Theoretical Studies of Microfluidic Dispensing Processes

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The understanding of electrokinetic transport phenomena in microfluidic dispensers, an important component of biochips, is very important for designing and controlling biochips. A theoretical model to study the electrokinetic transport processes in microfluidic dispensers was developed in the work to study the controlling parameters for the dispensing process. The electrical field, the flow field, and the concentration field during dispensing processes were obtained by solving this theoretical model numerically. The effects of the electroosmotic mobility of the buffer solution, the diffusion coefficient and the electrophoretic mobility of the sample, the applied electrical field strength, and the channel size on the dispensing process are examined in this paper. The investigations show that optimal controlling parameter values can be found by using this model for dispensing any desired amount of the sample. © 2002 Elsevier Science (USA)

INTRODUCTION

Biochips or lab-on-a-chip devices have drawn great attention over the past few years due to their ever-increasing applications in biomedical diagnosis and analysis, such as clinical detection, DNA scanning, and electrophoretic separation (1–7). Typically, a biochip is a thin glass plate with a network of microchannels etched into its surface. An important component of biochips is the microfluidic dispenser, which employs electroosmotic flow to dispense minute quantities of samples for chemical and biomedical analysis. The precise control of the dispensed sample amount in microfluidic dispensers is the key to the performance of biochips and other lab-on-a-chip devices in chemical and biomedical analysis applications.

Generally, all solid–liquid interfaces have electrical charges. These electrical charges will attract counterions from the electrolyte solutions, and bear an electrical charge on their surfaces. When an electrical field is applied to the liquid, the excess counterions in the diffuse layer will move under the applied electrical field. Because of the viscous drag force, the moving ions will pull the surrounding liquid with them and thus generate a bulk liquid motion. This is referred to as electroosmosis.

Most liquids involved in chemical and biomedical analysis systems contain biological particles, e.g., DNA strands or proteins. The presence of these particles makes the electrokinetic transport of bioliquids different from the electrolyte solutions. These particles are very big in size or mass compared to the ions in electrolyte solutions, and bear an electrical charge on their surfaces. When an electrical field is applied to the liquid, these charged particles will move under the applied electrical field relative to the medium. The motion of particles is referred to as electrophoresis (EP).

Extensive experimental and theoretical studies have been performed to investigate transport phenomena in biochips. Harrison et al. (8) integrated capillary electrophoresis and sample handling (sample injection and separation) system on a planar glass chip. In this study, they 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. Seiler et al. (9) presented improvements in the instrumentation and experimental method for the device described by Harrison et al. (8). Effenhauser et al. (10) 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. All these experimental studies focused on the design and testing of microfluidic devices, and did not investigate how to control the microfluidic processes in such devices. Ermakov et al. (11) presented a 2-D mathematical model to investigate electrokinetic focusing in a cross intersection of microchannels and sample mixing in a T-shape microchannel. Based on this model, the same authors (12) studied electrokinetic injection techniques in microfluidic devices. In this paper, they focused on studying the effect of the electric field distribution in the channels on the injected sample concentration. However, they did not investigate how to control the volume and the uniform distribution of the dispensed sample, which is the key to the performance of biochips. Patankar and Hu (13) simulated a 3-D electroosmotic flow in two crossing microchannels. The focus of this model study is the...
electroosmotic flow of buffer solutions, and sample transport was not considered.

The objective of this work is to study the controlling parameters of both the loading process and the dispensing process in microfluidic dispensers by numerical simulations. The size and the shape of the dispensed sample, the electrical field, the flow field and the concentration field were investigated. The effects of the applied electrical potential, the electroosmotic mobility of the solution, the diffusion coefficient and the electrophoretic mobility of the sample, and the channel size on the volume of the dispensed sample were examined.

**MATHEMATICAL MODEL**

The microfluidic dispenser studied in this work is formed by two crossing microchannels as shown in Fig. 1. The depth and the width of all the channels are assumed 20 and 50 µm, respectively, except as indicated otherwise. There are four reservoirs connected to the four ends of the microchannels. Electrodes are inserted into these reservoirs to set up the electrical field across the channels. Initially, a sample solution (a buffer solution with sample species) is filled in reservoir 1; the other reservoirs and the microchannels are filled with the pure buffer solution. When the chosen electrical potentials are applied to the four reservoirs, the sample solution in reservoir 1 will be driven to flow toward reservoir 3 passing through the intersection of the cross channels. This is the so-called loading process. After the loading process reaches a steady state, the sample solution loaded in the intersection can be dispensed into the dispensing channel by adjusting the electrical potentials applied to these four reservoirs. This is called the dispensing process. The volume of the dispensed sample is the key to this dispensing process. However, in order to obtain the information on the dispensed volume, the electrical field, the flow field and the concentration field during the loading and the dispensing processes have to be studied.

**Electrical Field**

We consider a thin double layer and no net charge density in the bulk liquid. According to the theory of electrostatics, the applied electrical potential, \( \phi \), can be described by the Poisson equation,

\[
\nabla^2 \phi = 0
\]

[1]

Because no electrical potential is applied in the \( z \)-direction (the direction of the channel depth), the electrical potential profile in this direction is constant. Therefore, Eq. [1] can be rewritten as

\[
\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0.
\]

[2]

Introducing the nondimensional parameters

\[
\phi^* = \frac{\phi}{\Phi}, \quad x^* = \frac{x}{h}, \quad y^* = \frac{y}{h},
\]

where \( \Phi \) is a reference electrical potential and \( h \) is the channel width, chosen as 50 µm in this paper, Equation [2] can be nondimensionalized as

\[
\frac{\partial^2 \phi^*}{\partial x^2} + \frac{\partial^2 \phi^*}{\partial y^2} = 0.
\]

[3]

Boundary conditions are required to solve this equation. We impose the insulation condition on all the walls of microchannels and the specific nondimensional values on all the reservoirs. Once the electrical field in the dispenser is known, the local electric field strength can be calculated by

\[
\vec{E} = -\hat{\nabla} \Phi.
\]

[4]

**Flow Field**

The basic equations describing the flow field are the continuity equation,

\[
\hat{\nabla} \cdot \vec{V}_{eo} = 0,
\]

[5]
and the momentum equation,

$$
\rho \left( \frac{\partial \mathbf{v}_{eo}}{\partial t} + (\mathbf{v}_{eo} \cdot \nabla) \mathbf{v}_{eo} \right) = -\nabla P + \mu \nabla^2 \mathbf{v}_{eo} + \rho_e \mathbf{E}, \quad [6]
$$

where \( \mathbf{v}_{eo} \) is the bulk electroosmotic velocity vector, \( \rho \) is the density of the liquid, \( P \) is the pressure in microchannels, \( \mu \) is the viscosity of the liquid, and \( \rho_e \) is the net charge density in the solution.

As mentioned earlier, the driving force in the liquid flow is the electrical force, \( \rho_e \mathbf{E} \), which appears as the third term of the right-hand side of Eq. [6]. For microchannels with a rectangular cross-section, a previous paper (14) has shown that the electroosmotic velocity component parallel to the wall has a flat profile. In other words, the velocity is constant everywhere except in the region very near the wall (i.e., within the double layer). However, when the concentration is higher (i.e., \( C \leq 2 \times 10^{-5} \) mol/l), the electrical double layer is very thin (i.e., less than 10 nm) as compared to the dimensions of the microchannel’s cross-section (i.e., 50 \( \mu \m)\). Therefore, we will neglect the electrical driving force term in Eq. [6] and consider the effect of electroosmotic flow as the slip wall boundary conditions to the equation of motion. The electroosmotic mobility is assumed to be \( \mu_{eo} = 5.5 \times 10^{-8} \) m²/V·s through all the tests except indicated otherwise. In the electroosmotic flow process, Reynolds number \( Re = \frac{v h}{\nu} \) (\( v \) is the kinematic viscosity, \( V \) is the electroosmotic velocity component and \( h \) is the channel width), which gives the ratio between the inertial forces and the viscous forces, is very small (e.g. \( Re \leq 0.1 \)). Hence, the viscous forces prevail and define the characteristic time scale at which the flow field reaches a steady state. Therefore, the time scale for electroosmotic flow to reach a steady state can be evaluated by

$$
i_{steady} = \frac{h^2}{v}, \quad [7]
$$

where \( h \sim 5 \times 10^{-5} \) m and \( v \sim 10^{-6} \) m²/s, thus \( i_{steady} \sim 10^{-3} \) s. This time scale is very small as compared to the characteristic time scales of the sample loading and sample dispensing. Hence, the electroosmotic flow here is approximated as steady state. In addition, the velocity component in \( z \)-direction, \( u \), is very small as compared to the velocity component in \( x \)-direction and \( y \)-direction, \( u \) and \( v \). Therefore, the dispensing process in the dispenser can be considered as a two-dimensional problem, which has been verified by Patankar and Hu (13). Taking into account of the above considerations, Eq. [5] and Eq. [6] can be rewritten as

$$
\frac{\partial u_{eo}}{\partial x} + \frac{\partial v_{eo}}{\partial y} = 0, \quad \frac{\partial u_{eo}}{\partial x} + v \frac{\partial^2 u_{eo}}{\partial x^2} + v \frac{\partial^2 u_{eo}}{\partial y^2} = -\frac{\partial P}{\rho} + \nu \frac{\partial^2 u_{eo}}{\partial y^2}, \quad \frac{\partial v_{eo}}{\partial x} + v \frac{\partial^2 v_{eo}}{\partial x^2} + v \frac{\partial^2 v_{eo}}{\partial y^2} = -\frac{\partial P}{\rho} + \nu \frac{\partial^2 v_{eo}}{\partial y^2} \quad \text{[8][9a][9b]}
$$

where \( u_{eo}, v_{eo} \) are the electroosmotic velocity component in the \( x \) and \( y \) directions, respectively.

Introducing the nondimensional parameters

$$
P^* = \frac{P - Pa}{\rho(v/h) \gamma}, \quad u_{eo}^* = \frac{u_{eo} - h}{v}, \quad v_{eo}^* = \frac{v_{eo} - h}{v},
$$

where \( P_e \) is the atmospheric pressure, Eqs. [8], [9a], and [9b] can be nondimensionalized as

$$
\frac{\partial u_{eo}^*}{\partial x} + \frac{\partial v_{eo}^*}{\partial y} = 0, \quad \frac{\partial u_{eo}^*}{\partial x} + v \frac{\partial^2 u_{eo}^*}{\partial x^2} + v \frac{\partial^2 u_{eo}^*}{\partial y^2} = -\frac{\partial P^*}{\rho} + \nu \frac{\partial^2 u_{eo}^*}{\partial y^2}, \quad \frac{\partial v_{eo}^*}{\partial x} + v \frac{\partial^2 v_{eo}^*}{\partial x^2} + v \frac{\partial^2 v_{eo}^*}{\partial y^2} = -\frac{\partial P^*}{\rho} + \nu \frac{\partial^2 v_{eo}^*}{\partial y^2} \quad \text{[10][11a][11b]}
$$

Boundary conditions are required in order to solve this set of equations numerically. The slip velocity conditions are applied to the walls of the microchannels, the fully developed velocity profile is applied to all the interfaces between the microchannels and the reservoirs, and the pressures in the four reservoirs are considered as the atmospheric pressure.

**Concentration Field**

In order to obtain the information about the volume of the dispensed sample, the sample’s concentration distribution has to be found. The distribution of the sample concentration can be described by the conservation law of mass, which takes the form of

$$
\frac{\partial C_i}{\partial t} + \left( u_{ eo} + u_{ epi} \right) \frac{\partial C_i}{\partial x} + \left( v_{ eo} + v_{ epi} \right) \frac{\partial C_i}{\partial y} = D_i \left( \frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} \right), \quad [12]
$$

where \( C_i \) is the concentration of the \( i \)-th species, \( u_{ eo} \) and \( v_{ eo} \) are the components of the electroosmotic velocity of the \( i \)-th species, \( D_i \) is the diffusion coefficient of the \( i \)-th species, chosen as \( D_i = 1.0 \times 10^{-11} \) m²/(s·V) in all the calculations unless specified otherwise, and \( u_{ epi} \) and \( v_{ epi} \) are the components of the electrophoretic velocity of the \( i \)-th species given by \( u_{ epi} = E \mu_{ epi} \), where \( \mu_{ epi} \) is the electrophoretic mobility. Since rhodamine dye will be used as a sample in our laser visualization experiments to verify the model predictions, rhodamine dye is chosen as a sample in all the simulations reported here. The electrophoretic mobility for the rhodamine dye was experimentally determined as \(-2.46 \times 10^{-8} \) m²/(s·V) (15) and \( \mu_{ epi} = -2.0 \times 10^{-8} \) m²/(s·V) was used in all computations in this paper unless specified otherwise.

In this work, we are interested in how to control the volume of the dispensed sample. This volume depends on the electroosmotic mobility of the solution, the diffusion coefficient, and the
electrophoretic mobility of the sample, the applied electrical potential and the dimensions of the dispenser. Introducing the nondimensional parameters

\[ C^* = \frac{C}{\bar{C}}, \quad \tau = \frac{t}{\bar{h}^2/\nu}, \]

where \( \bar{C} \) is a reference concentration, we can nondimensionalize Eq. [12] as

\[ \frac{\partial C^*_i}{\partial \tau} + (u^{*}_{eo} + u^{*}_{ep}) \frac{\partial C^*_i}{\partial x} + (v^{*}_{eo} + v^{*}_{ep}) \frac{\partial C^*_i}{\partial y} = D_i \left( \frac{\partial^2 C^*_i}{\partial x^2} + \frac{\partial^2 C^*_i}{\partial y^2} \right). \]  

[13]

Boundary conditions are required to solve the above equation. In the calculations, the concentration of the sample in reservoir 1 is the applied sample concentration; the sample concentrations in reservoirs 2 and 4 are zero, and the flux of the sample to reservoir 3 is zero. Since both loading and dispensing are unsteady processes, initial conditions are required to solve the above equation. For the loading process, the initial concentration in reservoir 1 is the applied sample concentration; the initial concentrations in the other reservoirs and the channels are zero. After the loading process reaches the steady state, the loaded sample in the cross intersection can be dispensed into the dispensing channel by adjusting the electrical potentials applied to all the reservoirs. Therefore, the concentration distribution for loading process at the steady state was used as the initial conditions for dispensing process.

Numerical Scheme

The complete set of nondimensional equations, Eq. [3], Eq. [10], Eq. [11a], Eq. [11b], and Eq. [13], were solved using the semimiplet method for pressure-linked equations (SIMPLE) algorithm developed by Patankar. The algorithm is based on a finite control volume discretization of the governing equations on a staggered grid. In order to capture all the features near the four corners of the dispensers shown in Fig. 1, a nonuniform grid 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. This numerical scheme has been verified by solving the problems given in Ref. (17) and by comparing the simulation results with those given in this paper.

RESULTS AND DISCUSSION

Electrical Field and Flow Field

Once the electrical potentials are applied to the four reservoirs, electrical fields are set up across the channels. These electrical fields exert an electrical force on the liquid to pump the solution containing the sample through the cross intersection of the channels (loading process) and then dispense the sample into the dispensing channel. We assume the chip is made of electrically insulating material and applied the insulation conditions to all the channel walls. Therefore, when the applied electrical potentials change or the channel sizes change, the electrical field will change and hence the velocity field will in turn change. Figure 2 shows a typical electrical field and flow field for the loading and dispensing processes, respectively. In this figure, the nondimensional applied electrical potentials are \( \phi^*(1) = 1.0, \phi^*(2) = 1.0, \phi^*(3) = 0.0, \phi^*(4) = 1.0 \) for loading process and \( \phi^*(1) = 0.2, \phi^*(2) = 2.0, \phi^*(3) = 0.2, \phi^*(4) = 0.0 \) for dispensing process, where \( \phi^*(i) \) represents the nondimensional electrical potential applied to the \( i \)th reservoir. For this specific case, the electrical field and the flow field for the loading process are symmetric to the middle line of the horizontal channel, and the electrical field and the flow field for the dispensing process are symmetric to the middle line of the vertical channel.

Diffusion Coefficient Effect

Under the same applied electrical field as specified in the above section, two different diffusion coefficients, \( D_1 = 1.0 \times 10^{-11} \text{m}^2/\text{s} \) and \( D_2 = 1.0 \times 10^{-10} \text{m}^2/\text{s} \) were tested. Figure 3 shows the concentration distribution during the dispensing process. In this figure, the black regions are the buffer solution; the white region represents the region where the sample concentration is higher than 80\% of the original sample concentration (the same for all other figures in this paper). Generally, the dispensed sample size decreases with the increase of diffusion coefficient, because more samples will diffuse into the buffer solution when the diffusion coefficient is larger, consequently the high concentration region of the sample is smaller. However, we found the effect of the diffusion coefficient is not significant for this particular case. As seen from Fig. 3, when the diffusion coefficient increases from \( 1.0 \times 10^{-11} \text{m}^2/\text{s} \) (Fig. 3a) to \( 1.0 \times 10^{-10} \text{m}^2/\text{s} \) (Fig. 3b), the volume of the dispensed sample decreases only by 2\% (i.e., from 390 to 383 pl in this particular case).

Electroosmotic Mobility Effect

Under the same applied electrical field as specified previously, two cases with the different electroosmotic mobility, \( \mu_{eo1} = 5.0 \times 10^{-8} \text{m}^2/\text{V} \cdot \text{S} \) and \( \mu_{eo2} = 6.0 \times 10^{-8} \text{m}^2/\text{V} \cdot \text{S} \), were examined. The simulation results show that when the electroosmotic mobility increases, the dispensed sample moves further downstream in the dispensing channel, as can be seen in Figs. 4a and 4b. This is because when the electroosmotic mobility increases, the average velocity of the bulk flow increases. Thus, during the same time period, the solution with high electroosmotic mobility is moved further than that with low electroosmotic mobility. The numerical results also reveal that when
the electroosmotic mobility increases, the size of the dispensed sample is smaller. For example, at time $t = 1.25$ s, the sample volume for the case of low electroosmotic mobility is 395 pl and that for the case of high electroosmotic mobility is 372 pl. This is because the velocity in the upstream of the dispensing channel is higher than that in the downstream of the dispensing channel, as shown in Fig. 2. When the sample is dispensed downstream in the dispensing channel, the front of the sample (in the downstream of the dispensing channel) moves relatively slower than the back of the sample (in upstream of the dispensing channel); consequently, the sample is compressed. When the electroosmotic mobility increases, the difference between the velocity in the upstream and the velocity in the downstream of the dispensing channel is larger. Indeed, our numerical results show that the difference between the velocities in the downstream and the upstream increases when the electroosmotic mobility increases. Consequently, the dispensed sample is more compressed and the volume of the dispensed sample is smaller for the case of high electroosmotic mobility.

**Electrophoretic Mobility Effect**

Under the same applied electrical field as described previously, two cases with different electrophoretic mobility, $\mu_{ep_1} = -2.0 \times 10^{-8} \text{ m}^2/\text{V} \cdot \text{S}$ and $\mu_{ep_3} = -3.5 \times 10^{-8} \text{ m}^2/\text{V} \cdot \text{S}$, were examined. Figure 5 shows that the concentration distribution during the dispensing process. From this figure, we can see that when the absolute value of the electrophoretic mobility increases from $2.0 \times 10^{-8} \text{ m}^2/\text{V} \cdot \text{S}$ to $3.5 \times 10^{-8} \text{ m}^2/\text{V} \cdot \text{S}$, the volume of dispensed sample at the same time (i.e., $t = 2.0$ s) increases from 332 to 406 pl. This is because, with the negative electrophoretic mobility, the electrophoretic motion of the charged sample species is against the electroosmotic flow. The net effect is a reduced bulk flow velocity. When the absolute value of the electrophoretic mobility increases (from $2.0 \times 10^{-8} \text{ m}^2/\text{V} \cdot \text{S}$ in Fig. 5a to $3.5 \times 10^{-8} \text{ m}^2/\text{V} \cdot \text{S}$ in Fig. 5b), the net flow velocity of the sample decreases, and the velocity difference between the front of the sample (in the downstream of the dispensing channel) and the back of the sample (in upstream of the dispensing channel) is smaller. Consequently, the compressing effect
 FIG. 3.  Effect of the diffusion coefficient on the concentration field of the sample in the dispensing process. The black regions are the buffer solution; the white region is the sample solution with a sample concentration higher than 80% of the original sample concentration. The diffusion coefficient: (a) $1.0 \times 10^{-11}$ m$^2$/s, (b) $1.0 \times 10^{-10}$ m$^2$/s.

Channel Size Effect

In this set of simulations, the nondimensional applied electrical potentials are $\phi^*(1) = 1.0$, $\phi^*(2) = 1.02$, $\phi^*(3) = 0.0$, $\phi^*(4) = 1.02$ for the loading process, and $\phi^*(1) = 0.2$, $\phi^*(2) = 2.0$, $\phi^*(3) = 0.2$, $\phi^*(4) = 0.0$ for the dispensing process.

Three pairs of channel sizes were used to test the channel size effect on the dispensing process. The results are shown in Fig. 6. The first case (Fig. 6a) is the same as that shown in Fig. 1, where the size of the horizontal channel is equal to that of the vertical channel. We describe this case by the ratio of these two channel sizes, $W_y/W_x = 1:1$, where $W_y$ is the width of the horizontal channel and $W_x$ is the width of the vertical channel. In the second case (Fig. 6b), the size of the horizontal channel is twice that of the vertical channel, i.e., $W_y/W_x = 2:1$. In the third case (Fig. 6c), the size of the horizontal channel is half that of the vertical channel, i.e., $W_y/W_x = 1:2$. All other parameters are same for these three cases.

As seen from Fig. 6, the channel size has significant effects on the dispensing process and on the dispensed sample volume. Under the same applied electrical field, the shape and the volume of the loaded sample at the intersection are very different for these three cases. The loaded sample volume in the case of $W_y/W_x = 1:1$ is the largest. Consequently, the shape and the volume of the dispensed sample are very different for these three cases. The dispensed sample volume in the case of $W_y/W_x = 1:1$ is the largest (the sample volume is approximately 113 pl). This is because under the same applied
FIG. 4. Effect of the electroosmotic mobility on the concentration field of the sample in the dispensing process. The black regions are the buffer solution; the white region is the sample solution with a sample concentration higher than 80% of the original sample concentration. The electroosmotic mobility is (a) $5.0 \times 10^{-8}$ m$^2$/V·s, (b) $6.0 \times 10^{-8}$ m$^2$/V·s.

electrical potentials and the same channel surface properties, if the channel size changes, the electrical field will change since we applied the insulation boundary conditions to all the walls. Since the flow field depends on the electrical field as shown in Fig. 2, the concentration field, in turn, is strongly dependent on the electrical field. When the electrical field changes due to the change of channel size, the concentration distribution will change.

**Electrical Field Strength Effect**

For a given set of properties of the sample and the buffer solutions and the specified microchannels' surface properties and dimensions, the applied electrical potentials are the key controlling parameters for the loading and dispensing processes. Two different combinations of nondimensional applied electrical potentials were tested, as shown in Figs. 7 and 8. The nondimensional applied electrical potentials for the two cases in Fig. 7 are: in Fig. 7a,

\[ \phi^*(1) = 1.0, \; \phi^*(2) = 1.0, \; \phi^*(3) = 0.0, \; \phi^*(4) = 1.0 \]

for the loading process,

\[ \phi^*(1) = 0.2, \; \phi^*(2) = 2.0, \; \phi^*(3) = 0.2, \; \phi^*(4) = 0.0 \]

for the dispensing process;

in Fig. 7b,

\[ \phi^*(1) = 3.0, \; \phi^*(2) = 1.895, \; \phi^*(3) = 0.0, \; \phi^*(4) = 1.895 \]

for the loading process,

\[ \phi^*(1) = 0.2, \; \phi^*(2) = 2.0, \; \phi^*(3) = 0.2, \; \phi^*(4) = 0.0 \]

for the dispensing process.
The nondimensional applied electrical potentials for the two cases in Fig. 8 are: in Fig. 8a,

\[
\phi^* (1) = 1.0, \quad \phi^* (2) = 1.0, \quad \phi^* (3) = 0.0, \quad \phi^* (4) = 1.0 \\
\text{for the loading process,}
\]

\[
\phi^* (1) = 0.2, \quad \phi^* (2) = 2.0, \quad \phi^* (3) = 0.2, \quad \phi^* (4) = 0.0 \\
\text{for the dispensing process;}
\]

in Fig. 8b,

\[
\phi^* (1) = 1.0, \quad \phi^* (2) = 1.0, \quad \phi^* (3) = 0.0, \quad \phi^* (4) = 1.0 \\
\text{for the loading process,}
\]

\[
\phi^* (1) = 1.0, \quad \phi^* (2) = 2.0, \quad \phi^* (3) = 1.0, \quad \phi^* (4) = 0.0 \\
\text{for the dispensing process.}
\]

The simulation results show that the loading electrical field strength has very important effects on the volume of the dispensed sample, as shown in Figs. 7a and 7b. Under the same dispensing conditions, if the applied electrical potential for the loading process is changed, the size of the loaded sample in the intersection of the microchannels changes and eventually the volume of the dispensed sample changes. Figures 7a and 7b clearly demonstrate the difference. The volume of the dispensed sample in the downstream of the dispensing channel changes significantly from 390 pl in Fig. 7a to 204 pl in Fig. 7b.

Comparing Figs. 8a and 8b, we see that under the same loading conditions, if the applied electrical potential for the dispensing process changes, the volume of the dispensed sample changes too. For example, during the dispensing process, while \( \phi^* (2) \) and \( \phi^* (4) \) keep constant, \( \phi^* (1) \) and \( \phi^* (3) \) are increased from 0.2
FIG. 6. Effect of the microchannel size on the concentration field of the sample in the dispensing process. The black regions are the buffer solution; the white region is the sample solution with a sample concentration higher than 80% of the original sample concentration. The channel width ratio is (a) \( W_y/W_x = 1:1 \); (b) \( W_y/W_x = 2:1 \); (c) \( W_y/W_x = 1:2 \).

In Fig. 8a to 1.0 in Fig. 8b, the volume of the dispensed sample increases (i.e., from 390 pl in Fig. 8a increases to 527 pl in Fig. 8b). This is because when \( \phi^*(1) \) and \( \phi^*(3) \) are bigger, the electrical field strength between the intersection and reservoir 1 and between the intersection and reservoir 3 is weaker. Consequently, less amount of the sample is drawn back toward these two reservoirs and a bigger portion of the sample is dispensed downstream in the dispensing channel (Fig. 8b).

Practical applications such as on-chip separation and detection require that the dispensed sample must be distributed
Effect of the applied electrical potentials in the loading process on the concentration field of the sample in the dispensing process. The electrical potentials for the dispensing process are the same for both cases (a) and (b). The black regions are the buffer solution; the white region is the sample solution with a sample concentration higher than 80% of the original sample concentration. The nondimensional applied electrical potentials are shown at the bottom of this figure.

uniformly across the channel cross-section or have an evenly cut plug shape. However, the shape of the dispensed sample strongly depends on the dimensions of the cross microchannels and the combination of the applied electrical potentials. The even plug shape of the dispensed samples presented in most figures in this paper is the results of carefully choosing the optimal controlling electrical potentials. Figure 6b shows an example of nonuniformly dispensed sample.
As discussed above, there are several parameters affecting the dispensing process and a certain combination of these parameter values are required for dispensing a specific sample volume. The theoretical model presented in this paper can simulate both the loading and dispensing process and predict the dispensed sample volume under any specific conditions. Therefore, it can find the optimal values of these controlling parameters for dispensing any specific volume of the sample.
SUMMARY

A theoretic model was developed in this work to simulate the sample loading and dispensing processes in microfluidic dispensers. The electrical potential field, the flow field, and the concentration field were obtained by numerically solving this theoretical model. The effects of several controlling parameters on the dispensing process were investigated. We found that the diffusion coefficient, the electroosmotic mobility, the sample’s electrophoretic mobility, the applied potentials, and the channel sizes have effects on the dispensing process. When the diffusion coefficient increases 10 times, the volume of the dispensed sample decreases by only about 2%. When the electroosmotic mobility increases, the average velocity of the bulk flow increases, and hence the sample is transported more quickly and has less chance to diffuse into the buffer solution. When the absolute value of the sample’s electrophoretic mobility increases, the region of high sample concentration increases and hence the dispensed sample volume increases. Because both the loading and the dispensing processes are electrokinetically driven processes, changes in the applied potentials and in the channel sizes will directly change the applied electrical field in the dispenser, and hence dramatically affect the effectiveness of the loading process and the size of the dispensed sample.

Overall, the results reported in this paper show that the size and the shape of the dispensed sample can be controlled by the channels’ dimensions and the applied electrical potentials. The model developed in this work can be used to find the optimal controlling parameter values for the loading and the dispensing processes.

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REFERENCES