Microchannel Cell

Introduction

This example was originally formulated by Albert Witarsa under Professor Bruce Finlayson's supervision at the University of Washington in Seattle. It was part of a graduate course in which the assignment consisted of using mathematical modeling to evaluate the potential of patents in the field of microfluidics.

This model treats an H-microcell for separation through diffusion. The cell puts two different laminar streams in contact for a controlled period of time. The contact surface is well defined, and by controlling the flow rate it is possible to control the amount of species transported from one stream to the other through diffusion.
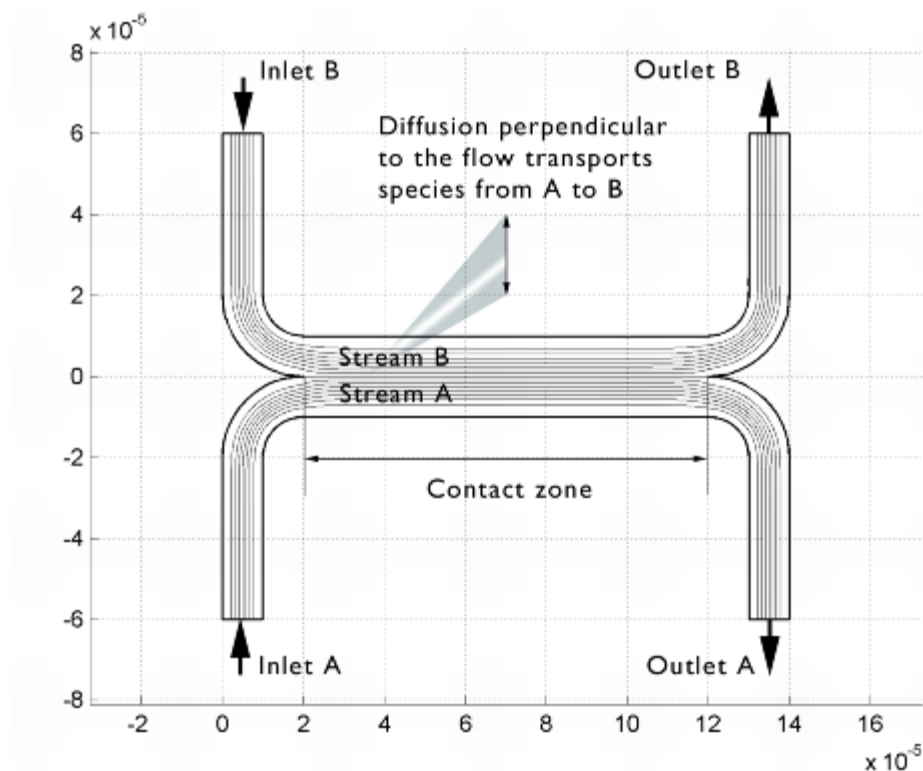

Figure 4-47: Diagram of the H-microcell.

Model Definition

The geometry of the microcell (Figure 4-43) is taken from Albert Witarsa's and Professor Finlayson's assignment. The cell geometry is divided in half because of symmetry. The design aims to avoid upsets in the flow field when the two streams, A and B, are united. This is to avoid the two streams mixing through convection, which would mix all species equally and lead to loss of control over the separation abilities. The transport of species between streams A and B should take place only by diffusion in order that species with low diffusion coefficients stay in
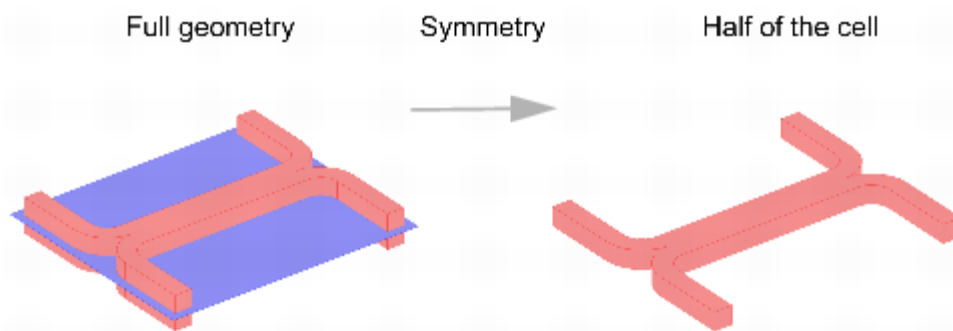
their respective streams.

Figure 4-48: Model geometry. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry.

The simulations involve solving the fluid flow in the H-cell. According to the specifications, the flow rate at the inlet is roughly 0.1 mm/s. This implies a low Reynolds number, well inside the region of laminar flow:

$$\text{Re} = \frac{d\rho u}{\eta} = \frac{1\cdot 10^{-5} \cdot 1\cdot 10^{3} \cdot 1\cdot 10^{-4}}{1\cdot 10^{-3}}$$
(4-12)

[Equation 4-12](#) gives a Reynolds number of 0.001 for a water solution and the channel dimensions given in [Figure 4-43](#), a value typical for microchannels. Thus it is easy to get a numerical solution of the full momentum balance and continuity equations for incompressible flow with a reasonable number of elements. The equations that you need to solve are the Navier-Stokes equations at steady state:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})]$$
$$\nabla\cdot\mathbf{u} = 0$$
(4-13)

Here ρ denotes density (kg/m^3), $\mathbf{u}$ is the velocity (m/s), η denotes viscosity (Pa·s), and p equals pressure (Pa).

Separation in the H-cell involves species in relatively low concentrations compared to the solvent, in this case water. This means that the solute molecules interact only with water molecules, and it is safe to use Fick's law to describe the diffusive transport in the cell. This mass-balance equation for a solute appears in the Convection and Diffusion application mode and reads

(4-14) $-\nabla\cdot(-D\nabla c + c\mathbf{u}) = 0$.

In this equation, D denotes the diffusion coefficient (m^2/s) and c represents the concentration (mol/m^3). In this model, you use the parametric solver to solve [Equation 4-14](#) for three different values of D—$1\cdot 10^{-11}$ m^2/s, $5\cdot 10^{-11}$ m^2/s, and $1\cdot 10^{-10}$ m^2/s— to simulate the mixing of different species.

You solve two versions of the model:

- In the first version, you assume that a change in solute concentration does not influence the fluid's density and viscosity. This implies that it is possible to first solve the Navier-Stokes equations and then solve the mass balance equation.

- In the second version, you include a correction term in the viscosity that dependes quadratically on the

concentration:

$$(4\text{-}15) \quad \eta = \eta_0(1 + \alpha c^2).$$

Here α is a constant of dimension $(\text{concentration})^{-2}$. An influence of concentration on viscosity of this kind is usually observed in solutions of larger molecules.

Next, consider the boundary conditions, starting with the Navier-Stokes equations. For the relevant boundary groupings, refer to .
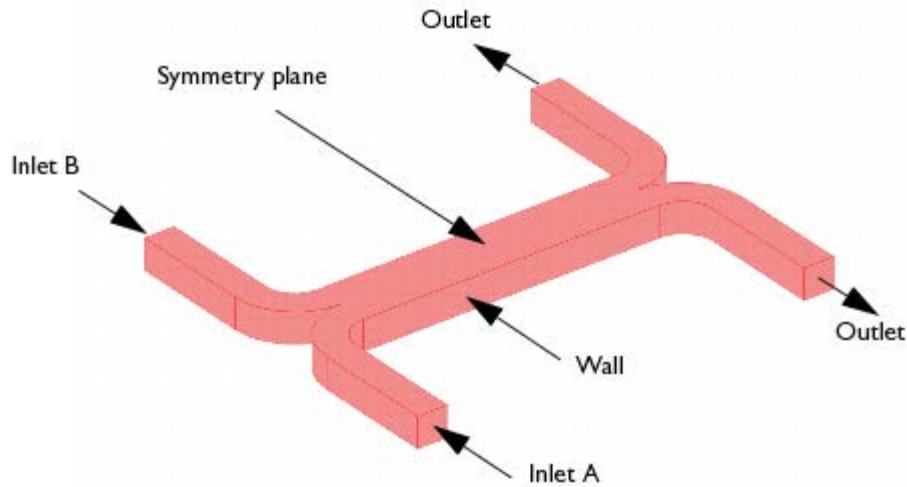

Figure 4-49: Model domain boundaries.

At the inlets and outlets, *Pressure* conditions apply along with vanishing viscous stress:

$$p = p_0$$
$$(4\text{-}16) \quad \mathbf{n} \cdot \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) = 0$$

Setting the pressure at the outlets to zero, the pressure at the inlets represents the pressure drop over the cell. These inlet and outlet conditions comply with the H-cell being a part of a channel system of constant width, which justifies the assumption of developed flow.

At the symmetry plane, choosing the boundary type *Symmetry boundary* sets the velocity component in the normal direction of the surface to zero:

$$\mathbf{n} \cdot \mathbf{u} = 0$$
$$(4\text{-}17) \quad \mathbf{t} \cdot \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\mathbf{n} = 0$$

At the walls, *No slip* conditions state that the velocity is zero:

$$(4\text{-}18) \quad (u, v, w) = (0, 0, 0) \quad \text{at the walls}$$

For the mass balances, the assumption that solute molecules interact only with water molecules implies that it is sufficient to consider a single species A of concentration c. At the inlets, use the *Concentration* boundary condition with the following values:

$$c = c_0 \quad \text{at inlet A}$$

$$(4\text{-}19)\; c = 0 \quad \text{at inlet B}$$

Model the symmetry plane and cell walls with the *Insulation/Symmetry* condition:

$$(4\text{-}20)\quad (-D\nabla c + c\mathbf{u}) \cdot \mathbf{n} = 0 \quad \text{at the symmetry plane and walls}$$

This equation states that the flux of species perpendicular to the boundary equals zero. At the outlets, the *Convective flux* condition applies, stating that the diffusive transport perpendicular to the boundary normal is negligible:

$$(4\text{-}21)\quad (-D\nabla c) \cdot \mathbf{n} = 0 \quad \text{at the outlets}$$

This condition eliminates concentration gradients in the flow direction.

Results

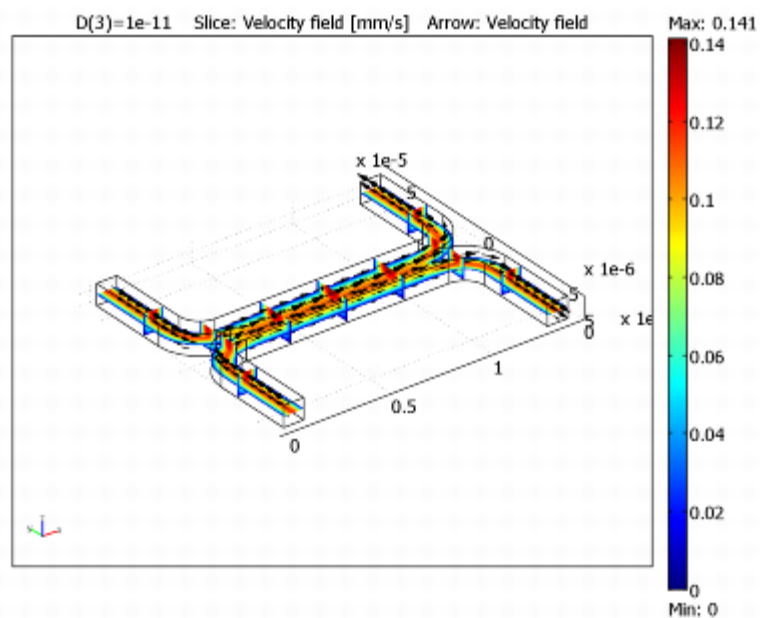Figure 4-44 shows the velocity field. The flow is symmetric and is not influenced by the concentration field.

Figure 4-50: Flow velocity field.

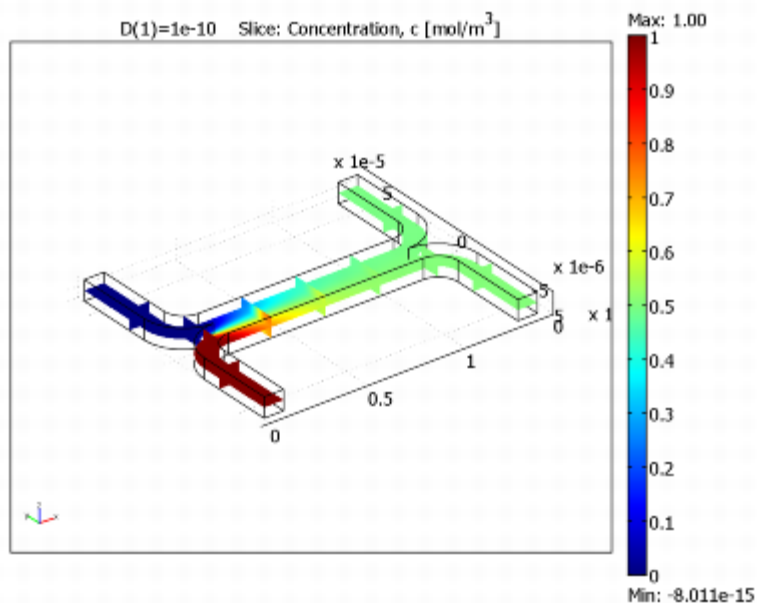Figure 4-45 shows the concentration distribution for the lightest species in this study.

Figure 4-51: Concentration distribution for a species with diffusivity $1 \cdot 10^{-10} m^2/s$.

Because of the relatively large diffusion coefficient, the degree of mixing is almost perfect for the lightest species. The species with a diffusion coefficient ten times smaller than that of the lightest species shows a different result.
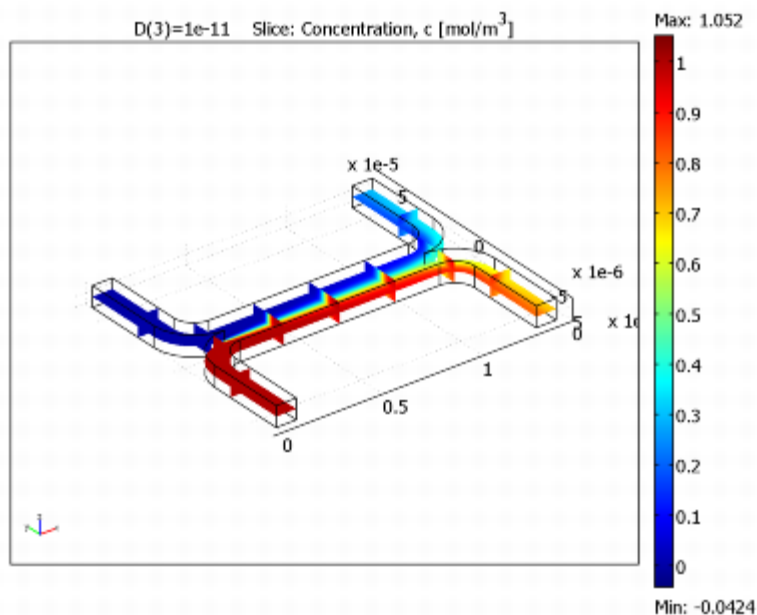

Figure 4-52: Concentration distribution for a species with diffusivity $1 \cdot 10^{-11} m^2/s$.

The concentration distribution in Figure 4-52 indicates that the diffusion coefficient for the species is low enough to avoid any significant mixing between streams A and B. The simulation clearly shows that the H-cell can separate lighter molecules from heavier ones. A cascade of H-cells can achieve a very high degree of separation.

In some cases, especially those involving solutions of macromolecules, the macromolecule concentration has a large influence on the liquid's viscosity. In such situations, the Navier-Stokes and the convection-diffusion become coupled, and they therefore must be solved simultaneously. Figure 4-53 shows the results of such a simulation, which you repeat in the second version of this model. You can see that changes in the concentration

influence the flow field. It is clear from this plot that the velocity becomes asymmetric due to changes in viscosity. As a consequence of the modified flow field, the transport of molecules to the outlet B is also different from the result using a constant flow field. You can see the difference by comparing Figure 4-54 with Figure 4-52 on page 361.
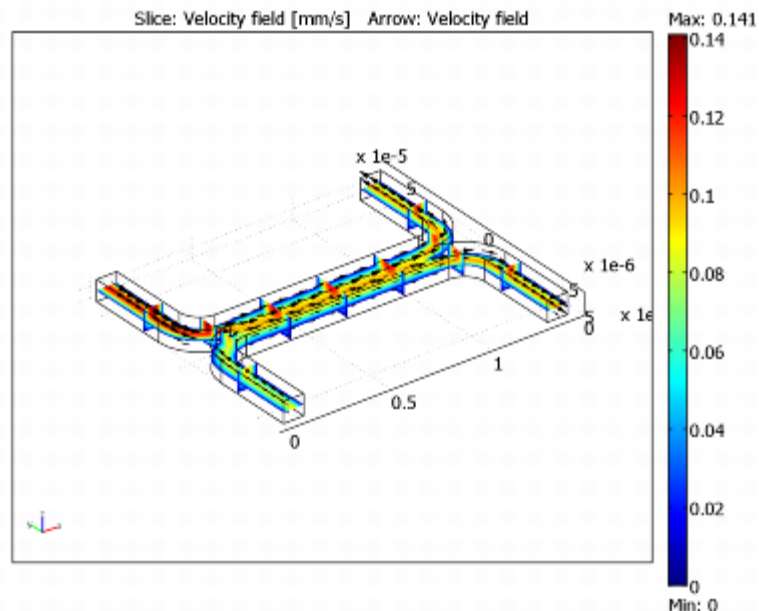
Figure 4-53: Velocity field. The viscosity varies with the concentration according to $\eta = \eta_0(1 + \alpha \ c^2)$ with $\alpha = 0.5 \ (m^3/mol)^2$. The figure shows that the velocity field is affected by variations in concentration. Compare it to the velocity field in Figure 4-44.

Figure 4-54: Concentration distribution for the species with diffusivity $1 \cdot 10^{-11} m^2/s$ for the case where the fluid viscosity varies with concentration. Comparison with the plot in Figure 4-52 shows that fewer molecules of the species are transported to outlet B.

Model Library path: `MEMS_Module/Microfluidics_Models/microchannel_h_cell`

Modeling Using the Graphical User Interface

1 Start COMSOL Multiphysics.

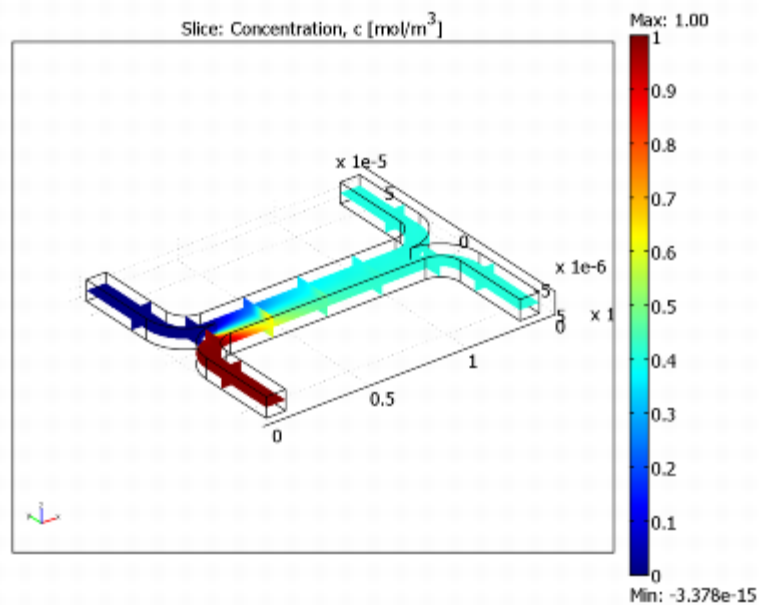**2** On the **New** page, set the **Space dimension** to **3D**.

3 From the list of application modes, select **MEMS Module>Microfluidics>Flow with Species Transport>Incompressible Navier-Stokes**.

4 Click the **Multiphysics** button, then click **Add**. As you can verify by inspection of the **Multiphysics** area on the right, this adds an Incompressible Navier-Stokes and a Convection and Diffusion application mode to the model. Later you will also see that a predefined coupling of the Navier-Stokes flow velocity has been included for the Convection and Diffusion application mode.

5 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, select **Constants**.

2 Enter the following variable names, expressions, and (optionally) descriptions in the **Constants** dialog box; when done, click **OK**.

NAME	EXPRESSION	DESCRIPTION
rho	1e3[kg/m^3]	Density
eta	1e-3[Pa*s]	Viscosity
D	1e-10[m^2/s]	Diffusion constant
p0	2[Pa]	Pressure drop
c0	1[mol/m^3]	Inlet concentration
alpha	0.5[(m^3/mol)^2]	Viscosity c^2-term prefactor

GEOMETRY MODELING

1 From the **Draw** menu, select **Work-Plane Settings**.

2 Use the default **Quick** work plane (the xy-plane at $z = 0$) by clicking **OK**.

3 From the **Options** menu, open the **Axes/Grid settings**.

4 On the **Axis** page, enter the following settings:

PROPERTY	VALUE
x min	-1
x max	15
y min	-7
y max	7

5 On the **Grid** page, clear the **Auto** check box and set both the **x spacing** and the **y spacing** to 1. Click **OK**.

6 Click the **Line** button on the Draw toolbar, then click the points with the x- and y-coordinates at (0, 6) and (0, 2).

7 Select the **2nd Degree Bezier Curve** tool on the Draw toolbar and click at the coordinate pairs (0, 0) and (2, 0).

Select the **Line** tool and click at the coordinates (12, 0).

8

9 Select the **2nd Degree Bezier Curve** tool and click at the coordinates (14, 0) and (14, 2).

10Select the **Line** tool and click at the coordinates (14, 6). Continue by clicking at the coordinates (13, 6) and (13, 2).

11Select the **2nd Degree Bezier Curve** tool and click at the coordinates (13, 1) and (12, 1).

12Select the **Line** tool and click at the coordinates (2, 1).

13Select the **2nd Degree Bezier Curve** tool and click at the coordinates (1, 1) and (1, 2).

14Select the **Line** tool and click at the coordinates (1, 6).

15Click the right mouse button to close the set of lines and create a solid object, CO1.

You have now created half of the 2D cross section and can use copy, paste, and rotate operations to create the other half.

1 Click first the **Copy** button and then the **Paste** button, both on the Main toolbar. Leave the **Displacement** components at 0 and click **OK** to create the composite object CO2.

2 Click the **Scale** button on the Draw toolbar. Change the **y** component of the **Scale factor** to −1 (leave the other parameters at their default values).

3 Click **OK** to flip CO2 over the x-axis.

4 From the **Edit** menu, choose **Select All**. (Alternatively, press Ctrl+A.)

5 Click the **Create Composite Object** button on the Draw toolbar.

6 Clear the **Keep interior boundaries** check box. Click **OK**.

The cross section is now finished and you can extrude it to the full 3D geometry.

7 Select **Extrude** from the **Draw** menu. Let the **Distance** remain equal to 1. Click **OK**.

The final geometry-modeling step is to scale the geometry to the correct scale.

8 Click the **Scale** button on the Draw toolbar.

9 Type 1e−5 in all three **Scale factor** edit fields. Click **OK**.

10Click the **Zoom Extents** button on the Main toolbar.

You do not need the 2D work plane any more, so you can remove it from the model:

1 From the **Multiphysics** menu, choose **Model Navigator**.

2 In the **Multiphysics** area to the right, select **Geom2 (2D)** and then click **Remove**.

3 Click **OK** to close the **Model Navigator**.

PHYSICS SETTINGS

Subdomain Settings

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Select Subdomain 1, then specify the settings in this table; when done, click **OK**.

PROPERTY	VALUE
ρ	rho
η	eta

4 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

5 From the **Physics** menu, select **Subdomain Settings**.

6 Select Subdomain 1.

7 In the **D (isotropic)** edit field, type D. Note that the velocity variables from the Incompressible Navier-Stokes application mode appear as predefined couplings.

8 Click **OK** to confirm the settings and close the dialog box.

Boundary Conditions

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 Specify boundary conditions as in the following table; when done, click **OK**.

SETTINGS	BOUNDARIES 2, 8	BOUNDARIES 20, 22	BOUNDARY 4	ALL OTHERS
Boundary type	Inlet	Outlet	Symmetry boundary	Wall
Boundary condition	Pressure, no viscous stress	Pressure, no viscous stress		No slip
p_0	p0	0	–	–

4 From the **Multiphysics** menu, select **2 Convection and Diffusion (chcd)**.

5 From the **Physics** menu, select **Boundary Settings**.

6 Specify the boundary conditions in the following table; when done, click **OK**.

SETTINGS	BOUNDARY 2	BOUNDARY 8	BOUNDARIES 20, 22	ALL OTHERS
Type	Concentration	Concentration	Convective flux	Insulation/Symmetry
c_0	c0	0	–	–

MESH GENERATION

1 From the **Mesh** menu, select **Free Mesh Parameters**.

2 From the **Predefined mesh sizes** list, select **Extra fine**.

3 Click the **Remesh** button.

4 When the mesher has finished, click **OK**.

COMPUTING THE SOLUTION

Start by first computing the solution for the velocity field and then use that solution for solving the mass transport problem.

1 Click the **Solver Parameters** button on the Main toolbar.

2 On the **General** page, select **Direct (PARDISO)** from the **Linear system solver** list.

3 Click **OK**.

4 Click the **Solver Manager** button on the Main toolbar.

5 On the **Solve For** page, select **Incompressible Navier-Stokes (mmglf)**.

6 On the **Initial Value** page, click the **Initial value expression** option button in the **Initial value** area.

7 Click **OK**.

8 Click the **Solve** button on the Main toolbar.

You have now computed the velocity field and can use that solution to make a parametric analysis for the mass transport problem with varying diffusivity.

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Convection and Diffusion (chcd)**.

3 Click the **Initial Value** tab, then click the **Current solution** option button in the **Initial value** area.

4 Click **OK**.

5 Click the **Solver Parameters** button on the Main toolbar.

6 From the **Solver** list, select **Parametric**.

7 In the **Parameter name** edit field, type D.

8 In the **Parameter values** edit field, type `1e-10 5e-11 1e-11`.

9 Click **OK**.

10 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To generate Figure 4-44 follow these steps:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

2 On the **General** page, select the **Slice** and **Arrow** check boxes in the **Plot type** area.

3 Clear the **Element refinement Auto** check box and type 5 in the associated edit field.

4 Click the **Slice** tab.

5 In the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

6 From the **Unit** list, select **mm/s**.

7 In the **Slice positioning** area, set **x levels** to 5, **y levels** to 2, and **z levels** to 1.

8 Click the **Arrow** tab.

9 On the **Subdomain Data** page, verify that **Velocity field** is selected in the **Predefined quantities** list.

10 In the **Arrow positioning** area, set the numbers of **x points**, **y points**, and **z points** to 14, 21, and 3, respectively.

11 In the **Arrow parameters** area, click the **Color** button. Select the black swatch from the palette in the **Arrow Color** dialog box, then click **OK**.

12 Select **3D arrow** from the **Arrow type** list.

13 Click **Apply** to generate the plot.

To generate Figure 4-45, continue with the following steps:

1 Clear the **Arrow plot** check box, then click the **Slice** tab.

2 From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

3 On the **General** page, select **1e-10** from the **Parameter value** list. Click **OK**.

Generate Figure 4-52 the same way as Figure 4-45, except use the parameter value **1e-11**.

PHYSICS SETTINGS—STUDY 2

1 From the **Multiphysics** menu, select **1 Incompressible Navier-Stokes (mmglf)**.

2 From the **Physics** menu, select **Subdomain Settings**.

3 Change the viscosity expression to eta*(1+alpha*c^2). Click **OK**.

COMPUTING THE SOLUTION—STUDY 2

When the viscosity is concentration dependent you must solve all equations simultaneously.

1 Click the **Solver Manager** button on the Main toolbar.

2 On the **Solve For** page, select **Geom1 (3D)** from the **Solve for variables** list. Click **OK**.

3 Click the **Solver Parameters** button on the Main toolbar.

4 From the **Solver** list, select **Stationary**. Click **OK**.

5 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION—STUDY 2

Finally, generate Figure 4-53 and Figure 4-54 with the following steps:

1 Click the **Plot Parameters** button on the Main toolbar.

2 On the **General** page, select the **Arrow** check box in the **Plot type** area.

3 Click the **Slice** tab.

4 In the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)> Velocity field**.

5 In the **Unit** list, select **mm/s**, then click **Apply** to generate <u>Figure 4-53</u>.

6 In the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**.

7 On the **General** page, clear the **Arrow** check box in the **Plot type** area.

8 Click **OK** to close the dialog box and generate <u>Figure 4-54</u>.