# MIXING, FLOW AND CHEMICAL REACTION OF PARTIALLY MISCIBLE COMPONENTS IN MICRO-SCALE CHANNELS

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**Abstract:** This paper addresses single- and two-phase flows in channels having widths in the range 0.1–10 microns. The focus is on differences in phenomena compared to mixing and flow in macro-channels. Major differences include the speed of cross-channel diffusion, the importance of axial diffusion, and effects due to the finite thickness of the interface between partially miscible phases and the chemical nature of the channel walls. Results and computational techniques are provided for estimating mixing times in initially striated flows, for the effects of combined cross-channel and axial diffusion on chemical reactions, and on the spatial-mean concentrations, convected-mean concentrations and relative flow rates of partially miscible components and the possibility of flow enhancement through the choice of wall chemistry.

**Keywords:** laminar flow; axial diffusion; radial diffusion; axial dispersion; micro-fluidics; micro-reactors.

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## INTRODUCTION

This paper envisions analytical instrumentation, presumably fabricated by hard lithography, in which channel dimensions are in the range 0.1–10 microns. This is in contrast to current devices fabricated by soft lithography with typical channel dimensions of 100–1000 microns. The motivation for smaller device sizes includes smaller smaple size, less by-product, improved safety, more functions per device and faster responce times. All these devices will operate in the laminar flow regime. Larger devices are sometimes limited by slow, cross-channel diffusion, and ingenious methods have been devised to disturb the flow in order to accelerate mixing (Deshmukh and Vlachos, 2005). Radial diffusion is 100–1 000 000 times faster for the smaller devices, solving the cross-channel mixing problem but new phenomena and new problems arise. The chemical nature of the wall relative to the bulk flow can be important. When the fluid is a multi-component mixture, there is the possibility of selective enrichment or depletion of one component near the wall, with subsequent consequences in flow and pressure drop. Also important is the width of the interface between partially miscible phases. When some of the components are polymers, the interfacial thickness can be an appreciable fraction of the channel width, invalidating the sharp-interface assumption conventionally used for two-phase flows.

### Mixing Times

Figure 1 allows estimates of the time required to achieve compositional uniformity for an initially striated minor component. This is a conventional result obtained by solving the diffusion equation for an inlet boundary condition corresponding to striated flow of non-reactive components:

$$v_z(y)\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial y^2} \qquad (1)$$

$$v_z(y) = 1.5\bar{u}(1 - y^2) \qquad (2)$$

The response of the system is governed by the initial distribution of components and a dimensionless diffusion number

$$D = \frac{Dt_{\mathrm{mix}}}{Y^2} \qquad (3)$$

where $D$ is the molecular diffusivity and $Y = W/2$ is the channel half-width. The mixing time is related to the mixing length by $L_{\mathrm{mix}} = \bar{u}t_{\mathrm{mix}}$. The results in Figure 1 apply to fluids with water-like properties and to asymmetric injection of the minor component along one wall. Composition uniformity is defined as a 99% response to the equilibrium concentration of the minor component at the opposite wall. The required value for $D$ is a very weak function of the concentration ratio, and $D = 1.6$ is adequate for minor component concentrations in the range 0.1–50%.

The key point is that radial mixing in micro-scale devices will be essentially

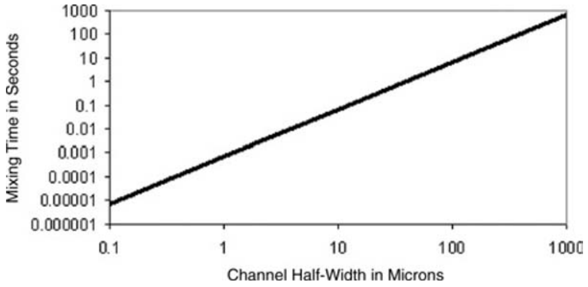

*Figure 1.* Mixing times for water-like fluids in ducts.

instantaneous for all but the fastest reactions. An acid-base titration will go to completion in 67 ms in a channel with width 2 $Y = W = 20$ microns and will go to completion in approximately one microsecond when $W = 0.2$ microns.

The results in this section apply to completely miscible components. When the components are partially miscible and are introduced as striated, pure components, they will quickly form an equilibrium interface as discussed subsequently in this paper.

### Axial Mixing

Figure 2 shows the effects of combined cross-channel and axial diffusion on the yield of a first order reaction with dimensionless rate constant $k\bar{t} = 1$. In this figure, the diffusion number is defined in terms of the mean residence time in the reactor, $D = \mathcal{D}\bar{t}/Y^2$ where $\bar{t} = L/\bar{u}$.

A version of Figure 2 has been reported previously (Nauman and Nigam, 2005). The current results eliminate a problem due to numerical ill-conditioning and extend the calculations into the region where the reactor performance approaches that of a CSTR. This is the region of interest for micron-scale reactors. For a water-like fluid in a 20 micron channel, $\mathcal{D}/Y^2 \approx 6\bar{t}(\text{time}^{-1})$, so that axial mixing will be significant for all but very fast reactions. For a 2 micron channel, reactor behavior will approximate that of a CSTR unless the channel is very long.

The results in Figure 2 use two different solution techniques that are matched at approximately the inflection points of the curves. For values of $D$ lower than the inflection point, the full diffusion equation is solved:

$$v_z(y)\frac{\partial c}{\partial z} = D\left[\frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right] - kc \tag{4}$$

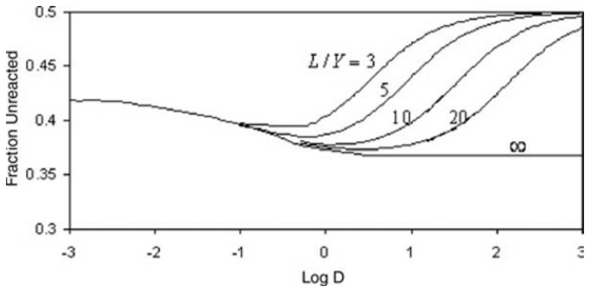

*Figure 2.* combined effects of radial and axial diffusion on the conversion of a first order reaction.

These solutions become ill-conditioned at high values of $D$ when the cross-channel concentration gradients have essentially vanished, but the axial dispersion model then becomes an excellent approximation, smoothly matching the earlier solution. Above the inflection point, the results in Figure 2 are from the analytical solution of the axial dispersion model

$$\bar{u}\frac{dc}{dz} = \frac{1}{\mathbf{Pe}}\left[\frac{d^2 c}{dz^2}\right] - kc \tag{5}$$

where the Peclet number **Pe** is related to $D$ by

$$\mathbf{Pe} = \frac{1}{D}\left[\frac{L}{Y}\right]^2 = \frac{\bar{u}L}{\mathcal{D}} \tag{6}$$

### PHASE SEPARATION IN SMALL SYSTEMS

Figure 3 shows the spatial distribution of concentration for a partially miscible binary mixture confined between flat plates. The calculation is based on minimization of the Landau–Ginzburg functional for the free energy of the system subject to a material balance constraint:

$$G = \int_0^W \left[g + \frac{\kappa}{2}\left(\frac{dc}{dy}\right)^2\right] dy \tag{7}$$

$$\bar{c} = \frac{1}{L}\int_0^L c(y)dy \tag{8}$$

Here, $g$ is the ordinary free energy of mixing scaled by RT and $\kappa$ is the gradient energy parameter. The ordinary free energy is approximated by Flory-Huggins or regular solution theory:

$$g = c\ln(c) + (1-c)\ln(1-c) + \chi c(1-c) \tag{9}$$

where $c$ is now the mole fraction or volume fraction of one component of the mixture and $\chi > 0$ is an interaction parameter that predicts phase separation in a macroscopic system if $\chi > 2$. The illustrated system assumes polymers solutions with $\bar{c} = 0.7$, $\chi = 3$ and $\kappa = 2R_g^2\chi/3$ where $R_g$ is the radius of gyration of the polymers. The channel width is 32 $R_g$ or about 1 micron for high molecular weight polymers. This system has binodal concentrations of 0.071 and 0.929 and these limits are closely approached throughout most of the domain. The interface occupies five $R_g$ or about 0.2 microns. Figure 3 assumes neutral wall that attracts mixture components equally. Because of this, the composition profiles have zero slope at the walls.

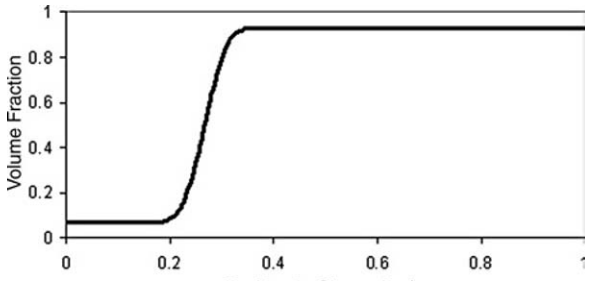

*Figure 3.* Example of cross-channel composition profile.

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