

# Supplementary notes on Taylor-Aris dispersion

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## 1 The flow profile $u(y, z)$ .

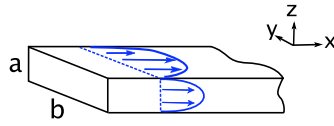


Figure 1: Geometry of our microfluidic flow chamber

For our micro-channel, we define the channel height as  $a$ , and the width as  $b$ . We choose our reference frame so that  $x$  increases in the direction of flow,  $z$  points up the channel, and  $y$  increases across the channel. See figure 1. The origin is centered in the center of the channel.

The low Reynolds number flow profile in the channel is given by

$$\nabla^2 u = \frac{1}{\mu} \frac{dP}{dx} \equiv -\alpha \quad (\text{S-1})$$

On the boundary,  $\Gamma$ , we have the no slip condition  $u = 0$ . The Fourier series for  $u$  then looks like

$$u(y, z) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} A_{mn} \cos \left[ \frac{\pi}{b} (2m+1)y \right] \cos \left[ \frac{\pi}{a} (2n+1)z \right], \quad (\text{S-2})$$

where

$$A_{mn} = \frac{4\alpha\gamma^2 a^2}{\pi^4} \cdot \frac{1}{(2m+1)(2n+1)} \cdot \frac{(-1)^m (-1)^n}{(2m+1)^2 + \gamma^2 (2n+1)^2}, \quad (\text{S-3})$$

and  $\gamma \equiv b/a$  is the aspect ratio.

For high aspect ratio geometries, we see that, over most of the channel, the flow is independent of the  $y$  coordinate. See figure 2. In the case of  $y$ -independence, the flow profile is parabolic in  $z$ . That is,

$$u(y, z) = u_0 \left[ 1 - \left( \frac{2z}{a} \right)^2 \right],$$

where  $u_0 = a^2 \alpha / 8$  is the maximum velocity. The average flow velocity  $\bar{u} = 2u_0/3$ .

When using microfluidics for physiological applications, shear stresses must be kept below certain limits [4, 3]. The wall shear stress is given by  $\tau = \mu \partial u / \partial n$ , where  $\partial / \partial n$  is the normal derivative. For high aspect ratio geometries, this becomes

$$\tau = 6\mu\bar{u}/a. \quad (\text{S-4})$$

In §6, we will present code to calculate the flow profile and wall shear stress for arbitrary aspect ratio micro-channels.

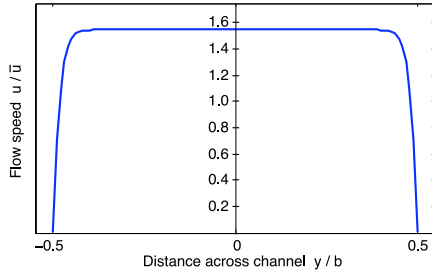


Figure 2: The flow profile across a high aspect ratio channel. Here  $\gamma = 20$  and  $z = a/2$ . Notice that for most of the channel, the flow is independent of the  $y$  component, with the maximum flow speed being close to the standard, flat plate, parabolic flow value of  $3\bar{u}/2$ .

## 2 The Taylor condition $a^2/4\pi^2D \ll l/\bar{u}$ .

In the theory of Taylor [8], convection by the parabolic flow profile in a cylindrical tube tries to spread a plug of diffusible solute laterally, but radial diffusion works against this effect, washing out the parabolic shape the plug of solute tries to take. For the theory of Taylor dispersion to hold, therefore, the radial (or in our case vertical) diffusion time must be much shorter than the longitudinal convective transport time.

The characteristic convective transport time,  $t_{\text{convect}} = l/\bar{u}$ , where  $l$  is the characteristic length scale. To calculate the characteristic vertical diffusion time, let us look at the evolution of a symmetric<sup>1</sup> concentration profile that only has  $z$  dependence:

$$\frac{\partial^2 c}{\partial z^2} = \frac{1}{D} \frac{\partial c}{\partial t}.$$

We can separate variables  $c(z, t) = c_z(z)c_t(t)$ :

$$\frac{1}{c_z} \frac{d^2 c_z}{dz^2} = \frac{a^2}{D c_t} \frac{dc_t}{dt} \equiv -\beta^2,$$

where  $\beta$  is a constant. We get that  $c_z = C \cos(\beta z)$  and  $c_t = \exp(-\beta^2 D t)$ . No flux boundary conditions tell us that  $dc_z/dz = 0$  at  $z = \pm a/2$ . It follows that  $\beta = 2\pi n/a$ , where  $n$  is an integer. The solution is

$$c(z, t) = \sum_{n=0}^{\infty} C_n \cos\left(\frac{2\pi n z}{a}\right) \exp\left(-\frac{4\pi^2 n^2 D}{a^2} t\right).$$

The slowest decaying mode,  $n = 1$ , has a time constant of

$$t_{\text{diffuse}} = \frac{a^2}{4\pi^2 D}.$$

Thus, we get the Taylor condition

$$\frac{a^2}{4\pi^2 D} \ll \frac{l}{\bar{u}}. \quad (\text{S-5})$$

## 3 On the geometric constant $\kappa = 1/210$ .

R. Aris [1] showed that the effective longitudinal diffusion coefficient describing a distribution of solvent is

$$K = D + \frac{\kappa a^2 \bar{u}^2}{D}, \quad (\text{S-6})$$

<sup>1</sup>We are interested in how quickly vertical diffusion removes the  $z$  dependence of a concentration profile generated by the flow. Since the flow itself is symmetric about  $z = 0$ , the concentration profile it generates is also symmetric.

where  $D$  is the diffusion coefficient of the solute,  $a$  is the characteristic dimension of the channel,  $\bar{u}$  is the mean flow velocity, and  $\kappa = \overline{\chi\bar{\varphi}}$  is a geometrical factor.<sup>2</sup> Aris defined  $\chi$  as the normalized deviation from the mean flow velocity

$$\chi(y, z) = \frac{u(y, z)}{\bar{u}} - 1,$$

and  $\varphi$  as the solution to<sup>3</sup>

$$\left. \begin{aligned} a^2 \nabla^2 \varphi &= -\chi, & \text{on } R \\ \frac{\partial \varphi}{\partial n} &= 0 & \text{on } \partial R \end{aligned} \right\}. \quad (\text{S-7})$$

Here,  $R$  represents cross-section,  $\partial R$  its boundary, and  $\frac{\partial}{\partial n}$  is the normal derivative.

We now calculate  $\chi$  for our high aspect ratio geometry:

$$\begin{aligned} \chi(y, z) &= \frac{1 - \left(\frac{2z}{a}\right)^2}{\int_{-1/2}^{1/2} [1 - (2\zeta)^2] d\zeta} - 1 \\ &= \frac{1}{2} - \frac{6z}{a}. \end{aligned}$$

The equations (S-7) for  $\phi$  now read

$$\left. \begin{aligned} a^2 \frac{d^2 \varphi}{dz^2} &= \frac{1}{2} - \frac{6z}{a}, & \text{for } -a/2 < z < a/2 \\ d\varphi/dz &= 0, & \text{at } z = \pm a/2 \end{aligned} \right\}.$$

The solution is

$$\varphi = \frac{1}{2} \left(\frac{z}{a}\right)^4 - \frac{1}{4} \left(\frac{z}{a}\right)^2 + \frac{7}{480}.$$

We can now calculate the geometric factor  $\kappa$ :

$$\begin{aligned} \kappa &= \int_{-1/2}^{1/2} \left( \frac{\zeta^4}{2} - \frac{\zeta^2}{4} + \frac{7}{480} \right) \left( \frac{1}{2} - 6\zeta^2 \right) d\zeta \\ &= \frac{1}{210}. \end{aligned}$$

Now we have the effective longitudinal diffusion:<sup>4</sup>

$$K = D + \frac{1}{210} \frac{a^2 \bar{u}^2}{D}, \quad (\text{S-8})$$

and provided that 1) lateral diffusion is negligible and 2) the Taylor condition holds, our problem essentially becomes one dimensional.

## 4 Advection-diffusion equation with uncaging source

Figure 3 shows the geometry of our uncaging setup when viewed from above (xy plane). A caged compound flows across an rectangular region illuminated by a UV light. This light activates (uncages) material by cleaving the bond between the active part and the caging group. The region is of length  $L$ . The cell that will be stimulated by the uncaged compound is a distance  $l$  downstream of the uncaging light.

<sup>2</sup>We denote averaging across the cross-section with an over-bar.

<sup>3</sup>Here we have assumed that solute's diffusibility is independent of concentration. Note also that these expressions define  $\varphi$  up to a constant, but the constant disappears when calculating  $\kappa$ . Aris defined this constant so that  $\bar{\varphi} = 0$ .

<sup>4</sup>This is the well known flat plate result [5].

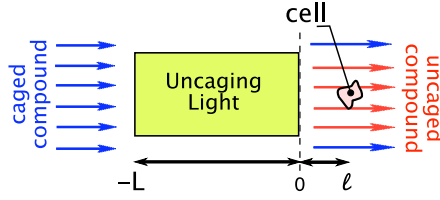


Figure 3: The uncaging geometry

If we turn on the uncaging light at  $t = 0$ , then we can describe the evolution of the concentrations for uncaged ( $c$ ) and caged ( $c_2$ ) material as follows:

$$\frac{\partial c}{\partial t} = -\bar{u} \frac{\partial c}{\partial x} + K \frac{\partial^2 c}{\partial x^2} + c_2 f(x, t) \quad (\text{S-9})$$

$$\frac{\partial c_2}{\partial t} = -\bar{u} \frac{\partial c_2}{\partial x} + K_2 \frac{\partial^2 c_2}{\partial x^2} - c_2 f(x, t) \quad (\text{S-10})$$

with the initial conditions

$$c(x, 0) = 0 \quad (\text{S-11})$$

$$c_2(x, 0) = c_0. \quad (\text{S-12})$$

The function  $f(x, t)$  describes the uncaging region:<sup>5</sup>

$$f(x, t) = \begin{cases} \sigma \phi I & \text{for } -L \leq x \leq 0 \text{ and } t > 0 \\ 0 & \text{otherwise} \end{cases},$$

here  $I$  is the light intensity,  $\sigma$  is the absorption cross-section, and  $\phi$  is the quantum yield.

If the diffusivity of the caged compound is markedly different from that of the uncaged species, (an example is caged calcium), we should solve the coupled equations (S-9) and (S-10) numerically.

If we can assume that the diffusion coefficients of the caged and uncaged substance are comparable, as is the case for many nucleotides, then  $K = K_2$ . By adding equations (S-9) and (S-10), we can see that the total concentration follows the advection-diffusion equation. Furthermore, we see that the initial condition is uniform—add (S-11) and (S-12) together. Therefore, the total concentration is constant in time and space:  $c + c_2 = c_0$ . We can rewrite (S-9) as

$$\frac{\partial c}{\partial t} = -\bar{u} \frac{\partial c}{\partial x} + K \frac{\partial^2 c}{\partial x^2} + (c_0 - c) f(x, t) \quad (\text{S-13})$$

We introduce the dispersive length scale  $\eta_K = K/\bar{u}$ , dispersive time scale  $\tau_K = K/\bar{u}^2$ , photolysis time scale  $\tau_p = (\sigma \phi I)^{-1}$ , and residence time  $\tau_r = L/\bar{u}$ . By expressing all lengths in units of  $\eta_K$ , all times in  $\tau_K$ , and concentration in units of  $c_0$  we get the dimensionless form of Eq. (S-13):

$$\frac{\partial c}{\partial t} = -\frac{\partial c}{\partial x} + \frac{\partial^2 c}{\partial x^2} + (1 - c) f(x, t), \quad (\text{S-14})$$

where

$$f(x, t) = \begin{cases} \tau_p^{-1} & \text{for } -\tau_r \leq x \leq 0 \text{ and } t > 0 \\ 0 & \text{elsewhere.} \end{cases}$$

Unless stated otherwise, we will use these units for the rest of this section. Note that in the dimensionless form used here,  $L = \tau_r$ . This treatment differs from the main text, in which we left  $\tau_p$ ,  $\tau_r$  and  $L$  in the original units.

<sup>5</sup>We have assumed that the time-scale for the bond cleavage is insignificant compared to the other time scales involved in the problem.

## 4.1 Steady state solution

We get the steady state solution by setting  $\frac{\partial c}{\partial t} = 0$ :

$$\frac{d^2 c}{dx^2} - \frac{dc}{dx} + (1 - c)f(x) = 0$$

The full solution to this equation, with the condition that  $c \rightarrow 0$  when  $x \rightarrow -\infty$ , is

$$c = \begin{cases} A_0 e^x & \text{for } x < -\tau_r \\ A_1 e^{\lambda_1 x} + A_2 e^{\lambda_2 x} + 1 & \text{for } -\tau_r \leq x \leq 0 \\ A_3 & \text{for } x > 0 \end{cases} \quad (\text{S-15})$$

Here,

$$\lambda_{1,2} = \frac{1}{2} \left( 1 \pm \sqrt{1 + 4/\tau_p} \right),$$

and the  $A_i$ 's are given by the continuity of  $c$  and  $dc/dx$  at  $x = -\tau_r$  and  $x = 0$ :

$$A_0 = \frac{\lambda_1(-\lambda_2)e^{\tau_r}(e^{-\lambda_2\tau_r} - e^{-\lambda_1\tau_r})}{\lambda_1^2 e^{-\lambda_2\tau_r} - \lambda_2^2 e^{-\lambda_1\tau_r}}$$

$$A_1 = -\frac{-\lambda_2}{\lambda_1^2 e^{-\lambda_2\tau_r} - \lambda_2^2 e^{-\lambda_1\tau_r}}$$

$$A_2 = -\frac{\lambda_1}{\lambda_1^2 e^{-\lambda_2\tau_r} - \lambda_2^2 e^{-\lambda_1\tau_r}}$$

$$A_3 = 1 - \frac{\lambda_1 - \lambda_2}{\lambda_1^2 e^{-\lambda_2\tau_r} - \lambda_2^2 e^{-\lambda_1\tau_r}}$$

We will now look at two limiting cases. The first case is when the uncaging light intensity is high, where we would expect everything to be uncaged. The second case is that of low light intensity, where we expect to see a linear dependence of the uncaged concentration with the length and brightness of the uncaging region.

### 4.1.1 Low Light Intensity Regime: $\tau_p \gg 1$

In this limiting case,  $\lambda_1 = 1 + 1/\tau_p$  while  $\lambda_2 = -1/\tau_p$ . Using this with  $|\lambda_1| \gg |\lambda_2|$ , we get the concentration to the right of the uncaging region

$$c(x > 0) = 1 - \exp\left(-\frac{\tau_r}{\tau_p}\right). \quad (\text{S-16})$$

Now, under the additional limiting condition that  $\tau_p \gg \tau_r$ , we get a linear relation between the uncaged concentration and residence time:

$$c(x > 0) = \frac{\tau_r}{\tau_p}. \quad (\text{S-17})$$

Restoring our original units for length, time, and concentration,

$$c(x > 0) = \frac{c_0 \sigma \phi I L}{\bar{u}}. \quad (\text{S-18})$$

### 4.1.2 Saturating Regime: $\tau_p \ll 1$

In this limiting case, we see that

$$\begin{aligned}\lambda_1 &= -\lambda_2 \\ &= \sqrt{\frac{1}{\tau_p}} \\ &\gg 1.\end{aligned}$$

The concentration to the right of the uncaging region

$$\begin{aligned}c(x > 0) &= A_3 \\ &= 1 - \frac{2\lambda_1}{\lambda_1^2(e^{\lambda_1\tau_r} + e^{-\lambda_1\tau_r})}\end{aligned}$$

The second term is negligible, and thus,

$$c(x > 0) = 1,$$

or in original units,  $c(x > 0) = c_0$ , as expected.

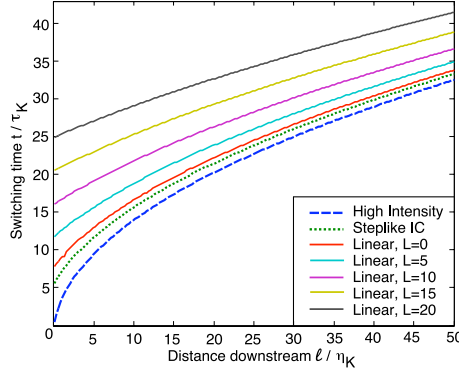


Figure 4: The time it takes for the concentration to rise from 5% to 95% of the final concentration, as a function of distance for the three cases of 1) low light intensity, 2) saturating light intensity, and 3) step-like initial conditions.

## 4.2 Time dependent solution

### 4.2.1 Low Light Intensity Regime: $\tau_p \gg 1$ and $\tau_p \gg \tau_r$ .

In the linear regime, the uncaged concentration is far from being saturated, i.e.  $c \ll 1$ . Then, equation S-14 reads

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} - \frac{\partial^2 c}{\partial x^2} = \begin{cases} \tau_p^{-1} & \text{for } -\tau_r \leq x \leq 0 \\ 0 & \text{elsewhere} \end{cases} \quad (\text{S-19})$$

We get the solution to this equation by convolving the inhomogeneous source term with the Green function:

$$\begin{aligned}c(x, t) &= \int_0^t \int_{-\tau_r}^0 \left\{ \frac{\tau_p^{-1}}{\sqrt{4\pi(t-\tau)}} \exp\left[-\frac{(x-\xi-t+\tau)^2}{4(t-\tau)}\right] \right\} d\xi d\tau \\ &= \frac{1}{2\tau_p} \int_0^t \left[ \operatorname{erf}\left(\frac{x+\tau_r-t+\tau}{2\sqrt{t-\tau}}\right) - \operatorname{erf}\left(\frac{x-t+\tau}{2\sqrt{t-\tau}}\right) \right] d\tau\end{aligned} \quad (\text{S-20})$$

#### 4.2.2 Saturating Regime: $\tau_p \ll 1$

In the high light intensity case, everything underneath the light source is uncaged, so we can find the concentration to the right of the uncaging light by solving the advection diffusion equation

$$\frac{\partial c}{\partial t} = -\frac{\partial c}{\partial x} + \frac{\partial^2 c}{\partial x^2},$$

with the boundary condition

$$c(0, t) = 1,$$

and the initial condition

$$c(x > 0, 0) = 0.$$

The equation can be solved by taking a Laplace transform in time and solving the ordinary differential equation in space.<sup>6</sup> The solution reads

$$c(x, t) = \frac{e^{x/2}}{2} \left[ e^{x/2} \operatorname{erfc} \left( \frac{x+t}{2\sqrt{t}} \right) + e^{-x/2} \operatorname{erfc} \left( \frac{x-t}{2\sqrt{t}} \right) \right]. \quad (\text{S-21})$$

#### 4.2.3 Valve based switching: $I = 0$ and $c(x, 0) = H(-x)$

We can treat switching in valve based systems as an initial value problem  $c(x, 0) = H(-x)$  with no source term,  $I = 0$ . Here,  $x = 0$  is the location where the valve opens and introduces the solute. The solution is

$$c(x, t) = \frac{1}{2} \operatorname{erfc} \left( \frac{x-t}{2\sqrt{t}} \right).$$

Irimia et al. [6] describe a system for switching a gradient of fluorescein in  $\sim 4$  s by using microfluidic valves. Let us apply the Taylor-Aris theory to this system.

Their channel is  $100 \mu\text{m}$  tall with an average flow speed  $\bar{u} = 370 \mu\text{m}/\text{s}$ . The diffusion coefficient of fluorescein  $D = 425 \mu\text{m}^2/\text{s}$  [2]. The observation window is a distance  $l \approx 1750 \mu\text{m}$  away from the valves.

With these values, we calculate that  $Pe_a = 87$  and  $Pe = 1524$ . The Taylor condition is satisfied, as  $Pe_a^2/Pe = 5.0$ . The effective diffusion coefficient

$$K = D \left( 1 + \frac{Pe_a^2}{210} \right) = 1.57 \times 10^4 \mu\text{m}^2/\text{s}.$$

We can write the distance as  $l = 42.5\eta_K$ . Referring to the dotted green line in figure 4, we see that the switching time

$$t = 31\tau_K = 3.5 \text{ s},$$

which is in good agreement with the experimentally observed switching time.

## 5 Measuring the diffusion coefficient of caged fluorophores

We filled a  $3 \text{ cm} \times 500 \mu\text{m} \times 26 \mu\text{m}$  channel with  $10 \mu\text{M}$  of 3000 MW, dextran conjugated caged fluorescein. The tubing we used to inject the caged fluorophore was removed from the microfluidic device, and excess fluid was wiped away from the inlet and outlet. The channel was mounted on an Olympus Fluoview 1000 dual scanner confocal microscope with a 40x objective. We adjusted the location of the sample and focus of the microscope so that we were looking near the middle of the channel. After waiting for the flow inside the device to stop, we imaged a  $78 \mu\text{m} \times 9 \mu\text{m}$  ( $125 \times 15 \text{ pixel}^2$ ) at a rate of  $0.037 \text{ s}/\text{frame}$  for 50 frames. After the tenth frame, we uncaged a vertical,  $75 \mu\text{m}$  (121 pixel) line through the middle of the imaging region. See figure 5. To obtain

<sup>6</sup>For example, see [7].

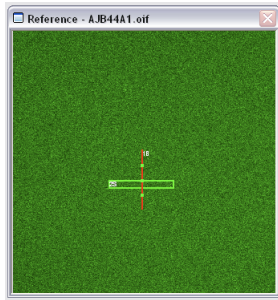


Figure 5: Regions of interest for diffusion coefficient measurements. The red line corresponds to a  $75\mu\text{m}$  uncaging region. The green rectangle corresponds to the  $78\mu\text{m} \times 9\mu\text{m}$  imaging window.

a better signal to noise ratio, we averaged over 20 measurements, and we collapsed the imaging region to one dimension by averaging over the height of the frame.

By looking how the fluorescence intensity profile, figure 6(a), evolves with time, we can determine the diffusion coefficient. Provided that the width of the intensity profile is considerably smaller than the height of the uncaging line, we can treat the problem as a one dimensional diffusion problem. If we model the uncaging (photobleaching) event as releasing  $C_0\delta(x-x_c)\delta(t-t_{\text{uncage}})$  of material, then concentration profile

$$c(x, t) = \frac{C_0}{\sqrt{2\pi}\sigma_t} \exp\left[-\frac{(x-x_c)^2}{2\sigma_t^2}\right],$$

where the variance of the distribution  $\sigma_t^2 = 2D(t - t_{\text{uncage}})$ . Assuming that the fluorescence intensity scales linearly with fluorophore concentration, the intensity should also have this form.

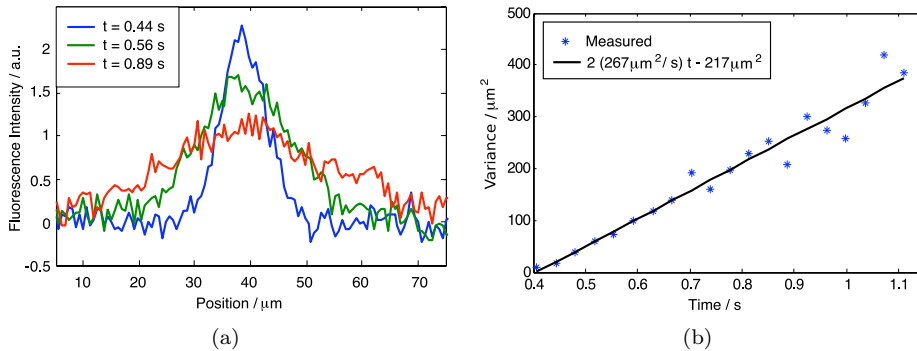


Figure 6: Determination of the diffusion coefficient for caged fluorescein. a) The fluorescence intensity profile at various times after a line of fluorescein has been uncaged;  $t_{\text{uncage}} = 0.37\text{s}$ . b) The squared width,  $\sigma_t^2$ , of the fluorescence distribution as a function of time.

In figure 6(b), we show with blue asterisks the variance of gaussian fits to the fluorescence intensity profile. The solid black line is a linear fit. From the fit, we get the diffusion coefficient of our caged fluorescein:

$$D_{\text{cfl}} = 267 \pm 8\mu\text{m}^2/\text{s}.$$

The error reflects the 95% confidence interval of the linear fit.

## References

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## 6 Matlab codes:

### 6.1 Calculating flow profile and shear stress

```
1 % ----- flowprofile.m ----- %
2 %
3 % This script calculates the flow profile and bottom wall
4 % shear stress inside a rectangular cross-section channel.
5 %
6 % ----- %
7
8 ubar = 104e-6;      % Speed (m/s)
9 a = 26e-6;         % Channel height (m)
10 b = 500e-6;       % Channel width (m)
11 visc = 1.0e-3     % Dynamic viscosity of water (Pa*s)
12 sumterms = 40;    % Number of entries to sum over in m and n
13
14 gam = b/a;        % Aspect ratio
15
16 [M,N] = meshgrid(0:sumterms,0:sumterms);
17 clear sumterms;
18
19
20 % First, let's get the average flow velocity normalization
21
22 ubar2=4/(ubar*pi^2)*sum(sum((1).^M./...
23     ((2*M+1).^2.*(2*N+1).^2.*(2*M+1).^2+...
24     gam*gam*(2*N+1).^2)));
25
26 % Next, we calculate the flow in the middle of the channel
27
28 i=1;
29 z=0;
30 for y=-0.5:0.01:0.5 % in units of channel width
31     u(i)=sum(sum((-1).^M.*(-1).^N.*cos(pi*(2*M+1)*y).*...
32         cos(pi*(2*N+1)*z)./((2*M+1).*(2*N+1).*(2*M+1).^2+...
33         gam*gam*(2*N+1).^2)));
34     i=i+1;
35 end
36 u=u/ubar2; % Normalize u to get the correct mean velocity
37
38 % Display the flow speed
39 y=-0.5:0.01:0.5;
40 plot(y,u); % Plot it
41 xlabel('y / b');
42 ylabel('Flow speed u / (m/s)');
43
44 % Next, we calculate the shear at the bottom of the channel
45
46 i=1;
47 z=0;
48 for y=-0.5:0.01:0.5
49     stress(i)=(pi/a)*sum(sum((-1).^M.*cos(pi*(2*M+1)*y)./...
50         ((2*M+1).*((2*M+1).^2+gam*gam*(2*N+1).^2)));
51     i=i+1;
52 end
53 stress=visc*stress/ubar2;
54
55 % Display the shear
56 figure
57 y=-0.5:0.01:0.5;
58 plot(y,stress);
59 xlabel('y / b');
60 ylabel('Wall shear stress \tau / Pa');
```

## 6.2 Calculating Taylor-Aris switching times

```

1  % ----- switchTimeExample.m ----- %
2  %
3  % This script demonstrates how to calculate the Taylor-Aris %
4  % switching time for valve based systems, linear regime and %
5  % saturating regime flow photolysis systems. %
6  %
7  % Note that all lengths are in units of eta.K = K/u, and %
8  % all times are in units of tau.K = K/u^2 %
9  % ----- %
10
11
12  l = 30; % The distance from the cell to the uncaging light (or valve)
13  L = 20; % The length of the uncaging region (for the linear case)
14
15  % First example is the valve based switching
16  t1 = fzero(@(t) (valveSwitchC(l,t)-0.05),l);
17  t2 = fzero(@(t) (valveSwitchC(l,t)-0.95),l);
18  swT1=t2-t1
19
20  % The next example is the linear regime photolysis
21  t1 = fzero(@(t) (LowIntensityC(L,l,t)-0.05),L,l);
22  t2 = fzero(@(t) (LowIntensityC(L,l,t)-0.95),L,l);
23  swT2=t2-t1
24
25  % The last example is the saturating regime photolysis
26  t1 = fzero(@(t) (HighIntensityC(l,t)-0.05),l);
27  t2 = fzero(@(t) (HighIntensityC(l,t)-0.95),l);
28  swT3=t2-t1

1  function y = valveSwitchC(x,t)
2      %Deal with problematic nonpositive t's
3      t=t.*(t>0);
4      t=t+(t<=0)*1e-50;
5
6      y = 0.5*erfc((x-t)/(2*sqrt(t)));

1  function y = LowIntensityC(L,x,t)
2      %Deal with problematic nonpositive t's
3      t=t.*(t>0);
4      t=t+(t<=0)*1e-50;
5      %High Intensity Uncaging concentration
6      y = quad(@(tau) (0.5*(erf((t-x-tau)/(2*sqrt(t-tau)))+...
7          erf((L-t+x+tau)/(2*sqrt(t-tau))))),0,t)/L;

1  function y = HighIntensityC(x,t)
2      %Deal with problematic nonpositive t's
3      t=t.*(t>0);
4      t=t+(t<=0)*1e-50;
5      %High Intensity Uncaging concentration
6      y = 0.5*exp(x/2).*(exp(x/2).*erfc((x+t)/(2*sqrt(t)))+...
7          exp(-x/2).*erfc((x-t)/(2*sqrt(t))));

```