

# Simulation of electrically–excited flows in microchannels for mixing application

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## ABSTRACT

In the present paper we propose a method for improved mixing in microchannels. The basic idea is to excite a secondary vortex flow around an obstacle within the micromixer by applying an external oscillatory electrical field. For a simple setup with a single cylindrical obstacle our numerical (FEM) simulations demonstrate the potential of this method. We find that mixing is improved due to an enlargement of the “interfacial” area between the liquids. Further, a dimensionless quantitative measure for the increase of the “interfacial” area is proposed.

**Keywords:** electrical double layer, electrohydrodynamics, microchannel, microflow, micromixer, vortex street

## 1 INTRODUCTION

Within microchips for chemical or biological analysis ( $\mu$ TAS) and within microreactors, mixing of liquids plays an important role. In general, efficient mixing of liquids can be viewed as a two step process: Firstly, the “interfacial” area between the liquids to be mixed is increased and the thickness of the liquid lamellae is reduced. Secondly, mass diffusion completes the mixing on the molecular length scale. Of course, between two miscible liquids no real interface exists. We nevertheless, term the area where both liquids are in contact “interfacial” area hereon. In macroscopic flows the channel Reynolds number  $Re = u_0 d_0 / \nu$  is typically large and thus, inertia forces and instabilities serve to increase the “interfacial” area between the liquids. Here,  $u_0$  is the mean velocity,  $d_0$  is the width of the microchannel and  $\nu$  is the kinematic viscosity of the liquid. In microchannels, in contrast, the channel Reynolds number is usually small, i.e. the flows remain laminar. Since we cannot rely on instabilities to create large “interfacial” areas for effective diffusion in microchannels, other means have to be considered.

A first class of approaches towards effective mixing engages the mixer geometry to tailor large “interfacial” areas. This method is called multilamination (see e.g. [1]). In general such mixer designs need complex three-dimensional structures, which hardly allow for cheap

production. A second class of approaches engages oscillating flows from side channels into the main channel for the creation of folded “interfacial” areas. The driving for the oscillating flows in the side channels is provided by mechanical devices (e.g. pumps, membranes).

The approach adopted in the present work is to apply an oscillating electrical field of appropriate frequency, amplitude and orientation to the flow field. This will induce time–dependent electrical forces in the electrical double layers at liquid/solid boundaries. These forces lead to a time–dependent flow even at low Reynolds numbers and likewise provide folding. Thus, by increasing the “interfacial” area the efficiency of mixing will be improved.

## 2 TREATMENT OF THE ELECTRICAL DOUBLE LAYERS

Usually liquids contain positive and negative charges (see e.g. [2]). In the liquid bulk cations and anions are homogeneously distributed and, thus, the liquid bulk appears to be electrically neutral. Since the walls consist of different molecules, charges will be present likewise at the walls. An excess of one type of ions, therefore, is induced in the liquid near the walls, resulting locally in a non–zero net charge. In the Debye–Hückel approximation the net charge distribution  $\rho_e$  varies exponentially from its value at the wall  $q_W$  to zero in the liquid bulk (cf. equation (1)). The length scale of the decay is given by the Debye length  $l_D$ , which is usually smaller than  $1 \mu\text{m}$ ;

$$\rho_e(y) = -\frac{q_W}{l_D} e^{-y/l_D}. \quad (1)$$

These non–neutral electrical layers at the walls are termed electrical double layers (EDL), cf. figure 1. Only within these layers can electrical forces be induced.

Even in microchannels the Debye length  $l_D$  is usually much smaller than the channel width  $d_0$ . Hence, in a numerical simulation the mesh near the walls would need substantial refinement to reasonably resolve the electrical double layers. This would make computations fairly expensive. Since the influence of the electrical forces is confined to the immediate vicinity of the walls, it appears straight forward to engage matched asymptotic expansions to infer an inner solution (valid near the

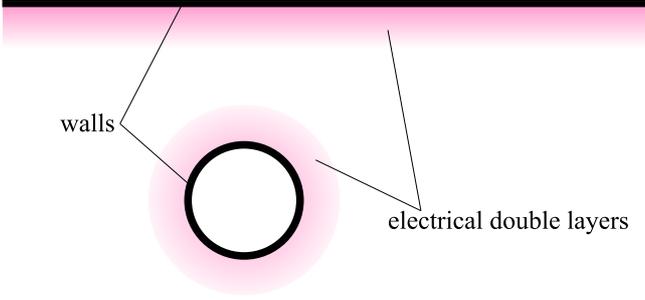


Figure 1: Electrical double layers at various walls.

wall) which is matched to an outer solution (in the liquid bulk), which may still be obtained numerically. Essentially, this method provides modified boundary conditions for the liquid bulk solution. For example, the conventional no-slip boundary condition at the walls will be replaced by tangential slip if tangential electrical forces act in the electrical double layer.

The governing equations for an incompressible, time-dependent and two-dimensional flow in the presence of an applied electrical field  $\mathbf{E}$ , are non-dimensionalized with the microchannel data, namely with the length scale  $d_0$ , with the velocity scale  $u_0$ , with the time scale  $d_0/u_0$  and with the viscous pressure scale  $\mu u_0/d_0$ . From the continuity equation and for the Navier–Stokes equations we obtain

$$U_X + V_Y = 0, \quad (2)$$

$$\begin{aligned} Re [U_T + UU_X + VU_Y] = \\ -P_X + U_{XX} + U_{YY} - \epsilon^{-2} \bar{\Pi}_x e^{-Y/\epsilon}, \end{aligned} \quad (3)$$

$$\begin{aligned} Re [V_T + UV_X + VV_Y] = \\ -P_Y + V_{XX} + V_{YY} - \epsilon^{-2} \bar{\Pi}_y e^{-Y/\epsilon}, \end{aligned} \quad (4)$$

where  $(X, Y)$  are the wall-tangential and wall-normal coordinates and  $(U, V)$  are the velocity components in tangential and normal direction. The origin of the coordinate system is at the wall and the capital indices denote partial derivatives with respect to the space variables  $(X, Y)$  and with respect to time  $T$ .  $\epsilon = l_D/d_0$  is the ratio of the length scales involved and due to  $l_D \ll d_0$  we have  $\epsilon \ll 1$ . Further,

$$\begin{pmatrix} \bar{\Pi}_x \\ \bar{\Pi}_y \end{pmatrix} = \frac{q_W l_D}{\mu u_0} \begin{pmatrix} E_x \\ E_y \end{pmatrix} \quad (5)$$

is a dimensionless group, expressing the ratio of electrical and viscous forces.  $q_W$  denotes the charge at the wall, it is linked via  $q_W = \tilde{\epsilon} \zeta / l_D$  with the zeta potential  $\zeta$  and the dielectrical constant  $\tilde{\epsilon}$  of the liquid.  $\mu$  is the dynamic viscosity of the liquid and  $E_x, E_y$  denote the tangential and normal components of the applied

electrical field  $\mathbf{E}$ . By rescaling the system (2-4) an approximate inner solution for the flow near the wall can be derived analytically. In the tangential direction the dominant balance is between electrical forces and viscous forces; in the normal direction the electrical forces are balanced by pressure forces. This inner solution near the wall is given by

$$U_W(X, \tilde{Y}) \simeq \bar{\Pi}_x (e^{-\tilde{Y}} - 1), \quad (6)$$

$$V_W(X, \tilde{Y}) \simeq 0, \quad (7)$$

$$P_W(X, \tilde{Y}) \simeq \epsilon^{-1} \bar{\Pi}_y e^{-\tilde{Y}} + P_B(T, X, 0). \quad (8)$$

In equations (6-8)  $\tilde{Y} = y/l_D$  is the rescaled wall-normal coordinate and  $P_B$  is the pressure from the outer solution in the liquid bulk.

The bulk flow is governed by the system (2-4), whereas the electrical terms can be ignored, since they decay rapidly as we move away from the immediate wall vicinity. This system of equations can be solved numerically by invoking standard computational fluid dynamics (CFD) codes. The boundary conditions for the computation of the liquid bulk solution can be derived from the inner solution (6-8) by considering the limit  $\tilde{Y} \rightarrow \infty$ . We obtain the kinematic boundary conditions

$$U_B(T, X, 0) \simeq -\bar{\Pi}_x, \quad (9)$$

$$V_B(T, X, 0) \simeq 0. \quad (10)$$

### 3 PRINCIPLE OF AN ELECTRICALLY-EXCITED MICROMIXER

The basic concept of an electrically-excited micromixer is shown in figure 2. Two liquids enter the mixer via two supply channels. Both liquids merge into a single channel, where mixing occurs, and through this common channel the mixture leaves the device. Within the mixing section an obstacle, e.g. a cylinder, is installed. Electrical double layers are present both around this obstacle and at the channel walls. An oscillating electrical field is applied with its orientation perpendicular to the main flow direction. As a consequence, an oscillatory secondary flow around the obstacle is induced by electrical forces, acting in the electrical double layer. Alternating periodically, detaching vortices arise and are swept downstream to form a vortex street. Due to the rotating vortices the “interfacial” area between the liquids is stretched and folded. This significantly increased “interfacial” area provides via more effective diffusion greatly improved mixing.

### 4 RESULTS AND DISCUSSION

In our time-dependent and two-dimensional Finite-Element simulations we investigate the pure flow field

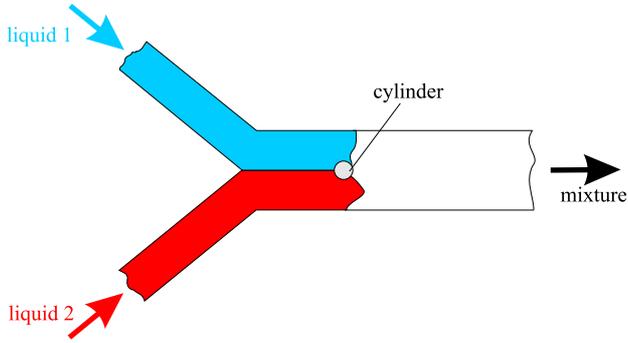


Figure 2: Principle of a simple micromixer with a cylinder as an obstacle for electrical excitation.

in a micromixer with and without electrical excitation. Diffusion between the liquids is not yet considered, all properties of both liquids are assumed identical. A single circular cylinder is positioned as an obstacle in the microchannel, while the ratio of cylinder diameter and channel width is  $d_{cyl}/d_0 \simeq 0.07$ . The Reynolds number  $Re_{cyl} = u_0 d_{cyl}/\nu$  based on the cylinder diameter  $d_{cyl}$  is  $Re_{cyl} = 10$ ; this is clearly below the threshold for a (naturally-excited) Karman vortex street and, thus, all time-dependent flow phenomena are due to the external electrical excitation. The amplitude of the electrical field is  $\hat{E} = 50 \text{ V/mm}$ , the field is oriented vertically ( $E_x = 0$ ). The excitation frequency can be expressed in non-dimensional form as a Strouhal number  $St_{cyl} = f d_{cyl}/u_0$  and we have  $St_{cyl} = 0.1$  in figure 3b. We visualize the time-dependent flow field by repeatedly adding coloured particles at fixed positions within both liquids in given time steps. This gives streak lines in both liquids, so the virtual “interfacial” area can be found where both colours meet.

As can clearly be seen in figure 3a, the flow without excitation remains steady and the “interfacial” area between the liquids, as visualized by the separation line between the upper blue and the lower red streak lines, remains small. Diffusion can only act along the “interfacial” plane downstream of the cylinder, which separates both liquids. In contrast, within the flow with electrical excitation, as shown in figure 3b, detaching vortices stretch and fold the separation line between both liquids repeatedly and, thus, the “interfacial” area is significantly increased. Therefore, diffusion is more effective and mixing is greatly enhanced.

It is, of course, of interest to optimize the excitation in such a flow. The optimal excitation will certainly occur if we excite in resonance with the inner time scale of the flow in a spatially-repeated fashion. There are two obvious parameters which have some potential in that respect, namely (i) the excitation frequency (or  $St_{cyl}$ ) and (ii) the multiple arrangement of obstacles at an optimal distance. To demonstrate the effect of the excitation

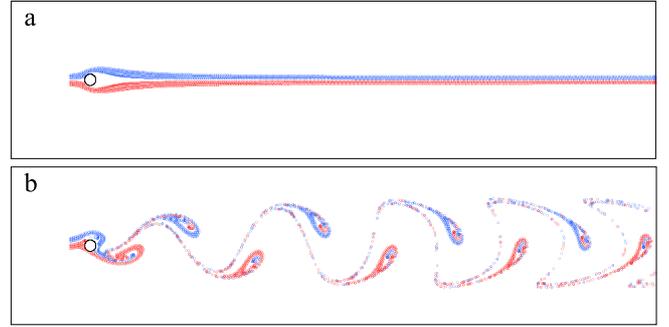


Figure 3: Results for  $Re_{cyl} = 10$ ,  $St_{cyl} = 0.1$  without (a) and with (b) electrical excitation.

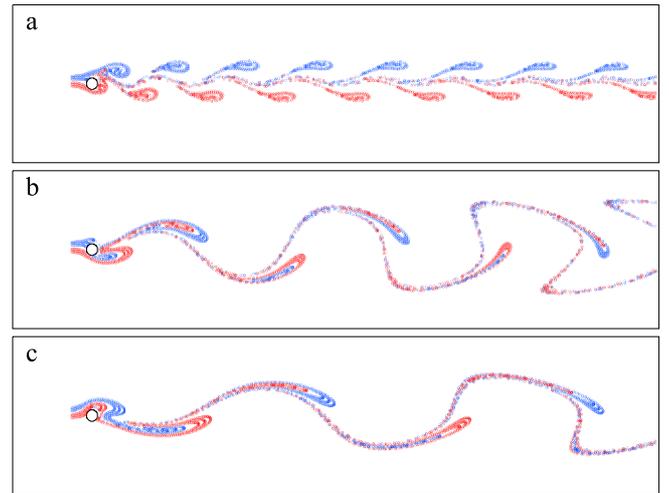


Figure 4: Variation of flow structures with excitation frequency. Parameters are  $Re_{cyl} = 10$  and (a)  $St_{cyl} = 0.167$ , (b)  $St_{cyl} = 0.067$ , (c)  $St_{cyl} = 0.05$ .

frequency, figure 4 in addition to figure 3b shows simulation results for  $Re_{cyl} = 10$  and various excitation frequencies. For fast oscillations of the electrical field with  $St_{cyl} = 0.167$ , figure 4a demonstrates that the detaching vortices hardly interact, and as a result the “interfacial” area barely increases. Likewise, the vertical extent of the vortex street remains small and, hence, the two liquid layers stay largely separated. For lower excitation frequencies the interaction enhances, as can be seen in figures 4b,c with  $St_{cyl} = 0.067$ ,  $0.05$ . We recognize the separation line between the liquids to be stretched and folded, providing thin liquid lamellae which allow for effective diffusion. Also, the vertical extent of the vortex street increases. On the other hand, as the excitation frequency is decreased, less vortices emerge from the cylinder per time period, which may ultimately lead to a decrease of the net “interfacial” area. This reasoning suggests that an optimal excitation frequency exists, which provides the largest possible “interfacial” area.

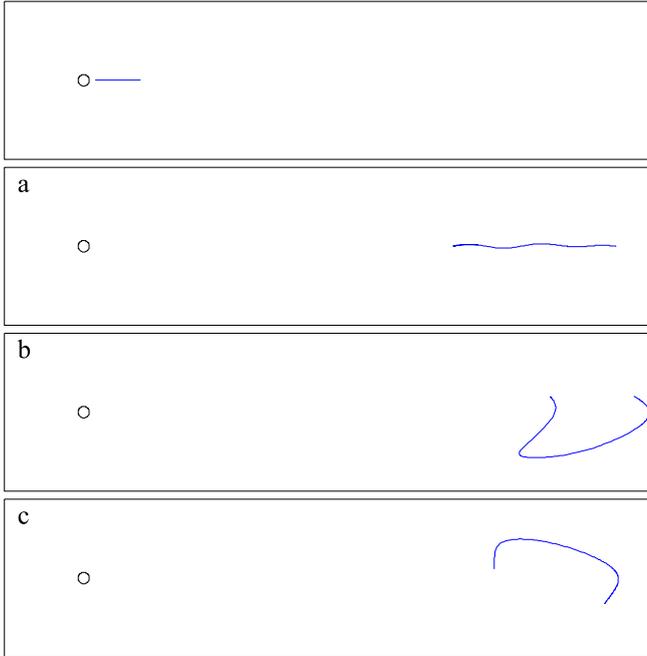


Figure 5: Comparison of separation lines for various excitation frequencies.  $Re_{cyl} = 10$  and (a)  $St_{cyl} = 0.167$ , (b)  $St_{cyl} = 0.067$ , (c)  $St_{cyl} = 0.05$ .

From figures 3,4 it is hardly possible to quantitatively evaluate the mixing improvement. For that reason we introduce a measure for the increase of the “interfacial” area by tracking a separation line of defined initial length. The line is stretched and folded while being swept downstream and, thus, the time evolution of the “interfacial” area between the liquids can be quantified. A line of particles is placed at the separation line at  $T = 0$ , cf. top of figure 5. Figures 5a-c show the shape of the separation lines at  $t = 45 d_{cyl}/u_0$  for the same parameters as in figure 4. It is obvious, that for high excitation frequencies (figure 5a) some stretching and little folding of the separation line occurs. More folding is observed if a lower excitation frequency is used, as seen from figures 5b,c. A dimensionless measure for the increase of the “interfacial” area is readily obtained by computing the ratio of the actual length  $l_{a,b,c}$  of the separation lines and its initial length  $l_0$ . We obtain for the three cases  $l_{a,b,c}/l_0 = 4.3, 5.6, 4.4$ . This supports our expectation concerning an optimal excitation frequency, which is around  $St_{cyl} = 0.067$  (case b).

## 5 SUMMARY AND OUTLOOK

In the present paper we proposed a method for improved mixing in microchannels. The basic idea is to excite a secondary vortex flow around an obstacle within the micromixer by applying an external oscillatory electrical field. An obstacle is required because the sur-

rounding electrical double layers allow induction of electrical forces. For a simple setup with a single cylindrical obstacle, numerical (FEM) simulations are engaged to evaluate the benefit of such an electrical excitation. Within the numerical simulations the electrical double layer is not really resolved. Instead, a matched asymptotic method is used to infer analytical approximate solutions for the immediate wall regions. The coupling of the wall solutions and the numerical bulk solution takes place via the boundary conditions: The bulk flow, e.g., experiences a slip boundary condition at solid boundaries if tangential electrical forces act within the electrical double layers.

The FEM simulations demonstrate the potential of this method. We find that mixing is improved due to an enlargement of the “interfacial” area between the liquids. Further, a quantitative measure for the increase of the “interfacial” area is introduced, which should allow one to optimize the parameters to achieve the best possible mixing.

The above simulations are, of course, only a first step in the development of an electrically-excited micromixer. The simulations are simplified in various respects. Simulations with two liquids of different properties, including interliquid diffusion, are certainly necessary to get more insight into the role of non-symmetric electrical effects and into the role of mass diffusion. Further, at some stage three-dimensional simulations may help to assess the (damping) influence of all channel walls. The latter point is particularly important with regard to a comparison of simulations and validation experiments, which are presently in preparation. Validation experiments are essential to prove the present theoretical modelling.

This first setup of a micromixer is only the simplest possible configuration, which allows for optimization in various directions. Given e.g. the above dimensionless measure of the “interfacial” area, or some other appropriate criteria, the optimal excitation frequency is readily inferred. Multiple obstacles, arranged at optimal distances are further strong candidates for a substantial improvement of the mixing. Other parameters, like obstacle geometries different from a simple cylinder, the obstacle material or the time function and amplitude of the electrical field  $\mathbf{E}(t)$  may likewise be helpful in that respect.

## REFERENCES

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