Structural evolution of self-expanding arrays of charged particulates

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Abstract
Self-expansion patterns of unconstrained assemblies of charged particulates are simulated by solution of their individual trajectories. The general behaviour of these systems is considered regarding their expansion shape and structure. As the particulates cannot be described, in general, in terms of massless charged entities, the complete equation of motion, inclusive of the inertial and other size effects, must be applied to each and every member of the assembly. It is shown that irrespective of the initial position of the particulates and the time dependent shape of the assembly, when expanding in free space or else the particulates are identical in size, shape and mass, they self-expand asymptotically into a circular or spherical shape with an inner structure that tends to uniformity. This behaviour persists irrespective of the size and charge level of the particulates, or whether they form a single or multiple separate groups in one, two and three dimensions. In this context, ionic gaseous assemblies that fit into the realm of continua, are included. Two- and three-dimensional examples of simulation outputs for different particulate assemblies, illustrate typical self-expansion patterns. Internal structures that evolve in two-dimensional self-expanding arrays are shown to be different compared to those obtained in three dimensions. These simulations show that models of particle capture by random self-expanding arrays of charged particulates, may lack physical grounds, as they contradict the asymptotic mode of uniform and ordered self-expansion that is expected from the array.

Keywords: Self-expansion; Charged particulates; Particle-capture

1. Introduction

The motion of charged particulates and ionic assemblies has been a long standing subject of research. Charged particulates occur frequently in nature, industry and clean as well as polluted environment. Well-known examples are natural clouds, industrial dispersions and airborne solid and liquid particulates. Different charging procedures are used to enhance and control the formation of sprays [1], and charged particles are collected electrostatically [2] on large scale in coal fired power stations. A considerable effort has been directed toward the solution of corona discharges and gaseous currents [3–6]. In particular, the ion drift regime was studied analytically and numerically [7].

A collection of very large volumes of dispersed droplets is required as part of the design of energy towers. In these towers, saline water, which is dispersed as droplets at the top, evaporates and cools dry air that flows gravitationally downwards [8]. This air flow drives electricity generating turbines. Randomly dispersed clouds are expected to behave differently compared to structured clouds. This applies to the hydrodynamics involved and their capacity to capture other arrays of dispersed particulates, as they fall down gravitationally. Of particular interest is the evolution of the degree of uniformity of self-expanding clouds. Higher degree of uniformity simplifies the system regarding its nature, operation and option of simulation. Therefore, it is desirable to determine if the self-expansion leads to higher degree of uniformity of the arrays, and the kinetics involved. This relates to the interaction between two or more clouds and the outcome of their overlap, merger and then coself-expansion. Such interaction governs the process whereby self-drifting charged particulates that are sprayed as separate clouds, tend to fill the space around them. In this work, we establish a fundamental physical behaviour of an unconstrained assembly of charge particulates that self-expands in zero gravity free space, or where gravity has no effect on the outcome of the expansion, i.e., when the particles are identical in size, shape and mass.
Single collector models are abundant in literature [9–11]. Multiple collector models have been presented [12]. However, these models are limited to a set up such as a few spherical or cylindrical collectors, arranged in line. Recently, the collection of aerosols by arrays of larger drops was studied by simulation of their trajectories [13,14]. Intricate trajectories and unexpected collection patterns were found and the meaning of collection efficiency was revised accordingly. Self-drifting effects are expected to be significant when finite clusters of charged collecting drops are used. The self-drifting of ionic clouds was studied by Jones, who considered the problem in the context of a continuum of massless ions [7].

In this work, we present an extension of our study on self-expansion of charged assemblies of drops [15]. We give the full scope in content and results of simulations of self-expansion of arrays of charged particulates, regarding their shape and internal structure. In Ref. [15], the basic phenomenon is described as a short letter that does not permit elaboration and an in-depth scope in content and results of simulations of self-expansion. Many relevant data was excluded from Ref. [15] because of space restrictions, and examples were limited to two figures. In contrast, this work, which is a full length paper, contains detailed theoretical considerations concerning: the nature of the self-expansion, the reason for the asymptotic tendency, the tendency to form ordered and uniform structure, the behaviour of different merging self-expanding groups, details of accuracy and its significance, three-dimensional simulations additional to the example of the perturbed line (which here includes a larger number of drops, thus corroborating previous results), the effect of size and charge distribution, expansion of centered hexagonal structured arrays, and comparative tests of theoretical and simulated velocities of particulates. In this context Ref. [15] is an introductory work in a short form of a letter. Here we expand the scope and content (10 figures) of the presented material, for the benefit of the reader who is interested to follow an in-depth study of the new findings, the related theory, results and their consequences. We consider self-drifting patterns of unconstrained charged particulates that qualify neither as continuum nor as massless objects. The term “unconstrained” implies the absence of driving forces (except for gravity) other than those originating from electric interactions between members of the particulate assembly. Thus, for example, the presence of external electromagnetic fields must be excluded [15].

It is shown that the asymptotic behaviour of two- and three-dimensional self-drifting arrays of charged particulates involves a tendency to form a structure of higher order and uniformity that is enclosed by a circle and a sphere, respectively. This agrees with the asymptotic drift patterns described by Jones for ionic gaseous clouds [7]. Furthermore, it extends this result to discrete assemblies of charged particulates moving with velocities that are not necessarily collinear with the local field.

2. Theory

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 [14]

\[
m\ddot{r} - m\dot{r}\dot{\theta}^2 - m\dot{r}\dot{\varphi}\sin^2\theta = mg \cos \theta + F_{D_0} + F_{E_0},
\]

\[
m\ddot{\theta} + 2m\dot{r}\dot{\theta} - m\dot{r}\dot{\varphi}^2 \sin \theta \cos \theta = -mg \sin \theta + F_{D_0} + F_{E_0},
\]

\[
m\ddot{\varphi} \sin \theta + 2m\dot{r}\dot{\varphi} \sin \theta + 2m\dot{r}\dot{\varphi} \cos \theta = F_{D_0} + F_{E_0},
\]

where \(r, \theta, \varphi\) denote spherical coordinates, \(m\) is mass, \(g\) gravity acceleration, and \(F_{D_0}\) and \(F_{E_0}\) drag and electric forces, respectively. Subscripts \(r, \theta, \varphi\) 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. Equations (1)–(3) do not account for hydrodynamic interactions, which may exist between neighbouring particulates.

The two-dimensional case is obtained at \(\varphi = 0\). The non-dimensional counterpart of Eqs. (1)–(3) depends on the flow regime characterizing the motion as follows:

**Stokes flow \(Re \leq 0.2\)**

\[
A\left[\ddot{r} - \dot{r}\dot{\theta}^2 - \dot{r}\dot{\varphi}^2 \sin^2 \theta\right] = \left[AB \cos \theta - (\vec{r} - \vec{u}_{\infty}) \right] + \sum_{i,j,k} \frac{1}{r_{ijk}^2} \mathbf{e}_{i,j,k} \cdot \mathbf{e}_{r}, \quad (4)
\]

\[
A\left[\ddot{\theta} + 2\dot{r}\dot{\theta} - \dot{r}\dot{\varphi}^2 \sin \theta \cos \theta\right] = -AB \sin \theta - (\vec{r} - \vec{u}_{\infty}) + \sum_{i,j,k} \frac{1}{r_{ijk}^2} \mathbf{e}_{i,j,k} \cdot \mathbf{e}_{\theta}, \quad (5)
\]

\[
A\left[\ddot{\varphi} \sin \theta + 2\dot{r}\dot{\varphi} \sin \theta + 2\dot{r}\dot{\varphi} \cos \theta\right] = -\left(\vec{r}\dot{\varphi} \sin \theta - \vec{u}_{\infty}\right) + \sum_{i,j,k} \frac{1}{r_{ijk}^2} \mathbf{e}_{i,j,k} \cdot \mathbf{e}_{\varphi}, \quad (6)
\]

\[
A = \frac{D_p^2 \rho_p u_{\infty}^2}{18 \mu t R_c}, \quad B = \frac{R_c g}{u_{\infty}^2}, \quad C = \frac{q Q}{12\pi^2 \epsilon_0 R_c^2 D_p \mu t u_{\infty}}. \quad (7)
\]

**Intermediate and turbulent flow \(Re > 0.2\)**

\[
A\left[\ddot{r} - \dot{r}\dot{\theta}^2 - \dot{r}\dot{\varphi}^2 \sin^2 \theta\right] = A' B' \cos \theta - C_D (\vec{r} - \vec{u}_{\infty}) \cdot \mathbf{e}_r + C' \sum_{i,j,k} \frac{1}{r_{ijk}^2} \mathbf{e}_{i,j,k} \cdot \mathbf{e}_r, \quad (8)
\]

\[
A\left[\ddot{\theta} + 2\dot{r}\dot{\theta} - \dot{r}\dot{\varphi}^2 \sin \theta \cos \theta\right] = -A' B' \sin \theta - C_D (\vec{r} - \vec{u}_{\infty}) \cdot \mathbf{e}_{\theta} + C' \sum_{i,j,k} \frac{1}{r_{ijk}^2} \mathbf{e}_{i,j,k} \cdot \mathbf{e}_{\theta}, \quad (9)
\]

\[
A'\left[\ddot{\varphi} \sin \theta + 2\dot{r}\dot{\varphi} \sin \theta + 2\dot{r}\dot{\varphi} \cos \theta\right] = -C_D (\vec{r} - \vec{u}_{\infty}) \cdot \mathbf{e}_{\varphi} + C' \sum_{i,j,k} \frac{1}{r_{ijk}^2} \mathbf{e}_{i,j,k} \cdot \mathbf{e}_{\varphi}, \quad (10)
\]

\[
A' = \frac{4D_p \rho_p}{3 \rho t R_c}, \quad B' = \frac{R_c g}{u_{\infty}^2}, \quad C' = \frac{q Q}{\pi^2 \epsilon_0 R_c^2 D_p \mu t u_{\infty}^2}. \quad (11)
\]

where \(ijk\) identifies the particulate exerting the force, \(Q = Q_{ijk}\) is assumed for the sake of simplicity for all \(ijk\), \(\mathbf{e}_r, \mathbf{e}_{\theta}, \mathbf{e}_{\varphi}\) are unit vectors in the \(r, \theta, \varphi\) directions, in the frame of the reference sphere, and differentiation (denoted by dot over the
variable) is with respect to the dimensionless time, $\tilde{t}$. The following dimensionless variables were defined, and then used to derive Eqs. (4)–(11):

\[ \tilde{\xi} = \xi / R_c, \quad \tilde{u}_t = u_t / u_\infty, \quad \tilde{u}_\phi = u_\phi / u_\infty, \quad \tilde{u}_{\phi_0} = u_{\phi_0} / u_\infty, \quad \tilde{t} = t u_\infty / R_c. \]

The variable $\tilde{\xi}$ denotes all relevant length variables, e.g., position vectors $r$ and $r_{ij,k}$, and radial distances $r$ and $r_{ij,k}$.

The last term on the right-hand side of Eqs. (4)–(6) and (8)–(10) stands for the dimensionless effect of the corresponding ($e.g., r, \theta, \phi$) component of the electric force, acting due to all $i,j,k$ particulates. $R_c$ denotes radius of the particulate, and $u_t$ and $u_\infty$ local and distant (at infinity) fluid velocity, respectively.

The equations of motion are valid for discrete particulates, solid or liquid, down to the size of ionic species, where the effect of mass can be neglected and diffusion is significant. If the number density of particulates is sufficiently large, then the use of continuum theory can be justified, as was done by Jones [7] for ionic clouds using the concept of ionic mobility in the form

\[ u_t(x,t) = \mu_i E(x,t). \] (12)

Here the mobility $\mu_i$ of the $i$th ionic species (which may be either positive or negative) 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 (12) holds provided that the effect of mass and size can be neglected. Otherwise, in cases where inertia, effect of size on flow, and gravity are significant, the equation of motion in its complete form must be applied. Jones showed that the asymptotic shape of a self-drifting ionic cloud is a sphere [7]. 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 expansion is unaffected by gravity. The particular and coordinate of the $i$th particulate and the $ij$th part.

The boundary conditions of the system are linked to the condition of its being unconstrained. This sets the electric field to zero at infinity, and imposes the absence of external electromagnetic fields. The simulation is carried out assuming that the particulates fall, in other words quiescent, at their terminal gravitational velocity and the only significant electric forces are Coulombic. The latter is justified when the ratio between the interparticle distance to their diameter is sufficiently large (say above 5, where the hydrodynamic forces turn less than few percent), as indeed is the case for the expanding assembly. At start of the simulation ($t = 0$), velocity of all particulates is set at their terminal fall velocity (due to gravity). The Particle–Particle method [16], in its simplest and accurate form, as described for small N-body systems, was used for calculation of electrical forces between aerosols. The total electric force on each aerosol was accommodated to a primary algorithm in order to develop and integrate a system of two first-order differential equations with appropriate definition of velocity and acceleration. The operation was repeated for all aerosols.

The numerical solutions were obtained by the Runge–Kutta routine which was also used elsewhere to solve intricate aerosol trajectories in arrays of charged collecting drops [13,14]. The time step, set initially at $dt = 2 \times 10^{-5}$ s, was adjusted in order to match changes in velocity along the trajectory, and thus expedite calculations at the same level of accuracy. Note that this time step is divided further by the Runge–Kutta routine. Convergence of trajectories proved that no further improvement in accuracy is expected when time steps smaller than 0.0001 s are applied. At each consecutive time step, all relevant variables in the equation of motion, Re included, were updated. The electric-
cally driven self-expansion, relative to a frame attached to their center of gravity (or simply to one of the particles), is independent of gravity provided that the particulates are identical. Otherwise, they are expected to have a distribution of terminal velocity, and a gravity dependent self-expansion. This was verified by simulation of self-expansion of nonuniform assemblies of drops. As most of the self-expanding assemblies simulated in this work consist of identical 10 µm water drops, their self-expansion is unaffected by gravity.

However, in general, the results are not limited to small particulates, or the type of material, i.e., fluid or solid, from which they are made. Note that in the following simulations $Re \leq 10$ applied, where $Re$ is defined by $Re = \frac{\rho (\dot{r} - u_f) D_p}{\mu_f}$.

Fig. 1 shows simulation of two-dimensional self-expansion of 132, 10 µm drops [15]. A 250 V charging potential (imposed during formation of drops from a jet) was assumed. See Eq. (14) for the relation between the charge $Q$ and charging potential $V_c$. This gives $Q = 1.391 \times 10^{-13}$ 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.

$$Q = 4\pi \varepsilon RV_c, \quad \varepsilon = 8.854 \times 10^{-12} \text{ Cm}^{-1} \text{ V}^{-1}. \quad (14)$$

This setting cannot be described uniquely as a continuum. Consequently, it must be treated as a system comprising discrete elements. Therefore, the latter approach was applied in the simulation. The tendency of the assembly to spread out evenly becomes clear after 0.04 s (plot b) and 0.3 s (plot c) from start of motion. The asymptotic tendency of the assembly, to form a circle, becomes evident after 7 s (plot not shown), where the number density of the charged drops turn nearly even within an imaginary circle that encloses them. At 7 s, this circle is approximately 4 times the size of the initial assembly, i.e., at $t = 0$. Plots b and c disclose another tendency of the expanding assembly, namely to increase its order in the form of internal structure. Increase of time enhances this tendency. Plot d shows the assembly at $t = 1557.4$ s, where the asymptotic approach
to the enclosing circle (dashed line) 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 $\sigma_r$ from the circle radius. The self-expansion between $t = 0.3$ and 1557.4 s decreased $\sigma_r$ from 12.45 to 2.16%, concurrent with a 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. Note that in the asymptotic phase of expansion the structural changes turn slow to the extent that excessive computer time may be required. For example, between 295.22 and 1557.4 s $\sigma_r$ changes by 0.23% from 2.39 to 2.16%. The relative change in number density across the circle was tested by comparing, at $t = 1557.4$ s, the average number density of drops that characterize different inner circles. The deviation of average number density pertaining to inner circles (for example, $R/2$, $R/4$) relative to that of the outer circle $R$, ranged between 6 and 12%. Recalling the initial random distribution and irregular shape of the assembly, and the low rate of change of the inner structure in the asymptotic expansion phase, this deviation level is rather small.

Fig. 2 shows the behaviour of the same charged assembly in three dimensions. Initially (plot a), the 132 drops are distributed randomly in the $x$, $y$ and $z$ dimensions. The tendency toward a shape of higher symmetry, which is observed after 0.25 s (plot b) and 1 s (plot c) leads to nearly a sphere after 70 s (plot d). A measure of the degree of uniformity achieved by the 132 droplets at $t = 70$ s, is shown in Fig. 3, where the
The theoretical number of drops is plotted vs the normalized radius of an inner sphere. In a perfectly uniform sphere of radius \( R_{\text{max}} \) containing \( N \) (uniformly distributed) droplets, the number enclosed by an inner sphere of radius \( R_i \) is \( (R_i/R_{\text{max}})^3 N \), \( 0 \leq R_i/R_{\text{max}} \leq 1 \). This theoretical relation is shown as a solid boldface line. The results of the simulation proved to follow the theoretical line rather closely except for the range around \( R_i/R_{\text{max}} = 0.8 \). Clearly, 70 s is insufficient to eliminate number density fluctuation in this range. In order to test the effect of size, and hence also charge distribution, on the expansion characteristics of the drop assembly, simulations were run with drop populations characterized by normal distributions. Fig. 4 shows the two-dimensional self-expansion pattern (perpendicular to gravity) of 132 drops distributed normally, with expectation of size set at 10 \( \mu \)m and standard deviation of 2.5 \( \mu \)m. The previously described behaviour persists. The tendency toward circular symmetry becomes evident after 1.4 s (plot b). As time elapses, higher degree of circularity is observed, see plot c at 7 s and plot d at 12.5 s, where the imaginary enclosing circle provides a measure for the shape of the assembly. The development of uniformity, and tendency toward internal structure, is evident despite the size and charge distribution. This provides evidence that when the effect of gravity is eliminated, the asymptotic tendency to form a circle persists irrespective of the size and charge distribution of the particles.

The model of asymptotic self-expansion of a single assembly of particulates can be extended so as to include nonuniform multiple assembly systems. The systems may consist of particulates with size and charge distributions under zero gravity conditions, or else identical particulates in a finite gravitational field. Figs. 5a–5d shows an example of self-expansion of two distinct assemblies of particulates in zero gravity field. Both assemblies have a normal size distribution which is characterized by 10 \( \mu \)m mean and standard deviation of 2.5 \( \mu \)m. The charge is a linear function of the size at the 250 V charging potential. Consequently, the charge is also normally distributed. The initial position \( (t = 0) \) of the two assemblies, which was set by a random number generator, is shown in Fig. 5a. The result of self-expansion of the two assemblies at \( t = 0.23 \) s is shown in Fig. 5b. Each assembly tends to expand in the expected way forming a more ordered structure which is enclosed by an imaginary boundary of increased degree of sphericity. This tendency still persists at \( t = 1.73 \) s, as the assemblies start to merge, see Fig. 5c where the increased uniformity of structure and number density of the particulates are illustrated. The new approximately bi-spherical system expands further into its asymptotic single spherical shape. For example, at \( t = 341.49 \) s, the assembly is shaped close to a sphere, as shown in Fig. 5d. Thus, the approach toward sphericity and ordered uniform inner structure is evident also in the case of self-expansion of two separate, nonuniform and interacting assemblies of particulates.

Fig. 6 shows self-expansion of an assembly consisting of 7 groups of 10 \( \mu \)m droplets. The initial, \( t = 0 \), setting and number \( N \) of droplets in each group is shown in plot a, which gives two planar, \( xz \) and \( yz \), and one three-dimensional views. Plot b shows the assembly at \( t = 0.2744 \) s, where the self-expansion produced merger of the groups into a single self-expanding unit of 200 droplets. Plot c shows a three-dimensional, \( xyz \), view of the assembly at \( t = 375.55 \) s. Planar views (\( xz \) in plot d, and \( yz \) not shown) of this assembly at \( t = 375.55 \) s confirmed that a good fit (within few percent) to an enclosing circle can be found. This simulation verifies the general self-expansion pattern in the asymptotic phase, also for an assembly comprising different groups set randomly with respect to each of its member drops, as well as to each other. The self-expansion mechanism involves three steps: self-expansion of individual groups, merger of the groups into one unit, and then self-expansion of this unit toward the asymptotic phase where the shape turns circular or spherical. In the first step, each group may deform into any shape, including spherical one, continue deformation in the merger phase, and then the merged unit continues to self-expand toward the asymptotic phase. The tendency toward uniformity exists already in the first step and persists in the merger and asymptotic phases.

An example of self-expansion driven by small perturbation from a one-dimensional array of drops is considered next. Fig. 7 shows self-expansion of 201, 10 \( \mu \)m drops that form initially a uniform and finite row on the \( z \) axis, in the \( -0.01 \) m \( \leq z \leq 0.01 \) 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 (each of diameter \( D = 10 \) \( \mu \)m) are displaced from the \( z \) axis, the first (number 60 from the bottom of the drop array) in the \( xz \) plane to \( x = 10D \), \( y = 0 \), and the second (number 170 from the bottom) in the \( yz \) plane to \( y = 10D \), \( x = 0 \). These two small perturbation in position induce a drift both in the \( xz \) and \( yz \) planes (plot b, \( t = 0.0041 \) s), and turn the geometry of the charge assembly closer to being spherical (plot c, \( t = 249.96 \) s). This was verified by the three-dimensional plot d, where the size of the sphere is over 20 times the initial length of the line segment. The latter result is remark-
Fig. 4. Simulated two-dimensional self expansion of 132 drops (set in a plane perpendicular to gravity) characterized by a normal size distribution (expectation $= 10 \, \mu m$, standard deviation $2.5 \, \mu m$), $Q = 1.391 \times 10^{-13} \, C$, at 10 $\mu m$ and 250 V. (a) Random initial positions, $t = 0$, (b) 1.4 s, (c) 7.0 s, and (d) 12.5 s.

Asymptotically, with respect to the geometrical instability of unconstrained charge assemblies of particulates, irrespective of their shape and size. It also confirms the previously obtained results for a shorter, 49 drops, row [15]. One- or two-dimensional 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. Thus, a line of charge drops set along the $z$ axis, which is perturbed in the $x$ direction is expected to turn into a circle in the $xz$ plane. A second perturbation, however small, in the $y$ direction is expected to turn the circle, which evolved from the initial line, into a sphere. This system cannot be described uniquely as a continuum and the individual equation of motion for each charged drop must be applied. Consequently, in order to prove that the asymptotic approach of discrete systems is toward a uniform and structured circular or spherical shape, we need to resort to force and energy considerations as applied to individual members of the system.

4. Energy force and structural considerations

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

\[
U = \frac{1}{2} \sum_i \sum_j \frac{q_i q_j}{4 \pi \varepsilon_0 r_{ij}}, \quad i \neq j. \tag{15}
\]

In this process, which takes place in a carrier fluid, maximum transfer of electric energy occurs in the form of dissipation. In Eq. (15), $r_{ij}$ 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. In this context, although the size of the sphere is time dependent, its shape uniformity and structural characteristics are time invariable. After establishing the features of the expanding sphere, we show that all other expanding shapes tend asymptotically to an expanding sphere [15].

Consider a finite assembly of identical, charged particulates distributed uniformly in an ordered pattern inside a sphere of radius \( r_0 \). The particulates do not form a continuum but their structure (which as shown below can be approximated as centered hexagonal) 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 [17]

\[
E_r = \rho_0 \frac{r}{3 \varepsilon_f}, \quad \rho_0 = \frac{3 Q_0}{4 \pi r_0^3}, \quad r < r_0,
\]

where \( Q_0 = \sum_i q_i \) denotes the total charge of the assembly in a sphere of radius \( r_0 \).

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, the drift velocity, \( u \), can be presented as

\[
u = ar, \quad \alpha = \frac{\rho_0 q}{3 \varepsilon_f D}, \quad D = f_D/u, \quad r \leq r_0,
\]

where \( f_D \) is drag force, given by \( f_D = 6 \pi a \eta u \) for Stokes flow (of fluid with viscosity, \( \eta \)), around a particulate of radius \( a \). The expressions for \( f_D \) in the intermediate and turbulent flow regimes are given elsewhere [14].

The change in charge density of particulates is given by

\[
\frac{d \rho}{dV} = \frac{-\rho}{V}, \quad \rho = \frac{3 Q_0}{4 \pi r_0^3}, \quad r < r_0,
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\]
at uniform number density of particulates across the expanding sphere,

$$\rho = \rho_0 \exp\left[-(\rho_0 q / \varepsilon f D)t\right].$$

Note, that in the asymptotic phase of expansion, the velocities, and hence even more so acceleration, are expected to be small. This supports the assumption that the radial component of inertia can be neglected. As already mentioned, there are no unbalanced angular forces as the sphere expands. Elimination of parts of the sphere, or its distortion into another shape, generates a state of unbalanced angular ($\theta$ and $\phi$) 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. If the perturbation is negative, then the same situation arises as previously described. If it is positive, then the rest of the assembly can be considered as being the region where the number density was lowered. Thus, any shape different than a sphere can be viewed as being derived from a sphere by elimination of parts therein. Consequently, a self-expanding assembly of charged particulates, of any shape, will tend to form a sphere.

The internal structure of the expanding assembly tends to minimize the local electric energy. The energy of a particulate is determined primarily by its closest neighbours. In the one-dimensional case, when a charged particulate is set between two equally charged particulates, the electric energy is minimized once it is placed in the center between its neighbouring particulates. In two dimensions, the energy of three charges confined to a circle will be minimized when they form an equilateral triangle. Six charged particulates placed on a circle will form a hexagon where all particles have the same distance from their closest neighbours. If a seventh particulate is allowed to move inside the circle, then the electric energy of the 7 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 neighbours.

Consider a two-dimensional structure (Fig. 8a) comprising the centered hexagonal unit cell as its fundamental structural unit. This two-dimensional structure can fit circles having radii
Fig. 7. Simulated self expansion of 201, 10 µm drops, set initially on the \( z \) axis as a uniform row \((-0.01 \text{ m} \leq z \leq 0.01 \text{ m})\), except for two drops, one shifted in the \( x \) direction (to \( x = 100 \mu\text{m}, y = 0 \)) and the other in the \( y \) direction (to \( x = 0, y = 100 \mu\text{m} \)), \( Q = 1.391 \times 10^{-13} \text{ C} \). (a) \( t = 0 \), (b) \( t = 0.0041 \text{ s} \), (c) \( t = 249.96 \text{ s} \), \( zy \) plot, (d) \( t = 249.96 \text{ s} \), \( xyz \) plot.
For example, if \( 0 \leq n a < 1 \) as the primary radius (of a primary circle) is one particulate at the center. Here \( a \) is the fixed distance between neighbouring particulates in an equilateral triangle, or the centered hexagonal unit cell. This centered hexagonal structure conforms (for large \( n \)) with the asymptotic model of uniformly expanding assembly that satisfies Eqs. (15) and (16). The radius \( na \), which corresponds to \( i = (n - \beta)/2 \), is defined as the primary radius (of a primary circle) \( n = 1, 2, \ldots \). All radii larger than \( (n - 1)a \) and smaller than \( na \), which correspond to \( 0 \leq i < (n - \beta)/2 \), are defined as intermediate radii (of intermediate circles). For example, if \( n = 3 \), then \( \beta = 1 \) gives \( 3a\sqrt{3}/2 \) as the intermediate radius and \( 3a \) as the primary one, for \( i = 0 \) and \( i = 1 \), respectively (Fig. 8b). The number of drops enclosed by a circle of radius \( na \) is \( 3n(n + 1) + 1 \).

The match between circles and the centered hexagonal structure is not perfect. The larger the \( n \) is, the smaller is the mismatch. If \( n \) is even, so that \( \beta = 0 \), then the closest radius to \( na \) is \( \sqrt{3n^2 + (n - 1)^2} \), the relative difference (RD) being

\[
\left( \frac{na - a}{2} \sqrt{3n^2 + (n - 1)^2} / na \right) \text{ or } \sqrt{3/4 + (1 - 1/n)^2/4}.
\]

Clearly, \( \lim_{n \to \infty} \text{RD} = 1 \), which gives a match between the centered hexagonal structure and the \( na \) primary circle. If \( n \) is finite, as in Fig. 8, the structure enclosed by a circle must first deform in order to increase the match with the circle and then proceed to regain the centred hexagonal structure, see Figs. 9a and 9b. The competition between the tendencies to form an outer circle on the one hand, and internal ordered structure on the other, produces structures that deviate from perfect centred hexagonal (Fig. 9a). These intermediate structures may contain unit cells that can range, for example, from centered square or pentagon to centred hexagonal. Note that after 150 s of expansion (Fig. 9b) the size of the assembly increased by more than two orders of magnitudes (compare Fig. 8a and Fig. 9b). At this stage the rate of expansion and change of structure are slow.

The drifting results in an increase of the characteristic inter-particle distance \( a \), at fixed number of particulates. In three dimensions, the structure of a self-expanding assembly of charged particulates is expected to evolve so as to dissipate the self-electric energy at the fastest rate. Consequently, the principle that each particulate is driven to a position wherein the distance from its closest neighbours becomes more uniform, applies also here. Isometric structures such as face-centered cube and its tetragonal equivalent (with \( b = 2^{1/2}a \), where \( b \) and \( a \) are the long and short axes, respectively) may qualify to this end.

The structure shown in Fig. 8 can be repeated in the third dimension by appropriate shifts of layers, set one on top of the other, so that the distance between 12 neighbouring particulates will be fixed. The optimum structure in three dimensions is yet to be determined and its identification needs further research. As there is no constraint on \( a \), the above results apply to particulates down to the size of ions, where thermal motion is expected to be important.

Theoretical results and outputs of the self-expansion model were compared in the following example. Fig. 10 shows calculated velocities vs radial distance within the sphere shown in Fig. 7d, at \( t = 249.96 \) s, of 10 \( \mu \)m drops, using Eq. (17) and the self-expansion model.

The linear plot of Eq. (17) is shown as a straight solid line and outputs of the self-expansion model by 6 different groups of symbols. Each group, comprised of 3 points, stands for a different direction, set inside the sphere at random. Despite the fact that the assembly, shown in Fig. 7d, has not yet reached a state of perfect spherical shape and uniformity of number density, there is good agreement between the predic-
Fig. 9. Self expansion of a finite centered hexagonal array of 55, 10 µm particulates (water drops in air) charged at 250 V: \( t = (a) 0.000025 \) and \( (b) 150 \) s. The initial \( (t = 0) \) array is identical to the one specified in Fig. 8a.

Fig. 10. Calculated velocities of 10 µm drops vs radial distance within the sphere shown in Fig. 7d, at \( t = 249.96 \) s. Solid line—Eq. (17). Each group of 3 symbols, obtained as an output of the self-expansion model, pertains to a different direction set at random inside the sphere.

We are now in position to formulate the following principle regarding the nature of self-expanding assemblies of particulates [15]. An unconstrained, self-expanding system of (charged) particulates, driven by its own energy, and being characterized by \( n \) degrees of freedom of motion, tends to reach steady state, or directional equilibrium, in each of them independently. Thus in finite assemblies of charged particulates, the angular degrees of freedom of a spherical frame of reference, approach their final steady state faster. This state is also defined here as partial or directional equilibrium. Clearly, as the angular degrees of freedom reach their final steady states, the motion turns purely radial. The notion of directional equilibrium conforms with a state where the sum of all forces projected in the given direction vanish.

The model used in this work for the description of self-expansion of an assembly of particulates, does not depend on their shape. This is readily observed by assigning, to shapes other than spherical, a shape factor that permits the use of their spherical equivalent. Thus, even if the drops are slightly distorted, their effective size can adjusted, with no effect on their tendency to self-expand into a circle or a sphere. The same applies to change of size of spherical particulates.

The existence of ordered or structured, self-drifting assemblies of charged particulates is significant with respect to their interactions with other particulates. This is true especially for those which penetrate the space they occupy. Such penetration may be desirable for the purpose of removal of particulates from air streams, e.g., by their capture in moving assemblies of larger charged particulates. The notion that assemblies of equally charged particulates can be kept random, as they expand by self-drifting, is contrary to the patterns simulated in this work. In particular, this applies for large assemblies. Consequently, models that rely on random distribution of charged self-drifting particulates, lack the structural and uniformity effects that become important as the assembly expands toward its asymptotic shape. The stability of shape, structure and uniformity permit the description of the self-expanding assemblies as well-defined units when their interactions with similar units are considered.

The asymptotic spherical shape of self-expanding identical and equally charged assembly of drops is unaffected by grav-
ity. This does not hold if the assembly is nonuniform and, for example, characterized by a size distribution of the drops.

5. Summary and conclusions

Self expansion of unconstrained assemblies of charged particulates is considered. In general, these assemblies, being comprised of discrete members, can neither be described as a continuum nor as massless moving entities. Simulation of these self-expanding assemblies requires solution of the complete equation of motion for each particulate. This gives the general case, where the system is discrete and the velocity is not necessarily collinear with the self-electric field of the expanding assembly. Two-dimensional simulations of self-expansion of random assemblies of uniform and nonuniform charged particulates, show patterns that involve ordered structures with uniform number density, and asymptotic tendency to form a circle. In three dimensions, the evolution into a sphere is faster than that of structures and uniformity of number density. Self expanding assemblies comprising separate groups of particulates, may first deform into general or spherical shapes, and then merge into one unit that continues to self-expand toward the asymptotic spherical shape. Here, the increase in uniformity of number density occurs already in the first phase of the self-expansion, before merger takes place.

A finite straight line of charges self-expands into a circle, or a sphere, once the position of at least one of its members undergoes perturbation (however small), perpendicular to the line. As the assembly self-expands it follows two major and sometimes competing tendencies to form a sphere and to evolve into an ordered and uniform structure. The latter can involve centered square, pentagonal and hexagonal unit cells.

A self-expanding finite, centered hexagonal structure, deforms first so as to better fit an enclosing circle, and then proceeds to regain its original centered hexagonal geometry. As the number density of particulates in the assembly increases, there is a better fit to an enclosing circle. Consequently, in the latter case, the two above mentioned tendencies can be satisfied simultaneously.

The results of this work conform with those of Jones, who predicted them for self-drifting systems of massless ions in a charged gas. Energy and force considerations are used to prove the asymptotic shape and structure of self-expanding charged particulate assemblies. The results of this work are significant for interacting self-expanding charged assemblies. In particular, their structure is important when one assembly is used to capture the other by interpenetration. The use of models of nonuniform random arrays of self-expanding charged particulates, for simulation of processes where smaller particles are captured by arrays of larger particles, may lack physical grounds, if the asymptotic tendency toward uniformity and internal structure is disregarded.

This applies in all cases where the self-expansion time is sufficient for the arrays to approach the asymptotic phase, prior to start of the capturing process. For example, if the array of larger particulates self-expands into the asymptotic phase, before sweeping the array of smaller particulates (as they fall gravitationally), then the model whereby the capturing process can be simulated needs to account for the internal structure acquired by the array of larger particulates, e.g., instead of relying on the initial random distribution of its members in space.

References