Micro-component flow characterization

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Introduction

Microfluidic devices involve fluid flow and transport of energy and species. When designing such devices it is useful for engineers to have correlations that allow predictions before the device is built, so that the design can be optimized. Unfortunately, most correlations in the literature are for high-speed, or turbulent, flow. Thus, it is useful to develop correlations for slower, laminar flow. While most three-dimensional flow situations can be modeled in laminar flow using computational fluid dynamics (CFD), the calculations are extensive and time-consuming. Correlations are especially useful when the CFD capability is not present. Due to the multi-dimensional character of microfluidics, it is important to understand both the power and the limitations of concepts based on simple one- or two-dimensional cases. In this chapter we outline correlations and pertinent theoretical concepts for slow speed flow and diffusion: pressure drop, entry length, and mixing due to convection and diffusion.

Most of the work is conducted using CFD with the program Comsol Multiphysics (formerly FEMLAB). This program is easy enough to use that undergraduates can perform useful work with only a bit of guidance. Undergraduates in the chemical engineering program at the University of Washington first solved the problems described here over the past five years. The cases have been recomputed using more elements to improve the accuracy using state-of-the-art computers and programs.

Pressure Drop

Friction Factor for slow flows. First consider flow of an incompressible fluid in a straight pipe. The pressure drop is a function of the density and viscosity of the fluid, the average velocity of the fluid, and the diameter and length of the pipe. The relationship is usually expressed by means of a friction factor defined as follows.

$$f \equiv \frac{1}{4}\frac{D}{L}\frac{\Delta p}{\frac{1}{2}\rho < v >^2} \tag{1}$$

The Reynolds number is

$$Re \equiv \frac{\rho < v > D}{\eta} \tag{2}$$

The usual curve of friction factor is given in Figure 1a in a log-log plot. For any given Reynolds number, one can read the value of friction factor, and then use Eq. (1) to determine the pressure drop. In the turbulent region, for $Re > 2200$, one correlation is the Blasius formula.

$$f = 0.0791/Re^{0.25} \tag{3}$$

In the laminar region, for$Re < 2200$, the correlation is

$$f = 16/Re \tag{4}$$

When the definitions are inserted into Eq. (4) for laminar flow, one obtains for the pressure drop

$$\Delta p = 32\frac{L}{D}\frac{\eta < v >}{D} \tag{5}$$

Thus, in laminar flow in a straight channel, the density of the fluid does not affect the pressure drop. To use the correlation for friction factor, or Figure 1a, one must know the density. This problem is avoided if one plots the product of friction factor and Reynolds number versus Reynolds number, since from their definition

$$fRe = \frac{\Delta p D^2}{2L\eta < v >} \tag{6}$$

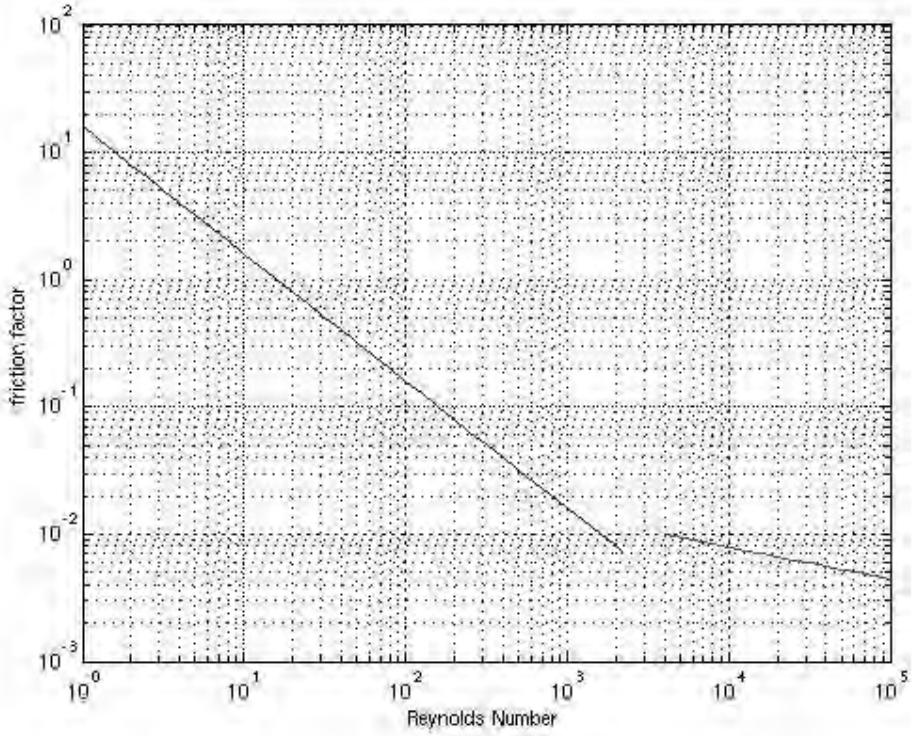
This is shown in Figure 1b. Notice that for $Re < 1$ the only thing needed is the numerical constant, here 16. For fully developed pipe flow, the quantity fRe does not change as the Reynolds number increases to 2200, but it does in more complicated cases. This covers the range that most microfluidic devices operate in. To predict the pressure drop, all that is needed is the single number for the geometry and flow situation in question. The way these numbers are determined is best illustrated by looking at the mechanical energy balance for a flowing system.

Mechanical energy balance for turbulent flow. Consider the control volume shown in Figure 2, with inlet at point 1 and outlet at point 2. In the following,•variable means the variable at point 2 (outlet) minus the variable at point 1 (inlet). The mechanical energy balance is [1]

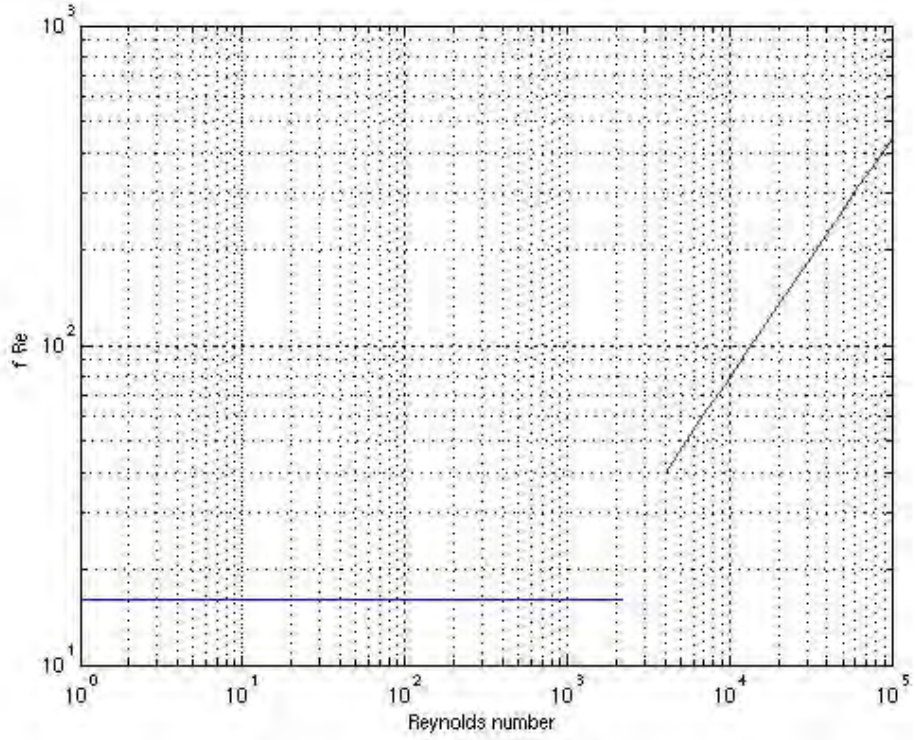
$$\Delta(\frac{1}{2}\frac{< v^3 >}{< v >} + g\Delta h + \int_1^2 \frac{dp}{\rho} = \dot{W}_m - \dot{E}_v \tag{7}$$

For no height change $g\Delta h = 0$; for no pump in the control volume $\dot{W}_m = 0$; for an incompressible fluid with constant density

$$\int_1^2 \frac{dp}{\rho} = \frac{1}{\rho}(p_2 - p_1) = \frac{1}{\rho}\Delta p$$



(a) Standard presentation of friction factor versus Reynolds number



(b) Low-Reynolds number presentation of *f Re*

Figure 1. Friction losses (pressure decreases) for fully-developed pipe flow

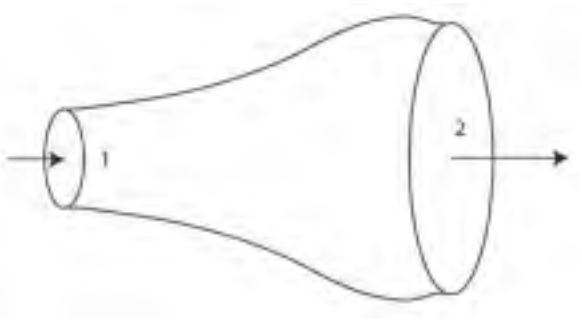


Figure 2. Geometry and notation for mechanical energy balance

Thus, under all these assumptions we have

$$\Delta\left(\frac{1}{2}\frac{<v^3>}{<v>}\right) + \frac{1}{\rho}\Delta p = -\hat{E}_v \tag{8}$$

By continuity the mass flow rate is the same, $w_1 = w_2$. The definition of the viscous losses is

$$E_v = -\int_V \boldsymbol{\tau} : \nabla \mathbf{v} dV = \int_V \eta[\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}}] : \nabla \mathbf{v} dV \geq 0 \text{ and } \hat{E}_v = \frac{E_v}{w}$$

Rewrite Eq. (8) in the form

$$\Delta\left(\frac{1}{2}\frac{<v^3>}{<v>}\right) + \hat{E}_v = -\frac{1}{\rho}\Delta p = \frac{p_1 - p_2}{\rho} \tag{9}$$

Dimensionless Mechanical Energy Balance

We make all variables non-dimensional by dividing them by a dimensional standard (which has to be identified in each case) and denoting the standard with a subscript *s*. For the velocity standard, use an average velocity somewhere in the system.

$$v' = \frac{v}{v_s}, \quad v_s \equiv <v>$$

We make the pressure non-dimensional by dividing it by twice the kinetic energy

$$p' \equiv \frac{p}{\rho v_s^2}$$

The units of viscous dissipation are

$$E_v \text{ [=] } \eta \frac{v_s^2 x_s^3}{x_s^2} = \eta v_s^2 x_s \quad \text{and} \quad \tilde{E}_v = \frac{E_v}{w} \text{ [=] } \frac{\eta v_s^2 x_s}{\rho v_s x_s^2} = \frac{\eta v_s}{\rho x_s}$$

Thus, define

$$\tilde{\tilde{E}}_v \equiv \frac{\tilde{E}_v \rho x_s}{\eta v_s}$$

The non-dimensional form of the mechanical energy balance is then

$$v_s^2 \Delta\left(\frac{1}{2}\frac{\langle v \rangle^2}{\langle v \rangle} + \frac{\eta v_s}{\rho x_s}\tilde{\tilde{E}}_v \equiv v_s^2 (p_1'' - p_2'')\right.$$

Dividing by v_s^2 gives

$$\Delta\left(\frac{1}{2}\frac{\langle v \rangle^2}{\langle v \rangle} + \frac{\eta}{\rho x_s v_s}\tilde{\tilde{E}}_v \equiv (p_1'' - p_2'')\right. \quad or \quad \Delta\left(\frac{1}{2}\frac{\langle v \rangle^2}{\langle v \rangle} + \frac{1}{Re}\tilde{\tilde{E}}_v \equiv (p_1'' - p_2'')\right. \tag{10}$$

where $Re = \rho v_s x_s / \eta$. This is the approach one uses for high-speed flow, including all turbulent cases.

For fully developed flow through a tube with a constant diameter, *D*, the kinetic energy does not change from one end to the other. We already have a formula for the pressure drop in terms of the friction factor, so that

$$p_1'' - p_2'' = \frac{\Delta p}{\rho \langle v \rangle^2} = 2f\frac{L}{D}$$

Thus the viscous dissipation term in Eq. (10) is also given by the friction factor for flow in a tube.

$$\frac{1}{Re}\tilde{\tilde{E}}_v \equiv 2f\frac{L}{D}$$

Mechanical energy balance for laminar flow. When the flow is slow and laminar, we use a different non-dimensionalization for the pressure. Divide the pressure by the viscosity times the velocity divided by a characteristic length.

$$p \equiv \frac{p}{p_s};\ with\ p_s \equiv \frac{\eta v_s}{x_s},\ \ p \equiv \frac{p x_s}{\eta v_s}$$

Then the mechanical energy balance is

$$v_s^2\Delta\left(\frac{1}{2}\frac{\langle v\rangle^2}{\langle v\rangle}\right)+\frac{\eta v_s}{\rho x_s}\hat{E}_v=\frac{\eta v_s}{\rho x_s}(p_1-p_2)$$

Multiply by $\rho x_s/\eta v_s$ to get another non-dimensional form of the mechanical energy balance.

$$\frac{\rho v_s x_s}{\eta}\Delta\left(\frac{1}{2}\frac{\langle v\rangle^2}{\langle v\rangle}\right)+\hat{E}_v=(p_1-p_2) \quad \text{or} \quad Re\,\Delta\left(\frac{1}{2}\frac{\langle v\rangle^2}{\langle v\rangle}\right)+\hat{E}_v=(p_1-p_2) \tag{11}$$

For fully developed flow through a tube with a constant diameter,*D*, the kinetic energy does not change from one end to the other. We already have a formula for the pressure drop in terms of the friction factor, so that

$$p_1-p_2=\frac{\Delta pD}{\eta\langle v\rangle}=32\frac{L}{D}$$

Thus the viscous dissipation term in Eq. (11) for laminar flow in a straight channel is:

$$\hat{E}_v=32\frac{L}{D}$$

Eq. (10) and Eq. (11) express the same physics. Eq. (10) is more useful at high velocity in turbulent flow when f is a slowly varying function of Reynolds number, and Eq. (11) is more useful at low velocity in laminar flow. The non-dimensional pressures in these two equations are different, but they are related

$$p=Re\;\;p''$$

Pressure drop for flow disturbances. Eq. (11) is the form of the mechanical energy balance that is useful in microfluidics. Note that a Reynolds number multiplies the term representing the change of kinetic energy, which is small in microfluidics. Consider the case when the Reynolds number is extremely small. Then any flow situation is governed by Stokes equation

$$\eta\nabla^2\mathbf{v}=-\nabla p$$

In non-dimensional form this equation is

$$\eta\frac{v_s}{x_s^2}\nabla^2\mathbf{v}=-\frac{p_s}{x_s}\nabla p \quad \text{or} \quad \nabla^2\mathbf{v}=-\frac{p_s x_s}{\eta v_s}\nabla p$$

Table I. Frictional loss coefficient for turbulent flow*

	$K = \Delta p_{excess} / \frac{1}{2}\rho < v >^2$
90º ell, standard	0.75
90º ell, long radius	0.35
180º bend,close return	1.5
Tee, branchng flow	1.0

* From Table 6-4, p. 6-18, Perry's Chemical Engineers' Handbook [2]

But with the definition of $p_s = \eta v_s / x_s$

$$\nabla^2 \mathbf{v} = -\nabla p$$

Thus, the non-dimensional flow does not depend upon the Reynolds number. This means that both

$$\Delta\left(\frac{\frac{1}{2} < v^2 >}{< v >}\right) \text{ and } \Phi_v$$

are constants, for the particular geometry being studied, since they can be calculated knowing the velocity field distribution. For turbulent flow, a reasonable approximation is that the velocity is constant with respect to radial position in the inlet and outlet ducts, and then $< v^2 > / < v > = < v^2 >$. This is not true for laminar flow, although both terms can be calculated for fully developed flow at the inlet and outlet. Furthermore, the kinetic energy term is negligible at small Reynolds number. To correlate the pressure drop, the main task is to correlate the viscous dissipation term, Φ_v.

A convenient way to correlate data for excess pressure drop when there are contractions, expansions, bends and turns, etc., when the flow is turbulent is to write them as

$$\Delta p_{excess} = K \frac{1}{2}\rho < v >^2$$

Then, to calculate the pressure drop for any given fluid and flow rate, one only needs to know the values of K, a few of which are tabulated in Table I.

As shown above, for slow flow the pressure drop is linear in the velocity rather than quadratic, and a different correlation is preferred. Write

$$\Delta p_{excess} = K_L \frac{\eta < v >}{D}$$

Values of K_L for different geometries are given in Table II as determined by finite element calculations.

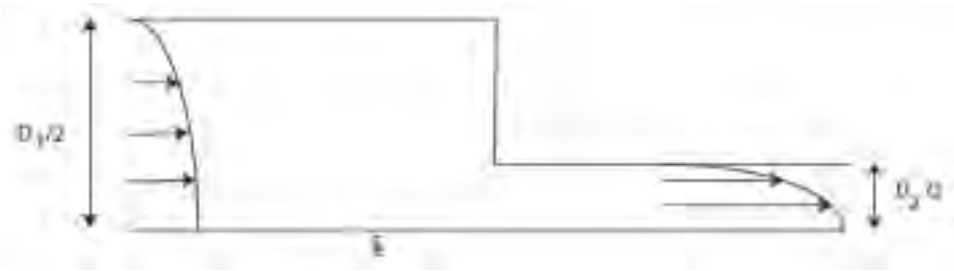


Figure 3. Contraction flow geometry

Table II. Coefficient K_L for Re negligbily small	Picture	K_L
Sharp bend, 2D		9.1
Smooth bend, 90 degrees, short radius, 2D (centerline radius = gap size)		19 (0.5)
Smooth bend, 90 degrees, long radius, 2D (centerline radius = 1.5 x gap size)		29 (0.36)
Bend, 45 degrees, sharp change, 2D		5.2 (0.2)
Bend, 45 degrees, long radius, 2D, (centerline radius = 1.5 x gap size)		14.3 (0.2)
Square corner, 3D		4.2 (-2.1)
Round pipe, 3D		75.2 (-0.2)

v_s = average velocity, x_s = thickness or diameter

The value in ( ) is the value if the entire length through the centerline is used to calculate the fully developed pressure drop. The excess pressure drop beyond this is negligible.

Pressure drop for contractions and expansions. Consider a large circular tube emptying into a smaller circular tube, as shown in Figure 3. The pressure drop in this device is due to viscous dissipation in the fully developed regions of the large and small channels, plus the extra viscous dissipation due to the contraction, plus the kinetic energy change. When the Reynolds number is small, the kinetic energy change is negligible. For the flow illustrated in Figure 3, we write the excess pressure drop for the contraction as the total pressure drop minus the pressure drop for fully developed flow in the large and small channels. The pressure drop for fully developed laminar flow is known analytically, of course [Eq. (5)].

$$\Delta p_{excess} = \Delta p_{total} - \Delta p_{large\ \ channel} - \Delta p_{small\ \ channel}$$

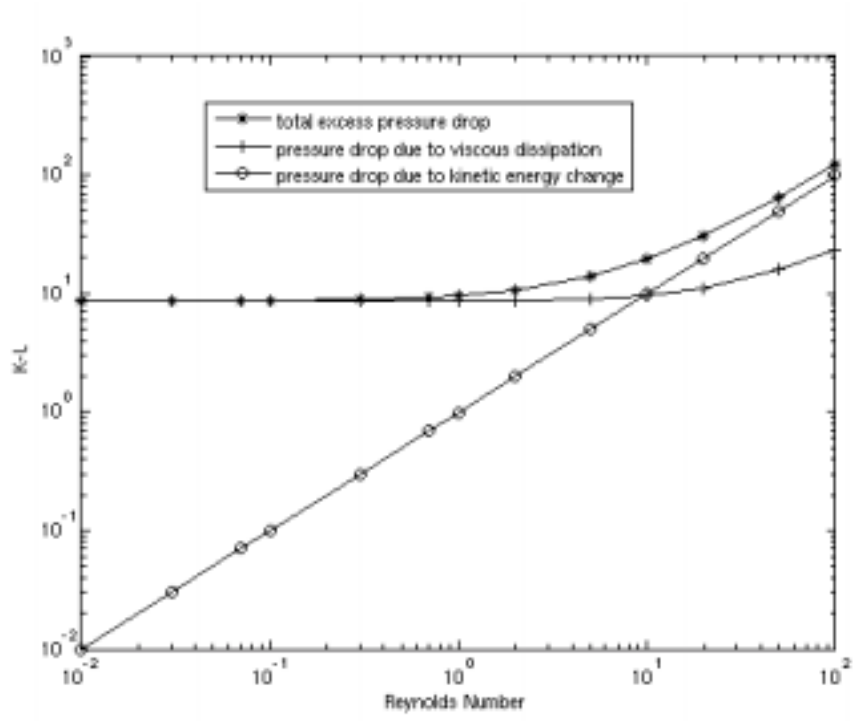


Figure 4. Laminar flow excess pressure drop for a 3:1 contraction in a circular channel. K-L is the total pressure minus the fully developed pressure drop in the two regions, expressed as $K_L = \Delta p_{excess} D_2 / \eta < v_2 >$.

Table III. Coefficient K_L for contractions and expansions for *Re* negligbily small

	Picture	K_L
2:1 pipe/planar		7.3/3.1
3:1 pipe/planar		8.6/4.1
4:1 pipe/planar		9.0/4.5
45 degrees tapered, planar, 3:1		4.9
28.07 degrees tapered, planar, 3:1		10.8
3:1 square (quarter of the geometry)		8.1

v_s = average velocity, x_s = thickness or diameter, both in the small section

The excess pressure drop is correlated using $\Delta p_{excess} = K_L \eta < v > / D$ and K_L can be determined from finite element calculations. Note that one must specify which average velocity and distance are used in this correlation, and the usual choices are the average velocity and the diameter or total thickness between parallel plates, all at the narrow end. The value of K_L depends upon the contraction ratio, too. Values are given in Table III, as determined from finite element calculations. Table III indicates that the value of K_L is approximately 8-15 depending upon the geometry.

When the Reynolds number is not vanishingly small, K_L depends on Reynolds number, too, and the dependence is easily determined using CFD. For example, for a 3:1 contraction in a pipe the results are shown in Figure 4. Note that K_L is approximately constant for $Re < 1$. The departure from a constant is due partially to extra viscous dissipation at higher Reynolds number, but mostly due to kinetic energy change.

For the axisymmetric pipe or channel case, in a contracting flow, the kinetic energy change is derived as follows. Let $\beta = D_2^2 / D_1^2$ be the area ratio ($D_2 < D_1$ for contraction), and use $v_i = v_{0i}[1-(r/R_i)^2]$ for the inlet and outlet. Then

$$\int_0^{R_1} v^3(r) r dr \; / \; \int_0^{R_1} v(r) r dr = \tfrac{1}{2} v_{01}^2 = 2 < v_1 >^2$$

By continuity

$$D_1^2 v_{01} = D_2^2 v_{02}, \text{ or } v_{01} = \beta v_{02}$$

The kinetic energy term is then

$$\tfrac{1}{2}[2 < v_{02} >^2 - 2 < v_{01} >^2] = < v_{02} >^2 (1-\beta^2)$$

The total balance, Eq. (11), is then

$$p_1 - p_2 = Re < v_2 >^2 (1-\beta^2) + \dot{E}_v \quad \beta = D_2^2 / D_1^2, \; \beta < 1 \tag{12}$$

If the velocity standard is the average velocity in the narrow tube, $< v_2 > = 1$. The viscous dissipation is $\dot{E}_v = K_L$. In dimensional terms Eq. (12) is

$$\frac{(p_1 - p_2) D_2}{\eta < v_2 >} = \frac{\rho < v_2 > D_2}{\eta} (1-\beta^2) + K_L$$

or

$$p_1 - p_2 = \rho < v_2 >^2 (1-\beta^2) + \frac{\eta < v_2 >}{D_2} K_L$$

When doing calculations or an experiment, it is the total pressure drop that is calculated or measured. When the analytic expressions for pressure drop in both tubes are subtracted, what remains is the excess pressure drop due to the contraction. The change of kinetic energy can be calculated so that the remaining term, viscous dissipation, is readily available. As seen in Figure 4, the viscous term predominates at low Reynolds numbers (i.e. in microfluidics) whereas the kinetic energy term predominates at high Reynolds number (>100). The equivalent expressions for other geometries are:

Flat plates, contraction, x_s = H_2 = thickness between plates, $v_s = < v_2 >$ so that $< v_2 > = 1$:

$$p_1 - p_2 = Re < v_2 >^2 \frac{27}{35}(1-\beta^2) + f_v \quad \beta = H_2/H_1, \ \beta < 1 \tag{13}$$

or

$$p_1 - p_2 = \rho < v_2 >^2 \frac{27}{35}(1-\beta^2) + K_L \frac{\eta < v_2 >}{H_2}$$

Flat plate with symmetry conditions upstream, contraction:

$$p_1 - p_2 = Re < v_2 >^2 (\frac{27}{35} - \frac{1}{2}\beta^2) + f_v \quad \beta = H_2/H_1, \ \beta < 1 \tag{14}$$

$$p_1 - p_2 = \rho < v_2 >^2 (\frac{27}{35} - \frac{1}{2}\beta^2) + K_L \frac{\eta < v_2 >}{H_2}$$

Expansions work in a similar fashion, and the viscous dissipation at negligible Reynolds number is the same in a contraction and an expansion. For expansion, the average velocity in the small tube is $<v_1>$ and we take $v_s = < v_1 >$ so that $< v_1 > = 1$.

Circular tubes, expansion:

$$p_1 - p_2 = Re < v_1 >^2 (\frac{1}{\beta^2} - 1) + f_v \quad \beta = \frac{D_2^2}{D_1^2} > 1 \tag{15}$$

or

$$p_1 - p_2 = \rho < v_1 >^2 (\frac{1}{\beta^2} - 1) + K_L \frac{\eta < v_1 >}{D_1}$$

Flat plates, expansion:

$$p_1 - p_2 = \mathrm{Re} < v_1 >^2 \frac{27}{35}(\frac{1}{\beta^2} - 1) + f_v \quad \beta = \frac{H_2}{H_1} > 1 \tag{16}$$

Flat plate with symmetry conditions upstream, expansion:

$$p_1 - p_2 = \mathrm{Re} < v_1 >^2 (\frac{27}{35}\frac{1}{\beta^2} - \frac{1}{2}) + f_v \quad \beta = \frac{H_2}{H_1} > 1 \tag{17}$$

However, in an expansion the kinetic energy change is opposite in sign to that in a contraction, causing the pressure to increase due to the kinetic energy and decrease due to the viscous dissipation.

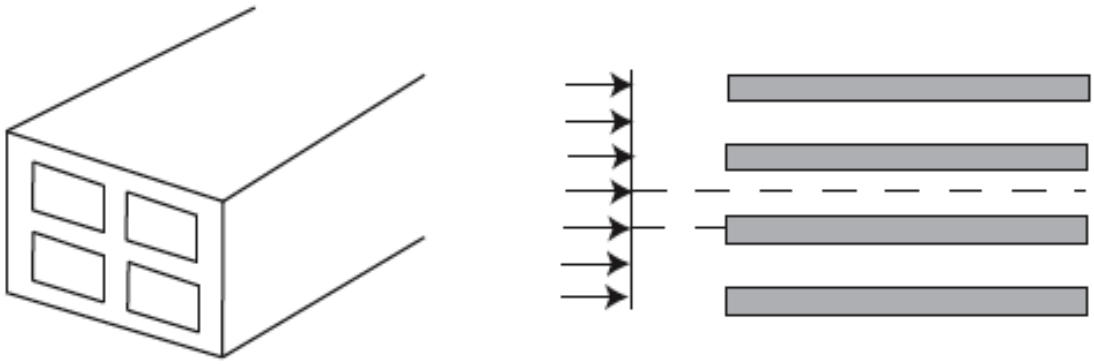


Figure 5. Manifold with square holes (left) or flat plates (right)

Manifolds. When a flowing stream is approaching a manifold, with many holes, there are other effects that must be considered. A typical situation is shown in Figure 5. Now calculations can be done for one cell of the manifold simply by using a symmetry condition upstream of the manifold, as illustrated. The case considered here is for a planar manifold, but 3D manifolds could be analyzed in the same way provided there was symmetry. Otherwise the entire device must be modeled. This situation has been analyzed by Kays [3] for turbulent flow, but he gives curves for laminar flow, too. Here we show that those curves are over-simplified for laminar flow.

Kays [3] presents results for a loss coefficient, K_c, defined as

$$\frac{\Delta p}{\frac{1}{2}\rho < v >^2} = K_c + 1 - \sigma^2 \tag{18}$$

where the loss coefficient depends upon σ, the ratio of free area in the channels to the free area upstream (see Figures 3, 6 in [3]). However, there is only one curve for laminar flow, although there are multiple curves for different Reynolds numbers in turbulent flow. The term $1-\sigma^2$ represents the kinetic energy change assuming a flat velocity profile, which is not true for laminar flow between flat plates. Since the flow will be considerably different at low Reynolds numbers (when the pressure changes are linear in velocity) from the flow at higher, but still laminar, Reynolds numbers (when the pressure changes are quadratic in velocity), multiple curves are expected for different laminar Reynolds numbers, too. Finite element calculations are performed for various contraction ratios and the K_c is calculated using Eq. (18) along with the computed excess pressure drop. Figure 6 shows that there are different curves for different Reynolds numbers, as expected, but that the curves for Re = 100 are close to those given by Kays. However, microfluidic devices seldom operate in this regime.

The same calculated results are plotted in Figure 7 in terms of K_L defined using Eq. (14) and the computed excess pressure drop. Now the values approach an asymptote at small Reynolds number, which is more useful for microfluidic flows.

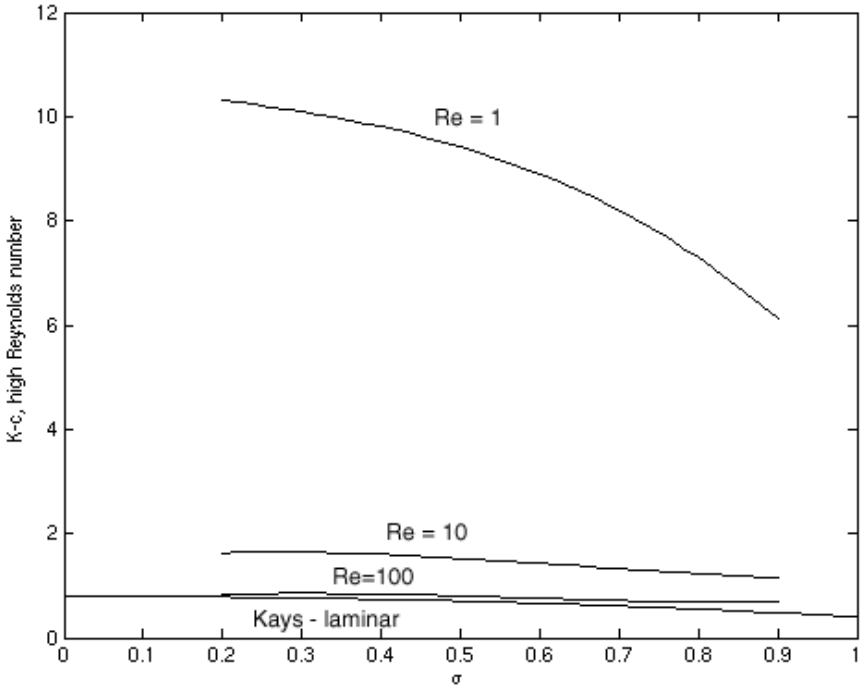


Figure 6. K_c defined by Eq. (18) for various planar contractions for a manifold

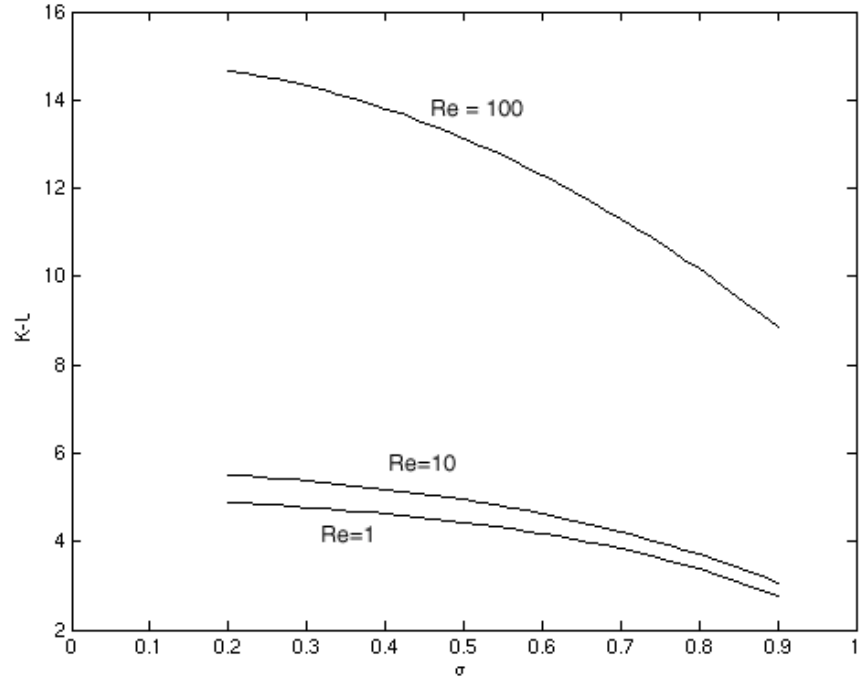


Figure 7. K_L defined by Eq. (14) for various planar contractions for a manifold; the curve for $Re = 0$ is indistinguishable from that for $Re = 1$.

Entry lengths

When the diameter or size of a flow channel changes, the velocity profile must change to adapt to the new size. It takes a certain length in the new size for the flow to become fully developed (if that is possible). In a microfluidic device, it is of interest to know how long that region is, so that the effect of a developing velocity field can be ignored if it is unimportant. The developing velocity field affects the pressure drop and it also complicates the diffusion of species in the device. In this section the approach length and entry length are explained for laminar flows.

Contraction flows. Consider flow into a circular channel or pipe with the velocity a constant at the entrance. As the fluid enters the channel, the velocity soon develops a parabolic profile. The velocity at the centerline increases from <v> (at the entrance) to 2<v> (far downstream) while the velocity at the wall decreases suddenly from <v> to zero. The entry length is defined as the length of channel it takes before the centerline velocity is 99% of its ultimate value, 2<v>. Sometimes the entry length is defined using a 98% or 95% criterion. Atkinson *et al*. [2, 4] solved this problem using the finite element method and correlated the results with the equation

$$\frac{L_e}{D} = 0.59 + 0.056Re, \text{ 1\% criterion}$$

This equation is based on the Stokes flow solution ($Re = 0$, giving the 0.59) plus a boundary layer solution (giving the 0.056 Re). It isn't actually a curve fit of the results for small Reynolds numbers. The calculation for $Re = 0$ in [4] and the experimental data in [5] give the following correlation.

$$\frac{L_e}{D} = 0.594 + 0.0024Re + 0.0036Re^2, \; Re \le 6.34, \; r^2 = 1.0, \text{ 1\% criterion}$$

For a 5% criterion, the correlation of Atkinson's data is

$$\frac{L_e}{D} = 0.43 + 0.0037Re + 0.0028Re^2, \; Re \le 6.34, \; r^2 = 0.9993, \text{ 5\% criterion}$$

It is impossible to realize a constant velocity at the inlet to the circular channel unless the wall is 'paper thin' and the flow can go past the outer wall, too. A more realistic case is where a larger channel decreases to a smaller channel as shown in Figure 3. Then a fully developed velocity profile can be used far upstream in the larger channel. The flow rearrangement occurs before the contraction, as shown in Figure 8. This is important in laminar flow because vorticity is generated at the corner and diffuses upstream. As the velocity increases, this region gets pushed against the inlet and becomes smaller. Thus, for turbulent flow the effect is much shorter. The approach length is presented in Figure 9 as a function of Reynolds number. Inside the pipe the entry length for a 4:1 contraction in a circular channel or pipe is derived from finite element calculations including the upstream segment.

$$\frac{L_e}{D} = 0.1264 + 0.0113Re + 0.0002Re^2, \; Re \le 10, \; r^2 = 1.0, \text{ 5\% criterion}$$

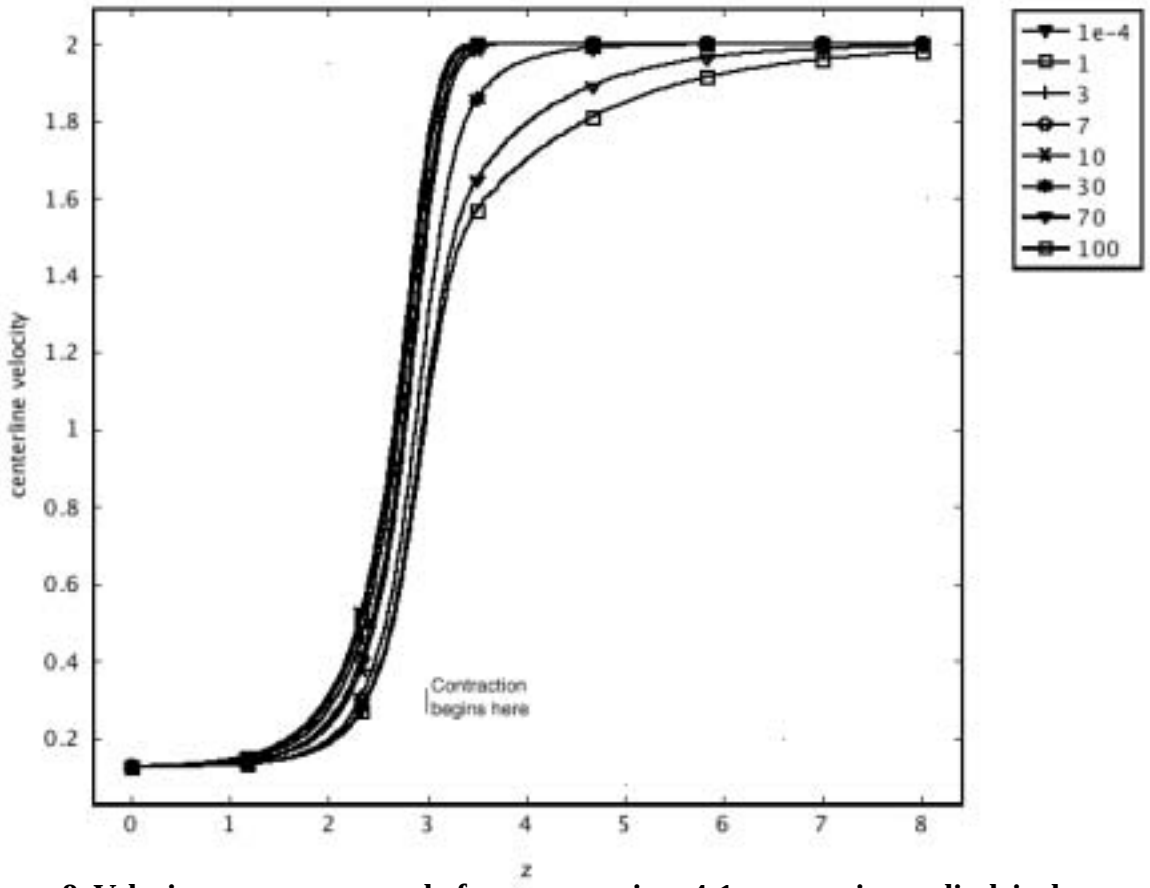


Figure 8. Velocity rearrangement before contraction, 4:1 contraction, cylindrical geometry for different Reynolds numbers based on the downstream section

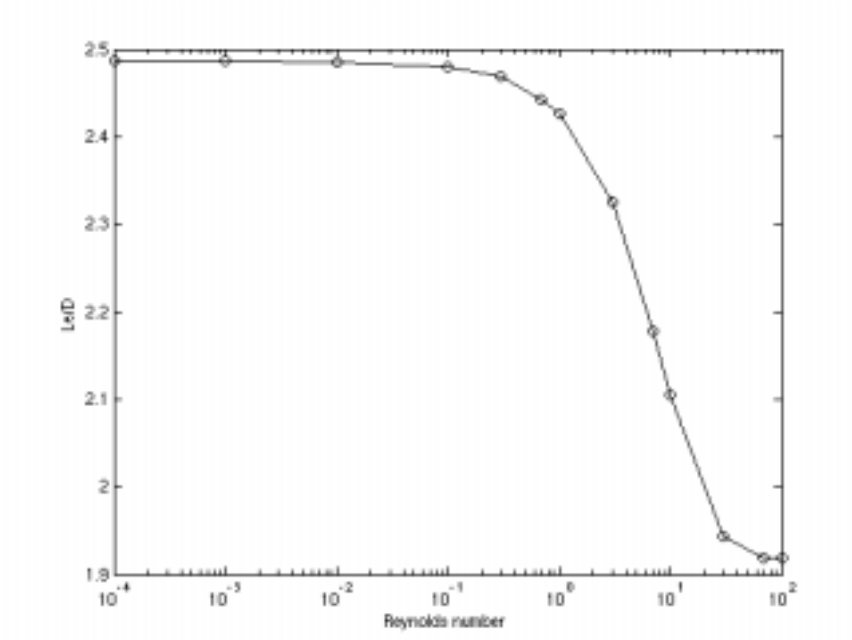


Figure 9. Approach length, 5% criterion, 4:1 contraction, cylindrical geometry

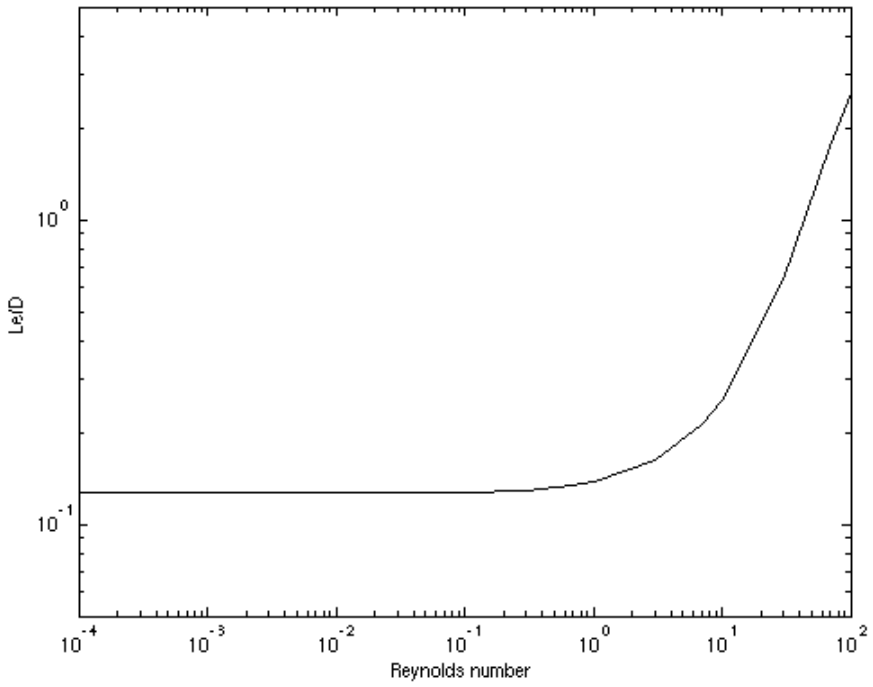


Figure 10. Entry length, 5% criterion, 4:1 contraction, cylindrical geometry

Figure 11. Diffusion in fully developed planar flow

The effect of Reynolds number is clearly displayed in Figure 10. When the upstream region is included the entry length is much shorter (L_e/D = 0.1264 rather than 0.43) since the velocity has already rearranged somewhat upstream.

Diffusion

Many microfluidic devices involve diffusion of concentration as well as fluid flow. The velocity crossing a plane normal to the flow is seldom uniform, so the diffusion must be examined in the midst of non-uniform velocity profiles. The simplest illustration of this effect is with Taylor dispersion.

For simplicity, consider flow between two flat plates as shown in Figure 11. The flow is laminar and the velocity profile is quadratic. Now suppose the entering fluid has a second chemical with the concentration shown, 1.0 in the top half and 0 in the bottom half. As this fluid moves downstream (to the right), the velocity is highest in the center, so the second chemical moves fast there. However, it can also diffuse sideways, and the chemical that does first diffuse sideways then

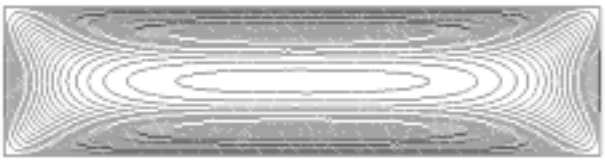


Figure 12a. Fully developed velocity profile in a 1 x 4 rectangular channel

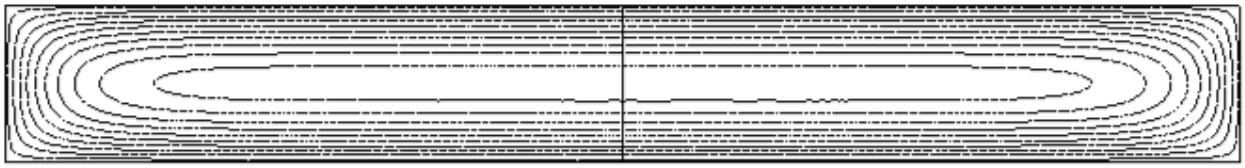


Figure 12b. Fully developed velocity profile in a 1 x 8 rectangular channel, $\langle v \rangle = 1$, $v(0,0)=1.628$

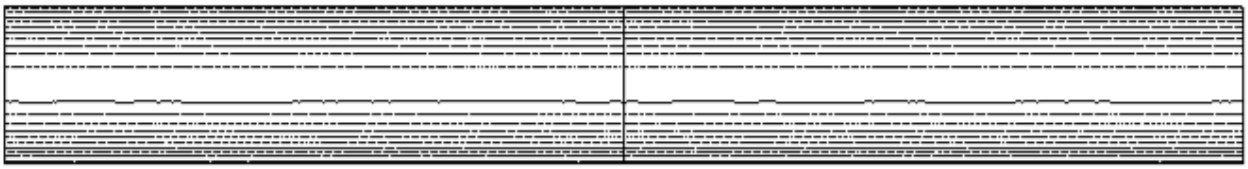


Figure 12c. Fully developed velocity profile in a 1 x 8 rectangular channel with slip on the side walls, $\langle v \rangle = 1$, $v(0,0)=1.500$

moves slower down the flow channel. At a point not on the centerline, the concentration is determined by this slower velocity in the flow direction and diffusion sideways because the concentration on the centerline is always higher than the concentration in adjacent fluid paths. This is called Taylor dispersion [6]. Taylor [7] and Aris [8] showed how to model the average concentration as a function of length using a simpler equation (dispersion in the flow direction only) and an effective dispersion coefficient given by

$$K = \mathcal{D} + \frac{\langle v \rangle^2 D^2}{192\mathcal{D}} \quad \text{or} \quad \frac{K}{\mathcal{D}} = 1 + \frac{\langle v \rangle^2 D^2}{192\mathcal{D}^2} = 1 + \frac{Pe^2}{192} \tag{19}$$

Next consider fully developed flow in a narrow channel, which is typical of a microfluidic device. The normal view is shown in Figure 12 with flow going into the paper. The velocity varies in x and y according to the equation

$$\eta\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = -\frac{\Delta p}{L}$$

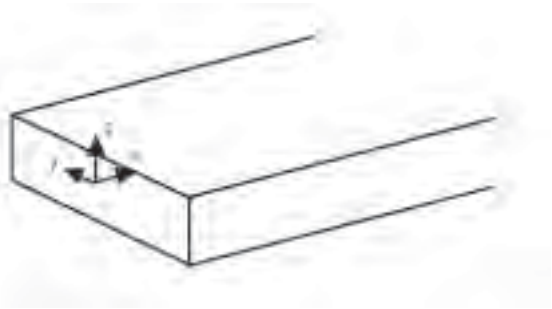


Figure 13. Three-dimensional rectangular channel

Figure 14. Concentration profile in channel; *Pe* = 100, width = 8, height = 1, length = 30, $\langle v \rangle = 1$. Fully developed velocity profile determined with 28,160 elements, 56,897 degrees of freedom. Concentration determined with 46,426 elements, 68,845 degrees of freedom

Typical solutions are shown in Figure 12(a,b). If one uses a model ignoring the edge effects, one is essentially using the velocity profile shown in Figure 12(c).

When diffusion is added into the problem, these two flow situations (b and c) are different. Take the three-dimensional flow situation shown in Figure 13, with the velocity profile being the same for all x. Let the material on one side have a dilute concentration of some species (taken = 1), and on the other side there is no concentration of that species (c = 0). What happens at different planes downstream? Typical concentration profiles are shown in Figures 14 and 15, and a quantitative description is given below.

Characterization of mixing. In order to evaluate mixing it is necessary to have a quantitative measure. The variance from the mean is appropriate, but in a flowing system some fluid elements have a higher velocity than others. The concept in chemical engineering that is used to account for this is the mixing cup concentration. This is the concentration of fluid if the flow emptied into a cup that was well stirred. In mathematical terms, the mixing cup concentration is

$$c_{mixing\ \ cup} = \frac{\int_A c(x,y,z)v(x,y)dxdy}{\int_A v(x,y)dxdy} \tag{20}$$

Note that the average velocity times the mixing cup concentration gives the total mole/mass flux through an area at position *z*. Then it is natural to define the variance of the concentration from the mixing cup concentration.

$$c_{\text{var iance}} = \frac{\int_A [c(x,y,z) - c_{mixing\ \ cup}]^2 v(x,y)dxdy}{\int_A v(x,y)dxdy} \tag{21}$$

Average concentration along an optical path. Optical measurements are frequently made through the thin layer of a microfluidic device. The average concentration is then determined by the integral along the path, such as

$$c_{optical} = \int_0^L c(x.y,z)dy / \int_0^L dy \tag{22}$$

When the velocity is variable in the *y*-direction some regions of the fluid are moving faster than others. Thus, the optical measurement, or integration along the optical path, may not be comparable to the mixing cup concentration. Indeed, it is entirely possible that several different flow and concentration distributions can give the same average along an optical path. In that case, computational fluid dynamics can be used to interpret the optical measurements.

Peclet number. The convective diffusion equation is

$$\frac{\partial c}{\partial t} + \mathbf{v} \sum \nabla c = \mathcal{D}\nabla^2 c$$

If this equation is made non-dimensional using

$$c \leftarrow \frac{c}{c_s},\ \ \mathbf{v} \leftarrow \frac{\mathbf{v}}{v_s},\ \ \nabla \leftarrow x_s \nabla,\ \ t \leftarrow \frac{t v_s}{x_s},$$

it is

$$Pe\frac{\partial c'}{\partial t'} + Pe\mathbf{v}' \sum \nabla' c' \leftarrow \nabla'^2 c' \text{ or } \frac{\partial c'}{\partial t'} + \mathbf{v}' \sum \nabla' c' \leftarrow \frac{1}{Pe}\nabla'^2 c' \tag{23}$$

where

$$Pe \equiv \frac{v_s x_s}{\mathcal{D}} \tag{24}$$

The Peclet number is a ratio of the time for diffusion, $x_s^2/\mathcal{D}$, to the time for convection, x_s/v_s. Typically, *Pe* is very large, and this presents numerical problems. The second form of Eq. (22) shows that the coefficient of the term in the differential equation with highest derivative goes to

zero; this makes the problem singular. For large but finite *Pe* the problem is still difficult to solve. For a simple one-dimensional problem it can be shown [9] that the solution will oscillate from node to node unrealistically unless

$$\frac{Pe\Delta x}{2} \le 1, \text{ or } \frac{v_s x_s}{2\mathcal{D}} \frac{\Delta x}{x_s} \le 1$$

This means that as *Pe* increases, the mesh size must decrease. Since the mesh size decreases, it takes more elements or grid points to solve the problem, and the problem may become too big. One way to avoid this is to introduce some numerical diffusion, which essentially lowers the Peclet number. If this extra diffusion is introduced in the flow direction only, the solution may still be acceptable. Various techniques include upstream weighting (finite difference [10]) and Petrov-Galerkin (finite element [11]). Basically if a numerical solution shows unphysical oscillations, either the mesh must be refined, or some extra diffusion must be added. Since it is the relative convection and diffusion that matter, the Peclet number should always be calculated even if the problem is solved in dimensional units. The value of *Pe* will alert the chemist, chemical engineer, or bioengineer whether this difficulty would arise or not. Typically v_s is an average velocity, x_s is a diameter or height, and the exact choice must be identified for each case.

Sometimes an approximation is used to neglect axial diffusion since it is so small compared with axial convection. If the flow is fully developed in a channel then one solves (for steady problems)

$$w(x,y)\frac{\partial c}{\partial z} = \mathcal{D}\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \tag{25}$$

This is a much simpler problem since the $\mathcal{D}$ can be absorbed into the length, *z*,

$$w(x,y)\frac{\partial c}{\partial(z\mathcal{D})} = \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

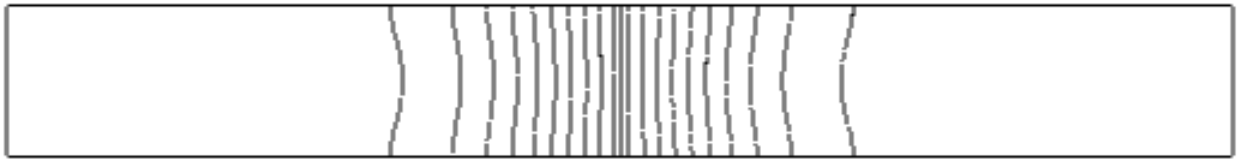
In non-dimensional terms the equation is

$$w(x,y)\frac{\partial c}{\partial(z/Pe)} = \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \tag{26}$$

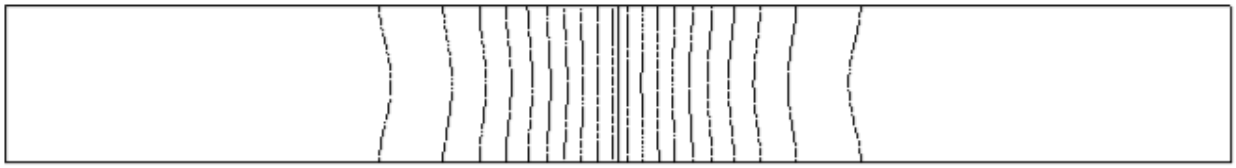
Then all results should depend upon z/Pe not z and *Pe* individually. The velocity is not a constant; it depends upon *x* and *y*. Thus, the problem is different from the following formulation

$$< w > \frac{\partial c}{\partial(z/Pe)} = \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \text{ or } \frac{\partial c}{\partial t'} = \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right), \text{ where } t = \frac{z}{< w > Pe} \tag{27}$$

where $< w > = \int_A w(x,y)\,dx\,dy / \int_A dx\,dy$.

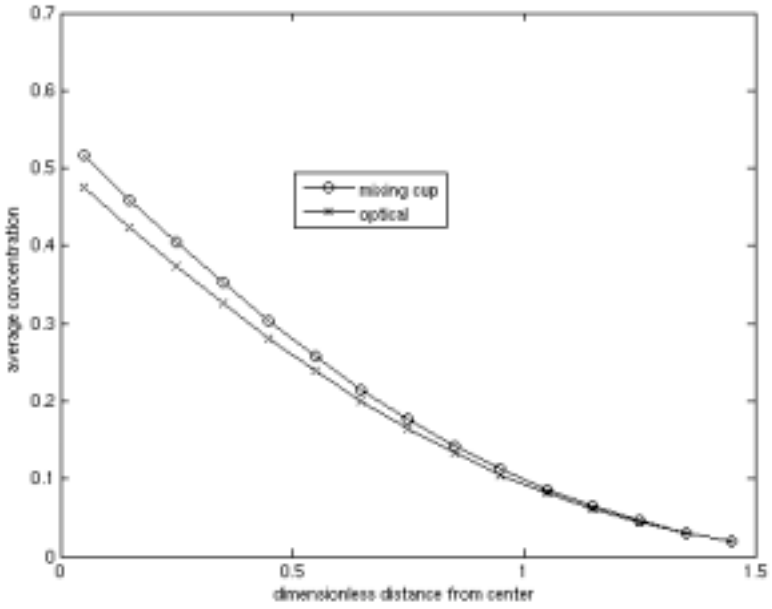


(a) Concentration at exit with fully developed velocity profile; variance = 0.193



(b) Concentration at exit with velocity profile allowing slip on the side walls, for the same average velocity as (a); variance = 0.195

(c) Concentration at exit with uniform velocity, for the same average velocity as (a); variance = 0.195



(d) Comparison of mixing cup and optical pathlength concentrations

Figure 15. Butterfly effect; concentration at exit at z = 30

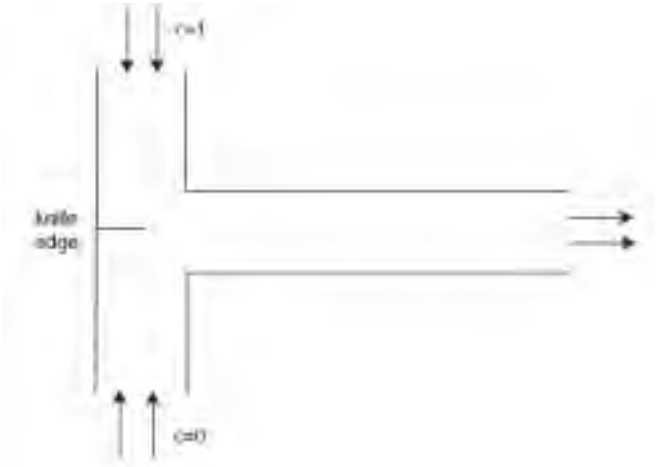


Figure 16. T-sensor; the knife edge can be added as shown

Diffusion in a rectangular channel. The quantitative measures are calculated for fully developed flow in rectangular channels. The concentration profile is shown in Figure 14. Figure 15a shows contours of the concentration on the exit plane. The material near the upper and lower surface has a slower velocity (see Figure 12b); thus it has a longer residence time in the channel and has more time to diffuse sideways. In fact, the concentration profile resembles a butterfly, and this effect was called the butterfly effect by Kamholtz *et al.* [12]. If the velocity is changed to that shown in Figure 12c, but with the same average velocity, the concentration profiles are altered slightly but the butterfly effect still exists, Figure 15b. The peak velocities are different in Figures 12b and 12c, though, even when the average velocities are the same, so that the butterfly effect would not be calculated correctly with a velocity allowing slip on the side walls (Figure 12c). When Eq. (27) is used with a uniform velocity, the butterfly effect disappears (Figure 15c) since every element of fluid has the same velocity, and hence the same residence time.

The difference between the mixing cup concentration and the optical path concentration is illustrated in Figure 15d. The differences are not large (maximum of 8% difference for this case).

Diffusion in a T-sensor [13, 14]. Consider next a two-dimensional case with flow coming in top and bottom on the left (see Figure 16). The fluid is mainly water, but a small concentration of a second species is in the upper flow. Along the top take $c = 1$, and along the bottom take $c = 0$. How will they mix? The variance is shown as a function of length/Peclet number in Figure 17. Points are computed when the problem is solved with different Peclet numbers and the curves are close to each other, justifying Eq. (26). If this problem is solved with a large Peclet number, oscillations appear ([15] p. 217) and the mesh must be refined or some stabilization (like Petrov-Galerkin or upstream weighting) must be applied. The stabilization, of course, smoothes the solution and adds unphysical diffusion. It is up to the analyst to decide if that effect can be tolerated.

The effect of placing a knife-edge in the device is very small; it is negligible because the amount of diffusion across the line where the knife-edge would be is a very small portion of the total mass transfer, and the flow field is affected only slightly.

Serpentine mixer. A serpentine mixer (Figure 18) can be used to mix two chemicals in a shorter length than happens in a straight channel. A typical solution for a Reynolds number of 1.0 and Peclet number of 1000 is shown in Figure 19. Comparing these data with those for a T-sensor

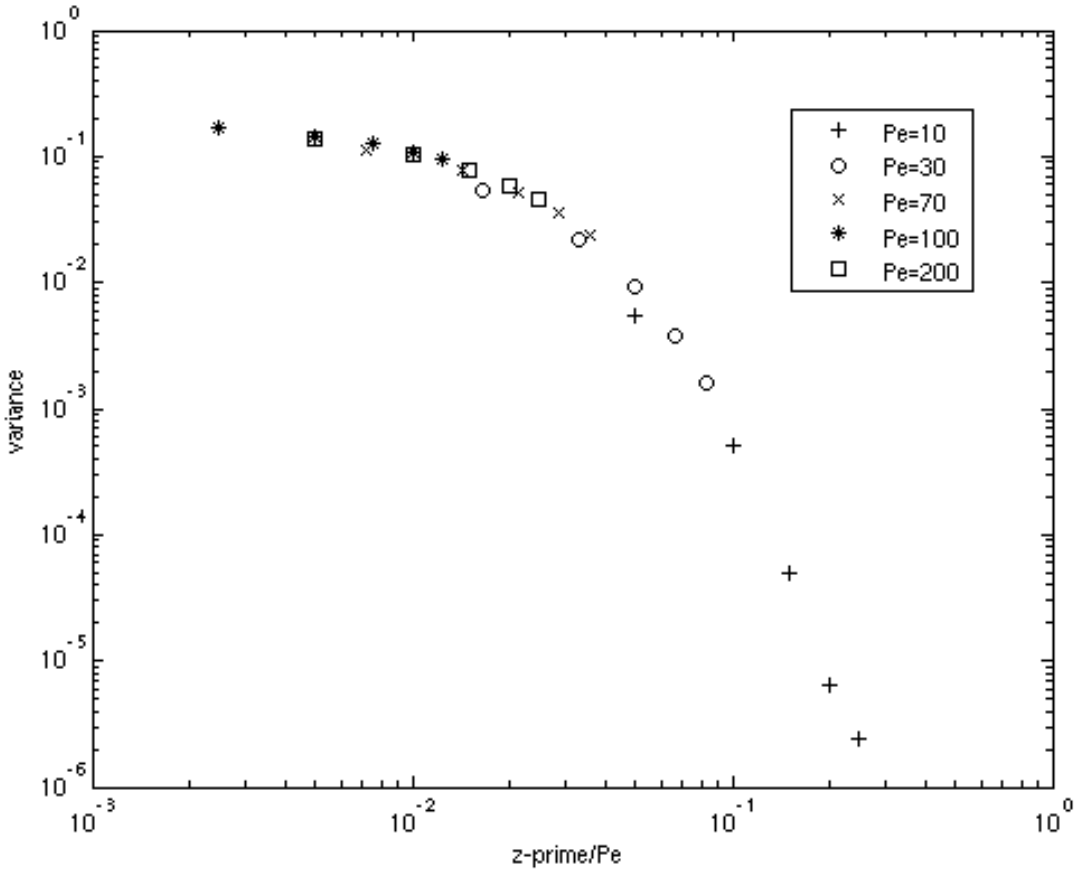


Figure 17. Variance for mixing in T-sensor

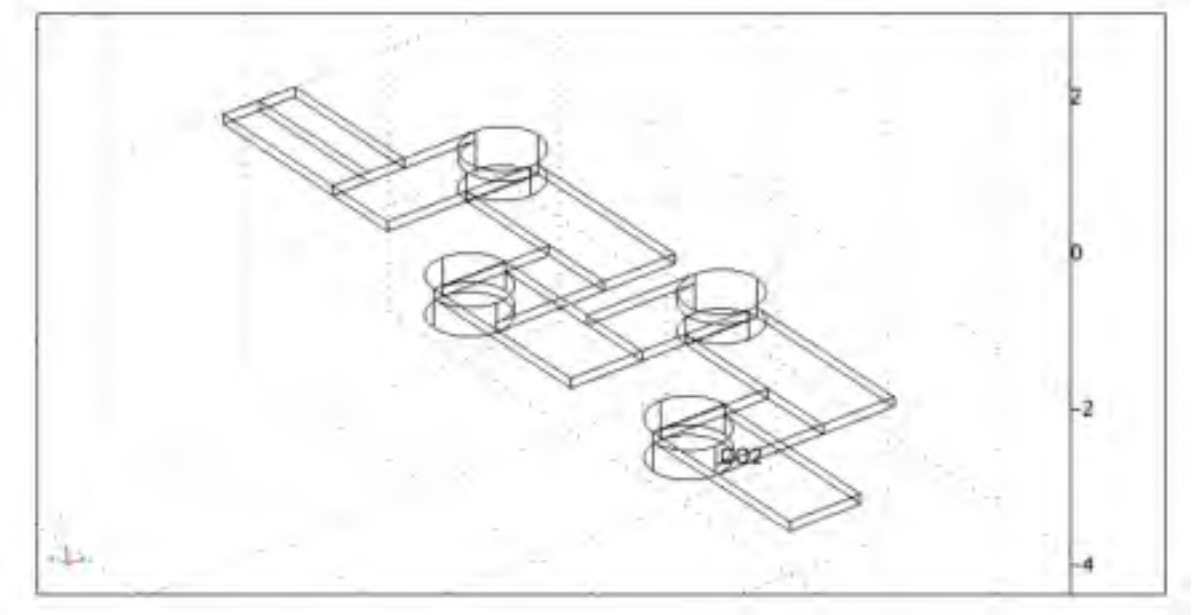


Figure 18. Serpentine mixer; width = 1, height = 1/8

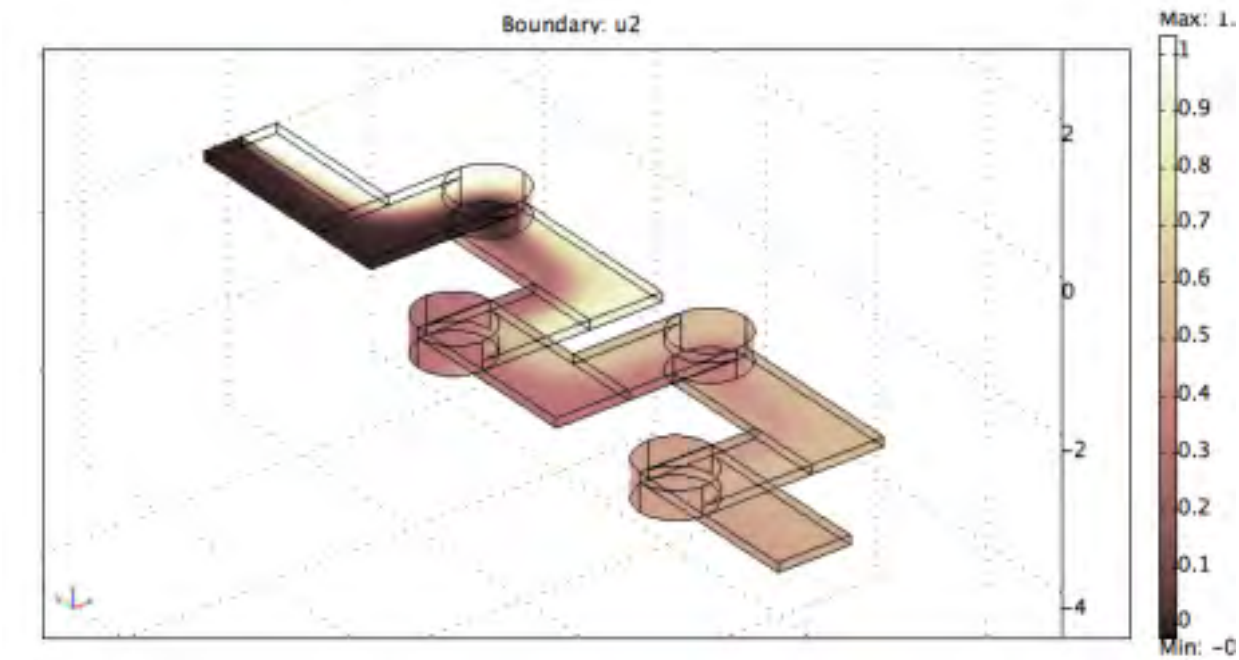


Figure 19. Concentration on surface of the serpentine mixer; *Re* = 1, *Pe* = 1000, 28,380 elements, 145,924 degrees of freedom for flow, 46,272 degrees of freedom for concentration; variance at exit is 2.6e-4

Table IV. Variance at different points in serpentine mixer

Re	*Pe*	variance	Equivalent length
0.25	250	5.31e-8	
0.5	500	1.56e-5	225
1.0	1000	2.60e-4	250
2	2000	1.12e-3	400
4	4000	2.10e-3	700
8	8000	3.03e-2	600

The equivalent length is the length of straight channel of the same dimensions that gives the same variance; the lengths are determined from Figure 17. All calculations have a dimensionless pressure drop of $\Delta p \Subset \Delta pH/\eta < v >$=2331, which means that the dimensional pressure drop increases linearly with Reynolds number. *Sc* = 1000. The case with *Pe* = 8000 is solved with 88,986 elements and 136,299 degrees of freedom for the concentration.

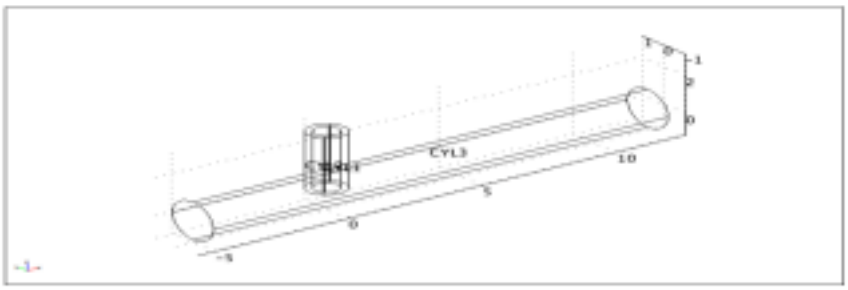


Figure 20. Reactor with two inlets for two reagents and a catalyst

(a) (b)

Figure 21. Outlet conditions, (a) velocity; (b) concentration of product

(Figure 17) shows that the total length/width necessary has been reduced from 250 to 19.6 when the variance is 2.6e-4.

Another aspect of the serpentine mixer is to define how much mixing occurs for a given pressure drop. The flow solution gives the pressure drop and the variance gives the mixing. Table IV shows results at different velocities for the serpentine mixer.

Reactor system. The importance of diffusion for mixing (or the lack of it) is illustrated by an example of a reactor system developed at Dow Chemical Company. The geometry of a small part of the device is shown in Figure 20. One chemical comes in at the left, and another chemical plus a catalyst comes in at the top inlet. The concentration distributions are found by solving the convection-diffusion-reaction equations for the two chemicals (*A* and *B*) plus the catalyst (*C*). The system is assumed to be dilute so that the total concentration does not change appreciably. The reaction is taken as

$$A + 2B \rightarrow D, \text{ in presence of } C$$

Needless to say, the reaction only occurs where both chemicals and the catalyst are all in the same place. Since little mixing occurs in laminar flow, and diffusion is slow, the product concentration

coming out is not uniform in space (Figure 21b)) even though the velocity is fully developed at the exit (Figure 21a). In this complicated three-dimensional case only CFD can give the details of mixing.

Conclusion

Engineering correlations have been presented for pressure drop and entry length in common geometrical flow channels with laminar flow. The correlations differ from their counterparts with turbulent flow (available in handbooks, depending upon density and velocity) since in slow flow the pressure drop is proportional to the velocity and the fluid viscosity. The entry length in laminar flow is also longer than is the case for turbulent flow, which means that some section of flow in microfluidics is in the entry region.

Mixing is more difficult to achieve in laminar flow than in turbulent flow. The mixing cup variance is introduced as a quantitative measure of mixing when there are flow and concentration variations. Diffusion is the mechanism in the T-sensor, and the amount of mixing depends upon the Peclet number. In the serpentine mixer, however, mixing is due primarily to the intertwining of flow streams, with diffusion across a short distance. A reaction system illustrated the importance of characterizing the flow and diffusion using computational fluid dynamics.

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Table of Nomenclature

c	[kmol m^{-3}]
D	[m] diameter of tube
$\mathcal{D}$	[m^2 s^{-1}] diffusivity
E_v	[Pa m^3 s^{-1}] viscous dissipation
$\hat{E}_v$	[Pa m^3 kg^{-1}] viscous dissipation per mass flow rate, = E_v /w
f	[–] friction factor, defined by Eq. (1)
g	[m s^{-2}] acceleration of gravity
h	[m] height above a datum
H	[m] distance between two flat plates
K	[–] friction loss coefficient, = $\Delta p_{excess} / \frac{1}{2}\rho < v >^2$
K_L	[–] friction loss coefficient for laminar flow, = $\Delta p_{excess} x_s / \eta v_s$
K_c	[–] friction loss coefficient for a manifold, defined by Eq. (18)
L	[m] length of channel
L_e	[m] entry length for velocity to come within a percentage of the fully-developed value
p	[Pa] pressure
Pe	[–] Pecle number, = $v_s x_x / \mathcal{D}$
r	[m] radial position
R	[m] radius of tube or correlation coefficient
Re	[–] Reynolds number, =– $\rho v_s x_x / \eta$
Sc	[–] Schmidt number, = $\eta / \rho \mathcal{D}$
t	[s] time
u	[m s^{-1}] velocity in the x-direction
v	[m s^{-1}] velocity, and velocity in the y-direction
V	[m^3] volume
$\boldsymbol{v}$	[m s^{-1}] vector velocity
w	[kg s^{-1}] mass flow rate or [m s^{-1}] velocity in z-direction
$\hat{W}_m$	[*Pa m^3 kg^{-1}*] work of pump per mass flow rate
x	[m] coordinate
y	[m] coordinate
z	[m] coordinate

Greek letters

β	[–] ratio of diameters or heights, defined by Eq. (12-17)
η	[Pa s] viscosity
ρ	[kg m^{-3}] Density

σ	[–] ratio of free area in manifold to area upstream
$\boldsymbol{\tau}$	[Pa] shear stress

Special symbols

©	non - dimensional pressure, using $p_s = \eta v_s / x_s$
"	non - dimensional pressure, using $p_s = \rho v_s^2$
< >	average over an area
∇	gradient operator
∇^2	Laplacian operator

Subscripts

mixing cup	concentration defined by Eq. (20)
optical	concentration defined by Eq. (21)
variance	variance defined by Eq. (22)
s	standard quantity
1	inlet value
2	outlet value
0	centerline value