An Analytical Solution on Convective and Diffusive Transport of Analyte in Laminar Flow of Microfluidic Slit

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Abstract— Microfluidic devices could find applications in many areas, such as BioMEMs, miniature fuel cells and microfluidic cooling of electronic circuitry. One of the important considerations of microfluidic device in analytical and bioanalytical chemistry is the dispersion of solute. In this study, we have developed an analytical solution, which considers the axial dispersion of a solute along the flow direction, to simulate convection and diffusion transport in a pressure driven creeping flow for a rectangular shape slit. During flow, the balance of competing effects of diffusion (especially cross-section diffusion) and convective diffusion in the flow direction are investigated.

Keywords— Diffusion/convection transport, Microfluidic, Pressure-driven flow, Taylor-Aris dispersion.

I. INTRODUCTION

Interests in microfluidc devices and components have recently been stimulated over the past decade by its potential applications in analytical and bioanalytical chemistry [1-2]. Examples of manipulations of fluid that are important include dynamic cell separations [3-4], surface patterning of cells and proteins [5], mass spectrometer delivery modules [6] and mixing of two different analytes. In nearly every microfluidic format, diffusion of the analytes or particles of interest is a fundamental aspect of the device operation.

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In microchannel, flow of liquids was usually driven by electrical field and/or pressure gradient for concentrationdependent processing in biochemical and chemical industry. Fluid flow driven by electric field is electrokinetically driven [7]. This approach was limited to polar solvent and may lead to sample damage by Joule heating in certain cases. Fluid flow driven by pressuregradient was designed to employ a branching mechanism [8]. This requires long mixing lengths and has comparatively large dead volumes and consumes relatively large amounts of precious analyte due to fast flow rates. However, it is preferable to use pressure-drvien flow due to its relative ease, flexibility of fabrication and insensitivity to surface contamination, ionic strength et al. Such kind of flow with continuous input in a microfluidic rectangular slit generates additional complexity in the distribution of analytes because of the parabolic velocity gradient across cross-sectional dimensions [9]. In addition, the breadth of such a distribution is decreased or increased by diffusion across the velocity gradient. Therefore, the distribution is highly dependent on dispersion mechanism of an analyte. The phenomena specific to pressure-driven side-by-side flow in a microchannel with continuous input are only beginning to be investigated [10-14,17].

One device in which diffusion plays a crucial role is the Yshape analytical device [11-13], which utilizes the interdiffuion of analyte from two or more input streams to produce an analyte concentration changes. The flow is strictly laminar and transport between analyte solution stream occurs side-by-side through interdiffusion since very low Reynolds number was employed. Brody et al.[5] presented some examples of the design of microfluidic device for biological processes. Kamholz et al. [10] presented an one-dimensional analytical model to quantitatively describe molecular diffusion in the microchannel of a T-sensor. Subsequently, a theoretical analysis of the scaling law in the absence of axial diffusion of the T-sensor based on molecular diffusion was proposed [11]. The molecular diffusion between two pressure-driven laminar flows at high Peclet numbers was experimentally and theoretically quantified by Ismagliov [14]. Finite element and finite difference method were employed to solve the coupled Navier-Stokes and diffusion-convection equation t o describe mass transport between fluid flows of two similar liquids [15-18]. However, the main difficulty in numerical calculation at high flow rates, which is associated with low values of diffusion coefficients, was encountered. Although very fine local mesh size can decrease numerical diffusion, but the resulting mesh would induce computational limitation.

Taylor dis persion [19-20] was widely proposed to be a phenomenon associated with the flow of two miscible fluids of similar properties. Taylor showed that even when the axial diffusion is small, the combined effects of axial convection and radial diffusion provides an axial diffusion equation governing the cross-section averaged concentration. Taylor's results were later verified and extended by Aris [21] and Barton [22] using the method of moments, and by Brenner [23] using multiple pole expansion.

In this study, we investigated analytically two miscible fluids of similar properties in a side-by-side pressure-driven creeping flow in the Yshape analytical device by using area-average method, which considered the axial dispersion of a solute along the flow direction. A two dimensional analytical solution in terms of enhanced axial dispersion is proposed to simulate long times convection and diffusion transport in a pressure driven creeping flow for a rectangular shape slit, which can overcome traditional numerical diffusion without time-consuming computational limitations.

II. MATHEMATICAL FORMULATIONS

A. Governing equations

Considering two streams pressure-driven flow side-byside between two parallel plates of a distance 2b apart (see Figure 1), with volumetric flow rate Q. A Cartesian coordinate system is utilized. In a microfluidic device, due to the low velocity of the flow and the micron size channels, the Reynolds number (Re) relating the inertial forces to the viscous forces, which is given by $\text{Re} = \overline{u}L/n$, is usually low [10]. This means that viscosity plays a dominant role in microchannels rather than inertia. When Re <<1, the Navier-Stokes equation in the absence of inertia effect can be employed to describe the Y-shape microfluidic device for incompressible flow [24]:



Figure 1 Simplified geometry of the Y-shape analytical device, with two fluids flow side-by-side. The analyte has diffused across the original interface (defined by dotted lines) between two fluids. The microfluidic device dimensions are L=4.5cm, W=150 mm, b=20 mm.

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

$$-\nabla p + \nabla \cdot \overline{\overline{t}} = 0 \tag{2}$$

$$\frac{\partial \mathbf{f}}{\partial t} + \vec{u}\nabla \mathbf{f} = D\nabla^2 \mathbf{f}$$
(3)

Considering a Newtonian fluid, the extra stress tensor \overline{t} is given by:

$$\overline{\overline{t}} = h\overline{\overline{g}}$$
(4)

where $\overline{\overline{g}}$ is the rate of strain tensor defined by $\overline{\overline{g}} = \nabla \overline{u} + (\nabla \overline{u})^T$. For pressure-driven slit flow, we have $\partial/\partial z \ll \partial/\partial x, \partial/\partial y; \quad u_x, u_y \ll u_z; \quad u_z = u_z(y)$ and p = p(z). Under these assumptions, the conservation equations (1)-(3) were greatly simplified to:

$$Q = 2W \int_{0}^{b} u_z dy$$
 (5a)

$$\frac{\partial p}{\partial z} - \frac{\partial}{\partial y} (\mathbf{h} \frac{\partial u_z}{\partial y}) = 0$$
(5b)

$$\frac{\partial \mathbf{f}}{\partial t} + u_z \frac{\partial \mathbf{f}}{\partial z} = D\nabla^2 \mathbf{f}$$
(5c)

B. Dispersion calculation with area average

The interplay of convection and diffusion is crucial in many microfluidic applications. The spreading of an injected analyte in a pressure-driven Poiseuille flow generally occurs much more rapidly than predicted if only molecular diffusion is considered. This Taylor dispersion occurs because molecular diffusion allows suspended particles to sample streamlines that have different speeds. In our investigation, we use an average analysis [24], wherein it is convenient to work with the cross-sectional

average
$$\overline{f} \equiv (2b)^{-1} \int_{-b}^{b} f dy$$
.

The low-Reynolds number velocity profile for flow in this geometry obtained from equation (5b) is:

$$u_{z}(y) = \frac{3\overline{u}}{2} [1 - (\frac{y}{b})^{2}]$$
(6)

where $\overline{u} = \frac{\partial P}{\partial z} \frac{b^2}{3h}$ is the cross-sectionally average velocity.

The concentration field of a dissolved solute evolves according to the convective-diffusion equation (5c):

$$\frac{\partial \mathbf{f}}{\partial t} + u_z(y)\frac{\partial \mathbf{f}}{\partial z} = D\nabla^2 \mathbf{f}$$
(7)

It is conceptually useful to work in terms of averages and deviations. Thus, we define $u_z(y) = \overline{u} + u'(y)$ and $\mathbf{f}(x, y, z, t) = \overline{\mathbf{f}}(x, z, t) + \mathbf{f}'(x, y, z, t)$, and substituting into equation (7) to give:

$$\frac{\partial \overline{\mathbf{f}}}{\partial t} + \frac{\partial \mathbf{f'}}{\partial t} + \overline{u} \frac{\partial \overline{\mathbf{f}}}{\partial z} + u' \frac{\partial \overline{\mathbf{f}}}{\partial z} + \overline{u} \frac{\partial \mathbf{f'}}{\partial z} + u' \frac{\partial \mathbf{f'}}{\partial z} =$$

$$D\nabla^2 \overline{\mathbf{f}} + D\nabla^2 \mathbf{f'}$$
(8)

Cross-sectional averaging of equation (7) leads to the mean convective-diffusion equation:

$$\frac{\partial \vec{F}}{\partial t} + \vec{u} \frac{\partial \vec{F}}{\partial z} = D\nabla^2 \vec{F} - \vec{u'} \nabla \vec{F'}$$
(9)

The additional contribution to the effective diffusion of the solute that arises from the "fluctuation" generated flux $\overline{u\nabla f'}$. u'(y) is given as:

$$u'(y) = \frac{\partial P}{\partial z} \frac{b^2}{6\mathbf{h}} [1 - 3(\frac{y}{b})^2]$$
(10)

In order to derive the equation governing f', we subtract equation (9) from equation (8) to obtain:

$$\frac{\partial \mathbf{f}'}{\partial t} + u' \frac{\partial \overline{\mathbf{f}}}{\partial z} + \overline{u} \frac{\partial \mathbf{f}'}{\partial z} + u' \frac{\partial \mathbf{f}'}{\partial z} = D\nabla^2 \mathbf{f}' + \overline{u'} \nabla \mathbf{f}'$$
(11)

Due to the long times characteristic of cross-stream diffusion being rapid relative to streamwise, i.e., $L \gg \overline{u}b^2/D$, and because $u' = O(\overline{u})$ while $\mathbf{f'} << \overline{\mathbf{f}}$, then equation (11) simplifies to:

$$u'\frac{\partial \overline{F}}{\partial z} \approx D \frac{\partial^2 f'}{\partial y^2}$$
(12)

Since u' is known, the solution of this equation satisfying $\partial \mathbf{f}' / \partial y = 0$ at y = 0 is given by:

$$\mathbf{f}'(x, y, z) = \frac{\partial P}{\partial z} \frac{b^2}{12\mathbf{h}D} [y^2 - \frac{y^4}{2b^2}] \frac{\partial \overline{\mathbf{f}}}{\partial z} + \mathbf{f}'(x, 0, z)$$
(13)

Thus, the additional contribution due to velocity variation from the average velocity can be written as:

$$\overline{u'\nabla f'} = \overline{u'\frac{\partial f'}{\partial z}} = -\frac{2}{105} \left\{ \left(\frac{\partial P}{\partial z}\right)^2 \frac{b^6}{9h^2 D} \right\} \frac{\partial^2 \overline{f}}{\partial z^2}$$
(14)

From equation (5c), it follows that the average concentration is governed by the two-dimensional convective-diffusion equation:

$$\frac{\partial \overline{F}}{\partial t} + \overline{u} \frac{\partial \overline{F}}{\partial z} = D \frac{\partial^2 \overline{F}}{\partial x^2} + D_{eff} \frac{\partial^2 \overline{F}}{\partial z^2}$$
(15)
where $D_{eff} = D + \frac{2}{105} \{ (\frac{\partial P}{\partial z})^2 \frac{b^6}{9\mathbf{h}^2 D} \}$

In regard to continuous species transport in microfluidic device, the steady flow species transport is assumed. Thus the steady species transport equation (15), by considering the Taylor-Aris dispersion, is reduced to:

$$\overline{u}\frac{\partial\overline{F}}{\partial z} = D\frac{\partial^2\overline{F}}{\partial x^2} + D_{eff}\frac{\partial^2\overline{F}}{\partial z^2}$$
(16)

The following initial and boundary conditions are considered:

B.C.1:
$$\mathbf{f}(x, z)\Big|_{z=0} = 0, \ 0 \le x < W/2$$
 (17a)

B.C.2:
$$\mathbf{f}(x, z)\Big|_{z=0} = \mathbf{f}_0, \quad W/2 < x \le W$$
 (17)

B.C.3:
$$\frac{\partial \mathbf{f}}{\partial z}\Big|_{x,z=L} = \frac{\partial \mathbf{f}}{\partial x}\Big|_{x=0,z} = \frac{\partial \mathbf{f}}{\partial x}\Big|_{x=W,z} = 0$$
 (17c)

with the following dimensionless parameters

$$\mathbf{f}^* = \frac{\overline{\mathbf{f}}}{\mathbf{f}_0}; \ z^* = \frac{z}{L}; \ x^* = \frac{x}{W}; \ Pe = \frac{\overline{u}L}{D}$$
(18)

In terms of the variables just defined, the dimensionless form of equation (16) can be written as:

$$Pe\left(\frac{W}{L}\right)^{2}\frac{\partial \mathbf{f}^{*}}{\partial z^{*}} = \frac{\partial^{2}\mathbf{f}^{*}}{\partial x^{*2}} + \frac{D_{eff}}{D}\left(\frac{W}{L}\right)^{2}\frac{\partial^{2}\mathbf{f}^{*}}{\partial z^{*2}}$$
(19)

Similarly, the boundary condition can also be written in a dimensionless form as:

B.C.1:
$$\mathbf{f}^{*}(x^{*}, z^{*})|_{z^{*}=0} = 0, \ 0 \le x^{*} < 1/2$$
 (20a)

B.C.2:
$$f^*(x^*, z^*)|_{z^*=0} = 1, 1/2 < x^* \le 1$$
 (20b)

B.C.3:
$$\frac{\partial \mathbf{f}^*}{\partial z^*}\Big|_{x^*,z^{*=1}} = \frac{\partial \mathbf{f}^*}{\partial x^*}\Big|_{x^*=0,z^*} = \frac{\partial \mathbf{f}^*}{\partial x^*}\Big|_{x^*=1,z^*} = 0$$
 (20c)

An analytical solution of equation (19) with boundary conditions (20) can be obtained by using a separation of variables technique.

$$\frac{\bar{F}}{F_0} = \frac{1}{2} - \frac{2}{p} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n-1)} \cos(\frac{(2n-1)px}{W}) \mathbf{y}_n(z)$$
(21)

where

$$\mathbf{y}_{n}(z) = \frac{e^{\mathbf{I}_{2}z} - (\mathbf{I}_{2} / \mathbf{I}_{1})e^{(\mathbf{I}_{2} - \mathbf{I}_{1})L + \mathbf{I}_{1}z}}{1 - (\mathbf{I}_{2} / \mathbf{I}_{1})e^{(\mathbf{I}_{2} - \mathbf{I}_{1})L}}$$
(22a)

$$\boldsymbol{l}_{1} = \frac{Pe}{2L} + \{(\frac{Pe}{2L})^{2} + (\frac{D}{D_{eff}})[\frac{(2n-1)\boldsymbol{p}}{W}]^{2}\}^{\frac{1}{2}}$$
(22b)

$$\boldsymbol{I}_{2} = \frac{Pe}{2L} - \{(\frac{Pe}{2L})^{2} + (\frac{D}{D_{eff}})[\frac{(2n-1)\boldsymbol{p}}{W}]^{2}\}^{1/2}$$
(22c)

7b) C. Two special cases

(a) Without axial diffusion and Taylor-Aris dispersion

Without axial diffusion and Taylor-Aris dispersion (D_{eff} is negligible), the streamwise diffusion is negligible compared to the spanwise diffusion (i.e. $\partial^2 \mathbf{f} / \partial z^2 \ll \partial^2 \mathbf{f} / \partial x^2$). Thus, equation (16) can be reduced to the following form :

$$Pe\left(\frac{W}{L}\right)^{2}\frac{\partial \mathbf{f}}{\partial z} = \frac{\partial^{2}\mathbf{f}}{\partial x^{2}}$$
(23)

With this simplification and the same boundary conditions (20), an analytical solution for equation (23) is obtained:

$$\frac{\overline{F}}{F_0} = \frac{1}{2} - \frac{2}{p} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n-1)} \cos(\frac{(2n-1)px}{W}) e^{-[(2n-1)p]^2 \frac{4z}{WPe}}$$
(24)

(b) With axial diffusion and without Taylor-Aris dispersion

With axial diffusion and without Taylor-Aris dispersion, equation (16) can be written in the following form:

$$Pe\left(\frac{W}{L}\right)^{2}\frac{\partial f}{\partial z} = \frac{\partial^{2} f}{\partial x^{2}} + \left(\frac{W}{L}\right)^{2}\frac{\partial^{2} f}{\partial z^{2}}$$
(25)

Analytical solution (21) is applicable to equation (25) with effective diffusivity D_{eff} replaced by D.

III. RESULTS AMD DISCUSSIONS

Figure 2 shows a comparison of concentration profile of analyte at the exit section with and without axis diffusion and Taylor-Aris dispersion. Through these concentration profiles, we observe that the diffusion in the spanwise direction changes drastically with consideration of Taylor-Aris dispersion. The reason is that the effective diffusivity can be orders of magnitude larger than it would have been in purely convective flow due to inhomogeneous velocity distribution in the gapwise direction. In fact, molecular diffusion in the major flow axis direction in purely convective flow has little effect on concentration profile ($W \ll L$), which is little difference from those obtained with $D_{eff} = D$.



Figure 2 Concentration profile with and without Taylor-Aris dispersion at the exit section of right side of device. The averaged velocity is 1cm/s, Molecular diffusion coefficient $D = 10^{-6} (cm^2/s)$

Figure 3 shows the evolution of concentration profile at three different sections (z=0, z=0.25L, z=L) along the flow direction. At entrance (z = 0.0), the two fluid inputs enter through the channel. The fluid on the right side contains diffusible analyte that is assumed to be uniform at the entrance. At position (z = 0.25L), there is a change of concentration due to interdiffusion between the two fluid side-by-side, see Figure 3. At the exit section (z = 1.0), interdiffusion is more pronounced. It could be observed that transverse diffusive broadening is proportional to the distance along the flow direction.

Figure 4 shows the concentration variation in the spanwise direction across the main channel. It is observed that the model presented can predict concentration variation in the spanwise direction with different average velocities. As the average velocity increases, the reduction in the mixing area of concentration profile across the contact interface can be observed. In addition, the evolution of interdiffusion zone during flow with different average velocities for the Yshape microfluidic device is shown in Figure 5. As expected, the diffusible analyte broadens at down stream due to longer resident time of diffusible analyte. As the averaged velocity decreases, the diffusible analyte also broadens at the contact interface of the two streams fluid. The reason is that the resident time of diffusible analyte with a slower flow rate is longer than that with a faster flow rate.





Figure 3 Evolution of concentration profile of analyte along the flow direction with Taylor-Aris dispersion at three different sections of right side of device. Averaged velocity = 2cm/s. Molecular diffusion coefficient $D = 10^{-6} (cm^2/s)$

Figure 4 Concentration profile across right hand side (the xdirection) of device. Molecular diffusion coefficient $D = 10^{-6} (cm^2/s)$, with Taylor-Aris dispersion.



Figure 5, Concentration evolution of interdiffusion zone with two different velocities (a) Um=1cm/s; (b) Um=0.5cm/s. Molecular diffusion coefficient $D = 10^{-6} (cm^2/s)$, with Taylor-Aris dispersion

The concentration distributions along the left and right walls are illustrated in Figure 6 for different values of the average fluid velocities at different height to width ratios of the channel. For Um=0.5cm/s and H/W=0.167, the mixing of the two solutions is complete at the end of the channel (C=0.5 at both walls, Figure 6a). For higher flow rate, the mixing efficiency is reduced due to shorter resident time. For Um=1cm/s and H/W=0.167, it can be observed that the mixing of the two solutions is incomplete at the end of the channel ($C_{left} = 0.459$, $C_{right} = 0.541$, as shown in Figure 6b). With an increase of the height of the channel, the mixing efficiency increases due to the increased contact surface of fluids, which will benefit process chemistry productivity.

IV. CONCLUSIONS

Since diffusion dominates spanwise transport and convection dominates streamwise transport, it is reasonable to simplify the three-dimensional model to two-dimensional mean convective-diffusion equations in high aspect ratio system based on effective dispersion coefficient, which can be several orders greater than the molecular diffusion coefficient. Two dimensional analytical solutions for pressure-driven side-by-side flow in Y-shape of microfluidic device are obtained based on convection and diffusion transport, with specific attention to the important Taylor-Aris mechanism due to transverse inhomogeneous velocity



(b) Um= 1 cm/s

Figure 6 Normalized concentration profile at the wall with different velocities and ratios of height to width of the channel. Molecular diffusion coefficient $D = 10^{-6} (cm^2/s)$, with Taylor-Aris dispersion

gradients, which can overcome the difficulty of numerical diffusion in numerical method.

NOMENCLATURE

- **h** = The viscosity of fluid ($Pa \cdot s$);
- \vec{u} =Velocity vector of the fluid (*cm*/*s*);
- \overline{u} = Averaged velocity of the fluid (*cm*/*s*);

u' = Velocity deviation from averaged velocity of the fluid (cm/s);

p = Pressure (Pa);

 \mathbf{n} = Kinetic viscosity (cm^2 / s);

f = an arbitrary function;

L = Length of rectangular slit in microfluidic device (*cm*);

D = Molecular diffusion coefficient of analyte (cm^2 / s);

x, y, z = Spanwise (width), gapwise (height) and flow

(length) direction of microfluidic flow respectively;

f = Sample concentration of analyte at any given point in microfluidic device;

 f_0 = Concentration of sample analyte inlet stream;

 \overline{f} = Averaged concentration of analyte;

f' = Concentration deviation from averaged concentration of analyte;

 D_{eff} = Effective dispersion coefficient of analyte (cm^2 / s);

 $\overline{\overline{t}}$ = Extra stress tensor;

 $\overline{\mathbf{g}}$ = Rate of strain tensor;

 u_x , u_y , u_z =The velocity component of the fluid in the x, y, z direction respectively (*cm*/*s*);

Q = Flow rate of the fluid (cm^3 / s);

W = Width of rectangular slit in microfluidic device ($\mathbf{n}m$);

H = Height of rectangular slit in microfluidic device ($\mathbf{m}m$);

b = Half height of rectangular slit in microfluidic device (**m***m*);

*f** = Dimensionless concentration of analyte;

 z^* = Dimensionless length of microfluidic device;

x * = Dimensionless width of microfluidic device;

Pe = Peclet number;

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