Convective Diffusion Equation Solved in Comsol 4.1.
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See also *Introduction to Chemical Engineering Computing*, Wiley (2006).

The T-sensor is described in Chapter 10, but its key use is to transfer a chemical from one flowing stream to the other. Thus, the convective diffusion equation must be solved, too. A fluid (such as water) comes in the top and bottom, but the top stream contains a dissolved chemical that needs is to be transferred. The bottom stream may contain a different chemical that will react and fluoresce, thus permitting a visual detection. Your goal is to predict how fast the transfer takes place.

Step 1: choose the problem. Open the Comsol file for the fluid flow problem in Ch. 10. First, we add physics by right clicking on Model, choosing Transport of Diluted Species, next; Stationary, finish.

Step 2: set the variables. Right click Definitions and choose Variables, and set Pe to 1.

Step 3: define the problem. Click on the Transport sub-node and choose Discretization. Change from Linear to Quadratic. Right click on Transport and choose Convection and Diffusion. Select the total domain, +, to add it to the Selection box. Change the velocity to u and v. The diffusivity is a stand-in for 1/Pe, so change it to 1/Pe.

Step 4: set the boundary conditions. To set the boundary conditions, right click on Transport and choose Inlet. Choose the top boundary, +, to add it to the Selection box. Keep the value as 0. Do the same thing for the bottom boundary, but set the Concentration to 1.0. Right click on Transport, choose Outlet; select the outlet boundary, +, to add it to the Selection box.

Step 5: solve the problem. To solve the problem, right click on Study 2 =.

Step 6: examine the solution. The velocity shows first in the graphics window. To see the concentration, right click on Results and choose 2D Plot Group. Right click on 2D Plot Group and choose Surface. The default expression is spf.U. Change it to c. Also change the Data set to Solution 2. Click the plot icon to see the plot of concentration, Figure 11.4.

Step 7: examine the solution. To check the mass balance, right click on the Derived Values under Results. and choose Line Integration. Integrate v*c over the top and bottom boundary (0.0 and 0.5000000). Integrate u*c over the outlet (0.4999998). Thus, the mass balance is quite good.

Step 8: change the Peclet number. Change the Peclet number to 50 and repeat. Click the Variables sub-node under Definitions and change 1 to 50. Right click Study 2 =. Change to the plot of concentration, Figure 11.5. Now there is good mixing, but not as good as when the Peclet number is smaller. The flow rates in and out are: 0.499959 and 0.5000000, which gives a quite accurate mass balance. Change the Peclet number to 500 and repeat, giving Figure 11.6. Now the mixing is not nearly as good. The mass balance numbers are the same as before, giving a good overall mass balance. Note, however, that the concentration (in the scale) goes from -0.019 to

1.0212. This indicates that there are oscillations in the solution, but they are on the order of 2%. This error can be decreased if desired by refining the mesh.

Step 9: plot two solutions. To plot outlet concentration profiles for Pe = 50 and 500, right click Global Definitions, choose Parameters, and use Pe (you can set a value). Now right click on Study2 and choose Parametric Sweep. When you click on the +, the Pe will appear in the window; select it and Add, OK. Click on the parameter icon and set the range from 50 to 500 with a step of 450. Right click Study 2 =. Right click on Results, choose 1D Plot Group; right click it an choose Line Graph. The two concentration profiles are plotted on one graph.
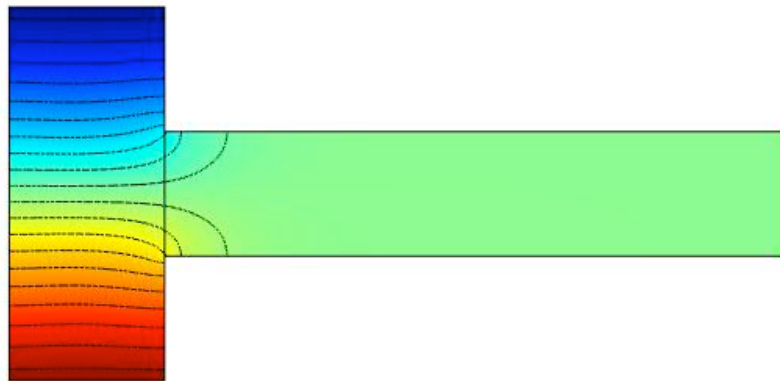

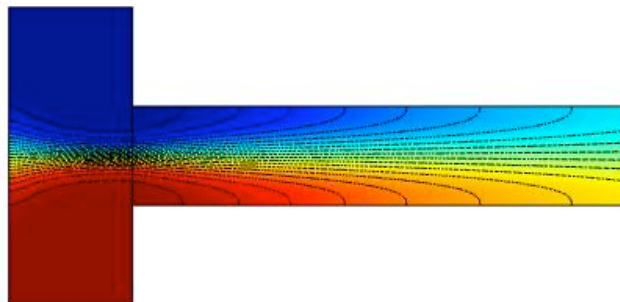**Figure 11.4. Solution to T-sensor diffusion/convection problem with D = 1**

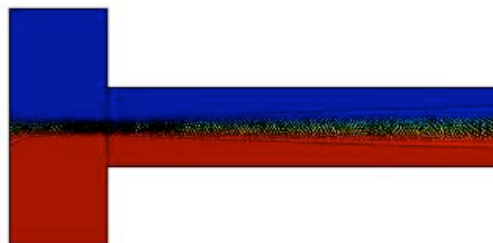**Figure 11.5. Solution to T-sensor diffusion/convection problem with D = 1/50**

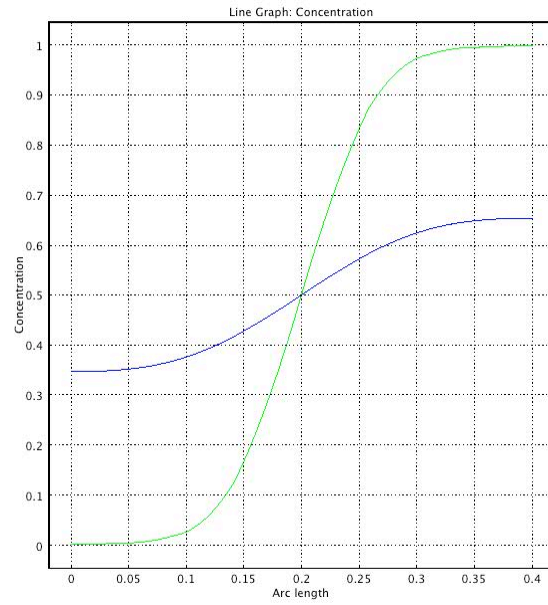**Figure 11.6. Solution to T-sensor diffusion/convection problem with D = 1/500**

Figure 11-7. Exit concentrations for Pe = 50 and 500 (D = 1/50 and 1/500).