Effects of spatial gradients of electrical conductivity on chip-based sample injection processes

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Abstract

The precise control of the loaded and dispensed sample amount in crossing microchannels is key to the performance of many lab-on-a-chip devices. The fundamental understanding of the complicated electrokinetic phenomena in such crossing type microchannels therefore is necessary. In the literature, a few theoretical models studying the transport phenomena in similar crossing microchannels did not consider the spatial gradients of conductivity due to its complexity. However, the spatial gradients of electrical conductivity of buffer solution often exist in many applications (i.e. pumping a large number of unknown species and stacking the interested sample species) and it was demonstrated that the presence of the conductivity gradients has significant influences on the on-chip microfluidic injection processes. A new theoretical model was developed in this paper to study the transport phenomena in crossing microchannels with the consideration of a large range of spatial gradient of electric conductivity. This developed model was used to simulate the potential field, flow field, and concentration field of the injection processes where the conductivity of the sample-carrying buffer differs significantly from that of the driving buffer. The transport phenomena are found to be very sensitive to the conductivity difference between the sample-carrying buffer and the driving buffer. The developed model here can be employed to find the optimal voltages for controlling the dispensed sample size and to provide guidance for designing such a crossing microchannel in lab-on-a-chip devices.

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1. Introduction

Microfluidic chips have drawn a great deal of attention recently due to the emerging applications in chemical and biomedical diagnosis and analysis, such as electrophoretic separation, clinical detection and DNA scanning [1–7]. Typically, a microfluidic chip is a thin glass plate, with a network of microchannels. The target analyte and buffer are transported through the microchannels according to the predefined routines. An important component of typical microfluidic chip is the microfluidic dispenser, which is a cross-type microchannel and employs electrokinetic flow to load samples into the intersection from one channel and dispense a minute quantity of sample into another channel. The precise control of the loaded and dispensed sample amount in microfluidic dispensers is key to the analysis processes.

However, the lack of understanding of the complicated transport phenomena in the dispensers makes it very difficult to precisely control the injected sample amount. Therefore, numerical modeling of the transport phenomena in such devices is especially valuable in order to provide guidance for conducting experiments in these microfluidic devices and to reduce the cost associated with building prototype chips. Sample transport in microfluidic dispensers is the result of three major mass transport mechanisms: convection, electrokinetic transport and diffusion. Bulk convective flow of liquid in the microchannel usually is one or a combination of the following flows: (a) electroosmotic-driven flow, which arises from the motion of net charge in the electrical double layer (EDL) induced by the axially applied electric field; (b) applied pressure-driven flow and/or induced pressure-driven flow due to the presence of axial gradient of flow velocity through the channel; and (c) thermal convention due to joule heating. Electrophoretic transport is the response of the charged particles, which exist commonly in chemical
and biomedical solutions (e.g. DNA strands or proteins), to the applied electric field. Diffusion takes place whenever a spatial gradient of the composition of solution exists. Extensive experimental and theoretical studies [8-13] have been performed to investigate the transport phenomena in microfluidic devices. Harrison et al. [8] examined and demonstrated the feasibility of using electroosmotic pumping to transport liquids in a manifold of channels and the possibility of conducting the electrophoretic separation on a planar substrate. Effenhauser et al. [9] performed a high-speed separation of antisense oligonucleotides on a micromachined capillary electrophoresis device on a glass plate, where electroosmotic flow was employed to inject the sample. Ermakov et al. [10,11] used a two-dimensional mathematical model to investigate the electrokinetic focusing in a cross-intersection of microchannels and the sample mixing in a T-shape microchannel. Patankar and Hu [12] simulated a three-dimensional electroosmotic flow in the intersection of a cross-type microchannel and investigated the effects of electric potential and pressure on the flow pattern. Bai et al. [13] examined the feasibility of using pressure-driven flow to inject the small amount of samples in a crossing microchannels. All the above-mentioned studies used the same solution (the same chemical composition and concentration) as the driving buffer, and the sample-carrying buffer did not consider any spatial gradient of electric conductivity in the liquid, and assumed negligible effects of samples on the bulk conductivity.

In many practical microfluidic systems, the gradient of electric conductivity exists in the liquid. For example, when a sample solution containing different sample species is required to be transported through microchannels without sample separation [14], a lower flow velocity in the sample zone is desirable during the loading process so that the electro-migration and the separation can be minimized by the slow motion. This can be achieved by using a high-conductivity buffer solution as the sample-carrying buffer (so the electroosmotic velocity is low) and a low conductivity buffer solution as the driving buffer (so the electroosmotic velocity is high). In such a case, the spatial gradient of electric conductivity exists. On the other hand, when a sample is required to be stacked in the system [15-18], the use of lower conductivity buffer solution in the sample region and higher conductivity buffer in the driving liquid region is a good choice to meet this need. This is because a higher velocity will be generated in the sample region and thus the sample can be stacked by the high conductivity buffer (low velocity) at the boundary of high- and low-conductivity buffer solutions.

The objective of this work is to develop a two-dimensional theoretical model to study the transient flow and mass transport phenomena in a crossing microchannel dispenser with a wide range of spatial gradient of electrical conductivity. It was demonstrated that the presence of the conductivity difference has significant influence on the on-chip microfluidic dispensing processes. The applied electrical potential field, the flow field and the concentration field in a microfluidic dispenser were predicted based on the simultaneous numerical solutions to this model. The effects of the conductivity gradient on the transport phenomena and particularly on the dispensed sample size were examined. Although the maximum difference of the conductivity between the sample-carrying buffer and the driving buffer is 10 times in our simulations, the developed model is not limited to this range.

2. Microfluidic dispenser

The microfluidic dispenser studied in this work has a cross-type microchannel as shown in Fig. 1. The depth and the width of all the channels are considered to be 20 and 50 μm, respectively. There are four reservoirs connected to the four ends of microchannels, in which the electrodes are inserted to set up the electrical field across the channels. The sample reservoir is R1, where a sample solution (the sample-carrying buffer) is initially loaded. The sample waste
The sample-carrying buffer and the driving buffer have the same chemical composites, but different ionic concentration as defined in Eq. (1) which defines the current flow due to diffusion and is found small as compared with the third term [20]. Consequently, for large ionic flows, one can write the electric current in terms of molar concentration

\[
\vec{i} = -\frac{e N_a \vec{\phi}}{kT} \sum_j z_j^n j D_j C_j
\]

where \(N_a\) is Avogadro number and the molar concentration is given by \(C_j = n_j/N_a\). For a given electrolyte solution, Eq. (2) can be rewritten as

\[
\vec{i} = \lambda \vec{\phi}
\]

where \(\lambda\) is the electric conductivity of electrolyte solution and takes the form of

\[
\lambda = \frac{e^2 N_a}{kT} \sum_j z_j^n j D_j C_j
\]

Eq. (4) is an expression of Ohm’s law for electrically neutral dilute solutions or solutions in a microchannel having large \(kD\), where \(C_j\) can be determined by a set of concentration equations. The charge conservation in the liquid has to be satisfied, which is described by

\[
\nabla \cdot \vec{i} = 0
\]

Substituting Eq. (3) into Eq. (5), the equation of the electrical potential field is obtained as

\[
\nabla \cdot (\lambda \vec{\phi}) = 0
\]

With the given concentration field and proper boundary conditions, Eqs. (4) and (6a) can provide the distribution of the applied electric field, \(\phi\), in the microchannel. It should be pointed out that if there is no spatial conductivity gradient, \(\lambda\) is a constant, and hence Eq. (6a) is reduced to

\[
\nabla \cdot (\lambda \vec{\phi}) = \nabla^2 \phi = 0
\]

3.2. Flow field

The flow field is described by the modified Navier-Stokes equations as follows:

\[
\rho \left[ \frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \nabla) \vec{V} \right] = -\nabla P + \mu \nabla^2 \vec{V} + \rho_s \vec{\phi}
\]

\[

\nabla \cdot \vec{V} = 0
\]
electric double layer results in a plug-like electroosmotic velocity profile cross the channel except in the double-layer region where velocity dramatically decreases to zero at the wall. For simplicity, we may treat the electroosmotic velocity as the boundary slip velocity and use it as the boundary condition for the momentum equation (Eq. (7a)). Mathematically, this slip boundary condition removes the last term in Eq. (7a) and includes its effects in the boundary condition:

\[ \vec{V}_{\text{wall}} = \mu_{\text{eo}} \vec{V}_0 \]  

(8a)

where \( \mu_{\text{eo}} \) is the electroosmotic mobility of the buffer solution. The other boundary conditions are:

\[ \frac{\partial u}{\partial n} = 0, \quad \vec{v} \cdot \vec{n} = 0 \quad \text{for reservoirs 1 and 3} \]  

(8b)

\[ \frac{\partial u}{\partial n} = 0, \quad \vec{v} \cdot \vec{n} = 0 \quad \text{for reservoirs 2 and 4} \]  

(8c)

\[ P_{\text{f2}} \big|_{x=1} = P_a \]  

(8d)

The initial boundary conditions are:

\[ u = 0, \quad v = 0, \quad P = P_a \]  

(8e)

### 3.3. Concentration field

In this study, we consider the spatial gradient of conductivity of the buffer solution. Therefore, the spatial gradients of buffer concentration exist and the gradients are time dependent, which have significant effects on the electrical potential field and the flow field during the injection process. Therefore, the buffer concentration field must be modeled simultaneously at each time step. The concentration field is governed by the mass conservation and can be described by:

\[ \frac{\partial C_i}{\partial t} + \vec{V} \cdot (\vec{V} C_i) = D_i \nabla^2 C_i \]  

(9a)

\[ \frac{\partial C_{\text{buffer}}}{\partial t} + \vec{V} \cdot \vec{V}_{\text{buffer}} C_{\text{buffer}} = D_{\text{buffer}} \nabla^2 C_{\text{buffer}} \]  

(9b)

where \( \vec{V}_{\text{epi}} \) is the electrophoretic velocity of the ith species, given by \( \vec{V}_{\text{epi}} = \mu_{\text{epi}} \vec{V}_0 \), where \( \mu_{\text{epi}} \) is the electrophoretic mobility of this species. Please note that Eqs. (9a) and (9b) describe the concentration fields of the sample and the buffer, respectively. The corresponding boundary conditions for sample at the loading step are:

\[ \frac{\partial C_{\text{sample}}}{\partial t} \big|_{x=0} = 0 \]  

(10a)

\[ C_{\text{sample}} \big|_{x=1} = C_{\text{sample,original}} \]  

(10b)

\[ C_{\text{sample}} \big|_{x=0} = C_{\text{sample}} \big|_{x=4} = 0 \]  

(10c)

\[ \frac{\partial C_{\text{sample}}}{\partial x} \big|_{x=0} = 0 \]  

(10d)

and initial conditions for sample at the loading step are:

\[ C_{\text{sample}} \big|_{t=0} = C_{\text{sample,original}} \]  

(10e)

The boundary and initial conditions for sample at the dispensing step are:

\[ \frac{\partial C_{\text{sample}}}{\partial t} = 0 \]  

(10f)

\[ C_{\text{sample}} \big|_{x=1} = C_{\text{sample,original}} \]  

(10g)

\[ C_{\text{sample}} \big|_{x=2} = C_{\text{sample}} \big|_{x=4} = 0 \]  

(10h)

\[ \frac{\partial C_{\text{sample}}}{\partial x} \big|_{x=1} = 0 \]  

(10i)

\[ C_{\text{sample}} \big|_{t=0} = C_{\text{sample,loading}} \big|_{\text{steady-state}} = 0 \]  

(10j)

The corresponding boundary conditions for buffer at the loading step are:

\[ \frac{\partial C_{\text{buffer}}}{\partial t} = 0 \]  

(11a)

\[ C_{\text{buffer}} \big|_{x=1} = C_{\text{sample-carrying-buffer,original}} \]  

(11b)

\[ C_{\text{buffer}} \big|_{x=2} = C_{\text{buffer}} \big|_{x=4} = C_{\text{driving-buffer,original}} \]  

(11c)

\[ \frac{\partial C_{\text{buffer}}}{\partial x} \big|_{x=1} = 0 \]  

(11d)

and initial conditions for buffer at the loading step are:

\[ C_{\text{buffer}} \big|_{t=0} = C_{\text{sample-carrying-buffer,original}} \]  

(11e)

\[ C_{\text{buffer}} \big|_{t=0} = C_{\text{driving-buffer,original}} \]  

(11f)

The boundary and initial conditions for sample at the dispensing step are:

\[ \frac{\partial C_{\text{buffer}}}{\partial t} = 0 \]  

(11g)

\[ C_{\text{buffer}} \big|_{x=1} = C_{\text{sample-carrying-buffer,original}} \]  

(11h)

\[ C_{\text{buffer}} \big|_{x=2} = C_{\text{driving-buffer,original}} \]  

(11i)

\[ \frac{\partial C_{\text{buffer}}}{\partial x} \big|_{x=1} = 0 \]  

(11j)

\[ C_{\text{buffer}} \big|_{t=0} = C_{\text{buffer,loading}} \big|_{\text{steady-state}} \]  

(11k)

### 3.4. Numerical scheme

The complete set of equations (Eq. (4) and Eqs. (6)–(11)) were normalized by introducing the following parameters:

\( \phi_i = \phi_i / 100 \text{V} \), \( \vec{u}_i = \mu_{\text{epi}} \vec{V}_0 \), \( \vec{p}_i = (P - P_a) / (\mu_{\text{epi}} / \text{H}^2) \), \( \text{H} = x / h \), \( C_{\text{sample}} = C_{\text{sample}} / C_{\text{sample,max}} \), and \( C_{\text{buffer}} = C_{\text{buffer}} / C_{\text{buffer,max}} \), where \( h = 50 \mu\text{m} \), \( v = 1.0 \times 10^{-6} \text{m}^2/\text{s} \), \( \rho = 1.0 \times 10^3 \text{kg/m}^3 \), and \( P_a = 1.0 \times 10^5 \text{N/m}^2 \). The normalized equations were then numerically solved using...
the semi-implicit method for pressure-linked equation (SIMPLE) algorithm developed by Pantakar [21]. The algorithm is based on a finite control volume discretization of the governing equations on a staggered grid. In order to capture all the detailed features near the four corners of the intersection shown in Fig. 1, the non-uniform grid system is employed. The control volume size next to the wall is minimum. The size of successive control volumes away from the walls is increased by a factor of 1.2. In this implementation, the solution to this set of equations is obtained by an iterative procedure. During each iteration procedure, the discretized equations are solved by a line-by-line iteration method. Due to the unsteady loading and dispensing processes, the numerical calculation of the potential field, flow field and concentration field must be converged at each iteration step and each time step.

4. Results and discussions

In this study, Rhodamine 110 standard is used as a sample with an electrophoretic mobility \(-2.0 \times 10^{-8} \text{ m}^2 / \text{V s}\) and a diffusion coefficient \(D_{\text{sample}} = 1.0 \times 10^{-9} \text{ m}^2 / \text{s}\), respectively, which are close to the measured value [22]. The driving buffer and the sample-carrying buffer have the same chemical composites, sodium carbonate, the same pH value (pH 9.0), the same diffusion coefficient, \(D_{\text{buffer}} = 1.0 \times 10^{-9} \text{ m}^2 / \text{s}\), but the different ionic concentrations and hence different electrical conductivities.

Two scenarios are studied here to investigate the effects of the conductivity gradient on the transport phenomena of the sample injection processes. In the first scenario, the driving buffer has a concentration of 10 mM and an electroosmotic mobility of \(5.5 \times 10^{-8} \text{ m}^2 / \text{V s}\). The concentration of the sample-carrying buffer is chosen to be 50 mM (five times that of the driving buffer) and its electroosmotic mobility is assumed to be \(5.0 \times 10^{-8} \text{ m}^2 / \text{V s}\). In this case, the driving buffer has a lower conductivity than that of the sample-carrying buffer and the relationship of the conductivity between these two solutions is approximated as \(\lambda_{\text{sample buffer}} / \lambda_{\text{driving buffer}} = 5\). In the second scenario, the driving buffer has a concentration of 50 mM and the electroosmotic mobility is assumed to be \(5.56 \times 10^{-8} \text{ m}^2 / \text{V s}\). The relationship of the conductivity between these two solutions is approximated as \(\lambda_{\text{sample buffer}} / \lambda_{\text{driving buffer}} = 1/10\).

The previous studies did not consider the spatial gradient of the electrical conductivity in the liquid during the injection processes. In these studies, the electric potential distribution is not affected by the conductivity (mathematically, the conductivity is not involved in the applied electrical potential equation, such as Eq. (6b)) and only need to be solved once prior to solving momentum and concentration equations. This simplicity, however, is not valid in this study where the spatial gradient of the conductivity exists. The equation of the electric potential, Eq. (6a), must be solved at each time step when the concentration distribution changes and in turn the conductivity distribution changes. Fig. 2(a) shows the normalized electric potential distribution of the first scenario \((\lambda_{\text{sample buffer}} / \lambda_{\text{driving buffer}} = 5)\) at

![Fig. 2. The effects of the conductivity difference on the applied electrical field in the dispenser. The iso-potential contours in the intersection in the steady-state loading step (left) and the corresponding dispensing step (right) for (a) \(\lambda_{\text{sample buffer}} / \lambda_{\text{driving buffer}} = 5\), (b) \(\lambda_{\text{sample buffer}} / \lambda_{\text{driving buffer}} = 1\).](image-url)
the loading and the dispensing step and Fig. 2(b), however, shows the normalized electric potential distribution without the consideration of spatial gradient of conductivity (i.e., \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1 \)) at the loading and dispensing step. In all the plots, the chip was oriented with channels from R1, R2, R3, and R4, counterclockwise from left and the same configuration is used for all the other plots in this paper, except stated otherwise. The normalized potentials applied to the reservoirs 1–4 are the same for all the plots in Fig. 2, \( \varepsilon_1 = 1.0, \varepsilon_2 = 1.0, \varepsilon_3 = 0.0 \) and \( \varepsilon_4 = 0.0 \) at the loading step and \( \varepsilon_1 = 0.2, \varepsilon_2 = 2.0, \varepsilon_3 = 0.2 \) and \( \varepsilon_4 = 0.0 \) at the dispensing step, respectively, where \( \varepsilon \) indicates the normalized applied voltages and subscripts correspond to reservoir numbers. The lines shown in these plots are equal potential lines. The potential drop between two lines is the same through all the plots and the electrical field strength can be evaluated by the ratio of the potential drop to the distance between the lines. The variation of the electric field strength is clearly demonstrated between the situations with and without the conductivity gradient.

During the loading process, the sample solution is pumped into channel 1 from the reservoir 1. Fig. 3(a) and (b) shows the concentration distribution of the sample near the intersection during the loading process for the above stated two scenarios, \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 5 \) and \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10 \), respectively. In all the plots, the concentration increases from black to white and the iso-concentration lines are 0.1, 0.3, 0.5, 0.7, and 0.9 of the original sample concentration. The lengths are scaled by the channel width, 50 \( \mu \)m. The sequence of plots shows the unsteady loading of the sample at different time. One can see that the conductivity gradient has significant effects on the unsteadying loading process. The time to reach the steady state is different for the two scenarios, \( t_{\text{steady}} = 12 \) s for the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 5 \) and \( t_{\text{steady}} = 6 \) s for the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10 \). That indicates that the average bulk velocity is affected significantly by the spatial gradient of conductivity. In addition, the concentration contour of the sample is distorted backward to the sample reservoir (R1) in the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10 \) as shown in the plot of \( t = 5 \) s in Fig. 3(b). This may be understood as follows. Because the conductivity of the sample region (the sample-carrying buffer and the sample) is much lower than that in the driving buffer region (\( \sim 1/10 \)), the voltage drop or the electric field strength in this region is bigger than that in the downstream of waste channel (from the intersection to right side reservoir 3). Additionally, the sample region has a lower ionic concentration and hence a much higher electroosmotic velocity. The combination of the high electrical field strength and the high electroosmotic mobility yields a much higher local electroosmotic velocity than that in the downstream. This intends to generate a higher flow.
rate in the upstream (sample-carrying buffer region) than the flow rate in the downstream (driving buffer region). For an incompressible liquid, the continuity condition requires the same flow rate throughout the microchannel. In order to achieve the same flow rate in both the upstream and the downstream, a negative pressure gradient (the pressure decrease in the flow direction) is induced in the downstream to increase the local flow rate, and a positive pressure gradient (the pressure increase in the flow direction) is induced in the sample region to decrease the local flow rate. This induced positive pressure gradient (the pressure increase in the flow direction) in the sample-carrying buffer region will add a backward pressure driven flow to the electroosmotic flow (plug-like velocity profile), resulting in the distorted backward velocity profile. Consequently, the sample concentration profile is distorted backward to reservoir 1 as well, because the sample concentration profile is dependent on the convection transport (bulk velocity).

One can also find that for the second scenario ($\lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10$), the sample is loaded slowly before $t = 4\ s$ (i.e. there are no sample present at the intersection before this moment); however, the sample concentration profile is distorted backward to reservoir 1 as well, because the sample concentration profile is dependent on the convection transport (bulk velocity).

In order to gain the insight into the transport phenomena behind the unsteady loading process, the sample concentration distribution at the centerline of the horizontal channel (from R1 to R3) and the vertical channel (from R2 to R4) are plotted in Fig. 4 for both scenarios. The
The time between each line is 1 s and the direction of the time increase is indicated in the figure. In all plots, the lengths are scaled by the channel width, 50 μm. Fig. 4(a) shows the sample concentration at the centerline of horizontal channel (left) and vertical channel (right), for the scenario of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 5 \), and Fig. 4(b) shows that for the scenario of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10 \). From Fig. 4(a) and (b), one can see that the sample is gradually pumped into channel 1 (0 < \( \tilde{x} < 50 \)) until a steady state is reached. A concentration drop is found at the inlet of the waste channel (51 < \( \tilde{x} < 101 \)), which is due to the flow of the driving buffer solutions in channels 2 and 4 into the water channel and the focus of the sample at the intersection.

Also, the sample concentration at the vertical centerline is symmetric to the center point, which is because the same voltages are applied to R2 and R4 and channels 2 and 4 have the same length. It is also clearly shown that the sample is focused by the driving buffers at the intersection of microchannels (200 < \( \tilde{y} < 201 \)). Note that the extent to which the sample is focused depends on the combination of the four applied voltages and can be adjusted.

As seen from Fig. 5((1) and (2)), with a strongly focused sample at \( \tilde{t} = 1.25 s \) (b) due to the small potentials applied to reservoirs 1 and 3 at the dispensing step (i.e. \( \varepsilon_1 = \varepsilon_3 = 0.2 \) compared to \( \varepsilon_2 = 2.0 \)).

As discussed above, the loading processes in the presence of the spatial conductivity gradient is different from that without the spatial conductivity gradient. It can be expected that the corresponding dispensing processes under the same applied voltages will be different. Fig. 5 shows the comparison of the loaded sample at the steady state (top row) and the dispersed sample at \( \tilde{t} = 1.25 s \) (bottom row) between the two cases with the conductivity difference and the case without the conductivity difference. For all the three cases, the normalized applied potentials \( \varepsilon_1 - \varepsilon_4 \) are 1.0, 1.0, 0.0, and 1.0 at the loading step and 0.2, 0.2, 0.2, and 0.0 at the dispensing step. In all the plots, the white region shows the sample solution with a concentration higher than 80% of the original sample concentration. Fig. 5(a) and (b) shows the loaded sample and the dispersed sample for the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 5 \), Fig. 5(c) and (d) shows that for the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10 \) and Fig. 5(e) and (f) shows that for the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1 \). The sensitivity of the loaded sample size (Fig. 5(a), (b) and (e)) and the dispersed sample size (Fig. 5(c), (d) and (f)) to the spatial conductivity gradient is clearly demonstrated. There is essentially no sample present in the dispensing channel shortly after the dispensing for the situations with the conductivity gradient.

This is because the loaded sample size in the intersection is small (see Fig. 5(a) and (b)) and the major part of the sample in the intersection is driven to reservoirs 1 and 3 when the dispensing is initiated (see Fig. 5(b) and (d)) due to the small potentials applied to reservoirs 1 and 3 at the dispensing step (i.e. \( \varepsilon_1 = \varepsilon_3 = 0.2 \) compared to \( \varepsilon_2 = 2.0 \)).

As seen from Fig. 5(1) and (2), with a strongly focused sample in the loading step, one cannot dispense or inject any sufficiently large sample in the dispensing channel. In order to obtain a sufficiently large dispersed sample, the size of the loaded sample at the intersection must be large at the end of the loading process. The applied voltages were found to be the most important parameter controlling the size of the loaded sample and the dispersed sample. Fig. 6(a) and (b) shows the effects of the applied voltages on the steady-state loaded sample for the case of \( \lambda_{\text{sample buffer}}/\lambda_{\text{driving buffer}} = 1/10 \). The normalized applied voltages, \( \varepsilon_1 - \varepsilon_4 \), for Fig. 6(a) and (c) are 1.0, 1.0, 0.0, and 1.0, and for Fig. 6(b) and (d) are 1.0, 0.2, 0.0, and 0.2, respectively. When the same normalized voltages applied to the reservoirs 2 and 4, \( \varepsilon_2 = \varepsilon_4 \), are decreased from 1.0 (Fig. 6(a) and (c)) to 0.2 (Fig. 6(b) and (d)), the loaded sample increases significantly for both scenarios because of
Fig. 6. The variation of the loaded sample’s size and shape at the intersection for different conductivity difference and different applied voltages. The loaded sample at steady state with \( \frac{\lambda_{\text{sample buffer}}}{\lambda_{\text{driving buffer}}} = 5 \) under the applied voltages, \( \varepsilon_1 - \varepsilon_4 \) of (a) 1.0, 1.0, 0.0, 1.0, and (b) 1.0, 0.2, 0.0, 0.2. The loaded sample at steady state with \( \frac{\lambda_{\text{sample buffer}}}{\lambda_{\text{driving buffer}}} = 1/10 \) under the applied voltages, \( \varepsilon_1 - \varepsilon_4 \) of (c) 1.0, 1.0, 0.0, 1.0, and (d) 1.0, 0.2, 0.0, 0.2. The white regions represent the solution with a concentration above 80% of the original sample concentration.

Fig. 7 shows the dispensed sample at different time for the case of \( \frac{\lambda_{\text{sample buffer}}}{\lambda_{\text{driving buffer}}} = 5 \) based on the different sizes of the loaded sample. The normalized applied voltages in the dispensing process are 1.1, 2.0, 1.1, and 0.0 for \( \varepsilon_1 - \varepsilon_4 \) in all the plots. Fig. 7(a) shows a loaded sample, and the corresponding dispensed sample at \( t = 0.9 \) s and \( t = 1.8 \) s, respectively. Fig. 7(b) shows a bigger loaded sample and the corresponding dispensed sample at the same dispensing time and under the same applied voltages. Indeed, the loaded sample size and hence the applied voltages in the loading step are critical in determining the dispensed sample size.

After the loading process reaches a steady state, the dispensing process can be initiated by changing the applied voltages to the four reservoirs. During the dispensing process, the loaded sample in the intersection is expected to be driven or dispensed into channel 4 and be surrounded by the buffer solutions from both the upstream and the downstream, providing a cut of sample for the subsequent chemical and biomedical analysis. This requires that the main flow direction in the dispensing process should be from R2 to R4 (perpendicular to the loading flow direction from R1 to R3), and the flow in channels 1 and 3 could be either from R1 (or R3) to R4 helping the major flow from R2 to R4 to provide a big sample or from R2 to R1 (or R3) splitting the major flow from R2 to R4 to provide a clear cut of sample in the downstream of channel 4. In order to perform this process, normally the voltage applied to reservoir 2 must be bigger than that applied to reservoirs 1 and 3. Otherwise, there will exist a flow from R1 to R2 or R3 to R2 as well besides the flow from R1 to R4 (R3 to R4 as well since R4 is grounded). This will split the loaded sample in the intersection to R2 and R4 and cannot provide a cut of sample (for the purpose of the dispensing) because the sample is continuously driven to R2 and R4 from the sample reservoir (R1). However, as we discussed earlier, when the voltages applied to reservoirs 1 and 3 are much smaller than that to reservoir 2 during the dispensing, there will be too much loaded sample flowing to reservoirs 1 and 3. This will result in a small dispensed sample size. In order to verify this, the same loaded sample as shown in Fig. 7(b) is dispensed using a new set of applied
voltage $\varepsilon_1 = 0.2$, $\varepsilon_2 = 2.0$, $\varepsilon_3 = 0.2$, $\varepsilon_4 = 0.0$, where the applied voltages to reservoirs 2 and 4 are the same as that used in Fig. 7(b); the applied voltage reservoirs 1 and 3 are much smaller (i.e. $\varepsilon_1 = \varepsilon_3 = 0.2$) than that used in Fig. 7(b) (i.e. $\varepsilon_1 = \varepsilon_3 = 1.1$). We found that there is essentially no sample dispensed in the dispensing channel at $t = 0.9$ s when using this new set of applied voltages ($\varepsilon_1 = \varepsilon_3 = 0.2$) in the dispensing step. Since no sample is present in the downstream of channel 4, the simulation results are not shown here. This indicates that when the applied voltages to reservoirs 1 and 3 are too low in the dispensing process, a significant amount of sample will be driven to reservoirs 1 and 3 when the dispensing process is initiated. The left small amount of the dispensed sample easily diffuses into the buffer solution in channel 4, consequently, no sample with a sufficiently high concentration appears. Therefore, in addition to the loaded sample size, the combination of the applied voltage in the dispensing process is another very important controlling parameter for the dispensed sample size.

From the above discussions, it is clear that the presence of the conductivity gradient has a strong effect on the sample loading and dispensing. The applied voltages can control the shape and the size of the loaded sample and hence the shape and the size of the dispensed sample. For a given sample–buffer system, there exists an optimal set of the controlling voltages in order to obtain a desired dispensed sample size. The model developed here is able to find such a set of the optimal voltages through the numerical simulation.

5. Conclusions

A theoretical model is developed to investigate the sample dispensing/injection processes in a crossing microchannel. The spatial conductivity gradient in the liquid is considered in this model, which requires solving all the coupled, transient governing equations simultaneously. This makes the numerical simulation very complicated as compared with the case without considering the spatial conductivity gradient. The developed model was used to simulate the potential distribution, consequently on the loaded and dispensed sample shape and size. It has been demonstrated that the shape and the size of the loaded and dispensed sample can be controlled by adjusting the applied voltages to the four reservoirs and this model can predict the optimized applied voltages.

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