ELECTROOSMOTIC INJECTION AND CHEMICAL KINETICS IN MICRO REACTORS

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INTRODUCTION
The study of fluid flow in microchannels is of significant interest due to its application in a wide area of fields ranging from microscale flow injection, cooling of microchips, fuel vaporizer and micro reactors for chemical and biological systems. Design of effective electrokinetic micro reactors requires in-depth understanding of the electrokinetic phenomena and bulk reactions of species in the micro reactor. Although electrokinetic flows are popularly used for applications in the field of capillary electrophoresis (CE) [1], the phenomena of electroosmosis can be conveniently used for bulk transport and mixing of reagents. Electroosmosis occurs when the electrical double layer (EDL) near a solid-liquid interface is created by an external electric field. The uniqueness of electroosmotic flow (EOF) is characterized by plug velocity profile having uniform flow. Devasenathipathy et al. [2] showed that EOF offers a number of significant advantages over conventional pressure driven flow like reduced sample diffusion and controlled sample movement.

The electrokinetic phenomena can be extended to micro reactor techniques such as micro total analysis systems (µTAS) and lab-on-a-chip (LOC). This work presents the numerical modeling of a liquid phase chemical reaction in a micro reactor using the principles of electroosmotic pumping.

METHODOLOGY
The design of the 2D model used in the simulation is shown in Fig. 1. The width of the channel is fixed at 50 µm and the length of each arm is 15 mm. The arrows indicate the direction of sample movement. The governing equations for EOF are equations 1 - 5:

Conservation of mass: \( \nabla \cdot \mathbf{u} = 0 \) \hspace{1cm} (1)

Conservation of momentum: \( \rho \left( \frac{Du}{Dt} \right) = \mu \nabla^2 \mathbf{u} - \nabla p + f_e \) \hspace{1cm} (2)

Coulomb force: \( f_e = \rho_e E = 0 \) \hspace{1cm} (3)

Poisson’s equation: \( \nabla^2 \Phi = 0 \) \hspace{1cm} (4)

Helmholtz- Smoluchowski eq.: \( U = \varepsilon_0 E / \mu \) \hspace{1cm} (5)

Conservation of species: \( \frac{DC_i}{Dt} = D_i \frac{\partial^2 C_i}{\partial x^2} + k_i C_i C_j C_k \), \( i = A, B, C \) \hspace{1cm} (6)

The last term \( f_e \) in the momentum equation is the Coulomb force arising due to the external electric field. As the bulk charge density, \( \rho_e \) is zero, the Coulomb force term is zero in our formulation (Eq. 3). The
pressure drop term is zero in Eq. 2 as constant pressure is maintained. The Poisson’s equation (Eq. 4) is coupled with the momentum through Helmholtz Smoluchowski equation (Eq. 5) which provides the EOF velocity, \( U \), for the applied potential, \( \Phi \), in V. For the liquid phase reaction we assume a bimolecular, irreversible reaction with a forward rate constant, \( k_f \), whereas the backward rate constant, \( k_b \), is considered negligible. Governing equation of the chemical reaction between reactants is shown in Eq. 6 where \( D_i \) and \( C_i \) are the diffusion coefficients and species concentrations of A, B and C respectively. The negative sign in the Eq. 6 corresponds to the depletion of reactants A and B while the positive sign corresponds to the formation of the product C [3].

The buffer used has a density, \( \rho \), of 1000 kg.m\(^{-3}\), dynamic viscosity, \( \mu \), of 1e-6 N.s.m\(^{-2}\) and relative permittivity, \( \varepsilon \), of 80. The zeta potential, \( \zeta \), is taken to be -0.1 V and the Debye-layer, \( \lambda_D \), is calculated to be 2.15 nm thick from our previous experimental studies [4]. An electric field, \( E \), of 250 V/cm is applied along the arms for pinching and switching. Initially the samples are focused at the center of microchannels 1 and 2. The samples at the centers of the microchannels 1 and 2 are injected into the reactor by sequential change of potential. Table 1 shows potential applied on the arms of the microchannel during pinching and switching.

### Table 1. Voltage values for pinching and switching.

<table>
<thead>
<tr>
<th>Pinching</th>
<th>Switching</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_2/S_3 )</td>
<td>( S_{av}/S_{in} )</td>
</tr>
<tr>
<td>750 V</td>
<td>Ground</td>
</tr>
<tr>
<td>250 V</td>
<td>250 V</td>
</tr>
</tbody>
</table>

**RESULTS AND DISCUSSION**

Figure 2 shows movement of samples A and B towards the reaction well at three different time intervals \( t_1 \), \( t_2 \), and \( t_3 \). By maintaining the same buffer concentration in both the microchannels and by applying the same electric fields, the samples A and B are dispensed into the well at the same time. The samples move with a velocity of 0.17 cm.s\(^{-1}\) which correlates with the theoretical value of 0.177 cm.s\(^{-1}\) and can be calculated from Eq. 4. It is seen from Fig. 3 that both samples A and B flow into the well at the same time and there is instantaneous product formation in the microreactor. From Fig. 3 it is seen that the concentration of the reactants in the microreactor decrease as time increases. This is due to the formation of product as well as convection of fluid. The reactant concentrations decrease by 23% within 0.02 s while the product concentration also varies with time indicating that the process is dynamic in nature. Figure 4 shows concentration of the final product C at different reaction rates. The plot of concentration versus reaction rate follows an logarithmic trend. At higher reaction rates the product concentration plateaus. It is observed that the concentration of the final product increases by 33% from 64.2 \( \mu \)M to 96.9 \( \mu \)M when the forward reaction rate \( k_f \) increases from \( 10^{0} \) L.mol\(^{-1}\).s\(^{-1}\) to \( 10^{3} \) L.mol\(^{-1}\).s\(^{-1}\) indicating that there can be better detection of products for higher reaction rates. However, the concentration increases only by 3.56% when the reaction rate \( k_f \) changes from \( 10^{0} \) L.mol\(^{-1}\).s\(^{-1}\) to \( 1.8 \times 10^{2} \) L.mol\(^{-1}\).s\(^{-1}\). This indicates that the product concentration reaches saturation above a certain reaction rate for the considered geometry and reactant concentrations.

**CONCLUSIONS**

Here, a numerical method to pinch and inject microliter samples into a common reaction well was developed. This method predicts when peak product concentration occurs for a selected geometry, electric field and reaction rates. Such microscale reactors offer advantages in automation, fast screening times, small sample volume and increased accuracy for medical diagnostics, drug dispensing, and screening of biological toxins.

**REFERENCES**