Supporting Information

Electrothermal flow effects in insulating (electrodeless) dielectrophoresis systems

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S2 Numerical Techniques

S2.1 Summary of Governing Equations and Boundary Conditions used in Numerical Simulations

We now simplify the general analytical expressions presented above to those solved numerically in our simulations. In our numerical work, we consider a DC-offset, AC electric field defined by:

\[ \mathbf{E} = \mathbf{E}_{AC} + \mathbf{E}_{DC} = (\alpha + 1)\mathbf{E}_{DC} \]  

and write the governing equations in terms of the DC field \( \mathbf{E}_{DC} \) and the scaling parameter, \( \alpha \), that relates the peak magnitude of the AC field to the magnitude of the DC field. The following steady-state governing equations were used in our simulations:

- **Electric Field** The equation for charge continuity was solved to determine the electric field.

  \[ \nabla \cdot (\sigma_{\infty} \mathbf{E}_{DC}) = 0 \]  

Electromagnetic boundary conditions are defined by specifying the potential at the channel inlet and outlet and specifying zero normal current at insulating channel walls.
Inlet: $\phi = V_{applied}$  \hfill (37)

Outlet: $\phi = 0 \quad$ \hfill (38)

Walls: $\hat{n} \cdot (\sigma_m E_{DC}) = 0 \quad$ \hfill (39)

where $\hat{n}$ is an outward-facing normal unit vector and $V_{applied}$ is the magnitude of the DC component of the electric potential at the inlet.

- **Fluid Velocity Field**

Equation 13 is simplified by setting $\omega = 0$ and $\omega_1 = \omega$. The incompressible Navier-Stokes equations with an electrothermal body force term and the continuity equation are solved to determine the fluid velocity field.

$$\rho_m (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \eta \nabla^2 \mathbf{u} + \langle \mathbf{f}_{ET} \rangle \quad$$ \hfill (40)

$$\langle \mathbf{f}_{ET} \rangle = \frac{1}{2} \text{Re} \left[ \left( \sigma_m \nabla \varepsilon_m - \varepsilon_m \nabla \sigma_m \right) \left( \frac{\alpha^2}{\sigma_m + i\omega\varepsilon_m} + \frac{2}{\sigma_m} \right) \cdot E_{DC} \right] E_{DC} \right]$$

$$- \frac{\alpha^2}{4} \text{Re} \left[ E_{DC} \cdot E_{DC} \right] \nabla \varepsilon_m \quad$$ \hfill (41)

$$\nabla \cdot \mathbf{u} = 0 \quad$$ \hfill (42)

The hydrodynamic boundary conditions applied in our numerical simulations are zero viscous stress at the inlet and outlet with no applied pressure gradient and an electroosmotic slip boundary condition at the channel walls.

Inlet: $\frac{\partial \mathbf{u}}{\partial n} = 0, p = 0 \quad$ \hfill (43)

Outlet: $\frac{\partial \mathbf{u}}{\partial n} = 0, p = 0 \quad$ \hfill (44)

Walls: $\mathbf{u} = -\frac{\varepsilon_m E}{\eta} \quad$ \hfill (45)
• **Temperature Field** The energy conservation and Joule heating equations are solved to determine
the temperature field.

\[ \rho_m C_p u \cdot \nabla T = k_m \nabla^2 T + q \]  \hspace{1cm} (46)

\[ q = \frac{\alpha^2 + 2}{2} \sigma_m E \cdot E \]  \hspace{1cm} (47)

Thermal boundary conditions are based on a 1mm-thick Zeonor (plastic) wall. The inlet boundary
c Condition is a fixed temperature, assuming that the fluid in the reservoir equilibrates to room
temperature. At the outlet, heat transfer is allowed via convective flux. This assumes that the outlet
reservoir is far from the constriction. Testing reveals that this boundary condition incurs less than 2%
error, comparing favorably with setting a fixed temperature condition as done in [58]. Heat transfer
through the channel walls is described in Section 2.3.3 and Section 4 in a linearized boundary
condition for the channel wall.

\text{Inlet : } T = 293 \hspace{1cm} (48)

\text{Outlet : } q = \rho_m C_p u \cdot \nabla T \hspace{1cm} (49)

\text{Walls : } q = -\frac{k}{l} \xi \zeta (T - T_0), T_0 = 293 \hspace{1cm} (50)

• **Particle Velocity Field** Electrophoretic and dielectrophoretic force fields are determined from the
electric field

\[ u_{ep} = \frac{\varepsilon_m \xi p}{\eta} E \]  \hspace{1cm} (51)
S2.2 Methods

Numerical simulations of the fully coupled system were performed using COMSOL multiphysics modeling software. A representative system was developed and tested in COMSOL and then scripted for parametric studies of geometry ($r$), AC-to-DC ratio ($\alpha$), particle zeta potential ($\zeta_p$), wall zeta potential ($\zeta_w$), and conductivity ($\sigma_m$) in MATLAB.

S2.2.1 Particle Deflection and Trapping

Particle deflection and trapping are two metrics used in this work to evaluate the impact of electrothermal flow on iDEP devices. Dielectrophoretic deflection refers to the movement of particles transverse to the direction of flow owing to a negative DEP (nDEP) force ($f_{CM} < 0$) pointing away from the corners of the constriction (localized peaks in the electric field magnitude). Consider a particle entering the channel in the middle (i.e., $y = 50 \mu m$ in a 100 $\mu m$-wide channel, Fig. 1): in the absence of electrothermal and DEP forces, this particle will pass the constriction and exit the channel at the same location. nDEP forces deflect the particle from this pathline, causing the particle to be displaced away from the constriction edge and exit at a different location (e.g., $y = 75 \mu m$). Particle deflection and deflection difference in the presence of an electrothermal body force are defined in Fig. 2. We calculated particle pathlines by balancing Equation 34 against Stokes' drag ($u_{DEP} = f_{DEP}/6\pi \eta a$) for a 1 $\mu m$ diameter particle:

\[ u_{DEP} = \frac{\varepsilon_m a^2}{6\eta} \left( \alpha^2 \Re[\bar{f}_{CM} (\omega)] + 2\Re[\bar{f}_{CM} (0)] \right) \nabla E_{DC}^2 \]  

(52)

\[ u_{particle} = u_{EP} + u_{DEP} + u = \frac{\varepsilon_m \zeta_p}{\eta} E + \frac{\varepsilon_m a^2}{6\eta} \left( \alpha^2 \Re[\bar{f}_{CM} (\omega)] + 2\Re[\bar{f}_{CM} (0)] \right) \nabla E_{DC}^2 + u \]  

(53)

where $u$ is the fluid velocity due to electroosmosis and electrothermal flow. For the purposes of comparison and to isolate the effects of electrothermal flow, the Clausius-Mossotti factor was −0.5 in
all simulations, with no frequency dependence. Deflection was calculated by subtracting the inlet position of the middle particle pathline from its outlet position. In cases where the particle did not exit the channel, no data is reported.

Dielectrophoretic trapping in insulating systems occurs when nDEP forces overcome linear electrokinetic and fluid drag forces, preventing particles from passing the constriction region. We consider a particle entering the channel in the middle (i.e., $y = 50 \mu\text{m}$ in a $100 \mu\text{m}$-wide channel) and calculate its path due to the combined effects of electrophoresis, DEP, and fluid drag (combined electroosmotic and electrothermal flow, Equation 53). If the final (stagnation) position of the particle is not past the constriction, then the particle is considered `trapped”. We quantify this phenomenon by recording the value of $\alpha$ where trapping first occurs, $\alpha_{\text{trapping}}$.

**S2.2.2 COMSOL**

Three packages — convection and conduction (heat transfer), conductive media DC (electrostatic), and incompressible Navier-Stokes — were combined to solve for stationary fluid and electrokinetic velocity fields. The convection and conduction package was selected from the COMSOL Multiphysics Heat Transfer toolbox. Conductive media DC and incompressible Navier-Stokes packages were selected from the MEMS Electrostatics and MEMS Microfluidics toolboxes, respectively. The MEMS toolbox includes boundary conditions that correctly handle simultaneous electroosmotic slip along, and thermal conductivity across, the channel boundary.

Specific boundary conditions and governing equations are discussed and expressed previously for electromagnetic, thermal, and fluid systems in Section 2.

**S2.2.3 Geometry Definition**

Device geometry was defined and varied parametrically using MATLAB. The geometry consisted of a 1 cm-long, 100 $\mu$-m-tall channel with a 100 $\mu$-m-long constriction in the middle. The corners of the
constriction were filleted (rounded) with a 5 \(\mu\)m radius of curvature. The height of the constriction varied from 25 \(\mu\)m to 95 \(\mu\)m. We describe the constriction using a \``\text{constriction ratio}'', \(r\), of the bulk channel depth vs the channel depth in the constriction region.

**S2.2.4 Mesh Resolution and Refinement**

Mesh resolution in COMSOL was specified using a free (unstructured) triangular mesh. Maximum element sizes were specified on both the boundary and subdomain. The computational domain was meshed using a 100 000-element triangular mesh with maximum element resolution specified as 25 \(\mu\)m in the domain and 2.5 \(\mu\)m on the boundaries. Element density was highest near the boundaries and in the constriction region (Fig. 1), consistent with the regions of interest in the computational domain.

A series of test simulations, with electrothermal body force, was run over a range of element sizes to qualitatively assess the sensitivity of the solution to mesh resolution. Element size for the unstructured triangular mesh in COMSOL was set by defining the maximum element size on the subdomain and boundaries. The coarsest mesh was defined using a 50 \(\mu\)m maximum boundary element size and a 500 \(\mu\)m maximum subdomain element size. The simulation was run over this mesh and four subsequent refinements. These simulations contained 1827, 4756, 16 566, 63 426, and 250 180 elements, respectively. The relative error was calculated using Equation 54 assuming that the finest resolution mesh was correct.

\[
\bar{\Omega}_n = \frac{\sum_{p} X_n - X_0}{P}
\]

where \(\bar{\Omega}_n\) is the average relative error at a resolution of \(n\), \(X_n\) is the value of a simulation variable (e.g., \(u\)) at a point \(p\) on the coarse, unstructured mesh, \(P\) is the total number of grid points, and \(X_0\) is the solution at the same point on the highest resolution mesh. Residuals calculated in this manner for
the $x$ and $y$ components of velocity and the fluid temperature were less than $1 \times 10^{-4}$ and indicate first-order convergence. Verification of the ODE formulation was performed by calculating a 1-D temperature distribution in a stagnant fluid and calculating the Laplace solution for electroosmotic flow in an isothermal case. Numerical results matched the analytical results in both cases.
Figure S1: The electrothermal body force is directed down gradients in fluid electrical parameters, i.e. down gradients in temperature. Arrows (red, color online) show the direction of the electrothermal force (Equation 13). Filled contours correspond to the magnitude of the electrothermal force and are logarithmic. The highest contour groups all electrothermal force magnitude values above 250N/m$^3$ for clarity (maximum, 1,865N/m$^3$). Simulation parameters are those listed in Table 2 with $\alpha = 40$ and include the electrothermal body force term in the Navier-Stokes equations.