

# Numerical and Analytical Studies of Electrothermally Induced Flow And Its Application For Mixing and Cleaning in Microfluidic Systems

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## ABSTRACT

This paper presents both analytic and simulation results of electrothermal flow in microfluidic systems. It also considers the application of this phenomenon to microscale mixing and cleaning. The basic operation requires application of an alternating electric field at high frequency and moderate amplitude to create thermal gradients. This in turn will induce both Columbic and dielectric forces to the bulk fluid due to the variation of electrical permittivity and conductivity of the buffer solution with respect to temperature. First, electrothermal flow in a simple two-electrode structure is investigated via analytical means. Subsequently, the detailed framework for a full-scale multiphysics simulation of electrothermal flow in complex devices is described. Using simulations, it is revealed that mixing can be increased dramatically due to the presence of electrothermal flows. Chaotic nature is established via exponential growth of the interface. Orders of magnitude improvement in the time required to washout contaminants trapped in microcavities is also demonstrated.

**Keywords:** electrothermal induced flow, micro-mixing, micro-cleaning

## 1 INTRODUCTION

Electrothermally induced flow often occurs when an electric field is applied to an electrolyte solution. The fluid is subjected to Columbic and dielectric forces due to variations in the dielectric properties of electrical permittivity and conductivity, respectively, as a function of temperature [1]. Though Joule effect is often the primary mechanism for heating the solution, other external sources, such as laser illumination, are also capable of inducing thermal gradients, and hence electrothermal flows. Recently, use of this phenomenon to enhance the biomolecular detection in an immunosensor [2] has been reported. The present paper focuses on analytical and numerical investigations of this flow phenomenon and its application, particularly in the context of mixing and cleaning in microsystems.

Electrothermally induced flow depends on a variety of physical and process parameters such electrical conductivity and permittivity, voltage and frequency of applied electric field, as well as geometric parameters such as electrode configuration and channel dimensions. To understand the underlying complex physics, one needs to solve the strongly-coupled equations that describe fluid

flow, temperature and electric field. In general, analytic solutions are extremely challenging to obtain. Computational methods must be employed to solve the governing equations, in practical situations. The present paper focuses on analytical and also develops full-scale computational solutions to electrothermal flow. The analytical solution is obtained via dual integral/series and Green's function methods [3, 4] applied to solve simplified governing equations. The simplification is affected by noting small temperature variations and heat conduction dominating convection. In the computational approach, the full set of governing equations is solved, using a finite volume approach [5].

Mixing and cleaning/wash-out are some of the fundamental and universal challenges that need to be addressed in developing integrated microsystems. Although the typical characteristic length scale associated with microdevices is small, diffusion alone does not provide adequate mixing. This often leads to inappropriate device dimensions, operational times or complex mixing devices/schemes. In the present paper, we demonstrate that electrothermally induced flow can be easily exploited (by simply adjusting geometry and/or field) to accomplish these tasks with considerable savings in real-estate and time. Using high-fidelity simulations, it will also be shown that this flow induces a chaotic mixing based on short term Poincare section and growth of a material segment. Sample application demonstrations include mixing in a T-Junction and cleaning of microcavities.

## 2 ELECTROTHERMAL FLOW

### 2.1 Formulation

The problem of onset of fluid flow due to temperature gradient in microfluidic systems has recently drawn attention [1]. It has been shown that even a small variation in the temperature has the potential to induce electrothermal flows that can be strong enough to shield other physical processes, for example dielectrophoresis [2]. The force density due to application of an electric field is given by [6]

$$\vec{f} = \rho_q \vec{E} - \frac{1}{2} E^2 \nabla \epsilon + \frac{1}{2} \nabla \left[ \rho_m \left( \frac{\partial \epsilon}{\partial \rho_m} \right)_T E^2 \right] \quad (1)$$

where  $\rho_e$  is the charge density,  $E$  is electric field,  $\epsilon$  is permittivity,  $\rho_m$  is material density. The first, second and third terms on the right side of the above expression are Coulomb force, DEP force and electrostriction force, respectively. For AC electric field, the averaged force density is approximately given by [1]

$$\langle \vec{f} \rangle = \frac{1}{2} \text{Re} \left[ \frac{\sigma \varepsilon (\alpha - \beta)}{\sigma + i \omega \varepsilon} (\nabla T \cdot \vec{E}_0) \vec{E}_0^* - \frac{1}{2} \varepsilon \alpha |\vec{E}_0|^2 \nabla T \right] \quad (2)$$

in which linear variation of electric properties are assumed. Here

$$\alpha = \frac{1}{\varepsilon} \frac{\partial \varepsilon}{\partial T}, \quad \beta = \frac{1}{\sigma} \frac{\partial \sigma}{\partial T} \quad (3)$$

where  $\sigma$  is electrical conductivity and  $T$  is temperature. In this paper, we focus attention only on Joule heating, which is expressed as:

$$j = \sigma E^2 \quad (4)$$

The conservation equation for heat is:

$$\rho_m c_p \frac{\partial T}{\partial t} + \rho_m c_p (u \cdot \nabla) T = k \nabla^2 T + \sigma E^2 \quad (5)$$

where  $c_p$  is the specific heat capacity,  $u$  is velocity vector, and  $k$  is thermal conductivity. The fluid flow is governed by Navier-Stokes and continuity equations:

$$\rho_m \left[ \frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right] = -\nabla p + \mu \nabla^2 \vec{u} + \vec{f} \quad (6)$$

$$\nabla \cdot \vec{u} = 0$$

where  $p$  is pressure and  $f$  is source due to electrothermal effect. The electric field satisfies

$$\vec{E} = -\nabla \Phi, \quad \frac{\partial \rho_e}{\partial t} + \nabla \cdot \vec{j} = 0 \quad (7)$$

$$\nabla \cdot \vec{D} = 0, \quad \vec{D} = \varepsilon \vec{E}, \quad \vec{j} = \sigma \vec{E}$$

where  $\phi$  is electric potential. Solutions to the coupled Equations (5) to (7) subjected to appropriate boundary conditions determine thermal, electric and flow fields.

In order to study mixing and cleaning of analytes in microfluidic devices, two modeling approaches are used. When the size of the analyte is very small (sub-micron) and inertial acceleration relative to the fluid can be neglected, a continuum-based advection/diffusion equation for the concentration of analytes is solved:

$$\frac{\partial c_i}{\partial t} + \frac{\partial J_{ij}}{\partial x_j} = 0, \quad J_{ij} = -D_i \frac{\partial c_i}{\partial x_j} + u_j c_i - z_i c_i \omega_i \frac{\partial \phi}{\partial x_j} \quad (8)$$

Here  $D_i$  is diffusion coefficient and  $\omega_i$  is electrophoretic mobility of the  $i^{\text{th}}$  analyte. For larger particles, where inertial acceleration must be accounted for we use

$$m_p \frac{du}{dt} = F_E + F_H, \quad u = \frac{ds}{dt} \quad (9)$$

Here  $m_p$  is particle mass,  $F_E$  and  $F_H$  represent electrothermal and hydrodynamic forces, respectively.

## 2.2 Exact Solution

Equations (5)-(7) are coupled non-linear PDEs that usually preclude analytic solutions. However, as has been noted [1], these governing equations can be simplified for steady state by careful examination of relative magnitude of each terms involved. In microfluidic systems, characterized by slow viscous flow, convection terms can be safely neglected. The resulting linear equations admit analytic solutions for simple electrode configurations. In this

section we briefly present exact solutions for a co-planar electrode structure as illustrated in Figure 1. For mathematical simplicity, we consider a DC field.

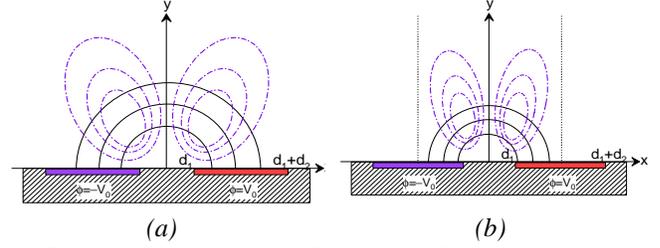


Figure 1 Electrothermal flow induced by (a) a pair of electrodes (b) array of equally spaced electrodes. The solid lines and the dashed lines illustrate electric field and streamlines, respectively

For a single pair of electrode, the normalized electric potential (by electrode potential  $V_0$ ) is given by the Fourier integral

$$\phi(x, y) = \int_0^\infty A(\lambda) \lambda^{-1} e^{-\lambda y} \sin(\lambda x) d\lambda \quad (10)$$

where

$$A(\lambda) = \frac{2}{K(a/b)} \sum_{n=1}^{\infty} (-1)^{n-1} P_{n-1}(\cos u) J_{2n-1}(\lambda b) \quad (11)$$

and

$$u = 2 \cos^{-1} a/b, \quad a = d_1, \quad b = d_1 + d_2 \quad (12)$$

Here  $P_n$  and  $J_n$  are Legendre and Bessel functions of order  $n$ , respectively.  $K$  is the complete elliptic function of the second kind.

The general solution to temperature is

$$T = -\frac{\sigma \phi^2}{2k} + Ax + By + C \quad (13)$$

where  $A$ ,  $B$  and  $C$  are constants and will be determined by physical considerations. Since the heat conduction on electrode is very high, we assume the temperature is constant. Thus we have

$$T = T_0 - \frac{\sigma V_0^2 \phi^2}{2k} \quad (14)$$

The electrothermal force is calculated by equation (2) and the solution for flow is obtained by Green's function method

$$u_i(x, y) = \iint_{S_0} G_{ij}(x_1, x_2, x_{0,1}, y_{0,2}) f_j(x_{0,1}, y_{0,2}) dS_0 \quad (15)$$

where  $G_{ij}$  is Green's function or Stokeslet in the presence of a planar boundary as given in [4]. Following a similar approach, we can also obtain an exact solution for a periodic array of electrodes, in which case, the electric potential is given in terms of Fourier series [3]

$$\phi(x, y) = \sum_{n=1}^{\infty} \frac{A_n}{\lambda_n} \cos \lambda_n e^{-\lambda_n y}, \quad \lambda_n = n - \frac{1}{2}; \quad A_n = \frac{P_{n-1}(\cos c)}{K(\cos \frac{c}{2})} \quad (16)$$

## 2.3 Numerical Method

In most practical devices, the electrode geometry as well as the operating conditions are substantially complex,

precluding the linearization assumption. In this scenario, the full-set of governing equations need to be solved using numerical methods. In this paper, finite volume method based solver has been developed [6] to solve Equations (5) to (7) in a coupled manner. In addition to these, Equations (8) and (9) are also solved to study mixing and cleaning phenomena. This computational capability is available in CFD-ACE+, CFDRC's commercial multi-physics simulation package. The numerical method has been validated by comparing the simulation results with that of analytical solution presented in previous section.

### 3 RESULT AND DISCUSSION

First, analytical results for the co-planar electrode array as shown in Figure 1(b) is presented. The electrode width and gap are  $50\mu\text{m}$  and DC signal of  $\pm 2\text{V}$  is applied to adjacent electrodes. The room temperature is kept at  $300\text{K}$ . In all simulations, KCl solution is used as running buffer. The electric and thermal properties of the solution are listed in the following table

**Table: Properties of Electrolyte Solution**

Property	Value
Density	$1000 \text{ kg/m}^3$
Viscosity	$10^{-6} \text{ m}^2/\text{s}$
Thermal Conductivity	$0.6 \text{ W/m-K}$
Heat capacity	$4100 \text{ J/kg-K}$
Electric Conductivity	$0.056/\text{Ohm-m}$
Relative Permittivity	78
$\alpha$	$-0.004 / \text{K}$
$\beta$	$0.02 / \text{K}$

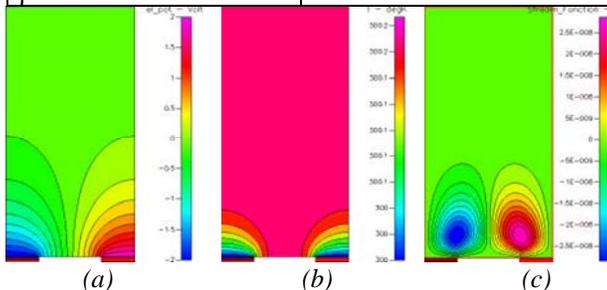


Figure 2 Contours of electric potential, temperature distribution and flow pattern for array of  $50\mu\text{m}$  electrodes.

The electric, thermal and flow fields are shown in Figure 2. The numerical and analytic results are graphically indistinguishable and the relative margin is less than 1%. A pair of circulation zones close to the electrode edges has been observed with a maximum velocity ( $\sim 4 \mu\text{m/s}$ ). This is achieved very close to the electrode edge. The maximum temperature difference is very small (0.2 K). From equation (1)-(7) we see the temperature and body force grow at least quadratically with the applied signal strength.

The circulation zones near the electrode edge created by the electrothermal effect appear to be universal. The flow direction is determined by dependency of electrical properties ( $\alpha$  and  $\beta$ ) on temperature. Such a rotational flow usually causes stretching of the material lines in the fluid. If the stretched material lines are folded back, and the process

repeated, it will lead to chaotic mixing. This concept has been explored by simulating the mixing of an analyte in a closed rectangular cavity of  $100 \times 200 \mu\text{m}$  as shown in Figure 3(a). Initially the analyte occupies only top half of the cavity. A passive scalar model (Eq. 8) is used in this simulation. Several electrodes are placed on cavity surfaces (locations shown in the figure) and are energized with a field of  $\pm 5\text{V}$  and  $10\text{kHz}$ . In the sample protocol, the bottom electrode is switched on for 2 seconds and then electrodes on two side surfaces are turned on, followed by the electrodes on the top surface. Figure 3(a) shows particle configurations, at  $T=0$  and  $12\text{s}$ . At 12 seconds, particles are distributed uniformly. In contrast diffusive mixing will take several minutes when the diffusion is on order of  $O(10^{-10} \text{ m}^2/\text{s})$  to achieve the same result

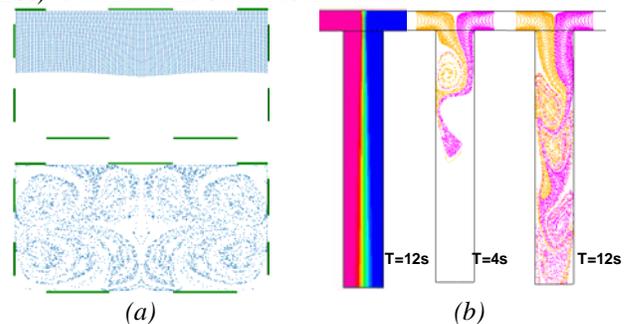


Figure 3 (a) Location of particles initially occupying top half of cavity for  $T=0.1$  and  $12\text{s}$ . (b) Mixing of two streams of analyte in a T-junction compared with pure diffusion.

The same concept is demonstrated in a continuous flow situation in Figure 3(b). Here in a T-junction, two streams of fluid containing samples are injected into the main channel at a flow rate of  $100 \mu\text{m/s}$ . The channel height is  $20\mu\text{m}$  and the main channel width is  $40\mu\text{m}$  and the electrodes are placed on side surfaces of the channel. Spreading of the interface by diffusion alone is very slow and takes hours. The closed cavity study is revisited with two analytes (SPA,  $c=1\text{nM}$ , SPB,  $c=3\text{nM}$ ) initially occupying the top and bottom halves. The top and bottom electrodes are subsequently energized for 5 seconds, with the same potential on the electrode. The concentration distributions, across the channel, are quantitatively examined in Figure 4. Uniform concentrations across the cavity are achieved within 5 seconds using electrothermal flow, while under diffusive action the concentration profiles are far removed from equilibrium even after 100 seconds. This establishes that mixing can be increased dramatically due to the presence of electrothermal flows.

In order to further investigate the mixing efficiency, the evolution of a tracer blob in the cavity is simulated. Due to the symmetry of the cavity, only half of the geometry is used in the simulation model. Results of advection-diffusion based continuum and particle dynamic models are shown in Figure 5. A blob of  $10 \times 10 \mu\text{m}$  is placed at  $30\mu\text{m}$  from bottom and symmetric plane. The signal is the same as used in Figure 3(a) and the system is energized and tracked for a period of 6 seconds. The particle lines (Figure 5(b)) and the concentration fields

(Figure 5(b)) clearly illustrate chaotic mixing. The short-term growth of the length of the sample-fluid interface (normalized by the initial interface) is shown in Figure 6. Exponential growth of this measure confirms the chaotic behavior.

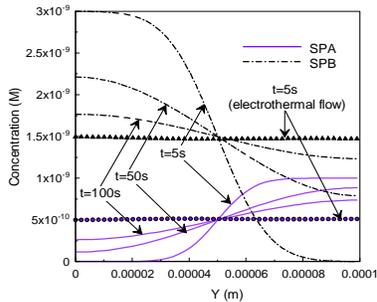


Figure 4 Comparison of concentration on a vertical line across the cavity with/without electrothermal flow

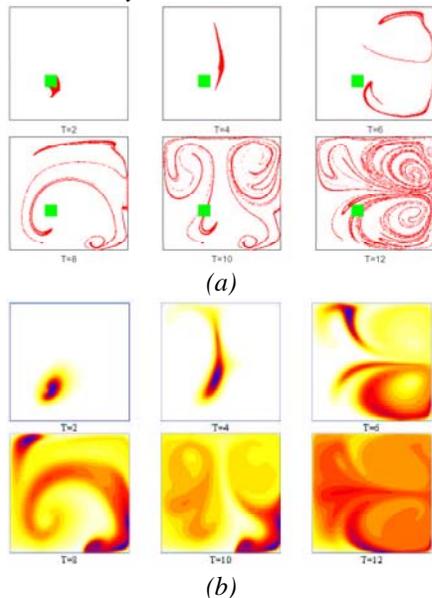


Figure 5. Evolution of a 10x10 mm material blob in a cavity Simulated via (a) Particle Tracking Model and (b) Advection-Diffusion Model

Another important application in microsystems is cleaning or removal of analytes. Contaminants are often trapped in nooks, crevices and intentionally designed cavities interfering with the accuracy of subsequent analyses. By combining electrothermal and pressure driven flow, it is possible to design an efficient cleaning mechanism which removes >99% of the trapped contaminants in a short period of time. We consider a cavity (Figure 7, 20x20 $\mu$ m) located at the bottom of a channel (height=20 $\mu$ m), where the contaminant (10,000 particles) is initialized. A pair of 10 $\mu$ m electrodes is placed as shown and energized by an AC signal. First a 5V/10KHz signal is applied for 0.5 second, followed by a pressure driven flow in the main channel at the rate of 50 $\mu$ m/s for 0.5 seconds. This process is repeated for 3 seconds. Figure 7 illustrates how the particles are levitated from the cavity (due to the electrothermal flow) and subsequently flushed-out by the pressure driven flow in the main channel. Defining the

efficiency of the removal process as (%) of initial particles flushed away, the combined electrothermal-pressure driven system has an efficiency of 80% (Figure 8). In comparison a pure pressure driven system has an efficiency of 10% over the same period. Relying on diffusion-alone to entrain the particles will take days.

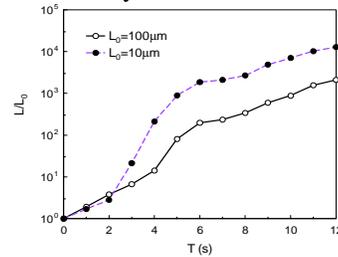


Figure 6. Short-term evolution of interface length

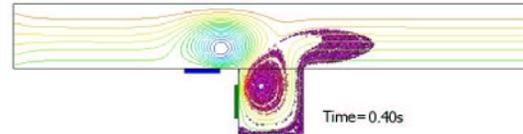


Figure 7 Removal of contaminant in a cavity

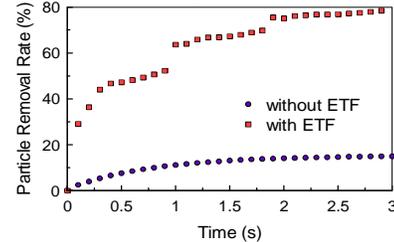


Figure 8 Contaminant removal rate for combining electrothermal and pressure driven flow system

## 4 SUMMARY

Electrothermal flow in microsystems has been analyzed using both analytical and full-scale numerical simulations. The simulations show that mixing can be effected in a very short period of time (reduced by at least three orders of magnitude) compared with diffusion-based mixing. Besides, this mixing also exhibits chaotic behavior. Combination of pressure-driven and electrothermal flow can be exploited to accomplish a fast and highly efficient cleaning (of trapped contaminants) in microsystems. Further investigations of this phenomenon are underway.

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