Self-expansion patterns of charged particulates and ionic assemblies

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(Received 14 July 2004; accepted 18 April 2005; published online 9 June 2005)

Self-expansion patterns of unconstrained assemblies of charged particulates are considered. As the assemblies cannot be described, in general, in the context of a continuum comprising massless charged entities, the complete equation of motion is applied for each member of the assembly. It is shown that irrespective of the initial positions of the particulates, when expanding in free space or else they are identical in size and mass, the assembly tends toward a spherical shape, with characteristic inner structure. Examples of simulations are presented to this end. © 2005 American Institute of Physics. [DOI: 10.1063/1.1938003]

The motion of charged particulates and ionic assemblies has been a long standing subject of research. A considerable effort has been directed toward the solution of corona discharges and gaseous currents.1–4

The self-drifting of ionic clouds was studied by Jones, who considered the problem in the context of a continuum of massless ions.5 In this work, we consider self-drifting patterns of unconstrained charged particulates that qualify neither as continuum nor as massless objects.

It is shown that asymptotic behavior of self-drifting assemblies of unconstrained charged particulates involves a tendency to form an ordered uniform structure that is enclosed by a sphere. This agrees with the asymptotic drift patterns described by Jones for ionic gaseous clouds.5

The self-drifting of an assembly of charged particulates is governed by the equation of motion of each of its members. The three-dimensional equation of motion (in spherical coordinates) of a single charged particulate in a fluid, is given by,6

\[ m\ddot{r} - mr^2\dot{\phi}^2 - mr\phi\dot{r}\sin\theta = mg\cos\theta + F_{D,\phi} + F_{E,\Sigma} \]  

(1)

\[ m\ddot{r} + 2mr\dot{\theta}\dot{\phi} - mr\phi\dot{r}\sin\theta = -mg\sin\theta + F_{D,\phi} + F_{E,\Sigma} \]  

(2)

\[ m\ddot{\phi} \sin\theta + 2m\dot{r}\dot{\phi}\sin\theta + 2mr\phi\dot{r}\cos\theta = F_{D,\phi} + F_{E,\Sigma} \]  

(3)

where \( r, \theta, \) and \( \phi \) denote spherical coordinates, \( m \) is mass, \( g \) is gravity acceleration, and \( F_{D,\phi} \) and \( F_{E,\Sigma} \) are drag and electric, forces, respectively. Subscripts \( r, \theta, \) and \( \phi \) denote the respective components of the forces, \( \Sigma \) signifies the contribution from all particulates to the electric force, and the dot stands for differentiation with respect to time.

If the number density of particulates is sufficiently large, then the use of continuum theory can be justified, as was done by Jones5 for ionic clouds using the concept of ionic mobility in the form:

\[ u_i(x,t) = \mu_i E(x,t). \]  

(4)

Here the mobility \( \mu_i \) of the \( i \)th ionic species is assumed fixed so that its position, \( x, \) and time, \( t, \) dependent velocity \( u_i(x,t) \) and the electric field \( E(x,t) \) are collinear. Equation (4) holds provided that the effect of mass can be neglected. Jones showed that the asymptotic shape of a self-drifting ionic cloud is a sphere.5 In this work, we show that this asymptotic behavior can be generalized to any unconstrained assembly of self-drifting charged particulates under the conditions where the expansion is unaffected by gravity. The general model considers charged particulates as discrete entities that drift according to the complete equation of motion. Solution of particulate trajectories discloses structural patterns, which develop as the number density of particulates tends toward uniformity. In what follows, results of simulation of expansion patterns are presented, and then, the asymptotic behavior of shape and structure of the drifting assembly are discussed.

The particulates are positively charged spherical water droplets dispersed in stationary air, at atmospheric pressure, and ambient temperature. No external constraint exists, so that the self-expansion of the charged drops assembly, from its initial setting, is solely due to electrostatic interactions between the drops. The simulations were carried out using a simplified three-dimensional equation of motion in Cartesian coordinates, for the \( i \)th particulate, as follows:

\[ m_i\ddot{\xi}_i = -6\pi R_i\mu_i (1 + 0.15 \text{Re}^{0.687})\dot{\xi}_i + \sum_{j\neq i} \frac{Q_j \xi_j}{4\pi\varepsilon_0 r_{ij}^2} + mg \varepsilon_i \cdot e, \]

(5)

where \( \xi_i \) stands for one of the coordinates \( x, y, \) or \( z, \) \( e \) is unit vector, being \( e_x, \) \( e_y, \) and \( e_z, \) respectively, the subscript \( i \) (\( i \neq j \)) was dropped for the sake of brevity, \( \text{Re} \) is the Reynolds number and \( m_i, R_i, Q_j, \mu_j, e_j, \) and \( r_{ij} \) denote, mass, radius, charge, viscosity, permittivity, and distance between the \( i \)th and \( j \)th drops. The mass, radius, and charge pertain to the \( i \)th drop, whereas the viscosity and permittivity are properties of the surrounding fluid, which here is air. \( Q_j \) and \( \xi_j \) denote charge of the \( j \)th drop and coordinate of the \( j \)th drop in the frame of the \( i \)th drop.

Figure 1 shows simulation of two-dimensional self-expansion of 132, 10 \( \mu \)m drops. A 250 V charging potential (imposed during formation of drops from a jet) was assumed [see Eq. (6) for the relation 7 between the charge \( Q \) and charging potential \( V_c \). This gives \( Q = 1.39 \times 10^{-13} \text{C} \) for each drop. The initial setting, at \( t = 0, \) of the drops (shown as dots) is given in plot a. The general shape of the drops assembly was arbitrary and all initial coordinates of the drops (within the framework of this shape) were set randomly:

\[ Q = 4\pi \varepsilon RV_c, \quad e = 8.854 \times 10^{-12} \text{Cm}^{-1} \text{V}^{-1}. \]  

(6)
The tendency of the assembly to spread out evenly becomes clear after 0.06 s and 0.3 s, from start of motion. Plot d shows the assembly at \( t = 1557.4 \) s, where the asymptotic approach to the enclosing circle is clear. The outermost, or peripheral drops, which were identified as being closest to the circle were used to calculate the average deviation of the assembly from being circular. To this end the radial distance of 23 drops was used to calculate their relative deviation from the circle radius. The self-expansion between \( t = 0.3 \) s and \( t = 1557.4 \) s decreased from 12.45% to 2.16%, concurrent with over tenfold increase in the circle radius, from 0.032 to 0.4602 m. The asymptotic approach to a structured circle is demonstrated by the decrease in distortion of the hexagons shown in plot c as compared to their shape in plot d. Figure 2 shows self expansion of 49 drops that form initially a uniform finite row on the z axis, in the \( -0.006 \leq z \leq 0.006 \) m range. This line segment of charged drops is unstable to the extent that perturbations, however small, from the z axis position of at least one drop, turns the expansion pattern two or three dimensional.

In plot a, two drops are displaced from the z axis, the first (second from the bottom of the drop array) in the \( xz \) plane and the second (19 from the top) in the \( yz \) plane. These two small perturbation in position induce a drift both in the \( xz \) and \( yz \) planes (plot b), and turn the geometry of the charge assembly closer to being spherical (plot c). The relative deviation from a sphere (see \( yz \) and \( xz \) views in plot c) is 3.92% for the six outermost drops. The latter result is remarkable with respect to the geometrical instability of unconstrained charge assemblies of particulates, irrespective of their shape and size. Charged assemblies of particulates, if unconstrained, will expand into a dimension, once the coordinates of at least one of its members is perturbed in this dimension.

Self-drifting of an unconstrained assembly of charged particulates is driven by their self-electric energy \( U \):

\[
U = \frac{1}{2} \sum_i \sum_j \frac{1}{4\pi\varepsilon_0 \ r_{ij}} q_i q_j, \quad i \neq j. \tag{7}
\]

In Eq. (7) \( r_{ij} \) is the distance between the \( i \)th and \( j \)th particulates having charges \( q_i \) and \( q_j \), respectively. If \( q_i > 0, q_j > 0 \) (or both are negative), then decrease of \( U \) involves increase in \( r_{ij} \) and hence self-expansion.

We show first that a uniformly structured sphere provides a stable form of expansion.

Consider a finite assembly of identical, charged particulates distributed uniformly in an ordered pattern inside a sphere of radius \( r_o \). The particulates do not form a continuum but their structure permits their uniform (or symmetrical) positioning on internal spherical surfaces, so that their action can be simulated by an equivalent charge at the center of the sphere. The electric field inside the sphere is radial and given by
$E_r = \frac{\rho_r}{3\varepsilon_f}, \quad \rho_o = \frac{3Q_o}{4\pi r_o^3}, \quad r < r_o,$

(8)

where $Q_o = \sum \Delta q$ denotes the total charge of the assembly in a sphere of radius $r_o$.

In this case, the drift velocity, which is governed by the equation of motion, is radial and hence does not involve angular acceleration. Consequently, assuming that in this case, the radial inertial effect may be neglected and the Stokes flow applies, the drift velocity, $u$, can be presented as,

$u = \alpha r, \quad \alpha = \frac{\rho_o D}{3\varepsilon_f D}, \quad D = f_D/u, \quad r < r_o,$

(9)

where $f_D$ is drag force, given by $f_D = 6\pi \eta a u$ for Stokes flow (of fluid with viscosity, $\eta$), around a particulate of radius $a$.

The change in number density of particulates is given by $d\rho = -pdV/V$, where $V$ is the volume of a sphere of radius $r \leq r_o$, and $dV = 4\pi r^2 dr, \quad dr = \alpha dt$. Hence, $d\rho = -3\rho a \alpha dt$ is independent of $r$ being uniform across the sphere from $o$ to $r_o$. Consequently, the change in $\rho$ is a sole function of time, at uniform number density of particulates across the expanding sphere. Elimination of parts of the sphere, or its distortion into another shape, generates a state of unbalanced angular ($\theta$ and $\varphi$) forces, while the radial ($r$) forces decrease. These forces drive the particulates into the vacant position until they fill them, so that the spherical shape is restored. In other words, stability of expanding shape is reached once the angular components of the electric forces vanish. This argument applies equally well to the effect of perturbations in number density of particulates.

The internal structure of the expanding assembly tends to minimize the local electric energy. Six charged particulates placed on a circle will form a hexagon. If a seventh particulate is allowed to move inside the circle, then the electric energy of the seven particulates will be minimized when it settles in the center. This gives a centered hexagon structure, where all particulates have the same distance (set equal to the radius) from their closest neighbors.