Dispersion Modeling in Microfluidic Channels for System-level Optimization

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ABSTRACT

Chip-based microfluidic separation systems often use serpentine channels to achieve long separation lengths in minimal area. Such designs suffer from the 'racetrack' effect due to the bends in the microchannel. In addition, the skew produced by a bend cannot be undone by an equal and opposite bend due to non-axial diffusion occurring in the inter-turn straight channel. This paper analyzes the non-axial diffusion of skewed bands of solute, in electrokinetic microchannels containing turns, to develop models which can be used for a system-level optimization of such designs. Distortion caused by transition and wall effects in the turn geometry and the inter-turn channel are also analyzed. Finite volume simulations are used to verify the proposed theory.

Keywords: turn induced dispersion, non-axial diffusion, effective diffusivity, electrokinetic separation, microfluidics, micro total analysis systems

INTRODUCTION

Microfluidic channels and turns are finding increasing use in micro total analysis systems (µTAS). Serpentine channels, commonly used due to the simultaneous need for long separation lengths and compact microchip area, suffer from the 'racetrack' effect. Previous analytical models predict that equal and opposite (complimentary) turns can cancel the 'racetrack effect' [1]. Recent studies indicate that non-axial diffusion of the band after the first turn cannot be undone in the equal and opposite second turn, and therefore, propose non-uniform width turns [2][3][4]. These device-level optimizations result in devices requiring high aspect ratio fabrication facilities and potentially suffer from increased dispersion due to Joule heating in the constricted portion of the turn. In contrast, this paper aims at a system-level approach to the optimization of microfluidic separation systems by developing a model of the non-axial dispersion introduced in microfluidic bends and inter-turn straight channels. Models capturing distortion induced by the channel wall and due to the field transition in the turn geometry are also proposed. Such models, and the resulting optimization of the microfluidic system as a whole, will lead to clearer trade-offs for µTAS designs.

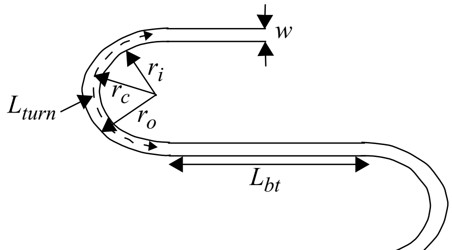

Figure 1: Geometrical parameters for a serpentine channel

BACKGROUND

Based on the advection-diffusion equation [5], the dispersion of solutes in a electrokinetic microchannel, due to turns in the microchannel, can be analyzed by considering three regimes [4] in the parameter space of dispersion Peclet number (Pe_{turn}) in the turn and ratio of axial length (L_{turn}) and width (w) (Figure 1). The dispersion Peclet number (Pe_{turn}) characterizes the relation between transport of solute due to advection and diffusion respectively and is given by $Pe_{turn} = (U_{turn}w)/D$ where D is the diffusivity of the solute. U_{turn} is the maximum velocity difference in a direction transverse to the channel and for an axial electric field whose magnitude is inversely proportional to radius is given by $2((wr_c)/(r_ir_o))U_c$ where, r_c, r_i and r_o are the radius of curvature at the center, inner side and outer side of the turn respectively, and U_c is the electric field at the center. When $Pe_{turn} < 1$, diffusion dominates over advection and hence the effect of turn induced dispersion is negligible compared to the dispersion due to axial diffusion. Similarly, when $L_{turn}/w > Pe_{turn} > 1$ (Taylor-Aris regime), the skew produced by the turn is masked by the non-axial diffusion and hence the behavior of the solute can be modeled using an effective diffusivity (D_{eff}). However, most microchannel system designs lie in the Pure Advection regime where $Pe_{turn} > L_{turn}/w$ [1][2]. Here the turn causes a well-defined skew (ΔL) in the solute band, causing an additional dispersion referred to as the 'racetrack' effect. The amount of skew (ΔL) [1] for a constant radius turn of angle θ is given by $\Delta L = 2\theta F$. F is a factor given by $F = w(1 - exp(t_D/t_t))$, where, w is the width of the channel, t_D is the transverse diffusion equilibrium time and t_t is the turn transit time. This implies that two equal and opposite turns should nullify such a skew. However as observed in [4], this cancellation depends on the distance between the two turns (L_{bt}) and the Peclet number in the channel (Pe_{bt}) given by $Pe_{bt} = (Uw)/D$ where, U is the velocity of the solute in the channel. Based on L_{bt}, the pure advection region can be further subdivided into two regions: (a) where the non-axial diffusion does not dominate ($Pe_{turn} > L_{turn}/w$ and $Pe_{bt} \gg L_{bt}/w$) and (b) where the non-axial diffusion dominates and hence the skew produced by a turn vanishes before reaching the second turn. In both these cases the diffusion of the band in the inter-turn channel is larger than predicted by the diffusivity of the solute. Separate additional effects (described below) cause distortion of the skewed band which cannot be undone by the second turn.

DISPERSION MODELS

To understand the diffusion process in the inter-turn channel, consider a plug-shaped band, of solute, which becomes skewed as it travels through the turn (Figure 2). To model the diffusion of the band we utilize the assumption that all diffusion occurs perpendicular to the face of the band. Before the turn, as the band travels from *a* to *b* it undergoes broadening due to axial diffusion which can be characterized by the diffusion length (L_d') given by $L'_d = \sqrt{2D(t_2 - t_1)}$. When this band flows through the bend, it undergoes a skew characterized by the angle α which for a turn of constant radius is given by $tan\alpha = 1/(2\theta)$, θ being the angle of the bend. This skewed band undergoes a diffusion perpendicular to it's face, *i.e.*, along the ordinate (x') of the local reference system of the band which is characterized by the diffusion length (L_d) given by $L_d = \sqrt{2D(t_4 - t_3)}$ in the local reference system. This leads to an effective axial diffusion length (L_{deff}) given by $L_{deff} = L_d/(sin\alpha)$ which can be modeled using an effective axial diffusivity (D_{eff}) of $D/(sin\alpha)^2$, which can be re-expressed as $D(1 + 4\theta^2)$. The resulting increase in the variance ($\Delta\sigma^2$) is then given by $\Delta\sigma^2 = 2D_{eff}t$, where t is the transit time.

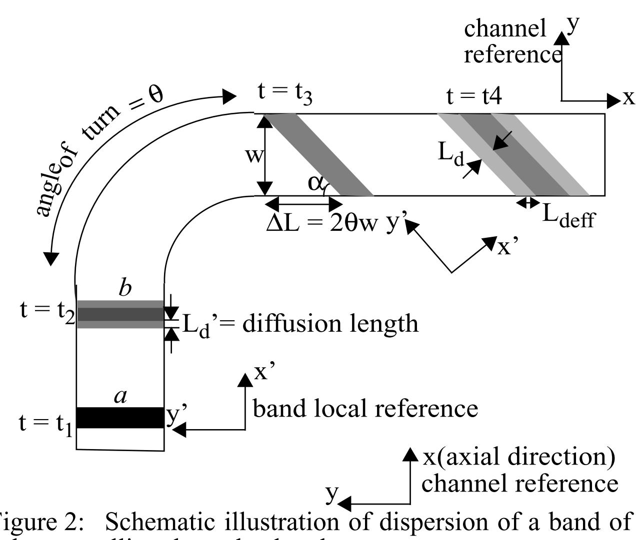

Figure 2: Schematic illustration of dispersion of a band of solute travelling through a bend

In addition to the increased diffusivity for a skewed band, as described above, wall-related effects also take place. For an un-skewed band (orthogonal to the channel), the diffusion behavior of the solute can be approximated as diffusion of a plug in an infinite channel. Hence the concentration profile, after diffusing for time *t*, is given by a gaussian having a standard deviation (σ) of *2Dt*. However, this assumption is not true for the acute-angled corners of a skewed band (Figure 3(a)). Here the resulting concentration profile can be obtained by assuming the walls to be reflecting surfaces which folds the portions of the ideal gaussian profile that lie outside the walls. This results in an increased concentration of the solute at the corners of the skewed band (as shown by the plot of the concentration profiles at different regions of the band in Figure 3(b)). Also, in order to maintain continuity of mass, the obtuse-angled corners of the skewed band tend to pull the expanding face of the band backward, resulting in a rounding of the face of the band at these corners. Both these effects result in a distortion of the face of the band (line of same solute concentration) and hence change the effective diffusivity (D_{eff}). Moreover, they tend to twist the skewed band to bring it back to its original shape (orthogonal to the direction of flow). When diffusion in the inter-turn length is small (*i.e.*, when $Pe_{turn} > L_{turn}/w$ *and* $Pe_{bt} \gg L_{bt}/w$) and the skew is small (*i.e.*, the skew angle α is large), such second order effects can be neglected and the diffusion in the inter-turn channel can be modeled using a single value of effective diffusion. If these conditions are not met then the diffusion in the inter-turn channel needs to be modeled by an effective diffusivity which varies with time.

In addition to the wall effects described above, micro-channels containing turns also suffer from distortion caused by the transition region of the electric field between the straight channel and the turn. As the electric field changes

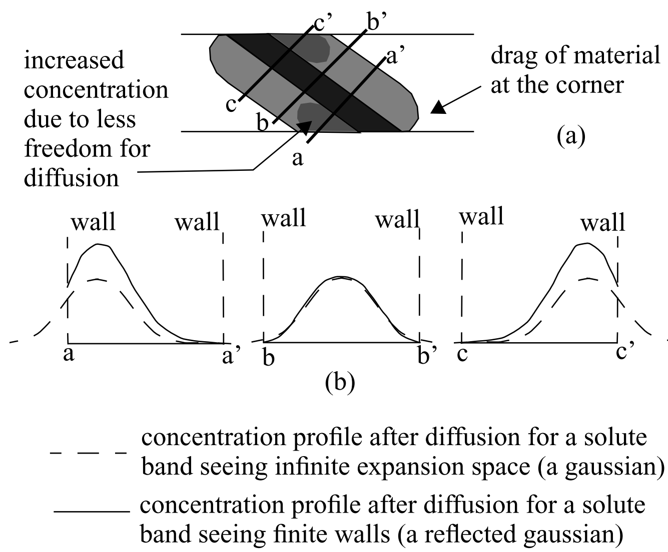

Figure 3: Wall effects in the diffusion of a skewed band. (a) the distorted band face after diffusion, (b) the concentration profile at various regions of the band

from a uniform field in the straight section to a radially decreasing circumferential field in the turn (Figure 4(a) and (b)), it passes through a transition region in which the field is not purely axially directed. The extent of this transition region varies with position along the width of the turn (Figure 4(c)). When the solute passes through two complimentary turns, it encounters two transition electric fields which are not equal (*e.g.*, the portion of solute which faces the transition region of the outer curve of the first bend encounters the transition region of the inner curve of the second bend). This causes an effective delay in the motion of the solute near the walls of the channel and produces a curved profile of the band after the complimentary turns and hence causes an additional dispersion. This effect is additive and the distortion increases as the number of complimentary turns in the microchannel increases.

RESULTS

This section presents results from finite volume (FVM) simulations of different geometries, using CoventorWare [6], to demonstrate the various dispersive effects in a microchannel described in the previous section. The skew angle (a) produced due to a 180^o turn is 9.0^o and that produced by a 90^o turn is 17.7^o. Hence for the analyzing a skewed band in a straight channel, the values for skew angle (α) have been approximated as 10^o and 20^o. This helps us imitate the two types of turns commonly used (a U turn and a right angle turn) while maintaining the ease of fast mesh generation for these test cases. Simulations for the worst and best case using these values have been shown. Finally the analytical results are verified for a serpentine channel.

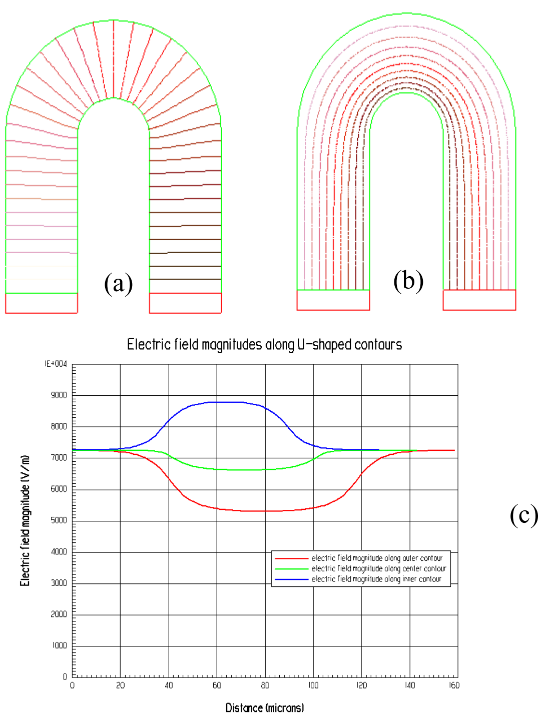

Figure 4: Numerical simulation showing the electric field in transition region of a microfluidic bend. (a) Plot of equipotential lines, (b) Plot of the streamlines, (c) Plot of electric field magnitude with distance along different inverted U-shaped contours. The channel width here has been exaggerated in order to show the effect of the transition region.

Skewed band in a straight channel

Figure 5(a) shows the dispersion of a skewed band in a straight channel for $(Pe)/(L/w) = 107$ and $\alpha = 20^o$. The diffusivity for the solute was assumed to be 3 $\mu m^2/s$. Figure 5(b) compares the standard deviation (σ) obtained from simulation with the value predicted using an effective diffusivity ($D_{eff} = D/(sin20)^2 = 25.6$). The standard deviation predicted from the derived analytical formula was found to be within 3% of the standard deviation obtained from numerical simulation). However when $Pe/(L/w)$ is reduced to 7 and the skew angle decreased to 10^o, the effects described above become more prominent (Figure 6(a)) and the standard deviation predicted by the formula using constant effective diffusivity no longer matches the value obtained from numerical simulation. As seen in Figure 6(b), the change in standard deviation (slope of the curve) obtained from simulation

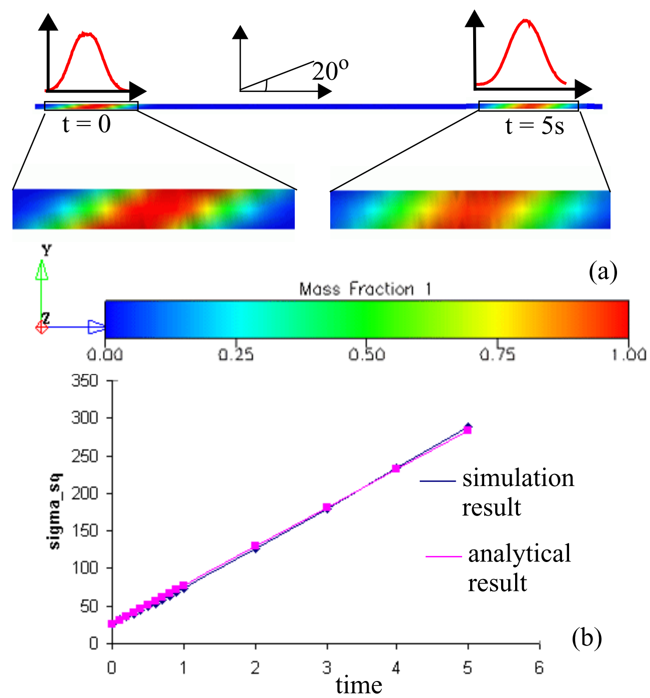

Figure 5: Comparison of FVM simulation data with analytical formula proposed for $(Pe)/(L/w) = 107$ and $\alpha = 20^o$. (a) shape of the band at start and after 5s, (b) plot of standard deviation (σ) obtained from simulation and from analytical formula using effective diffusivity

decreases with time implying that the effective diffusivity decreases with time as predicted, due to the wall effects.

Complementary turn channel

To demonstrate the system-level use of the proposed models, we compare the sum of the effective dispersion in the turns and the straight channels between the turns to numerical simulation of a serpentine channel having a pair of complimentary turns of radius 80 mm. Pe_{bt} and Pe_{turn} were set to 120 and the diffusivity of the species was set to 100. The initial and final values of standard deviation were found to be 1.4 and 79.7 respectively. Using the species diffusivity for travel within the turn and effective diffusivity ($100/\sin^2(9.0^o)$) for the skewed band in the inter turn channel the analytically predicted standard deviation is 81.5, which differs from the FVM simulation by only 2.3%.

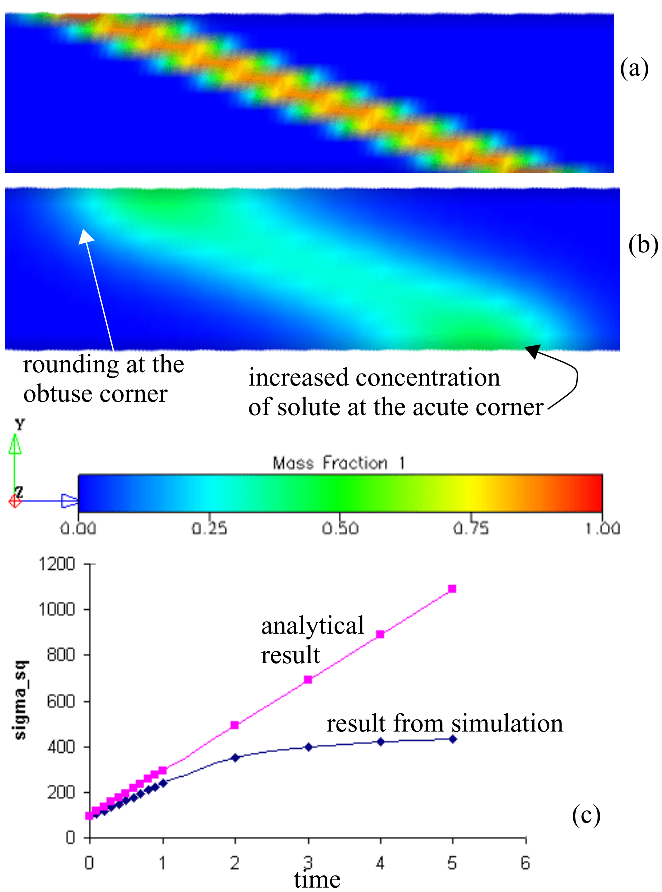

Figure 6: Comparison of FVM simulation data with analytical formula proposed for $(Pe)/(L/w) = 7$ and $\alpha = 10^o$. (a) shape of the band at start, (b) shape of the band after 5s, (c) plot of standard deviation (σ) obtained from simulation and from analytical formula using effective diffusivity.

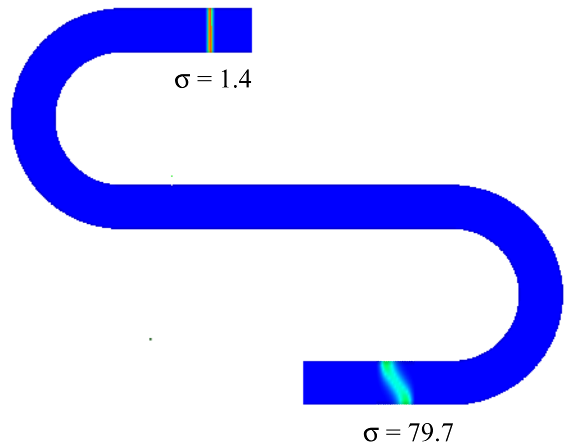

Figure 7: Dispersion in serpentine channel from FVM simulation.

CONCLUSION

A system level approach towards understanding the dispersion of solute bands in electrokinetic microchannels containing turns has been described. An analytical formula for diffusion in inter-turn channel for the commonly observed flow regime has been derived and verified using finite volume simulations. Additional effects in such channels have been identified and their presence verified using numerical simulations. Analytical models for such effects are currently being formulated, so as to describe dispersion in microchannels for all regimes. Such analytical models should facilitate system level optimization of microfluidic channels, resulting in better designs for micro total analytical systems.

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