Numerical Simulation of Single Microparticle Trajectory in an Electrodynamic Balance*

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Abstract By introducing Oseen's formula to describe the viscous drag force, a more complete motion equation for a charged microparticle levitated in an electrodynamic balance (EDB) has been put forward and solved numerically by the classic Runge-Kutta method in this paper. The theoretical results have firstly demonstrated the existence of the particle oscillations and their characteristics, especially of the springpoint oscillation at large amplitude. And through the comparisons of theoretical and experimental trajectories, the adopted motion equation has proved to be able to rigorously describe the particle motion in non-Stokes region—the shape of trajectory and frequency characteristics are fairly consistent and the deviations of amplitude can usually be less than 10%.

Keywords electrodynamic balance, microparticle oscillation, trajectory, numerical simulation

1 INTRODUCTION

Based on the principle of Millilkan Condenser, Davis $et\ al.^{[1-3]}$ have developed the technology of electrodynamic balance (EDB) by the superposition of DC and AC electric field within a specially configured chamber. Of which the adjustable DC field in the vertical direction levitates a charged microparticle mainly against the gravity and the AC field stabilizes it dynamically. Under their combined effects, the particle can be levitated in a gas flow, thus by some modern measuring techniques, such as light scattering and linescan etc., the studies on the surface transfer phenomena of a particle can be carried out conveniently. So the EDB technology has been extensively applied in aerosol research and has become an ideal technology for manipulating aerosol particles for in-situ analysis.

In the previous EDB studies^[4-7], the investigated microparticle was usually levitated at rest and the viscous drag force exerted on particle was mostly limited in the Stokes regime. Breaking through the limitation, Zhu et al.^[8] have recently extended the EDB study to the enhanced mass transfer from an oscillating microsphere. To facilitate this research and other EDB studies further, the precise description of the particle motion is very necessary.

The purposes of this paper are: (1) to analyze and determine the viscous drag force in non-Stokes regime, (2) to propose a more complete and reasonable motion equation for a trapped particle in EDB, (3) to obtain the particle trajectory by solving the motion equation numerically, and (4) to verify the rationality and ve-

racity of the equation through the comparison with the experimental observation.

2 EXPERIMENTAL OBSERVATION

In this experimental study, Zhu et al.^[8,9] use an octopole EDB to realize the stable or springpoint oscillation of particle only in the vertical direction by changing the AC field parameter. The technology of high-speed linscan has been applied to trace, observe the particle motion. The overhead view of the EDB and peripheral equipments is shown in Fig. 1. And the experimental observation of particle oscillation trajectories is shown in Fig. 2.

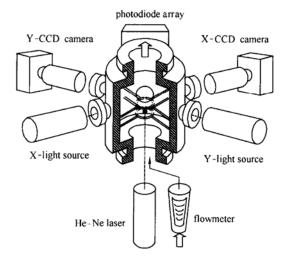


Figure 1 Octopole EDB electrode structure and its peripheral instruments

(ring half spacing $Z_0 = 1.98 \,\mathrm{mm}$, ring radius $r_0 = 5.56 \,\mathrm{mm}$)

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Demonstrated by Fig. 2, for the stable oscillation, its amplitude is usually small (herein just 2.70 times of $d_{\rm p}$) and its frequency can be kept identical with the driving AC frequency $f_{\rm AC}$, but for the springpoint oscillation, the amplitude becomes much larger (herein 10—11 times of $d_{\rm p}$) while the frequency is just half of $f_{\rm AC}$. And for a stable-oscillating particle, the springpoint oscillation can be achieved by increasing $V_{\rm AC}$ or decreasing $f_{\rm AC}$ appropriately in this experiment.

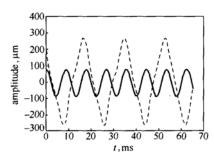


Figure 2 Particle oscillation experimental observation for a dodecanol microdroplet with $\rho_{\rm p} = 830.9\,{\rm kg\cdot m^{-3}}$

--- springpoint Osci.: $d_{\rm p}=24.48\,\mu{\rm m},\,f_{\rm AC}=110.64\,{\rm Hz},\,$ $V_{\rm DC}=0.3615\,{\rm V},\,V_{\rm AC}=1519.50\,{\rm V}$

3 PARTICLE MOTION TRAJECTORY MODEL

The specific mode of particle motion mainly depends on the concrete motion equation, which can directly be determined by the 3D forces exerted on the charged particle. In the previous studies^[10-12], the trajectory of the levitated particle in an EDB is usually governed by the following motion equation

$$m\frac{\mathrm{d}^{2}z}{\mathrm{d}t^{2}} = -mg + |q|C_{0}\frac{V_{\mathrm{DC}}}{Z_{0}} + 2|q|C_{1}\frac{V_{\mathrm{AC}}\cos(\omega t)}{Z_{0}^{2}}z + \frac{\pi}{6}\rho_{\mathrm{g}}gd_{\mathrm{p}}^{3} + F_{\mathrm{d}} + F_{\mathrm{p}}$$
(1)

where $F_{\rm d}$ is the viscous drag force and $F_{\rm p}$ is any other forces (such as thermophoretic, photophoretic forces or radiation pressure) exerted on the particle.

For a spherical particle with diameter $d_{\rm p}$ moving in a slow gas flow at a low Reynolds number ($10^{-4} < Re < 0.1$), the viscous drag force complies with the Stokes law

$$F_{\rm d} = -3\pi\mu d_{\rm p} \frac{{\rm d}z}{{\rm d}t} \tag{2}$$

While for an increased Re range, the drag force can usually be expressed better by Oseen's formula

$$F_{\rm d} = -3\pi\mu d_{\rm p} \frac{\mathrm{d}z}{\mathrm{d}t} \left(1 + \frac{3Re}{16} \right) \tag{3}$$

where

$$Re = \frac{d_{\rm p}|{\rm d}z/{\rm d}t|\rho_{\rm g}}{\mu} \tag{4}$$

Note that Eq. (3) is valid for $Re \leq 5$, which is much larger than the applied Re range for the Stokes's law, and has been applied in some EDB studies^[13,14].

By applying Oseen's formula to solve the viscous drag force, the particle trajectory equation become into

$$\begin{split} m\frac{\mathrm{d}^{2}z}{\mathrm{d}t^{2}} &= -mg + |q|C_{0}\frac{V_{\mathrm{DC}}}{Z_{0}} + 2|q|C_{1}\frac{V_{\mathrm{AC}}\cos(\omega t)}{Z_{0}^{2}}z - \\ 3\pi\mu d_{\mathrm{p}}\frac{\mathrm{d}z}{\mathrm{d}t} - \frac{9\pi}{16}d_{\mathrm{p}}^{2}\rho_{\mathrm{g}}\left|\frac{\mathrm{d}z}{\mathrm{d}t}\right|\frac{\mathrm{d}z}{\mathrm{d}t} + \frac{\pi}{6}\rho_{\mathrm{g}}gd_{\mathrm{p}}^{3} + F_{\mathrm{p},z} \end{split}$$
(5)

In absence of other external forces, Eq. (5) can be rearranged and reduced to

$$\frac{\mathrm{d}^2 z}{\mathrm{d}t^2} = A \left| \frac{\mathrm{d}z}{\mathrm{d}t} \right| \frac{\mathrm{d}z}{\mathrm{d}t} + B \frac{\mathrm{d}z}{\mathrm{d}t} + C \cos(\omega t) z + D \tag{6}$$

where

$$A = -\frac{9\pi}{16m}d_{\rm p}^2\rho_{\rm g} \tag{7}$$

$$B = -3\pi\mu d_{\rm p}/m \tag{8}$$

$$C = \frac{2|q|C_1 V_{AC}}{Z_0^2 m}$$
 (9)

$$D = \left(\frac{\pi}{6} d_{\rm p}^3 g(\rho_{\rm g} - \rho_{\rm p}) + |q| C_0 \frac{V_{\rm DC}}{Z_0}\right) / m \qquad (10)$$

4 SIMULATION RESULTS AND DISCUSSION

4.1 Numerical simulation to particle trajectory

Equation (6) is a second order, nonlinear, coefficient varying and inhomogeneous ordinary differential equation (ODE) and the analytical solution does not exist as usual. The classic Runge-Kutta method is introduced to simulate and analyze the particle trajectory here.

The results of numerical simulation for stable and springpoint oscillation of particle, respectively, are directly depicted into trajectory curves, and for comparison the experimental data under the same conditions are also shown in Figs. 3 and 4. In particular, by relating the theoretical amplitude to experimental results, the error analysis has been developed to further investigate the suitability of the trajectory model to springpoint oscillation (shown in Fig. 5).

The comparison results show the numerical calculation trajectories and experimental observation can be in excellent agreement for both stable oscillation and springpoint oscillation. The shape of trajectory and frequency characteristics for theoretical and experimental results are fairly consistent. And the error analysis illustrates the deviations for theoretical and experimental amplitude can usually be kept less than

10%. Thus the veracity and validity of the adopted motion equation has adequately been verified. It is more important that the numerical results have theoretically proved the existence of particle oscillation, especially of the springpoint oscillation.

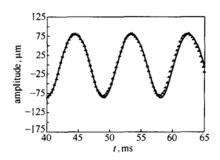


Figure 3 Comparison between numerical calculation trajectory and experimental observation for a dodecanol microdroplet in stable oscillation

$$\begin{split} (\rho_{\rm p} = 830.9\,{\rm kg\cdot m^{-3}}, \, q &= 1.60\times 10^{-14}{\rm C}, \, d_{\rm p} = 32.70\,\mu{\rm m}, \\ f_{\rm AC} &= 111.07\,{\rm Hz}, \, V_{\rm DC} = 0.8366\,{\rm V}, \\ V_{\rm AC} &= 2507.31\,{\rm V}, \, C_0 = 0.358, \, C_1 = 0.1977) \\ &\triangleq {\rm exp. \ curve;} \qquad {\rm cal. \ curve;} \\ {\rm cal. \ initial \ conditions:} \, \, ({\rm d}z/{\rm d}t)_0 = 0, \, z_0 = -177.53\,\mu{\rm m} \end{split}$$

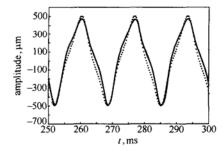


Figure 4 Comparison between numerical calculation trajectory and experimental observation for a dodecanol microdroplet in springpoint oscillation $(\rho_{\rm p}=830.9\,{\rm kg\cdot m^{-3}},\,q=2.12\times10^{-14}{\rm C},\,d_{\rm p}=28.27\,\mu{\rm m},\\f_{\rm AC}=120.87\,{\rm Hz},$

 $V_{\rm DC} = 0.54902\,{\rm V},\ V_{\rm AC} = 2162.67\,{\rm V},\ C_0 = 0.358,\ C_1 = 0.1977)$ \blacktriangledown exp. trajectory; —— cal. trajectory; cal. initial conditions: $({\rm d}z/{\rm d}t)_0 = 0,\ z_0 = -128.59\,\mu{\rm m}$

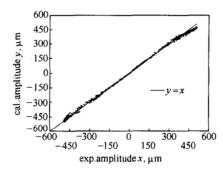


Figure 5 Amplitude comparison between theoretical and experimental results for springpoint oscillation

4.2 Effect of viscous drag force on the simulation to particle trajectory

For the stable oscillation, the particle motion still belongs to the Stokes regime (herein Re = 0.063), so

both Stokes's law and Oseen's formula can describe the viscous drag force correctly at that time. But it is different for the case of springpoint oscillation. By the above- mentioned simulation method, the effects of viscous drag force, determined by Stokes's law and Oseen's formula respectively, on the springpoint oscillation, have been investigated numerically and the comparison results are showed in Fig. 6.

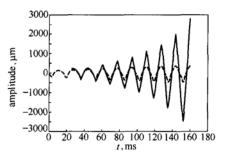


Figure 6 Effects of viscous force on numerical trajectory for a dodecanol microdroplet in springpoint oscillation

$$\begin{split} (\rho_{\rm P} = 830.9\,{\rm kg\cdot m^{-3}},\, q = 2.12\times 10^{-14}{\rm C},\, d_{\rm P} = 28.27\,{\rm mm},\\ f_{\rm AC} = 120.87\,{\rm Hz},\, V_{\rm DC} = 0.54902\,{\rm V},\, V_{\rm AC} = 2162.67\,{\rm V},\\ C_0 = 0.358,\, C_1 = 0.1977)\\ ----- & {\rm Stoke's\ law;\, ---- Oseen's\ formula;}\\ {\rm cal.\ initial\ conditions:}\,\, ({\rm d}z/{\rm d}t)_0 = 0,\, z_0 = -128.59\,\mu{\rm m} \end{split}$$

Compared with the experimental result (shown in Fig. 4), Fig. 6 demonstrates that for the springpoint oscillation (herein Re=0.435) Oseen's formula can still be used to describe the viscous drag force precisely but Stokes's law is no longer valid, which predicts by mistake that the particle will fly lost. Actually that is because the oscillation has become to non-Stokes motion. Thus it has been proved that Oseen's formula can describe the drag force for particle motion in EDB more accurately and completely than Stokes's law.

NOMENCLATURE

C_0	EDB levitation strength constant
C_1	EDB stabilization strength constant
$d_{ m p}$	diameter of microparticle, m
$f_{ m AC}$	AC frequency, Hz
m	mass of microparticle, kg
q	charge on microparticle, C
$V_{ m AC}$	amplitude of the ac field potential, V
$V_{ m DC}$	half of the DC potential difference between
	the two rings, V
Z_0	half spacing of the two rings, m
z	displacement of particle relative to EDB null, m
z_0	initial displacement for numerical simulation
$(\mathrm{d}z/\mathrm{d}t)_0$	initial velocity for numerical simulation
ω	angular frequency, Hz
μ	viscosity of gas fluid, Pa·s
$ ho_{ t g}$	density of gas fluid, kg·m ⁻³

REFERENCES

1 Davis, E.J., Process in Chemical Engineering, Vol.18, Academic Press Inc., New York (1992).

- 2 Davis, E.J., "A history of single aerosol particle levitaion", Aerosol Sci. Technol., 26, 212—254 (1997).
- 3 Zheng, F., Qu, X., Davis, E.J., "An octopole electrodynamic balance for three-dimensional microparticle control", Rev. Sci. Instrum., 72 (8), 3380—3385 (2001).
- 4 Iwamoto, T., Itoh, M., Takahashi, K., "Theoretical study on the stability characteristics of a quadrupole cell", Aerosol Sci. Technol., 15, 127 (1991).
- 5 Vehring, R., Aardahl, C.L., Davis, E.J., "Electrodynamic trapping and manipulation of particle clouds", Rev. Sci. Instrum., 68 (1), 70-78 (1997).
- 6 Davis, E.J., Buehler, M.F., Ward, T.L., "The double-ring electrodynamic balance for microparticle characterization", Rev. Sci. Instrum., 61 (4), 1281—1286 (1990).
- 7 Loyalka, S.K., Tekasakul, P., Tompson, R.V., Warder, R.C., "Computation of electric fields and particle motion in electrodynamic balance", J. Aerosol Sci., 26 (3), 445—458 (1995).
- 8 Zhu, J.H., Zheng, F., Mary, L.L., Davis, E.J., "Mass transfer from an oscillation microsphere", J. Colloid Interface Sci., 249, 351—358 (2002).

- 9 Zheng, F., Laucks, M.L., Davis, E.J., "Areodynamic particle size measurement by electrodynamic oscillation techniques", J. Aerosol Sci., 31 (10), 1173—1185 (2000).
- 10 Aarddahl, C.L., Vehring, R., Davis, E. J., Schweiger, G., Swanson, B.D., "Trapping two-particle arrays in a doublering electrodynamic balance", J. Aerosol Sci., 28 (8), 1491—1505 (1997).
- 11 Davis, E.J., Schweiger, G., The Airborne Microparticle: Its Physics, Chemistry, Optics and Transport Phenomena, Springer, New York (2002).
- 12 Maloney, D.J., Lawson, L.O., Monazam, E.R., "Measurement and dynamic simulation of particle trajectories in an electrodynamic balance: Characterization of particle drag force coefficient/mass ratios", Rev. Sci. Instrum., 66 (6), 3615—3622 (1995).
- 13 Davis, E.J., "Electrodynamic balance stability characteristics and application to the study aerocolloidal particle", Langmuir, 1, 379—387 (1985).
- 14 Xiang, Z.F., "On calculation of the drag coefficient and the fall velocity of spherical bodies", J. Hydrodynamics, 4, 16—27 (1994).