**ME141C:** **Spring 2007**
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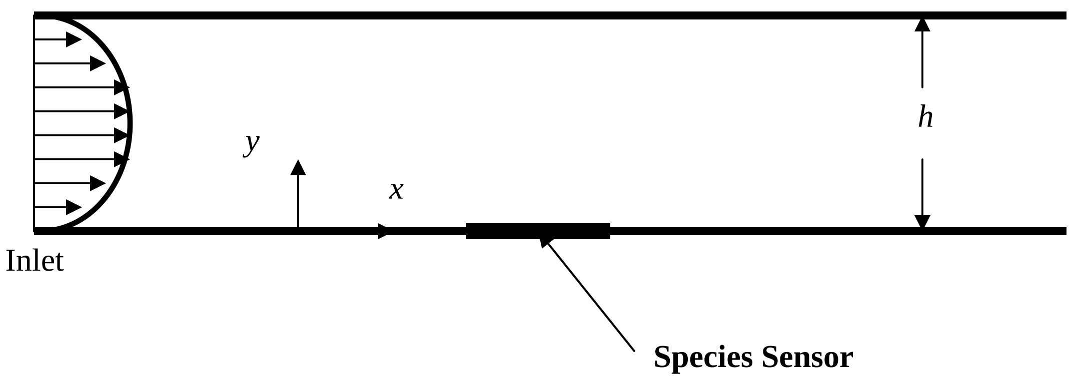
**Home Work 2**
Due: 3 May 2007

**Surface Binding Model**
**Problem Formulation:**

Consider a BioMEMS sensor, where the flow is between two parallel plates that extend to infinity into the *z* direction.




For this flow the Navier-Stokes equations can be simplified to the *x*-component of Stokes equation

$$\frac{dp}{dx} = \mu \nabla^2 u \qquad (1)$$

which has the solution

$$u = -\frac{1}{2\mu}\frac{dp}{dx}\left[y/h - \left(y/h\right)^2\right] = 4u_{\max}\left[y/h - \left(y/h\right)^2\right] \qquad (2).$$

For time $t < 0$ the channel is devoid of any concentration of species $c$. At time $t = 0$, a uniform concentration of species $c$ ($c = c_0$ is the initial concentration) is introduced at the inlet. The transport of $c$ in the channel is governed by the following equation:

$$\frac{\partial c}{\partial t} + \left(\vec{u}\cdot\nabla\right)c = \nabla\cdot\left(\vec{\vec{D}}\nabla c\right) + R_i \qquad (3)$$

where $D$ is the diffusion tensor of species $c$, and $R_i$ is the homogeneous rate of reaction which is zero. Since the velocity is purely in the *x*-direction, i.e. $\vec{u} = u\,\hat{e}_x$, we can simplify Eq. (3)

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]c\,. \qquad (4)$$

For design purposes, we may want to change the depth of the microchannel, to optimize the binding rate. It is convenient to keep the simulation geometry constant, and change the physical depth by introducing a stretching parameter α, such that $y = \alpha \hat{y}$, where $\hat{y}$ is the fixed simulation coordinate. Equation (4) becomes

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \left[ D\frac{\partial^2}{\partial x^2} + \frac{D}{\alpha^2}\frac{\partial^2}{\partial \hat{y}^2} \right] c \,. \tag{5}$$

This can be simulated by introducing an anisotropic diffusivity tensor into COMSOL

$$\vec{\vec{D}} = \begin{bmatrix} D & 0 \\ 0 & D/\alpha^2 \end{bmatrix}. \tag{6}$$

The height of the microchannel in the simulation is $\hat{h} = 100\mu m$. Therefore, an *h* = 50 μm wide channel can be simulated by setting, $\alpha = 0.5$.

On the sensor surface, species *c* reacts with antibodies placed upon the surface and forms species *B* which can be detected by a variety of methods, including optical, electrical, etc. The rate of reaction is governed by the rate of association minus the rate of dissociation

$$\frac{\partial B}{\partial t} = k_{on} c (R_t - B) - k_{off} B \,, \tag{7}$$

where $R_t$ is the total number of available antibodies immobilized on the sensor surface, $k_{on}$ is the on rate constant, and $k_{off}$ is the dissociation constant.

The rate of reaction at the binding site is equal to the rate of diffusion at the microchannel surface, just above the sensor,

$$\frac{\partial B}{\partial t} = D\left.\frac{\partial c}{\partial y}\right|_{y=0} \tag{8}$$

**Simulation:**

Modify the example given on the class website to meet the conditions of this problem.

**Solution:**

The default simulation uses the following parameters:

$C_0$ = 1e-9, $k_{on}$ = 1e8 $k_{off}$ = 0.02 $R_t$ = 1.67e-11 $D$ = 1e-11

*u*_max = 1e-3 $\alpha$ = 1 time steppping = [0 : 0.05 : 2].

A. For the default simulation parameters, plot to species concentration at *t* = 2 seconds. Create an animation to visualize the motion of the species.

B. For the default simulation parameters, plot the bound concentration *B* as a function of *x* along the sensor surface. Put multiple times on a single graph to show the trend.

C. For the default simulation parameters, plot the average bound concentration over the sensor area "*B_ave*" as a function of time.

D. Compare the slope of "*B_ave*" versus time curves for different values of channel height *h* = 200, 50, and 25 microns. This is accomplished by changing the stretching parameter alpha = 2, 0.5, 0.25, in the add/edit constants under the options menu. For advanced users, you can vary alpha as a parameter, using the parametric option, under solution parameters.

E. Compare the slope of "*B_ave*" versus time curves for different values of maximum velocity. Use values of *u_max* = 1e-2 to 1e-3. Do higher or lower velocities make the sensor more responsive? Note you may need to adjust the time the model runs, corresponding to the various velocities.

F. Compare the slope of "*B_ave*" versus time curves for different values of concentration of antibodies. Use values of *R*t = 100, 500, and 5000. Is your sensor more accurate with higher or lower antibody concentrations?

G. Compare the slope of "B_ave" versus time curves for different values of the diffusion coefficient. Use values of D = 1e-3 to 1e-6. Is your sensor more accurate with higher or lower diffusion?