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Dielectrophoretic choking phenomenon in a converging-diverging microchannel

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Experiments show that particles smaller than the throat size of converging-diverging microchannels can sometimes be trapped near the throat. This critical phenomenon is associated with the negative dc dielectrophoresis arising from nonuniform electric fields in the microchannels. A finite-element model, accounting for the particle-fluid-electric field interactions, is employed to investigate the conditions for this dielectrophoretic (DEP) choking in a converging-diverging microchannel for the first time. It is shown quantitatively that the DEP choking occurs for high nonuniformity of electric fields, high ratio of particle size to throat size, and high ratio of particle's zeta potential to that of microchannel. [doi:10.1063/1.3279787]

I. INTRODUCTION

An accelerated electrokinetic transport of particles is usually expected in a converging-diverging microchannel due to the electric field enhancement in the throat region.[1–4] Depending on the gradual enhancement in the particle velocity through the converging section, deformable biological entities, such as individual DNA molecules, can be stretched for genomic analysis.[5–7] In some other applications, particles experience a cross-stream motion due to a negative dielectrophoretic (DEP) force, successfully exploited to focus particle flows,[8–10] and separate particles and cells based on their sizes.[11–15]

Recently, a particle choking phenomenon in converging microchannels or nanopores due to the negative DEP effect is experimentally observed[10,12,16,17] and numerically predicted.[18] Dielectrophoresis refers to a nonlinear electrokinetic phenomenon in which a force is exerted on a dielectric particle when it is subjected to a spatially nonuniform electric field. The negative DEP force is always pointed from high electric field to low electric field. When a charged particle migrates toward a converging microchannel driven by electrophoresis and electro-osmosis, the negative DEP force, however, retards the particle transport owing to an enhanced electric field in the converging channel. As the DEP force increases with the electric field faster than electrophoresis and electro-osmosis,[18] it could prevent the particle from moving further into the converging channel at some certain conditions, which is in the present study named as DEP choking phenomenon. Usually, this kind of phenomenon should be eliminated in applications such as electrophoretic stretching of deformable particles and particle focusing. However, it is considered to have broad biomedical and environmental applications associated with particle trapping, concentration, and sorting.[19–28]

So far, a comprehensive understanding of the DEP choking phenomenon in a converging-diverging microchannel is still limited. Chen *et al.*[29] numerically studied the DEP choking criteria

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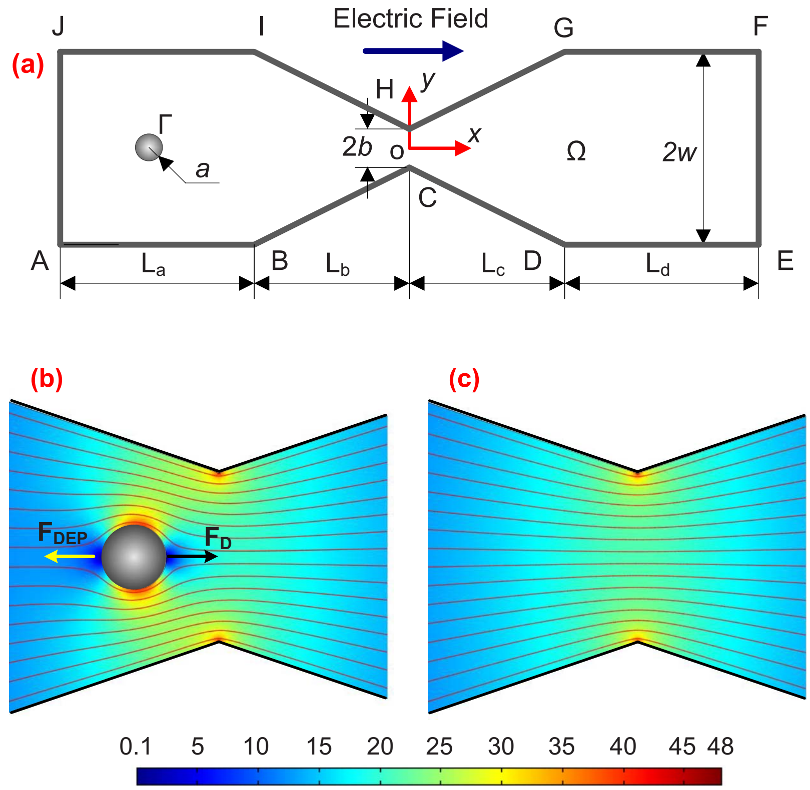

FIG. 1. A 2D schematic view of a circular particle electrophoretically migrating in a converging-diverging microchannel (a). The origin of the Cartesian coordinate system (x,y) locates at the center of the throat where the cross section is minimal. Distribution and streamlines of the dimensionless electric field within a converging-diverging microchannel in the presence (b) and absence (c) of a particle. F_D and F_{DEP} shown in (b) represent the electrokinetic driving force and the negative DEP force exerting on the particle, respectively.

of infinitesimal particles in a sawtooth microchannel consisted of successive converging-diverging sections. However, in most microfluidic applications, the particle size is comparable to the channel width, which could induce a significant distortion in the electric field and thus, generate a considerable DEP force on the particle.[30] As a result, distortions of electric and flow fields due to the presence of particles must be considered for an accurate prediction on the electrokinetic behavior of particles. In the present study, the DEP force is obtained by integrating the Maxwell stress tensor (MST) over the particle surface, which is considered to be the most rigorous method for the DEP force calculation.[31–33] To account for the particle-fluid-electric field interactions simultaneously, a verified transient finite-element method is used. For the first time a parametric study is performed to obtain the conditions for the DEP choking phenomenon in a converging-diverging microchannel.

II. MATHEMATICAL MODEL

The remarkable agreement between the numerical predictions of electrokinetic particle transport in a converging-diverging[18] and an L-shaped microchannel[34] obtained from a two-dimensional (2D) mathematical model and experimental data suggests that a 2D model is sufficient to capture the essential physics of the electrokinetic particle transport process, as explained further by Ai *et al.*[35] The numerical experiment of Davison and Sharp[36] with 2D, axisymmetric, and three-dimensional modeling also reveals less than 4% relative error for an electrophoresis problem. A 2D mathematical model is thus adopted in this study.

We consider a uniformly charged particle of radius a in a converging-diverging microchannel, as shown in Fig. 1(a). The computational domain Ω, enclosed by the channel boundary ABCDEF-

GHIJ and the particle surface Γ, is filled with an incompressible and Newtonian fluid of density $\rho=1\ \mathrm{g/cm^3}$, dynamic viscosity $\eta=1e^{-3}$ Pa s, and permittivity $\varepsilon_f=7.08\times10^{-10}$ F/m. The channel walls, ABCDE and FGHIJ, bear a uniform zeta potential $\zeta_w=-80$ mV, and are rigid and nonconducting. The converging-diverging section of the channel is constructed to be symmetric, $L_b=L_c=400\ \mu$m, with respect to the throat where the cross section is minimal. The half widths of the uniform section of the channel and the throat are w and $b=27.5\ \mu$m, respectively. The particle, considered to be rigid and nonconducting, bears a uniform zeta potential ζ_p on its outer surface Γ, and is initially located in the upstream uniform section of the channel. A dc electric field is applied between the inlet and outlet, denoted by AJ and EF, respectively. The effects of Brownian motion and gravity are ignored. The half width of the throat, b, the zeta potential of the channel wall, ζ_w, and the electrophoretic velocity, $U_\infty=(\varepsilon_f\zeta_w/\eta)(\zeta_w/b)$, are used as the characteristic length, characteristic electric potential, and characteristic velocity to normalized the governing equations, respectively. Figure 1(b) illustrates a highly distorted electric field due to the presence of a particle with a comparable size to the channel width, compared to the electric field in the absence of the particle, as shown in Fig. 1(c). Therefore, the effect of the particle on the electric and flow fields must be fully considered in the current study. The detailed mathematical model for this particle-fluid-electric field coupled system and its numerical implementation defined in arbitrary Lagrangian–Eulerian (ALE) frame are detailed previously.[18,37] Rigorous mesh-refinement tests are performed to confirm that all generated results are fully converged and grid independent.

III. RESULTS AND DISCUSSION

It is found that the minimum DEP force exists along the center line of the channel using the MST method. It is thus reasonable to study the particle transport along the center line in order to obtain conditions for the DEP choking. The effects of the four parameters, namely, the dimensionless particle radius, a^*, the electric field intensity, $\mathbf{E}^*$, the constriction ratio, w^*, and the zeta potential ratio, $\gamma=\zeta_p/\zeta_w$, on the DEP choking phenomenon are investigated in this study. The electric field intensity, $\mathbf{E}^*$, is calculated by dividing the dimensionless electric potential difference between the inlet and outlet over the dimensionless length of the entire microchannel. In the following, combinations of two of them are investigated to achieve the DEP choking based on the verified ALE finite-element model in our previous work.[18,34] In each combination, both parameters are discretized into 20 equally spaced points along their own interested ranges, generating 400 conditions in each combination. The DEP choking criterion in the numerical simulation is specified as the ratio of the particle's translational velocity to that in the upstream uniform section of the channel less than $1e^{-4}$ ($U_p^*/U_{up}^*<1e^{-4}$). As a result, a 20×20 binary matrix is obtained to distinguish the parametric regions for the DEP choking from nonchoking ones. The boundaries between choking and nonchoking regions are drawn with their corresponding best fitting curves based on the obtained matrix.

A. Electric field versus particle size

The nonuniformity of the electric field, depending on the constriction ratio and the magnitude of the electric field intensity, is the essential reason of the DEP choking phenomenon. Figure 2(a) shows the parametric ranges for the DEP choking in a constriction ratio versus particle size plane for different electric field intensities, $\mathbf{E}^*$, of 3.44 (solid line), 10.31 (dashed line), and 17.19 (dashed-dotted line). The zeta potential ratio, γ, is 0.4. The choking occurs in the region above each bounding curve. Straight uniform microchannels are impossible to induce the DEP choking phenomenon, no matter how large the particle size and the electric field intensity are. Smaller particles require a higher constriction ratio to obtain a higher nonuniformity of the electric field for the DEP choking. Hence, sequential converging-diverging channels with different constriction ratios can be utilized to selectively trap particles with different sizes and thus separate mixtures of complex biological particles,[28] which is usually necessary prior to the biological analysis.[38] Under

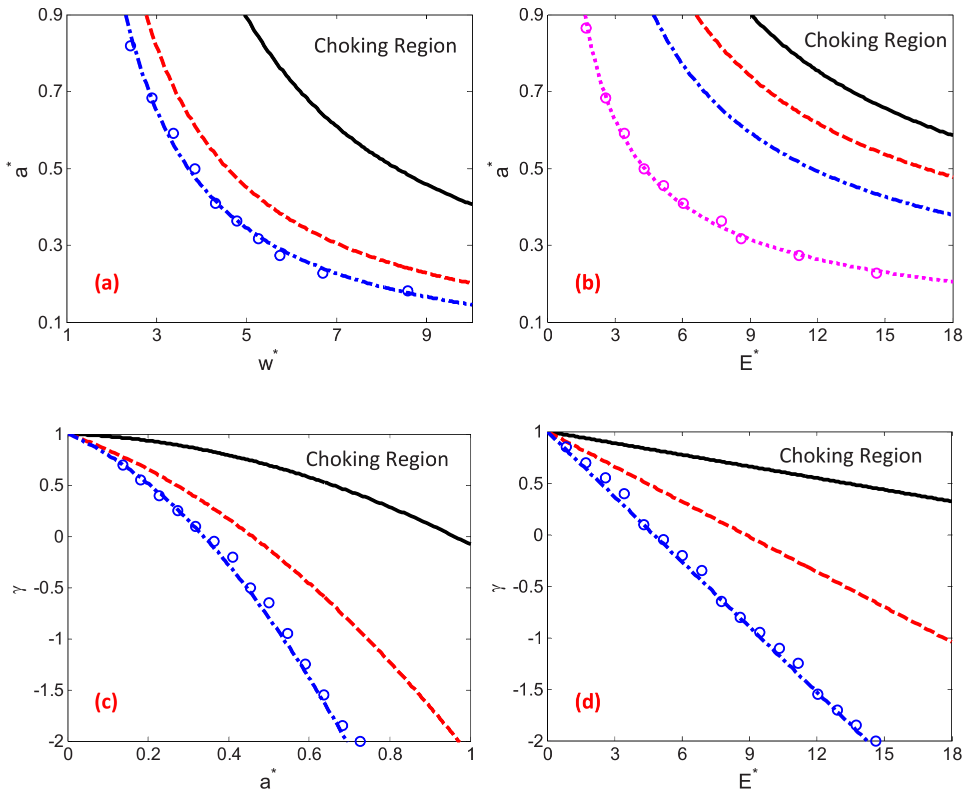

FIG. 2. DEP choking regions in a constriction ratio vs particle size plane for different electric field intensities (a); in an electric field vs particle size plane for different zeta potential ratios (b); in a particle size vs zeta potential ratio plane for different electric field intensities (c); in an electric field vs zeta potential ratio plane for different particle sizes (d). Circles represent the actually numerical results used to draw these fitting curves as the boundaries between choking and nonchoking regions. The choking occurs in the region above each bounding curve.

a specified constriction ratio, the nonuniformity of the electric field increases with the magnitude of the electric field intensity, $\mathbf{E}^*$. Thus, under a fixed constriction ratio, higher electric field intensities are required to trap smaller particles.

Figure 2(b) depicts the detailed DEP choking regions in an electric field, $\mathbf{E}^*$, versus particle size, a^*, plane for zeta potential ratios, γ, of -1.2 (solid line), -0.6 (dashed line), 0 (dashed-dotted line), and 0.6 (dotted line). The constriction ratio is fixed to $w^*=5.9$. It is also shown that smaller particles require larger electric field intensity for the DEP choking. When the particle radius, a^*, approaches zero, the electric field, $\mathbf{E}^*$, required for the DEP choking approaches infinity. Hence, the critical particle size for the DEP choking under a specified constriction ratio can be controlled by adjusting the electric field intensity. For a fixed particle size, the critical electric field increases as the particle zeta potentials deviate from that of the channel wall toward opposing polarity, which is consistent with the increase in the electrokinetic driving force, which will be discussed in Sec. III B.

B. Particle size versus zeta potential ratio

Figure 2(c) shows the DEP choking regions in the particle size versus zeta potential ratio plane for three different electric fields, $\mathbf{E}^*=3.44$ (solid line), 10.31 (dashed line), and 17.19 (dashed-dotted line). The constriction ratio, w^*, is 5.9. It is consistently shown that the choking region expands with the increase in the electric field intensity. When the zeta potential ratio is positive, both the particle and the channel wall are negatively charged. As a result, the particle electrophoresis retards the particle motion toward the converging-diverging channel. By contrast, a negative zeta potential represents the particle electrophoresis and accelerates the particle motion.

Therefore, the electrokinetic driving force decreases as the zeta potential ratio increases until it vanishes at $\gamma=1$. The critical particle size for the DEP choking thus decreases as γ approaches unity. It is to be noted that the choking is not achieved by the DEP effect but by the geometrical constraint when $a^* > 1$, beyond the scope of the current study.

C. Electric field versus zeta potential ratio

Figure 2(d) shows the DEP choking regions in an electric field versus zeta potential ratio plane with the particle size, a^*, fixed to 0.27 (solid line), 0.55 (dashed line), and 0.82 (dashed-dotted line). The constriction ratio, w^*, is 5.9. As electrophoresis and electro-osmosis are proportional to the electric field intensity, while DEP is proportional to the square of the electric field intensity, the critical electric field for the DEP choking thus increases linearly with the decrease in the zeta potential ratio for all particle sizes studied. The choking region is shown to expand with the increase in the particle size, which is consistent with other predictions in the present study.

IV. CONCLUDING REMARKS

The dc DEP choking phenomenon of particles through a converging-diverging microchannel, arising from the interactions between the spatially nonuniform electric field and the dielectric particles, is quantitatively predicted using a transient ALE finite-element model. A rather comprehensive parametric study reveals that a high nonuniformity of the electric field, a high particle size ratio, and a high zeta potential ratio could lead to the DEP choking of particles through a nonuniform microchannel. Although the DEP choking phenomenon may fail many electrokinetic operations, such as stretching of deformable particle,[5–7] particle focusing,[8–10] and particle separation,[11–15] it has extensive biomedical applications associated with the particle trapping, concentration, and sorting.[19–28] Parametric ranges for the DEP choking thus must be known prior these operations, and the present study explicitly shows how these ranges can be obtained and how some of these parameters are interrelated in creating the DEP choking. In the present study the particle size is assumed to be much larger than the thickness of the electric double layer (EDL) in the vicinity of the charged particle and the channel wall. The results thus are not applicable for nanoparticles, for which the hydrodynamics and the electrokinetics in the EDL must be fully resolved.[3,4,39,40]

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