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Higher order dielectrophoretic force characterisation of non-spherical particles

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Abstract. A numerical method is presented for determination of higher-order dielectrophoretic forces on non-spherical particles. The method is applied to ellipsoidal particles of different dimensions subjected to electric fields with different degrees of non-uniformity. The results are compared against net force calculations using the Maxwell stress tensor method. The contribution from higher-order forces is shown to exceed the dielectrophoretic force based only on the dipole approximation when particle dimensions are comparable to the length scale of electric field non-uniformity. It is also shown that individual contributions from quadrupolar and octupolar dielectrophoretic forces strongly depend on particle aspect ratio.

1. Introduction

Dielectrophoresis (DEP) [1] is one of the most commonly used techniques for manipulation and characterisation of micrometre and sub-micrometre particles suspended in fluid media [2-4]. The DEP force on particles arises from the interaction of a non-uniform electric field and polarisation charges at the particle/electrolyte interface. The dipole approximation that ignores all but the first-order of force terms is commonly invoked for determining the DEP force on spherical and non-spherical particles.

While competent in many circumstances, the dipole approximation is expected to provide an accurate account of the DEP force only when particle dimensions are much smaller than a characteristic length scale of electric field non-uniformity [5]. With the current trend towards micro-electrode geometry, there are an increasing number of instances where particle dimensions are indeed comparable to field non-uniformity length scales. Furthermore, most biological particles are non-spherical in which case shape-dependent polarisation gives rise to the induction of higher-order moments.

This paper presents a numerical method for determining higher-order DEP forces on particles of arbitrary shape. The method is applied to spherical and ellipsoidal particles of different dimensions subjected to electric fields with different degrees of non-uniformity to quantify the significance of higher-order forces in different cases of particle and field geometry. The results are compared against total force calculations made using the rigorous Maxwell stress tensor method both for verification and for determination of the contribution of individual force terms to the total DEP force.

2. Background and theory

Based on the dipole approximation, the dielectrophoretic force is given by [1]:

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$$\mathbf{F}_{DEP} = \mathbf{p} \cdot \nabla \mathbf{E} \tag{1}$$

where $\mathbf{p}$ is the effective dipole moment and $\nabla \mathbf{E}$ the gradient of the applied electric field $\mathbf{E}$. In general, the DEP force consists of an infinite number of terms with the nth-order term given by [6]:

$$\mathbf{F}^{(n)} = \frac{1}{n!}\mathbf{p}^{(n)}\left[\cdot\right]^{(n)}\nabla^{(n)}\mathbf{E} \tag{2}$$

where $\mathbf{p}^{(n)}$ is the nth-order effective moment, $\nabla^{(n)}\mathbf{E}$ is the nth gradient of the electric field and $\left[\cdot\right]^{(n)}$ is the nth-order dot product. There is no analytic method for deriving higher-order moments of non-spherical particles. However, in the case of axial symmetry, where the effective multipoles are linear, the moments can be found numerically by an integration of the potential due to the particles over a spherical enclosing surface [7]:

$$p^{(n)} = 4\pi\varepsilon_m R_t^{n+1}\int_0^{\pi}\varphi_{R_t}P_n(\cos\theta)\sin\theta d\theta \tag{3}$$

where ε_m is the dielectric constant of the suspending medium, R_t is the radius of the spherical integration surface, and $P_n(\cos\theta)$ are the Legendre polynomials. The following expressions, consistent with the charges on and positions of the poles of the first three linear multipoles, represented in figure 1, were used to calculate the field derivatives:

$$\nabla^{(1)}E = \frac{d}{dz}E(z) = \frac{E(z+\frac{d_1}{2}) - E(z-\frac{d_1}{2})}{d_1} \tag{4a}$$

$$\nabla^{(2)}E = \frac{d^2}{dz^2}E(z) = \frac{E(z+d_2) - 2E(z) + E(z-d_2)}{d_2^2} \tag{4b}$$

$$\nabla^{(3)}E = \frac{d^3}{dz^3}E(z) = \frac{E(z) - 3E(z-d_3) + 3E(z-2d_3) - E(z-3d_3)}{d_3^3}\ . \tag{4c}$$

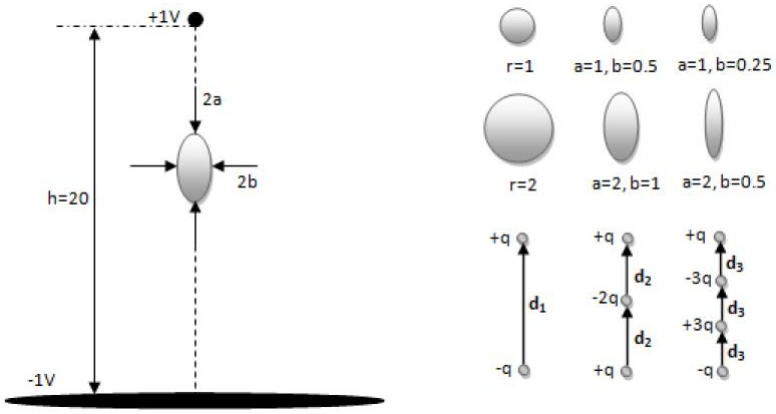

Figure 1. The electrode geometry (point-plane) and particle shapes and dimensions analysed in this work, and a representation of the first three linear multipoles

Using values of the first three effective moments obtained from equation (3) and values of the field derivatives obtained from equations (4a)-(4c), the first three terms of the DEP force on the particles were calculated from equation (2). Calculation was also made in each case of the total DEP force on the particles by integrating the Maxwell stress tensor over the surface of the particle [8]:

$$\mathbf{F}_{DEP} = \frac{1}{2}\varepsilon_m \oint E_m^2 \cdot \mathbf{n} dA . \quad (5)$$

In equation (5), E_m is the field magnitude inside the medium and **n** is the vector normal to the integration surface *A*. The Maxwell stress tensor (MST) method is known as the most unassailable in calculating field-induced force.

Figure 1 shows the particle shapes studied in this work and the way they are positioned within the electrode geometry. The particle and the medium are assigned dielectric constants of 3 and 80, respectively. With no loss of generality, the simulations were performed without considering units for the dimensions. Force values were calculated at fifteen different particle centre heights above the plane electrode: 2, 3, ..., 17 with higher points corresponding to a higher degree of field non-uniformity. We used FlexPDE (FlexPDE Inc) to numerically solve the electric field in each case.

3. Results and discussion

Figures 2 and 3 show the results for spherical and ellipsoidal particles, respectively. Contributions to the total DEP force from the first three force terms when the particles are at h = 17 (highest point above the plane electrode where the field gradient is strongest) are summarised in Table 1.

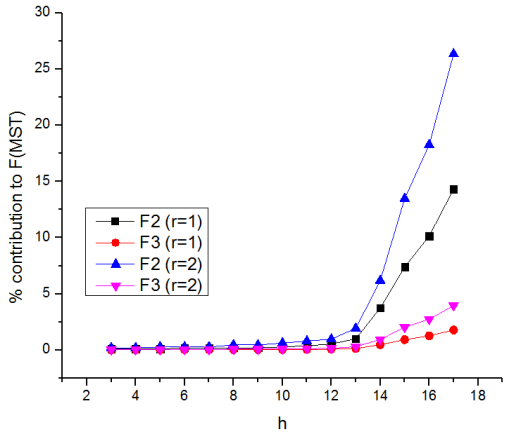

Figure 2. Variations with particle height (h) above the plane electrode of the contributions from the first three DEP force terms to the total DEP force on spherical particles of radii r = 1 and r = 2

Table 1. Contribution from the first three force terms to the total DEP force on the particles in figure 1 when they are at h = 17 where the field gradient is strongest

Particle	$F^{(1)}/F^{(MST)}$	$F^{(2)}/F^{(MST)}$	$F^{(3)}/F^{(MST)}$	$F^{(2)}+F^{(3)}/F^{(MST)}$
r = 1	83.5%	14.3%	1.8%	16.1%
r = 2	69.3%	26.4%	3.9%	30.3%
a = 1, b = 0.5	65.2%	24.9%	9.2%	34.1%
a= 2, b = 1	39.1%	43.6%	16.9%	60.5%
a = 1, b = 0.25	66.0%	20.2%	13.5%	33.7%
a = 2, b = 0.5	38.8%	35.9%	25.0%	60.9%

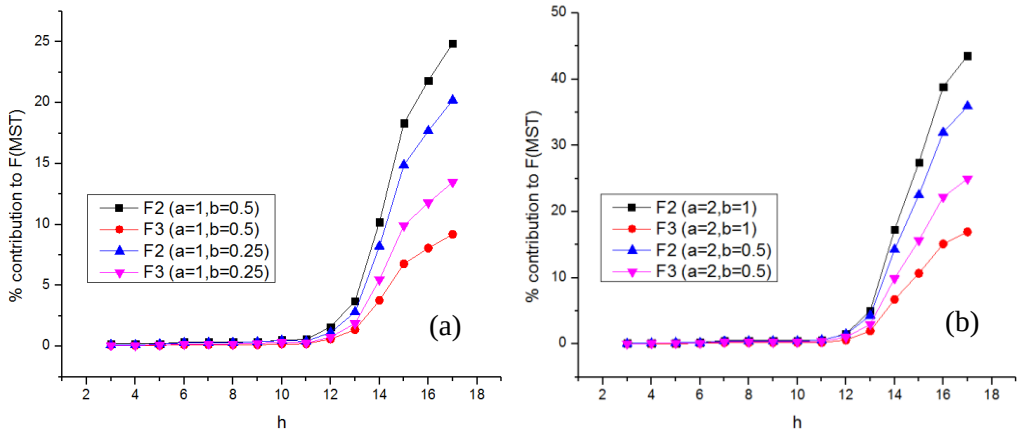

Figure 3. Variations with particle height (h) above the plane electrode of the contributions from the first three DEP force terms to the total DEP force on ellipsoidal particles with dimensions along the symmetry axis equal to (a) a = 1, and (b) a = 2

As suggested by the plots and the table, higher-order forces are less significant for spheres compared to ellipsoids of similar dimensions. The data confirms that higher-order forces become increasingly significant as particle dimensions become comparable to the length scale of electric field non-uniformity. At h = 17 where the field is most strongly divergent, higher-order contribution to ellipsoids of a = 1 is almost equal to 34% - interestingly, this is the same for both ellipsoids of a = 1 indicating that the parameter controlling the significance of higher-order DEP forces is the particle dimension along the axis of symmetry – whereas for ellipsoids of a = 2, higher-order contribution is a significant 61% exceeding the dielectrophoretic force based only on the dipole approximation.

It may also be seen from the data that although the overall contribution from higher-order forces is similar – to within an error of <1% - for particles with equal dimensions along the symmetry axis, individual contributions from second- and third-order force terms strongly depend on particle aspect ratio. The quadrupolar and octupolar DEP forces show inverse and direct relationships with particle aspect ratio, respectively.

4. Conclusion

A method was presented for determining higher-order dielectrophoretic forces on particles of arbitrary shape subjected to an axially symmetric electric field. The method was applied to spherical and ellipsoidal particles of different dimensions in electric fields with varying gradients. It was shown that higher-order forces are more significant for ellipsoidal particles and that it is the particle dimension along the axis of symmetry that controls the significance of higher-order contribution to the total force. It was also shown that unlike the overall higher-order contribution, quadrupolar and octupolar forces are strongly dependent on particle aspect ratio with the quadrupolar force decreasing and the octupolar force increasing with increasing aspect ratio. The results were validated against total force calculations using the Maxwell stress tensor method.

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