Dependence of ion wake characteristics on experimental conditions

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Abstract
Two-dimensional microparticle crystals can be formed in the sheath of a gas discharge plasma. Ions from the bulk plasma are accelerated in the sheath electric field, flowing past the grains to create a positive ion wake downstream from the grains. Interaction between the ion wake and neighboring grains creates additional coupling between oscillation modes and can trigger mode-coupling instability (MCI). In order to better understand MCIs, the interaction between dust grains and ion wakes must be understood; however, the relationship between the discharge parameters and ion wake characteristics is unknown. A molecular dynamics simulation of ion dynamics and dust charging is used to self-consistently determine the dust charge and ion wake characteristics for different synthetic experimental conditions. It is found that the ion wake is strongly dependent on the background gas pressure but not affected much by the discharge power.

Keywords: ion, wake, plasma, microparticles

(Some figures may appear in colour only in the online journal)

1. Introduction
Dusty (complex) plasmas are ionized gas that include micron-sized dust grains. In low pressure environments typical of laboratory experiments, the dust grains generally become negatively charged and can self-organize into crystalline structures [1–5]. Since these dust grains are easily imaged, dusty plasma crystals can be used to study phenomena such as phase transitions at the kinetic level [6–10]. Experiments investigating phase transitions with dusty plasmas are often performed in a capacitively coupled radio frequency (rf) cell. The dust grains levitate above the lower electrode where the electrostatic force acting on the dust grains in the sheath is balanced with the gravitational force. While the confinement in the vertical direction is strong, the weaker horizontal confinement, provided by a ring or cavity on the lower electrode, allows the dust grains to disperse uniformly in a 2D plane forming a hexagonal lattice. Ions from the bulk plasma are accelerated by the sheath electric field and flow past the dust grains creating a region of excess ion density downstream from each grain called the ion wake [11–18].

Ion wakes act as an independent body in the interaction between two dust grains, and can cause the interaction to appear nonreciprocal when the attractive force applied by the wake of one grain on a second grain does not equal the attractive force applied by the wake of the second grain to the first [19]. In a 2D complex plasma monolayer, this asymmetric attraction arising from the positively charged ion wake interacting with a negatively charged neighboring dust particle
can cause the in-plane (horizontal) and out-of-plane (vertical) oscillation modes to couple in an unstable hybrid mode. Thus, the energy transferred to the dust monolayer from the ions flowing past the dust grains can cause microparticles to gain energy and trigger the mode-coupling instability (MCI). When the grains are in a crystalline state, the energy transferred to the dust grains can lead to the breaking of symmetry and cause the structure to melt [19]. When in a fluid state, the dust particle energy (or kinetic temperature) has been observed to continue to increase, suggesting that MCIs continue to act after the crystal has melted unless suppressed by damping [20].

While the additional heating can cause a crystallized monolayer to melt, it also makes it more difficult for particles initially in a fluid state to crystallize. Previous experiments have shown that for microparticle monolayers levitating in the sheath of a rf discharge at a fixed discharge power there are two threshold pressures [21–23]: an upper threshold, \( p_{\text{crys}} \), above which the monolayer always has a crystalline structure, and a lower threshold, \( p_{\text{MCI}} \), below which the monolayer always undergoes MCI causing the monolayer to melt. Between these two pressures, the monolayer can exist in either a crystalline or fluid state depending on the initial state when entering the intermediate pressure regime. If the monolayer is initially in a fluid state, it will remain a fluid as pressure is increased from \( p_{\text{MCI}} \) to \( p_{\text{crys}} \), at which point it will crystallize. Similarly, if the monolayer is initially in a crystalline state, it will remain a crystal until the pressure is decreased to \( p_{\text{MCI}} \), at which point it will become a fluid.

In a simplified model, the ion wakes can be thought of as fixed, positive point charges with charge \( q_w \) at a distance \( l \) downstream of each dust particle. This point charge model for the ion wake adequately represents the system if grains remain far enough apart that the wake charge and location relative to the dust grain are constant [16]. While previous studies have used the point charge model to study MCIs [16, 20–29], the impact of changing discharge parameters, such as rf power and neutral gas pressure, on the ion wake characteristics remains largely unknown. The nonreciprocal interaction between the dust particles due to ion wakes are also related to other types of phenomena in complex plasma such the Schweigert instability in bi-layer complex plasma crystal [30–33] or the vertical pairing of dust particles [34]. However, in these studies, the structure of the ion wake and its dependence on the experimental conditions was also largely unknown. In this work, we model the ion wake downstream from a dust grain levitated in the plasma sheath and analyze the dependence of ion wake characteristics on experimental parameters.

The molecular dynamics simulation dynamic response of ions and dust (DRIAD) [16, 35–37] is used to determine dust charge and ion wake characteristics for a set of parameters simulating the different experimental conditions described in Couédel and Nosenko [23]. Plasma parameters that are unknown or not easily measured (including the sheath electric field, electron temperature, ion and electron number density, and ion flow speed) are determined through the iterative approach described in section 3. This method self-consistently optimizes the balance between the resultant electrostatic and gravitational forces on a dust grain for each set of parameters, allowing the wake characteristics to be evaluated as a function of system power and pressure. Discharge parameters for stable levitating dust grains have been experimentally determined many times in the past, yet the relationship between these parameters and the characteristics of the resulting ion wake is unknown. The ion wake dependence on different experimentally relevant conditions is therefore the focus of the present article.

This paper is organized as follows. Section 2 describes the experiment from which the input parameters were chosen. Section 3 describes the numerical model, DRIAD, and the process by which the additional plasma parameters are obtained. The results of the simulated discharge conditions are presented in section 4 along with the calculated wake characteristics such as the total wake charge and the distance between the dust grain and the ion wake’s center of charge. Section 5 is a discussion of the results and conclusions.

2. Experimental background

The experiments described in [23] were performed in a capacitively coupled rf cell. Particles are confined in the horizontal direction by a shallow circular depression in the lower electrode. The grounded ring electrode above the powered electrode allows the direct visualization of the 2D monolayer from the top windows of the vacuum vessel. An illustration depicting relevant components from the experimental setup is provided in figure 1 for reference. The experiments were performed using argon gas with pressure between 0.5 and 2 Pa and forward rf power between 5 and 25 W. Spherical melamine-formaldehyde microparticles with a diameter of 9.19 ± 0.09 μm were used to form a dust monolayer suspended in the plasma sheath. The experimental setup used in ref has been extensively described in other articles.

Threshold values of \( p_{\text{MCI}} \) and \( p_{\text{crys}} \) were experimentally determined for various rf powers (experimental procedures can be found in [23]), and discharge conditions for a stable two-dimensional crystal between these threshold pressures were reported for a range of power settings in [23]. For convenience, the experimental rf power, neutral gas pressure, and effective dust charge are reproduced in the first three columns of table 1. The stability of a crystalline monolayer was experimentally shown to increase with rf power and argon pressure. Additionally, the numerical models of the MCI mode coupling presented in [23] found the MCI pressure threshold to be strongly dependent on the amount of charge contained in the ion wake, a parameter that is experimentally unknown. Therefore, the goal of this study is to characterize the evolution of ion wake parameters as a function of rf power and neutral gas pressure.

Table 1 provides the neutral gas pressure, power, and measured effective grain charge (taken to be the excess charge on
the dust grain relative to the ion wake) for the 24 experimental conditions from the first and second sets of experiments. The experimental measurement of the dust particle charge was derived from the longitudinal and transverse sound speeds and the interparticle distance, assuming in first approximation, screened Coulomb interactions (with further details provided in [23]). The errors in the experimentally measured charge are included in table 1.

3. DRIAD and use of experimental data for model inputs

The molecular dynamics simulation DRIAD is capable of modeling the dynamics of the ions and dust and self-consistently calculating the dust charge [16, 36, 37]. To a good approximation, the electrons can be treated as having a Boltzmann distribution if the dust surface potential is negative enough to reflect most electrons [38]. This is taken into account in the DRIAD model by assuming that the electrons are depleted in the vicinity of the dust grain, such that the ions interact with the dust grain through a Coulomb potential. Far from the dust grain, the ions interact through a shielded Yukawa potential [17].

The charge on a dust grain is determined from the electron and ion currents to the dust grain surface. Since electrons are not directly simulated by DRIAD, the electron current

\[ \vec{F}_{\text{E}}(z) \] is the force from the sheath field, \( \vec{F}_{\text{in}} \) represents the ion-neutral collisions, and \( \vec{F}_{\text{bound}}(r,z) \) represents the force from ions outside the simulation boundary. The ion time step was set to \( \Delta t_i = 10^{-10} \) s to resolve the ion-neutral collisions, calculated using the null collision method [39]. In order to improve computational efficiency, DRIAD models a number of ions as a single superion with the same charge-to-mass ratio (and, therefore, obeying the same equation motion) as one ion. The exact number of ions per superion is determined by user input when a simulation is initialized, based upon the ion density and simulation size. The present results were obtained using approximately 74 000 superions, where each superion represents 20–40 individual ions.

In this work, the wake region of a single, fixed dust grain was studied. To fully resolve the elongated wake structure, the dust grain was placed at the center of a \( 10 \lambda_{De} \times 1 \lambda_{De} \) (height \( \times \) radius) cylindrical simulation region, where \( \lambda_{De} = \sqrt{\varepsilon_0 k_B T_e / (n_e e^2)} \) is the electron Debye length calculated for the electron density in the sheath. The potential of ions outside the simulation region is calculated numerically by finding the Yukawa potential of a homogeneous distribution of ions with density \( n_0 \) within the simulation region and subtracting it from a constant uniform background potential. The electric field due to the outside ions (which provides \( \vec{F}_{\text{bound}}(r,z) \) for ions inside the simulation) is then calculated by taking the negative gradient of this potential. Ions that leave the simulation boundary or are collected by the dust grain are inserted on the simulation boundary with a velocity consistent with the ion flow conditions [16].

The charge on a dust grain is determined from the electron and ion currents to the dust grain surface. Since electrons are not directly simulated by DRIAD, the electron current

\[ m_i \ddot{r} = \vec{F}_g + \vec{F}_{\text{ID}} + \vec{F}_{\text{E}}(z) + \vec{F}_{\text{bound}}(r,z) + \vec{F}_{\text{in}} \]  (1)

where \( \vec{F}_g \) is the Yukawa force between ions (with the electrons providing the shielding), \( \vec{F}_{\text{ID}} \) is the force from the Coulombic interaction between the dust grain and the ion,
is calculated from orbital-motion limited (OML) theory [40], with the current to a spherical grain given by

\[ I_e = 4\pi r_d^2 n_e \left( \frac{k_B T_e}{2\pi m_e} \right)^{\frac{1}{2}} \exp \left( \frac{e\Phi_d}{k_B T_e} \right). \]  (2)

where \( r_d \) is the radius of the dust grain, \( n_e \) is the electron density, and \( \Phi_d \) is the dust surface potential. The ion current to the dust grain is calculated self-consistently in DRIAD by counting the number of ions \( N_i \) with charge \( q_i \) that cross the dust collection radius \( b_c \),

\[ b_c = r_d \left( 1 - \frac{2q_i \Phi_d}{n_i v_s^2} \right)^{\frac{1}{2}} \]  (3)

where \( v_s \) is the characteristic velocity of ions

\[ v_s = \left( \frac{8k_B T_e}{\pi m_i} + v_i^2 \right)^{\frac{1}{2}} \]  (4)

and \( v_i \) is the drift speed of an ion. The charge collected per time step is then \( \Delta Q_d = N_i q_i + I_e \Delta t \).

The considered experimental conditions are such that the ratio of the plasma screening length to the ion mean free path \( \lambda_p/\ell_i \approx 0.1 \), which is in the range of collisionality for which ion collisions are important in determining the dust charge [41]. The dust charge found in the simulation is different from that predicted by OML theory in that (1) the charge is affected by the ion flow, (2) the ion current to the dust grain is enhanced as a result of ion-neutral collisions, and (3) the ion distribution is not homogeneous. However, the results for the charge of a single dust grain are found to be consistent with predictions based on OML theory which have been corrected to account for flowing ions and the presence of ion-neutral collisions [16].

Input parameters for the DRIAD simulation were based upon experimental conditions reported in [23] and shown in table 1. These include the rf power, neutral gas pressure, and effective dust grain charge \( Q_{\text{eff}} \), which was derived by consideration of particle conservation at low to intermediate pressures. Here \( K_u(T_e) = 2.34 \times 10^{-14}T_e^{0.59} \exp(-17.44/T_e) \) is the ionization rate fit determined in the range \( 1 \leq T_e \leq 7 \) eV for the \( e + \text{Ar} \rightarrow \text{Ar}^+ + 2e \) reaction reported in [42], \( u_B(T_e) \) is the Bohm velocity, \( n_g = PV/k_B T_g \) is the neutral gas density, and \( d_{\text{eff}} = 0.5R/\rho_{\text{eff}} + \ell/\rho_{\text{eff}} \) is the effective plasma size, with \( h_\ell \approx 0.86(3 + \ell/(2\lambda_\ell))^{-1/2}, h_g \approx 0.80(4 + R/(\lambda_\ell))^{-1/2}, \) and \( R, \ell \), and \( \lambda_\ell \) representing the plasma radius, length, and ion-neutral mean free path, respectively.

The electric field in the sheath was determined using an iterative process which is illustrated in figure 2. The initial estimate of the axial electric field strength, \( E \), was calculated based on the force balance equation \( Q_dE = mg \) using the reported dust charge for each set of experimental conditions. Once the interpolated electron density, calculated electron temperature, and maximum axial electric field strength were determined, these values were used to calculate the electron and ion Debye lengths. These values, combined with the reported experimental conditions, comprised the first set of input parameters for the DRIAD simulations (indicated by gray boxes on the far left of figure 2).

For each of the 24 cases, DRIAD was used to determine the dust charge and wake characteristics (indicated by the yellow box in figure 2). The results from DRIAD were evaluated

![Figure 2. Flowchart of the iterative procedure used to determine input parameters used in DRIAD simulations.](image-url)
Table 1. Data associated with experiment. Experimental settings for discharge power and pressure, calculated parameters for the sheath electric field, electron temperature, ion density, electron Debye length, and ion Debye length, and simulation results for ion flow speed, dust charge, and the ion wake characteristics as described in the text.

| Experimental conditions | Simulation inputs | Simulation results |
|-------------------------|-------------------|-------------------|
| Power (W) | Pressure (Pa) | $Q_{d,\text{i}}$ (10$^4$ e$^-$) | $E$ (V/m) | $T_e$ (eV) | $n_{i0}$ ($10^3$ m$^{-3}$) | $\lambda_{De,\text{e}}$ ($\mu$m) | $\lambda_i$ ($\mu$m) | Mach | $Q_d$ (10$^4$ e$^-$) | $L$ ($\lambda_i$) | $q_{\text{eff}}$ (e) |
|-------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| 25 | 1.58 | 1.05 ± 0.29 | 2185 | 2.15 | 8.00 | 385 | 45.5 | 1.80 | 1.79 | 1.06 | 3548 |
| 1.17 | 1.01 ± 0.24 | 2100 | 2.26 | 5.91 | 460 | 53.0 | 1.65 | 1.95 | 1.40 | 3231 |
| 0.75 | 1.46 ± 0.30 | 1850 | 2.44 | 3.80 | 596 | 66.1 | 2.00 | 2.16 | 1.41 | 1258 |
| 22 | 1.63 | 1.11 ± 0.30 | 2200 | 2.13 | 7.86 | 387 | 45.9 | 1.90 | 1.80 | 1.08 | 3708 |
| 1.17 | 1.43 ± 0.51 | 2000 | 2.26 | 5.61 | 472 | 54.4 | 1.65 | 1.92 | 1.23 | 3241 |
| 0.83 | 1.41 ± 0.60 | 1900 | 2.40 | 4.01 | 575 | 64.3 | 1.75 | 2.07 | 1.33 | 1660 |
| 19 | 1.70 | 1.00 ± 0.21 | 2350 | 2.12 | 7.72 | 390 | 46.3 | 1.60 | 1.76 | 1.20 | 3583 |
| 1.17 | 1.17 ± 0.23 | 2030 | 2.26 | 5.29 | 486 | 56.0 | 1.75 | 1.95 | 1.20 | 3031 |
| 1.00 | 1.25 ± 0.17 | 2035 | 2.32 | 4.53 | 532 | 60.5 | 1.70 | 2.06 | 1.54 | 2769 |
| 0.83 | 1.21 ± 0.28 | 1920 | 2.40 | 3.77 | 593 | 66.3 | 1.80 | 2.10 | 1.57 | 1585 |
| 16 | 1.80 | 0.98 ± 0.10 | 2390 | 2.10 | 7.61 | 391 | 46.7 | 1.62 | 1.74 | 1.22 | 3801 |
| 1.25 | 1.07 ± 0.17 | 2230 | 2.23 | 5.28 | 484 | 56.0 | 1.65 | 1.88 | 1.31 | 2950 |
| 1.00 | 1.34 ± 0.21 | 1900 | 2.32 | 4.23 | 551 | 62.6 | 1.80 | 2.00 | 1.24 | 2110 |
| 16 | 1.47 | 1.09 ± 0.11 | 2250 | 2.17 | 6.21 | 440 | 51.7 | 1.55 | 1.82 | 1.49 | 3847 |
| 1.17 | 1.21 ± 0.21 | 2030 | 2.26 | 4.93 | 503 | 58.0 | 1.95 | 1.93 | 1.13 | 2185 |
| 0.75 | 1.31 ± 0.32 | 1790 | 2.44 | 3.17 | 653 | 72.3 | 2.05 | 2.14 | 1.22 | 1046 |
| 13 | 1.50 | 1.04 ± 0.19 | 2250 | 2.17 | 5.84 | 453 | 53.3 | 1.70 | 1.84 | 1.30 | 3068 |
| 1.17 | 1.04 ± 0.12 | 2100 | 2.26 | 4.54 | 525 | 60.4 | 1.80 | 1.98 | 1.37 | 2397 |
| 0.75 | 1.42 ± 0.37 | 1800 | 2.44 | 2.92 | 680 | 75.4 | 1.55 | 1.82 | 1.93 | 1000 |
| 10 | 1.73 | 1.06 ± 0.19 | 2260 | 2.11 | 6.11 | 437 | 52.1 | 1.65 | 1.74 | 1.17 | 3369 |
| 1.17 | 1.15 ± 0.17 | 2140 | 2.26 | 4.12 | 551 | 63.4 | 1.75 | 1.96 | 1.51 | 2101 |
| 0.97 | 1.31 ± 0.37 | 1825 | 2.33 | 3.42 | 614 | 69.6 | 1.95 | 2.02 | 1.35 | 1749 |
| 7 | 1.83 | 1.14 ± 0.20 | 2250 | 2.09 | 5.76 | 448 | 53.7 | 1.80 | 1.74 | 1.16 | 3210 |
| 1.25 | 1.16 ± 0.12 | 2240 | 2.24 | 3.93 | 561 | 65.0 | 1.65 | 1.88 | 1.39 | 2475 |

to determine if the electrostatic force would be sufficient for the dust grain to levitate in the sheath (using the condition $Q_dE/mg \approx 1$) based on the input electric field strength and the dust grain charge resulting from the simulation (indicated by the blue box in figure 2). If the ratio $Q_dE/mg$ varied by more than 10% from 1, the electric field was adjusted and the simulations were repeated (indicated by the orange box in figure 2). As a further check, the effective dust charge, which is the sum of the dust grain charge and the charge in the ion wake, was required to be consistent with experimental measurements within ±10%. The iterative process consisting of running the simulations, checking the results, and adjusting the input parameters was repeated until the electrostatic force necessary to levitate the dust grains was met ($Q_dE/mg \approx 1 \pm 0.1$), at which point the iterative process was terminated (indicated by the final green arrow at the right of figure 2).

4. Results

Simulations were run for each of the conditions listed in table 1 and a dust grain of size $a = 4.6 \mu$m. The simulation time corresponded to a physical time of 8 $\mu$s, which covers 4–8 ion plasma periods, $\tau_i = 2\pi/\sqrt{e^2n_0/(\varepsilon_0 m_i)}$, depending on the plasma conditions simulated. The system was allowed to reach equilibrium during the first half of the simulation run, corresponding to two to four ion plasma periods. Results for the dust charge, ion density, and time-averaged electric potential from ions inside the simulation were then averaged over the final half of the simulation run time. The time-averaged wake structure and potential in the $xz$-plane were obtained by mapping the ion density and electric potential contributions to a grid with 64($x$) by 320($z$) grid points and $\lambda_{De}/32$ mesh size (where $\lambda_{De}$ varies for each case, as shown in table 1). At the end of the simulation, the contribution of the Yukawa potential from the ions outside the simulation region and the Coulomb potential of the dust grain was added to the time-averaged potential from ions inside the simulation region to obtain the total electric potential.

The resulting charge on the dust grain for each set of conditions is given in table 1. Theoretically, the surface potential of a grain with radius $a$ in a flowing plasma is given by the numerical solution of the OML electron current and the current of flowing ions [16, 43, 44]

$$I_e = 4\pi a^2 n_e e \left( \frac{kT_e}{2\pi m_e} \right)^{1/2} \exp \left(-\frac{e\Phi_d}{k_B T_e}\right)$$  \hspace{1cm} (6)

$$I_i = \pi a^2 n_i q_i v_{de} \left[ \left( 1 + \frac{1}{2\xi^2} - \frac{q_i\Phi_d}{k_B T_i \xi} \right) \text{erf} (\xi) + \frac{1}{\sqrt{\pi}} \exp \left(-\xi^2\right) \right]$$  \hspace{1cm} (7)

where $\xi = v_{de}/\sqrt{2k_B T_i/m_i}$, $n_{i,e}$, $m_{i,e}$, and $T_{e,i}$, are the electron and ion density, mass, and temperature, respectively, and $\Phi_d$...
Figure 3. Ion density in the vicinity of the dust grain. The power decreases from left to right whereas the pressure decreases from top to bottom. The grayscale image shows the wake region \((n_i - n_0)/n_0 > 0\). The contour lines indicate the potential from \(-0.1\) to \(0.15\) V in steps of \(0.05\) V, where dashed lines are contours of positive potential and solid lines indicate negative potential contours. The black diamond is the location of the center of charge, and the white dot is the location of the center of the dust grain, size not to scale. For clarity, the additional case at power 19 W and pressure 1.00 Pa is not depicted in this figure.

is the dust surface potential. The predicted dust charge is then

\[ Q_d = 4\pi \varepsilon_0 a \Phi_d. \] (8)

The dust charge predicted using equations (6)–(8) for a dust grain with radius \(a = 4.6\) \(\mu\)m is about 1.5 times larger than the dust charge obtained in the simulation, which is consistent with the reduction in charge expected from the enhanced ion flux due to ion-neutral collisions [45].

The ion densities in the wakes for the 24 experimental conditions are shown in figure 3. The rf power decreases moving from left to right, and pressure decreases from top to bottom in the figure. The location of the dust grain is indicated by a white circle with the center of charge in the ion wake indicated by a black diamond. At the very low discharge pressures used in the present study, the ion wake is greatly attenuated and stretched in the direction of the ion flow. In this work, we define the ion wake to be the region where \(n_i - n_0 > 0\). As shown in figure 3, the ion density in the wake region tends to decrease as both the power and pressure decrease. The solid and dashed black contour lines imposed on figure 3 are the equipotential lines in the region around the dust grain ranging from \(-0.1\) to \(0.15\) V in \(0.5\) V increments, with solid lines representing negative values and dashed lines indicating positive potential.

The number of ions within the ion wake is calculated by finding the number of ions in the region \(dx dz\) associated with each grid point and using azimuthal symmetry to calculate the total number of ions in a half ring at radial distance \(x\) from the \(z\)-axis.

\[ N_i = \pi \left( x + \frac{dx}{2} \right) (n_i - n_0) dx dz \] (9)
Figure 4. Wake characteristics as a function of power. (a) The ratio between wake charge and dust charge, \( q_w/Q_d \), (b) the distance between the center of charge and the dust grain \( l \), and (c) the electron Debye length, \( \lambda_{De} \). Different colors correspond to different pressure ranges. The blue diamonds are for pressures less than 1 Pa, the purple squares are for pressures between 1 and 1.4 Pa, and the orange circles are for pressures higher than 1.4 Pa. The shading of each color corresponds to different power values, with darker shades indicating higher powers.

where \( x \) is the horizontal distance from the dust grain to the grid location, and \( dx \) and \( dz \) are the grid spacings in the \( x \)- and \( z \)-directions.

The wake charge is commonly modeled by treating the ion wake as a positive point charge \( q_w \), located a distance \( l \) downstream of a dust grain, with the point charge assumed to be located at the center of charge of the wake region. The values describing the wake characteristics are determined by calculating the dipole moment of the wake relative to the position of the dust grain

\[
p = \sum q_i N_r (\bar{r}_r - \bar{r}_{dust})
\]

where \( q_i \) is the charge of a single ion, \( r_r \) is the location of the grid cell, and \( r_{dust} \) is the location of the dust grain. The location of the center of charge downstream of the grain is given by

\[
l = \frac{\sum r_r N_r}{\sum N_r}.
\]

The magnitude of the dipole moment is then divided by the magnitude of the distance between the dust grain and center of charge, which gives the charge in the wake. \( q_w = p/l \). Although the \( x \)-components of both the dipole moment and center of charge are computed, these values are negligible due to the azimuthal symmetry of the single dust grain case, with typical values on the order of \( p_x \sim 10^{-3} \) e\( \lambda_{De} \) and \( l_x \sim 10^{-3} \lambda_{De} \).

Characteristic parameters of the wakes are plotted as a function of power and pressure in figures 4 and 5. The electron Debye length \( \lambda_{De} \) for each set of conditions is also shown. The ratio \( q_w/Q_d \) and the distance to the center of charge \( l \) are relatively independent of the power (figures 4(a) and (b)). Note that due to the time-varying ion density and dust charge, the standard deviation of the values of \( l \) and \( q_w/Q_d \) is about 10%.

However, as seen in figure 5, \( q_w/Q_d \) increases with the pressure while \( l \) slightly decreases indicating that at higher pressures more ions are concentrated in the wake.

As shown in figure 3 the potential contours at distinct \( z \)-levels directly downstream of the grain exhibit local maxima. As a general trend, the contours of positive potential move upstream towards the dust grain as the power increases. In contrast to other numerical simulations of ion wakes, the equipotential lines downstream of the dust grain do not define distinct positive potential regions relative to the background potential [16, 17, 46, 47]. The primary difference in this set of simulations is the much smaller dust size, \( a \approx 5 \) \( \mu \)m, leading to weaker ion focusing. Given that the wakes in this pressure and power regime, for these small grain sizes, are very extended in the direction of the ion drift, the point charge model of the wake does not accurately capture the electrostatic potential of the system, as illustrated in figure 6.
Figure 5. Wake characteristics as a function of pressure. (a) The ratio between wake charge and dust charge, $q_w/Q_d$, (b) the distance between the center of charge and the dust grain $l$, and (c) the electron Debye length, $\lambda_{De}$. Different colors and symbols correspond to different pressure ranges. The blue diamonds are for pressures less than 1 Pa, the purple squares are for pressures between 1 and 1.4 Pa, and the orange circles are for pressures higher than 1.4 Pa. The shading of each color corresponds to different power levels, with darker shades indicating higher powers.

Figure 6. Contour plots of the electric potential around the dust grain. (a) The electric potential calculated by estimating the ion wake as a point charge. (b) The electric potential as outputted from the numerical simulation DRIAD. The contour lines indicate the potential from $-0.1$ to $0.15$ V in steps of $0.05$ V, where dashed lines are contours of positive potential and solid lines indicate negative potential contours. The black diamond is the location of the center of charge, and the white dot is the location of the center of the dust grains. These plots are generated for the 25 W power and 1.58 Pa pressure case.
5. Discussion and conclusions

Utilizing a molecular dynamics simulation of ions flowing past a stationary dust grain, the equilibrium dust charge and ion wake characteristics are determined for varying experimental conditions. An iterative method (outlined in figure 2) was used to self-consistently determine the sheath electric field that was able to balance the gravitational force while also providing the appropriate ion flow velocity to achieve the expected effective dust charge reported by the experiments [23]. The effective dust charge determined by DRIAID simulations, which is the sum of the charge in the ion wake and the dust grain charge, was required to be consistent with experimental measurements within ±10%.

The dust grains were experimentally observed to levitate near the sheath edge at a height of ~10 mm above the lower electrode. Particle-in-cell (PIC) simulations modeling the (dust-free) experimental conditions representative of those in [23]. Provide electric field values in the sheath region which are used for comparison with the present results (figure 7). The PIC results for 5–20 W rf power at 1–2 Pa show that increasing rf power at the same pressure (or decreasing pressure at the same rf power) increases the magnitude of the electric field at a given height above the lower electrode. The range of values for the electric field necessary to self-consistently charge and levitate a dust grain determined by this study using an iterative method are indicated by the horizontal shaded bar in figure 7. These correspond to the electric field determined from PIC simulations at a distance 10–14 mm above the lower electrode, which is consistent with experimentally observed dust levitation heights near the sheath edge [48].

The simulation results include the dust charge, ion density, and electrostatic potential in the region surrounding the grain for 24 combinations of rf power and neutral gas pressure. These results were utilized to calculate ion wake characteristics such as the equivalent wake charge for a point charge model, \( q_w \), and distance between the dust grain and the center of charge, \( l \). As shown in figure 5, the charge contained in the wake \( q_w/Q_d \), is proportional to the neutral gas pressure, ranging from 5% of the dust charge at pressures less than 1 Pa to 20% of the dust charge at pressures of 1.8 Pa. The charge contained in the wake is largely independent of rf power as shown in figure 4. The normalized distance between the dust grain and the location of the point wake charge varies little with power and pressure, and for all the conditions presented here is in the range of 1 < \( l/\lambda_{De} < 1.6 \).

Transitions between states, as caused by MCIs, can be studied utilizing N-body simulations of a cloud of dust grains, with wake charges \( q_w \) located a distance \( l \) downstream from each dust grain. It is known that the point-wake model is not self-consistent and is only a crude approximation. However, the point charge ion wake model has been employed in many studies to model nonreciprocal particle interactions [19, 24, 49–61]. The present results indicate that the point-wake model is inadequate for modeling the dynamic conditions with this power and pressure regime.

Simulations where both parameters are allowed to evolve as rf power and neutral gas pressure change can be used to further understand these non-reciprocal interactions and their effects on the system dynamics. While the wake characteristics as presented above will allow for better modeling of MCIs, the point charge model may not be suitable for describing ion wakes. In addition, the wake structure will evolve in the proximity of a second grain. A model that treats ion wakes as extended clouds of positive charge with location and magnitude depending on power, pressure, and the positive relative to close grains would more closely capture wake characteristics and allow utility across a larger range of discharge parameters. This is a subject ripe for development using machine-learning techniques to characterize the wakes.

Data availability statement

The data that support the findings of this study are available upon request from the authors.

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