \times 8d_p$. Initially, the particles at $x < 96d_p$ are charged positively $Q_p = Q_0$ and the particles at $x \geq 96d_p$ are charged negatively $Q_p = -Q_0$. We are going to neglect all the external forces (gravity, drag force, electrostatic, etc.). An initial granular temperature is imposed, and it remains constant during the simulations. We are also going to drop the triboconductivity effect. With these hypotheses, the charge transport equation can be simplified to a one-dimensional diffusion equation:

$$n_p \frac{\partial Q_p}{\partial t} = (\kappa_p^{\text{coll}} + \kappa_p^{\text{kin}}) \frac{\partial^2 Q_p}{\partial x^2} \quad (57)$$

This equation can be solved analytically:

$$Q_p = \sum_{n=1}^{\infty} \lambda_n e^{-\frac{\kappa_p^{\text{coll}} + \kappa_p^{\text{kin}}}{n_p} \left(\frac{2\pi n}{L}\right)^2 t} \sin\left(\frac{2\pi n x}{L}\right) \quad (58)$$

$$\lambda_n = \frac{2Q_0}{n\pi} (1 - (-1)^n) \quad (59)$$

Where $L = 192d_p$ is the box length in the x direction.

This equation allows to study the evolution of the electric charge in function of time. For the simulation, we set all the values specified in table 1 and $\alpha_p = 0.25$ and we plot the particle charge spatial profile for different values of the non-dimensional time $t^* = (\sqrt{\Theta}/d_p) t$ (Figure 2). As we can see the electric charge diffuses inside the domain as the time passes, and it tends to reach the equilibrium value $Q_p = 0$.

Table 1: Parameters used in the test case

Parameter	Value
d_p	250 μm
ρ_p	1500 kg/m^3
ε_0	$8.85 \cdot 10^{-6} \text{ F}/\text{m}$
Θ	$0.01 \text{ m}^2/\text{s}^2$
Y	$0.5 \cdot 10^6 \text{ Pa}$
ν	0.41

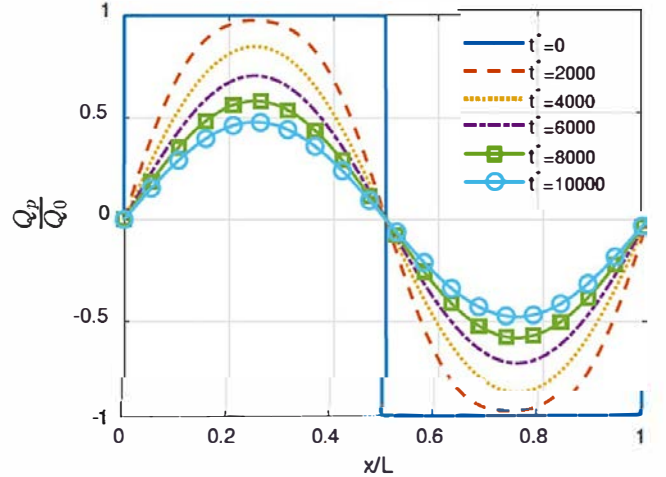


Figure 2: Particle charge profile as a function of x/L at different times $t^* = (\sqrt{\Theta}/d_p) t$

A more interesting analysis can be performed if we separate the kinetic and collisional contribution in the dispersion coefficient. Figure 3, 4 and 5 show the particle charge profile at $t^* = 4000$ for a dense system ($\alpha_p = 0.45$) a dilute system ($\alpha_p = 0.10$) and an intermediary system ($\alpha_p = 0.25$). The squares markers represent the dispersion created by the kinetic contribution, the circle markers account for the collisional contribution, and the solid line is the sum of both contributions. As we can see, for dilute systems, the dispersion comes almost exclusively from the kinetic contribution of the dispersion coefficient. On the contrary, for dense system the collisional terms is the dominant parameter. However, we can see that for intermediate values, both coefficient

are of the same order of magnitude, they both need to be taken into account in order to accurately predict the dispersion phenomenon.

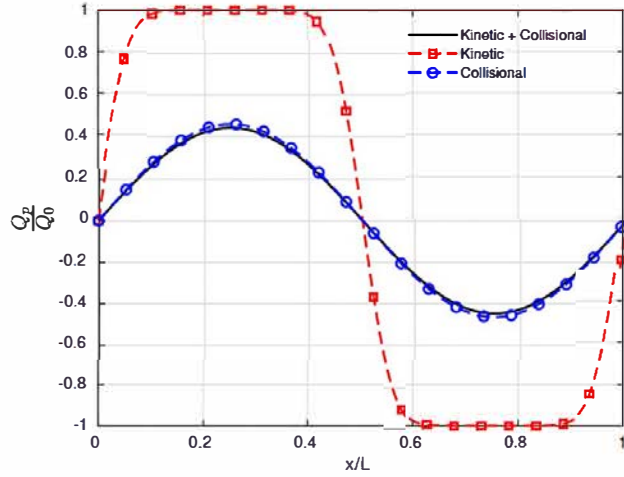


Figure 3: Particle charge profile at $t^* = 4000$ for $\alpha_p = 0.45$

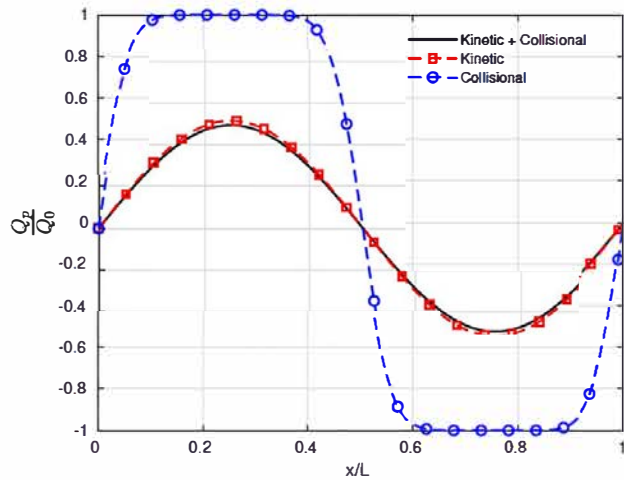


Figure 4: Particle charge profile at $t^* = 4000$ for $\alpha_p = 0.10$

Triboconductivity effect

One of the effects found on the collision integrals is the so called triboconductivity, characterize by σ_p . When the global charge distribution produces an electric potential difference, the positive charged particle tend to move against the potential gradient and the negative charged particles tend to move towards the gradient (Ohm's law). Taking the charge transport equation (equation 56) and the Maxwell's equations (equations 2 and 3) we can derive the following transport equation for the electric charge:

$$n_p \frac{\partial Q_p}{\partial t} = -\frac{\sigma_p}{V_p \epsilon_0} Q_p + \frac{\partial}{\partial x} \left((\kappa_p^{\text{coll}} + \kappa_p^{\text{kin}}) \frac{\partial Q_p}{\partial x} \right) \quad (60)$$

If we apply this equation to the same problem described before, we find the analytic solution (equation 61). Using the

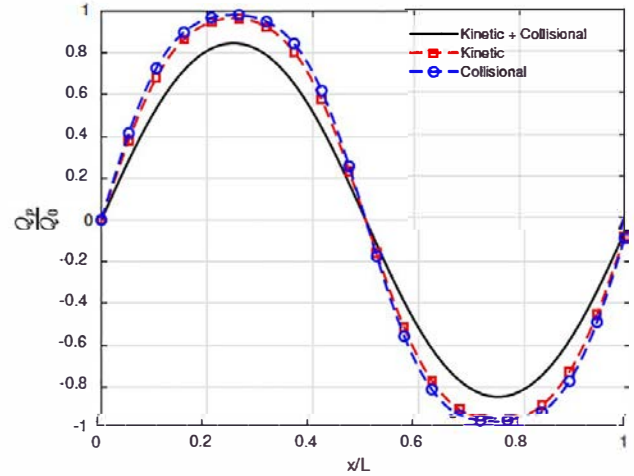


Figure 5: Particle charge profile at $t^* = 4000$ for $\alpha_p = 0.25$

same parameters as before, we can determine the dynamic evolution of the electric charge (figure 6). As we can see, the electric charge reaches the equilibrium value faster, which confirms that fact that the triboconductivity helps to the redistribution of the electric charge. However, it is worth noting that the triboconductivity effect seems to be more important than the diffusion process, this was also reported in the literature (Kolehmainen, J. et al. 2018).

$$Q_p = \sum_{n=1}^{\infty} \lambda_n e^{\left[-\frac{\sigma_p}{V_p \epsilon_0 n_p} - \frac{\kappa_p^{\text{coll}} + \kappa_p^{\text{kin}}}{n_p} \left(\frac{2\pi n}{L} \right)^2 \right] t} \sin \left(\frac{2\pi n x}{L} \right) \quad (61)$$

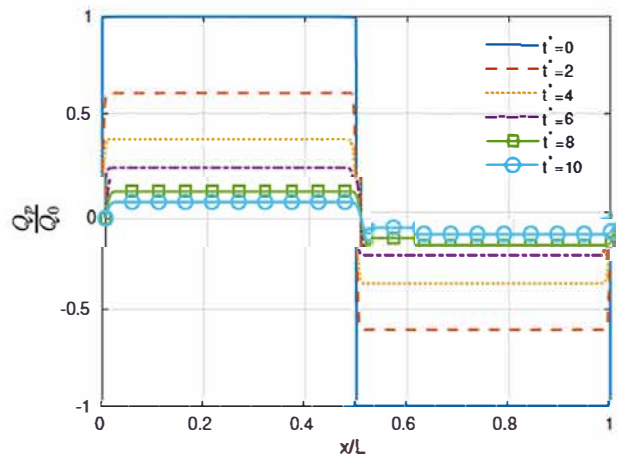


Figure 6: Particle charge profile as function of x/L at different times $t^* = (\sqrt{\Omega}/d_p) t$

In order to verify this, we are going to rewrite the equation 60, so we make appear the characteristic times for the dispersion (τ_κ) and the triboconductivity τ_σ . Taking l as the diffusion characteristic length, we have:

$$\frac{\partial Q_p}{\partial t} = -\frac{1}{\tau_\sigma} Q_p + l^2 \left(\frac{1}{\tau_\kappa^{\text{kin}}} + \frac{1}{\tau_\kappa^{\text{coll}}} \right) \frac{\partial^2 Q_p}{\partial x^2} \quad (62)$$

$$\tau_{\sigma} = \frac{n_p V_p \varepsilon_0}{\sigma_p} \quad (63)$$

$$\tau_{\kappa}^{\text{coll}} = \frac{n_p l^2}{\kappa_p^{\text{coll}}} \quad (64)$$

$$\tau_{\kappa}^{\text{kin}} = \frac{n_p l^2}{\kappa_p^{\text{kin}}} \quad (65)$$

$$\frac{1}{\tau_{\kappa}} = \frac{1}{\tau_{\kappa}^{\text{coll}}} + \frac{1}{\tau_{\kappa}^{\text{kin}}} \quad (66)$$

If we chose $l = L$, then we can represent them as function of the solid volume fraction (figure 7). We remark that the triboconductivity characteristic time is much smaller than the dispersion characteristic time for almost all values of α_p . It is only in very dilute (where there are almost no collisions) cases where the kinetic diffusion process is more efficient. This can be shown if we perform a simple analysis between the characteristic times of the dispersion and triboconductivity phenomena:

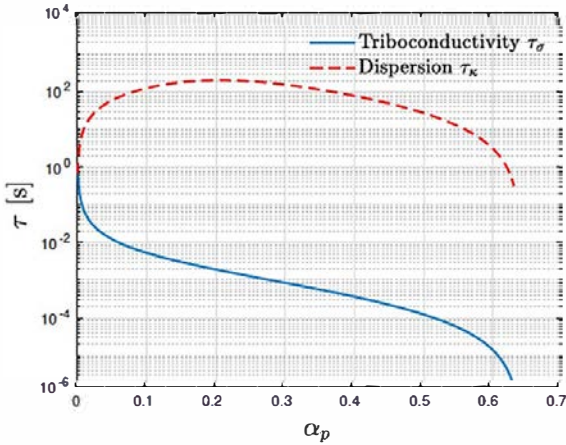


Figure 7: Triboconductivity and dispersion characteristic times in function of solid volume fraction for $\Theta = 0.01 \text{ m}^2/\text{s}^2$

$$\frac{\tau_{\sigma}}{\tau_{\kappa}^{\text{coll}}} \propto \left(\frac{d_p}{l} \right)^2 \quad (67)$$

$$\frac{\tau_{\sigma}}{\tau_{\kappa}^{\text{kin}}} \propto \frac{d_p^2 Y^{2/5}}{\rho_p^{3/5} \eta g_0^2 \alpha_p^2 l^2 (q_p^2)^{2/5}} \quad (68)$$

Where ρ_p is the particle density.

This shows, that for dense systems, the dispersion effect is only comparable to the triboconductivity when the dispersion characteristic length is of the same order of magnitude as the particle diameter. For dilute systems, the ratio between the characteristic times is more complex, because it depends on the particle physical properties (Young's module and density). However, we can say that when $\alpha_p \rightarrow 0$ the kinetic dispersion is dominant, because there are not enough collision for the triboconductivity to take place.

Conclusions

An eulerian model for the electric charge transport has been derived following the kinetic theory of granular flows. Assuming a correlated form between the electric charge and the particle velocity, we have been able to fully close the collision integrals without having to presume the expression for the particle electric charge distribution. This model have shown the main mechanisms involved in the electric charge dynamics. First of all, the dispersion phenomenon can be classified in two: a collisional dispersion that accounts for the charge transfer during a particle-particle collision, and a kinetic dispersion that due to the random motion of the particles. For both types of dispersion an expression was fully derived. We have shown that the collisional dispersion coefficient is predominant in dense regimes and that the kinetic dispersion coefficient is the most important in dilute configurations. There is, nevertheless, an intermediary region where both coefficient have to taken into account in order to accurately predict the dispersion effect.

The second mechanism responsible for the electric charge transfer, is the triboconductivity effect. The global charge distribution can create a electric potential difference. When two particles touch each other, they behave like a conductor material and therefore the electric charge flows following the potential gradient. In order to characterize which effect is more important between the dispersion and the triboconductivity, we have derive their characteristic times. These parameters have allowed us to show that, for dense regimes, the triboconductivity and the dispersion are of the same order of magnitude if the characteristic dispersion length is comparable to the particle diameter. For dilute regimes, the expression is more complicated. It depends on the particle geometrical and physical properties, solid volume fraction and the particle agitation.

Acknowledgments

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