

A Mean Field Approach to Many-particles Effects in Dielectrophoresis

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Abstract: One of the major applications for dielectrophoresis is selective trapping and fractionation in lab-on-a-chip devices. Nevertheless, many-particles effects due to high concentration of biological material around electrodes can cause a rapid decrease of trapping efficiency in dielectrophoretic devices. In this contribution we present a new approach based on a drift-diffusion dynamics to study the particles behavior near electrodes surroundings. Within this approach we easily introduce many-particles effects by invoking the effective medium approximation (EMA). In this framework electrodes can saturate losing their capability to attract further particles thus leading to a more realistic scenario never discussed in past literature. The complete system of non-linear PDEs employed represents a good example of multiphysics simulation to be solved by using COMSOL.

Keywords: Dielectrophoresis, mean-field, many-particles effects, lab-on-a-chip, drift-diffusion.

1. Introduction

In recent years dielectrophoresis (DEP) has emerged as an important technique for the manipulation of micro- and nano-sized particles suspended on a liquid medium [1,2]. Highly non-uniform electric field at a length scale comparable to cell size can be generated easily at low voltages. Since the relative dielectric responses (DEP spectrum) of the cells are dependent on the driving frequency of the applied electric field, an alternating electric field is usually applied to generate dielectrophoretic forces of different magnitudes and directions. Therefore, DEP devices may be easily employed for separating different cell types by simply modifying field frequency. In order to generate a spatially non-uniform electric field, essential ingredient for DEP separation, an array of metal

electrodes is embedded inside a micro-channel network. Starting point for any DEP separation strategy is the cell's DEP spectrum which can be computed via electrical models or obtained from data on electro-rotation experiments [3,4]. Many physical parameters can affect DEP spectra and we refer the reader to the past literature [1-3,5] for a better introduction. Nevertheless, there is a strong evidence that many-particles effects, coming from high concentration of cells in the surroundings of electrodes, can be an important source of indetermination for the knowledge of separation (or trapping) efficiency.

In the past decades different numerical approaches based on the direct solution of the equations of motion for a system of N particles have been used to account for many-particles effects in dielectric suspensions [6]. Due to the limited number of particles (i.e. $N \sim 100$) considered, these techniques are no feasible in view of the simulation of real devices. In this letter we suggest a method to include many-particles effects in the calculation of DEP trapping by mean of the effective medium approximation (EMA) for electric parameters of the suspension [7], where the local value of the volume fraction of dispersed particles is ruled by a drift-diffusion dynamics. We will demonstrate the reliability of the method and the importance of the many-particle corrections discussing a simulation example in a realistic DEP device geometry.

This paper is organized as follows. After a brief introduction on dielectrophoresis and trapping strategies in DEP devices in section 1, we discuss in section 2 the model employed in a standard dielectrophoresis simulation for cell trapping and the modifications we propose for the introduction of many-particle effects in the framework of EMA. In section 3 we show the simulation results for both dynamical and stationary cases and finally we draw the conclusions.

2. The Model

Most part of the physical information on dielectrophoresis resides in the DEP spectrum, known also as the Clausius-Mossotti factor [3], which in general is a complex quantity depending on the electrical field frequency ω , this factor reads:

$$f_{CM}(\omega) = \frac{\tilde{\epsilon}_2 - \tilde{\epsilon}_1}{\tilde{\epsilon}_2 + 2\tilde{\epsilon}_1} \quad (1)$$

where $\tilde{\epsilon}_j = \epsilon_j - i\sigma_j / \omega$ ($j=1,2$) represent respectively the complex dielectric functions of liquid medium and particles. However, if the local particle density is high the dipole-dipole particle interaction can significantly alter the DEP response [6]. We can approximately correct the DEP spectrum, embedding the many particle effects in the medium complex dielectric functions using the EMA for the dielectric properties of heterogeneous two-component composite materials [7]. The EMA approach allows to calculate the electrical conductivity σ and the dielectric function ϵ for various shapes of composite materials as function of the hosted material (ϵ_2, σ_2) and the host material (ϵ_1, σ_1) properties. In the case where the material 2 is included by means of a random formation of spherical clusters, the dielectric function ϵ is given by [7]:

$$\epsilon(\phi) = \frac{1}{4} \left[2\epsilon_p - \epsilon_p' + \sqrt{(2\epsilon_p - \epsilon_p')^2 + 8\epsilon_1\epsilon_2} \right] \quad (2)$$

with:

$$\begin{aligned} \epsilon_p &= (1-\phi)\epsilon_1 + \phi\epsilon_2 \\ \epsilon_p' &= \phi\sigma_1 + (1-\phi)\sigma_2 \end{aligned} \quad (3)$$

where ϕ represents the volume fractions of cluster inclusions. This scenario is analogous to that of a liquid medium where spherical particles (cells) are dispersed with a fraction of volume locally variable, like the case we are going to discuss. The generalization of (1) to include the EMA is straightforward and can be obtained by simply performing the following substitutions:

$$\begin{cases} \epsilon_1 \rightarrow \epsilon(\phi) \\ \sigma_1 \rightarrow \sigma(\phi) \end{cases} \quad (4)$$

In Fig.1 we present an example of DEP spectrum obtained from experimental data on latex micro-spheres given in [4]. As expected the effect of EMA in the DEP spectrum, shown in Fig.1, is a gradually flattening to zero of both real and imaginary part of Clausius-Mossotti factor as the volume fraction ϕ approaches one. For dielectrophoresis induced by electrical field gradients only the real part of (3) is relevant and we deal with it throughout this paper.

Once the electrical properties of the mixture (particles plus liquid medium) are determined as

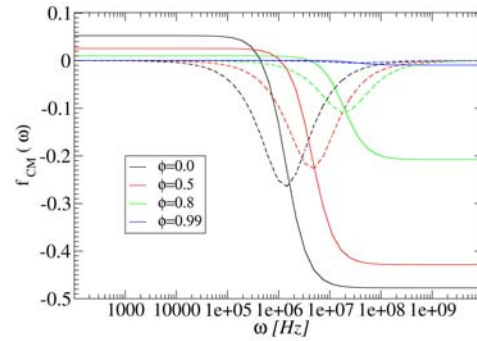


Figure 1. DEP spectrum of latex micro-spheres obtained from data given in [4]. Straight and dashed lines refer respectively to the real and imaginary parts of the Clausius-Mossotti factor. Colors refer to different values of particle volume fraction ϕ (see legend).

a function of the volume fraction, we introduce the equations needed for a complete description of trapping in DEP devices. The governing equations for a DEP device usually concern those for electrostatic and viscous fluid dynamics, and according to [5] each particle subjected to the DEP force reaches a steady regime of motion very quickly so that electric and fluid parts result completely uncoupled. In other words the particle's velocity field induced by DEP force, counterbalanced by drag force due to the liquid, \vec{u}_{DEP} can be expressed by the following relation:

$$\vec{u}_{DEP} = \mu_{DEP} \nabla |\vec{E}|^2 \quad (5)$$

where μ_{DEP} is called the DEP mobility and for a spherical particle of radius R and immersed in a liquid of viscosity η and it reads:

$$\mu_{DEP} = \frac{\varepsilon(\phi)R^2\Re[f_{CM}(\omega, \phi)]}{3\eta} \quad (6)$$

In addition the electric potential V can be computed by solving the Laplace equation:

$$-\vec{\nabla} \cdot \varepsilon_0 \varepsilon_r \nabla V = 0 \quad (7)$$

Subjected to the voltage boundary conditions or the continuity conditions for the normal component of the dielectric displacement at the internal boundaries. In particular, in the computational subdomain regarding the liquid medium with dispersed particles we must employ the value for the dielectric constant $\varepsilon_r(\phi)$ obtained within the EMA approach.

Since in this paper we assume that particles reach quickly a steady motion regime, the computation of the liquid medium velocity field \vec{u}_{fluid} is done completely apart from the rest of the simulation and consists of solving the Navier-Stokes equation (NSE) for a steady and incompressible fluid [9]. The vector composition of \vec{u}_{fluid} with the particle's velocity \vec{u}_{DEP} field represents the main goal in a standard DEP simulation, since this quantity gives all information on the particle motion inside the DEP device allowing us to compute particles trajectories.

The introduction of EMA in the simulation requires the knowledge of the local value of the particle volume fraction which is not easily tractable in the framework of a simple particle tracing. Therefore, the complete system of governing equations has to be enriched and consequently the way of representing particles inside a DEP device should be changed too. Since the total velocity field acts as a drift towards the electrodes, we can choose as physical quantity representing particles that of a drift-diffusion current \vec{J} of the following form:

$$\vec{J} = -D\nabla\phi + \vec{u}_{tot}\phi \quad (8).$$

In Eq.(8) the drift term, completely determined by the total velocity field $\vec{u}_{tot} = \vec{u}_{DEP} + \vec{u}_{fluid}$, dominates with respect to the diffusion one. We note, that for particle's dimension in the micrometer scale and in the diluted limit, D has only the meaning of a numerical diffusion, introduced to stabilize the entire calculation, while for the high density case D can effectively include the scattering events between particles or the limit threshold of ϕ for the packing (see

Eq. 10 below). In this picture the equation governing the time evolution of the particle volume fraction ϕ is the one in the following flux-conservative form:

$$\frac{\partial\phi}{\partial t} = -\vec{\nabla} \cdot \vec{J} \quad (9)$$

The latter equation (with the usual boundary conditions for \vec{J} or ϕ) coupled with Eqs.(1-7) represent the new set of governing equations, ready to be solved. The dependence on particle volume fraction of some electric constants makes the system highly non-linear since many physical parameters are now solution dependent.

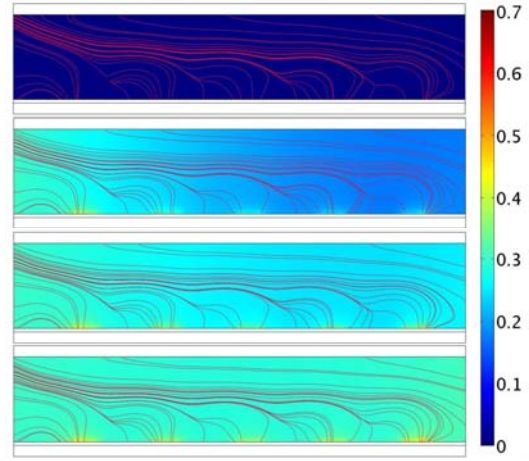


Figure 2. Snapshots taken at times 0, 2, 3, 4 seconds (from upper to lower) regarding the time evolution of particle volume fraction ϕ (color field) and the streamlines of the total velocity field $\vec{u}_{tot} = \vec{u}_{DEP} + \vec{u}_{fluid}$ (red lines). The color bar on the right gives the correspondence between colors and values of ϕ . Particles and fluid enter from the left (initial fluid velocity of $15\mu m/s$) where at the boundary ϕ is fixed to 0.3, in the other boundaries we employ the condition $\hat{n} \cdot \vec{J} = 0$ for Eq.(9). Electrodes (in number of 10) are separated from the fluid by a silicon layer $3\mu m$ thick and they are taken at a voltage of 0 or +5 Volt in an alternate sequence (see [5]).

3. Results

As simulation example of our model we considered the device geometry described in Ref.

[5], i.e. a two-dimensional trap with an array of parallel interdigitated electrodes placed at the base of a rectangular channel where the dispersed liquid medium flows. Copper electrodes are deposited on a glass substrate. Eqs. (7) and (9) and the NSE have been solved by using the COMSOL computational platform [8] which employs the standard finite element method for solving partial differential equations in a wide range of interests and types. For the simulation example shown in this letter we consider spherical latex particles of radius $R = 5.87 \mu m$ and dielectric constant and conductivity respectively equal to $2.4\epsilon_0$ ($\epsilon_0 = 8.8542 \times 10^{-12} F/m$) and $7.0 S/m^2$. Particles are dispersed in a saline solution (viscosity $\eta = 10^{-3} Pa \cdot s$) whose dielectric constant and conductivity are respectively $78\epsilon_0$ and $6.0 S/m^2$. During the calculation the electric field frequency ω is fixed to $10 kHz$ (see Fig.1). In order to prevent the volume fraction exceeds the threshold value for the packing fraction of 0.74, we introduce a diffusion coefficient D depending on ϕ by the following formula:

$$D(\phi) = \frac{9.6 \times 10^{-9}}{\sqrt{1 - \frac{\phi}{0.74}}} \quad (10)$$

From Eq.(10) one can argue that for values of ϕ well below 0.74 the diffusion coefficient is too high for a coherent treatment of diffusion for such a big particle, nevertheless in our simulation we choose as boundary value for ϕ that of 0.3, which turns out to be large enough to justify a possible enhancement of diffusion due to particle-particle collisions. In addition the non-linearity of the governing equations makes the computation very delicate and a concentration-dependent diffusion coefficient helps in achieving convergence.

Concerning Eq.(10) two additional remarks are worthy of note. The first regards the effect of Eq.(10) in the final results, since the introduction of a ϕ -dependence on D with a cut-off at 0.74 slightly reduces many-particles effects as will be clear later. The second has to do with the choice of Eq.(10) which is suggested only by intuitive arguments thus requiring further investigation on

this point. A possible assessment for the latter can come from Monte Carlo diffusion simulations of hard spheres.

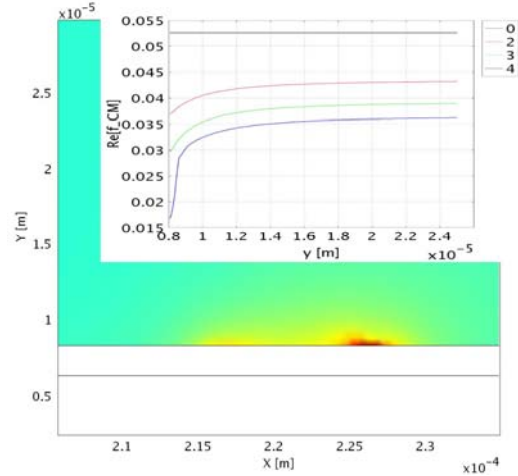


Figure 3. An enlarged portion of snapshot at $t = 4$ sec of Fig.2. The color field represents the particle volume fraction ϕ at the surroundings of an electrode where ϕ reaches its maximum value (colors are the same as in Fig.2). Abscissa and ordinate are spatial coordinates. In the inner panel the cross-section, taken just above the red region at $X = 2.26 \times 10^{-4} m$, of the Clausius_Mossotti factor as a function of the ordinate is shown, colours of the curves refer to the same times of the snapshots of Fig.2 (see the legend).

In Fig.2 some snapshots of the solution at different times are reported, in particular the color field represents the particle volume fraction ϕ while red lines are streamlines representing the total velocity field \vec{u}_{tot} acquired by the suspended particles. The real part of the Clausius-Mossotti factor decreases as ϕ increases, leading to a non-negligible many-particles effects in trapping efficiency. As expected the increasing particle fraction at the electrodes surroundings determines an evident reduction of trapping capabilities. This aspect becomes also more clear in Fig.3 where we focus in a small region around one electrode in order to show better the behavior of both ϕ and DEP spectrum. Note, indeed, the time dependence of $f_{CM}(\omega, \phi)$ near the electrode shown in the inset of Fig. 3.

In Fig.4 the stationary solution is shown as in the previous pictures the color field represents the particle volume fraction ϕ . In addition we report also a contour plot (second panel from above) regarding the real part of the Clausius-Mossotti factor which varies together with ϕ throughout the device according to the EMA prescription.

Nevertheless, the stationary solution reported in Fig.3 is obtained imposing slightly different conditions with respect to the dynamical ones. In this case indeed, maintaining the same apparatus as before for the electrostatic and fluid dynamic sectors, the value of ϕ is fixed at a value of 0.5 in both left and right walls of the computational domain. Moreover, the initial value of ϕ is chosen constant and non-zero throughout the computational domain. In other words before stating the simulation the device's channel is filled uniformly with the dispersed medium at a value of 0.5 for the particle volume fraction ϕ .

Even in Fig.4 results show an evident decrease of trapping capabilities due to many-particle effects which is stressed in the lower two panels focusing the neighbors of the last electrode, where a rapid increase of ϕ (lower left panel) determines consequently a decrease of the Clausius-Mossotti factor (lower right panel).

4. Conclusions

The simulation results here discussed show the importance of the inclusion of the many particle corrections for a reliable prediction of the trapping efficiency in devices aimed at the manipulation of micro- and nano-sized particles. The formalism should be applied in all the case where the diluted limit locally fails. This situation is rather common (not only for devices working in trapping configuration) since high particle density can be achieved in device geometry where tight regions are built to suitably tailor the electric field [10].

The combination of EMA and drift-diffusion opens the possibility to study carefully how many-particles effects can influence the features dielectrophoresis based devices. The formalism here presented represents only a first step toward a complete description of the possible complex particle kinetics in these devices and advances

are still needed. Indeed, the diffusion formalism can be easily generalized to a reaction-diffusion one in order to considered particle's stitching and clustering. Work in this direction is still in progress.

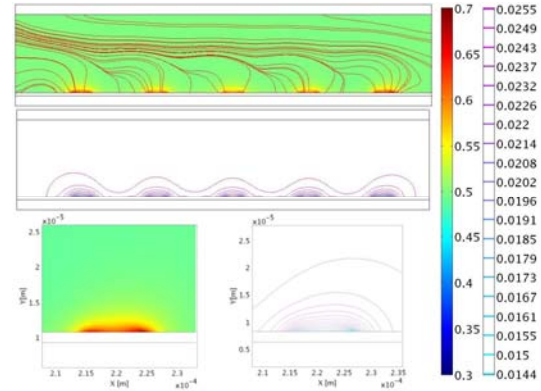


Figure 4. Plot regarding the stationary solution. The first two panels (from above) represent respectively the particle fraction ϕ (colour field) and the contour plot regarding the real part of the Clausius-Mossotti factor. Enlarged portions in the neighbors of the last electrode for both plots are shown in the lower part of the figure.

5. References

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