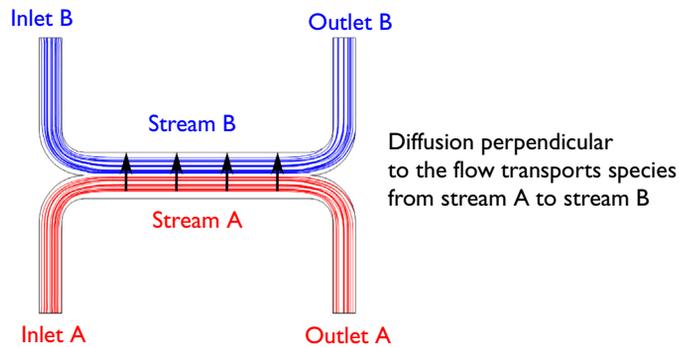


# Controlled Diffusion Micromixer<sup>1</sup>

## *Introduction*

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This model treats an H-shaped microfluidic device for controlled mixing through diffusion. The device 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. The device concept is illustrated in [Figure 1](#).



*Figure 1: Diagram of the device (dimensions in meters).*

## *Model Definition*

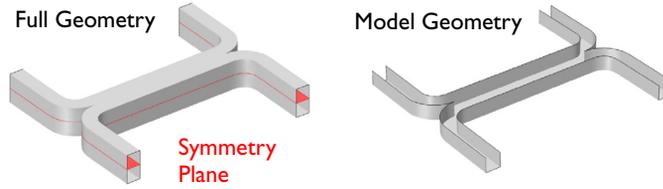
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The geometry of the device is shown in [Figure 2](#). The device geometry is split in two because of symmetry. The design aims to maintain a laminar flow field when the two streams, A and B, are united and thus prevent uncontrolled convective mixing. The

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1. 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.

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 2: 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, so the actual channel is twice as high in the z-direction.*

The flow rate at the inlet is approximately 0.1 mm/s. The Reynolds number, which is important for characterizing the flow is given by:

$$\text{Re} = \frac{\rho UL}{\mu} = 0,001$$

where  $\rho$  is the fluid density (1000 kg/m<sup>3</sup>),  $U$  is a characteristic velocity of the flow (0.1 mm/s),  $\mu$  is the fluid viscosity (1 mPa·s) and  $L$  is a characteristic dimension of the device (10 mm). When the Reynolds number is significantly less than 1, as in this example, the Creeping Flow interface can be used. The problematic convective term in the Navier-Stokes equations can be dropped, leaving the incompressible Stokes equations:

$$\begin{aligned} \nabla \cdot (-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) &= 0 \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

where  $\mathbf{u}$  is the local velocity (m/s) and  $p$  is the pressure (Pa).

Mixing in the device involves species at relatively low concentrations compared to the solvent, in this case water. This means that the solute molecules interact only with water molecules, and Fick's law can be used to describe the diffusive transport. The mass-balance equation for the solute is therefore:

$$-\nabla \cdot (-D\nabla c + c\mathbf{u}) = 0 \quad (1)$$

where  $D$  is the diffusion coefficient of the solute (m<sup>2</sup>/s) and  $c$  is its concentration (mol/m<sup>3</sup>). Diffusive flows can be characterized by another dimensionless number: the Peclet number, which is given by:

$$\text{Pe} = \frac{LU}{D}$$

In this model, the parametric solver is used to solve Equation 1 for three different species, each with different values of  $D$ :  $1 \times 10^{-11} \text{ m}^2/\text{s}$ ,  $5 \times 10^{-11} \text{ m}^2/\text{s}$ , and  $1 \times 10^{-10} \text{ m}^2/\text{s}$ . These values of  $D$  correspond to Peclet numbers of 100, 20 and 10 respectively. Since these Peclet numbers are all greater than 1, implying a cell Peclet number significantly greater than 1, numerical stabilization will be required when solving Fick's equation. COMSOL automatically includes the stabilization by default, so no explicit settings will be required.

Two versions of the model are solved:

- In the first version, it is assumed 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, the viscosity depends quadratically on the concentration:

$$\mu = \mu_0(1 + \alpha c^2)$$

Here  $\alpha$  is a constant of dimension  $\text{m}^6/(\text{mol})^2$  and  $\mu_0$  is the viscosity at zero concentration. Such a relationship between concentration and viscosity is usually observed in solutions of larger molecules.

### *Results and Discussion*

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[Figure 3](#) shows the velocity field for the case where viscosity is concentration independent. The flow is symmetric and is not influenced by the concentration field. [Figure 4](#) shows the corresponding pressure distribution on the channel walls that

results from the flow.

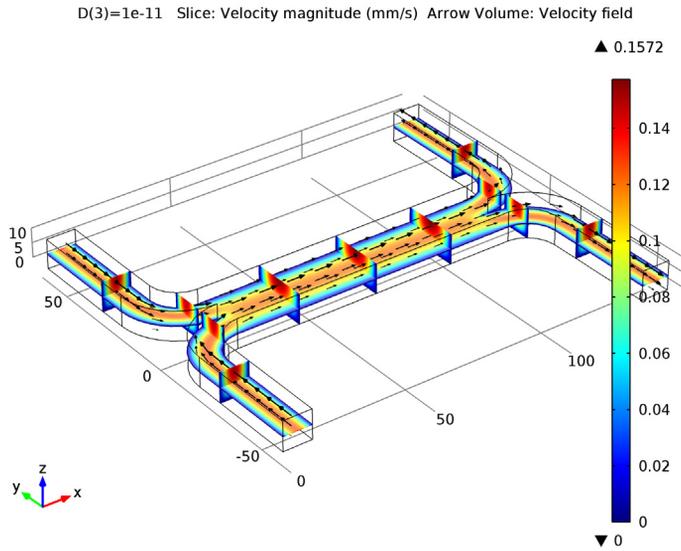


Figure 3: Flow velocity field.

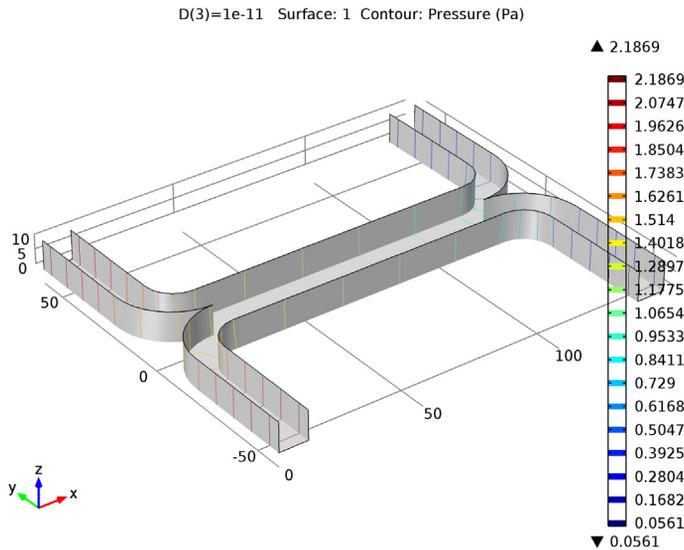


Figure 4: Pressure distribution on the channel walls.

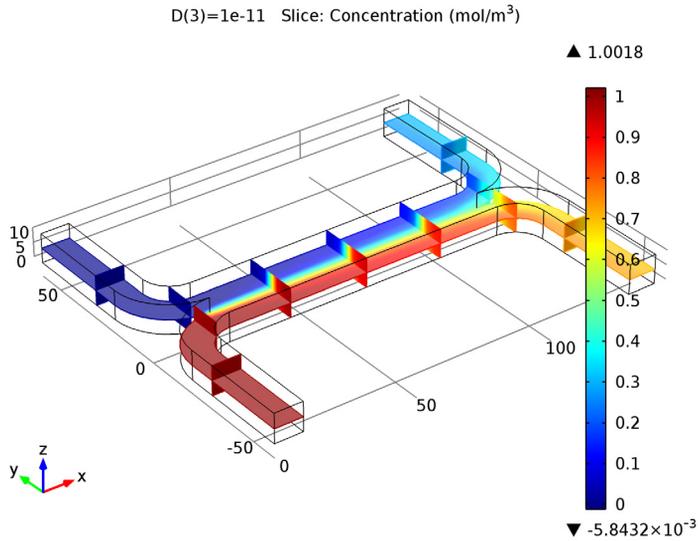


Figure 5: Concentration distribution for a species with diffusivity  $1 \cdot 10^{-11} \text{ m}^2/\text{s}$ .

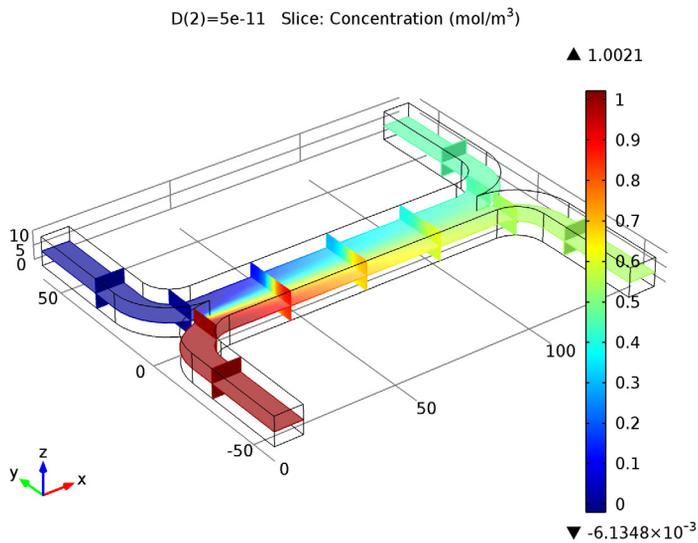


Figure 6: Concentration distribution for a species with diffusivity  $5 \cdot 10^{-11} \text{ m}^2/\text{s}$ .

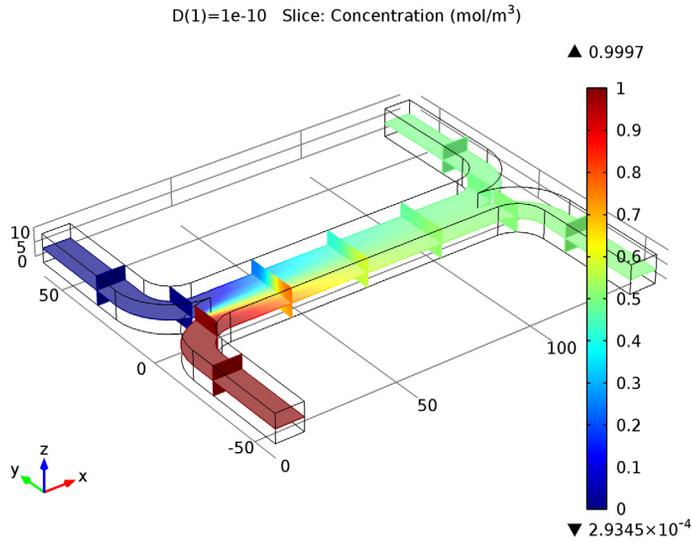


Figure 7: Concentration distribution for a species with diffusivity  $1 \cdot 10^{-10} \text{ m}^2/\text{s}$ .

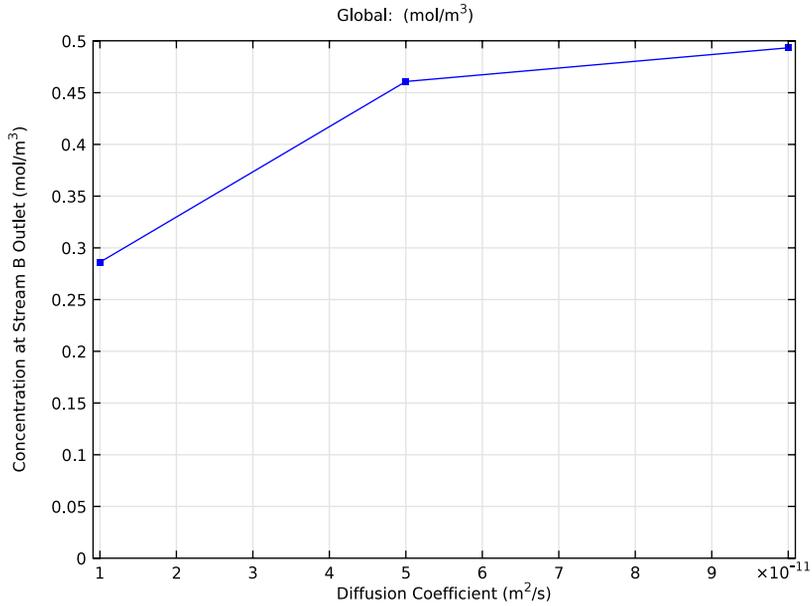
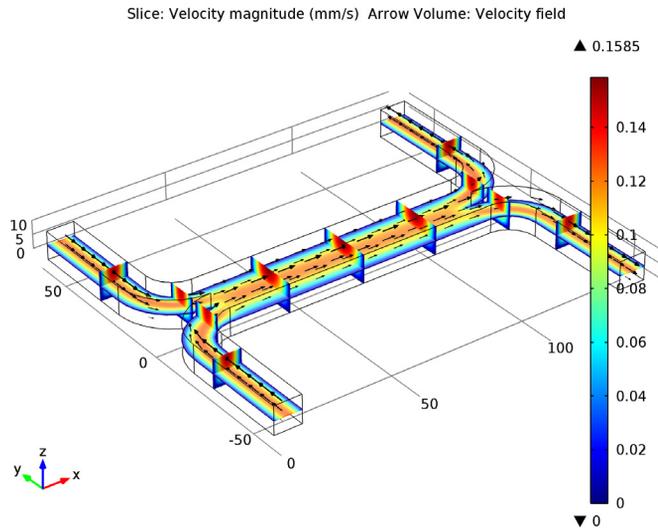


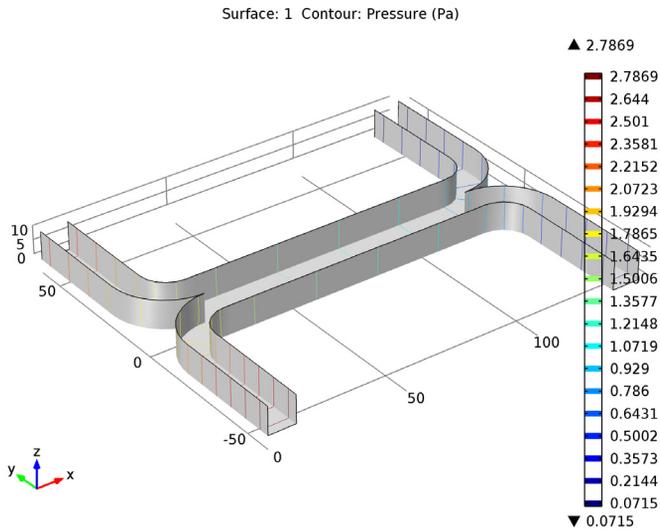
Figure 8: Average concentration at the outlet of stream B as a function of the diffusion coefficient.

Figure 5, Figure 6 and Figure 7 show the species concentration for the each of the three diffusion coefficients. For the heaviest species, which has the smallest diffusivity, there is almost no significant mixing between streams A and B (Figure 5). For the lightest species, which has the largest diffusion coefficient, the mixing is almost perfect (Figure 7). Figure 8 shows how the mean concentration of the species at the outlet of stream B varies for the different species diffusion coefficients. The simulation clearly shows that the device could be used to separate lighter molecules from heavier ones. By placing a number of these devices in series, a high degree of separation could be obtained.

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 equations become coupled, and so they must be solved simultaneously. Figure 9, Figure 10, and Figure 11 show the results of such a simulation, in which the Navier Stokes equations are solved with a concentration dependent viscosity. In this case the species with for the species with diffusivity  $5 \cdot 10^{-11} \text{ m}^2/\text{s}$ . The velocity field is altered slightly by the concentration dependent viscosity (see Figure 12) but this has little effect on the mean stream A outlet concentration, which changes only slightly from 0.450 to 0.451. Much more serious is the effect of the non-uniform viscosity on the pressure distribution required to maintain the two streams at the same flow rate. A larger pressure is required at the inlet of stream B to drive the higher viscosity fluid through the system. This asymmetry in the pressure distribution makes placing several devices in series much more difficult.



*Figure 9: Velocity field. The viscosity varies with the concentration according to  $\mu = \mu_0(1 + \alpha c^2)$  with  $\alpha = 0.5 \text{ (m}^3/\text{mol)}^{-2}$ . It is difficult to see the differences between this figure and that in Figure 3, but careful inspection reveals a slight change in the velocity profile. This is highlighted further in Figure 12.*



*Figure 10: Pressure distribution. The viscosity varies with the concentration according to  $\mu = \mu_0(1 + \alpha c^2)$  with  $\alpha = 0.5 \text{ (m}^3/\text{mol)}^{-2}$ . This figure should be compared to Figure 4. There are significant differences between the two cases.*

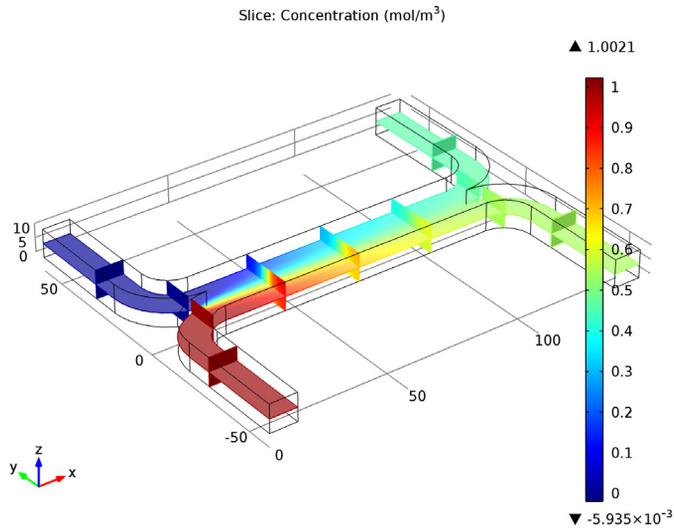


Figure 11: Concentration distribution for the species with diffusivity  $5 \cdot 10^{-11} \text{ m}^2/\text{s}$  for the case where the fluid viscosity varies with concentration. This plot is very similar to the corresponding plot for an uncoupled flow, shown in Figure 6.

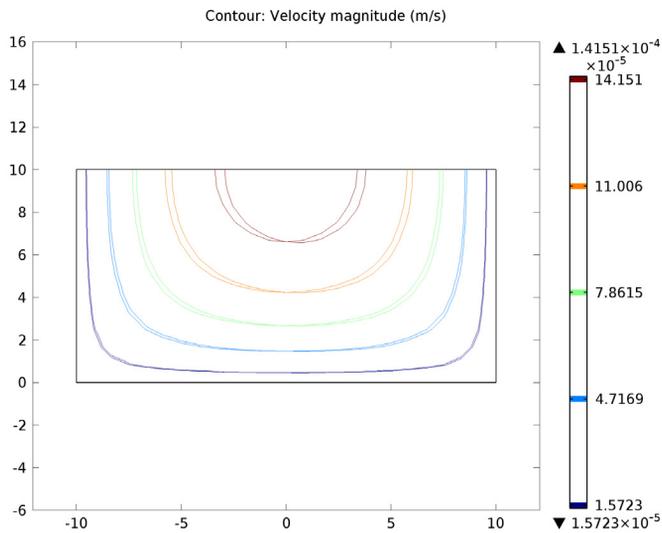


Figure 12: Comparison of the velocity field for the uncoupled and coupled flow simulations showing the difference between the two cases. The coupled flow, in which the fluid viscosity is a function of concentration, is asymmetric.

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**Model Library path:** Microfluidics\_Module/Micromixers/  
controlled\_diffusion\_micromixer

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### *Modeling Instructions*

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#### **NEW**

**1** In the **New** window, click the **Model Wizard** button.

#### **MODEL WIZARD**

- 1** In the **Model Wizard** window, click the **3D** button.
- 2** In the **Select physics** tree, select **Fluid Flow>Single-Phase Flow>Creeping Flow (spf)**.
- 3** Click the **Add** button.
- 4** In the **Select physics** tree, select **Chemical Species Transport>Transport of Diluted Species (chds)**.
- 5** Click the **Add** button.
- 6** Click the **Study** button.
- 7** In the tree, select **Preset Studies for Selected Physics>Stationary**.
- 8** Click the **Done** button.

#### **GEOMETRY I**

For many microfluidic devices it is convenient to specify the geometry dimensions using micrometers.

- 1** In the **Model Builder** window, under **Component I** click **Geometry I**.
- 2** In the **Geometry** settings window, locate the **Units** section.
- 3** From the **Length unit** list, choose **µm**.

The geometry can be constructed by extruding a 2 dimensional workplane. First draw a top down view of the structure in the workplane.

- 4** On the **Geometry** toolbar, click **Work Plane**.

#### *Rectangle I*

- 1** In the **Model Builder** window, under **Component I >Geometry I>Work Plane I** right-click **Plane Geometry** and choose **Rectangle**.
- 2** In the **Rectangle** settings window, locate the **Size** section.

- 3 In the **Width** edit field, type 140.
- 4 In the **Height** edit field, type 60.
- 5 Click the **Build Selected** button.

#### *Rectangle 2*

- 1 Right-click **Plane Geometry** and choose **Rectangle**.
- 2 In the **Rectangle** settings window, locate the **Size** section.
- 3 In the **Width** edit field, type 120.
- 4 In the **Height** edit field, type 50.
- 5 Locate the **Position** section. In the **xw** edit field, type 10.
- 6 In the **yw** edit field, type 10.
- 7 Click the **Build Selected** button.

#### *Difference 1*

- 1 On the **Work plane** toolbar, click **Difference**.
- 2 Select the object **r1** only.
- 3 In the **Difference** settings window, locate the **Difference** section.
- 4 Select the **Objects to subtract** toggle button.
- 5 Select the object **r2** only.
- 6 Click the **Build Selected** button.

#### *Fillet 1*

- 1 On the **Work plane** toolbar, click **Fillet**.
- 2 On the object **dif1**, select Points 3 and 5 only.
- 3 In the **Fillet** settings window, locate the **Radius** section.
- 4 In the **Radius** edit field, type 10.
- 5 Click the **Build Selected** button.

#### *Fillet 2*

- 1 On the **Work plane** toolbar, click **Fillet**.
- 2 On the object **fil1**, select Points 1 and 9 only.
- 3 In the **Fillet** settings window, locate the **Radius** section.
- 4 In the **Radius** edit field, type 20.
- 5 Click the **Build Selected** button.

*Mirror 1*

- 1 On the **Work plane** toolbar, click **Mirror**.
- 2 Select the object **fil2** only.
- 3 In the **Mirror** settings window, locate the **Input** section.
- 4 Select the **Keep input objects** check box.
- 5 Locate the **Normal Vector to Line of Reflection** section. In the **xw** edit field, type 0.
- 6 In the **yw** edit field, type 1.
- 7 Click the **Build Selected** button.

*Union 1*

- 1 On the **Work plane** toolbar, click **Union**.
- 2 Select the objects **mir1** and **fil2** only.
- 3 In the **Union** settings window, locate the **Union** section.
- 4 Clear the **Keep interior boundaries** check box.
- 5 Click the **Build Selected** button.  
Extrude the 2D geometry to create a 3 dimensional geometry.

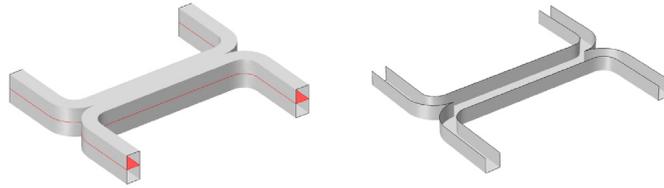
*Extrude 1*

- 1 On the **Geometry** toolbar, click **Extrude**.
- 2 In the **Extrude** settings window, locate the **Distances from Plane** section.
- 3 In the table, enter the following settings:

<b>Distances (<math>\mu\text{m}</math>)</b>
10

- 4 Click the **Build Selected** button.

- Click the **Zoom Extents** button on the Graphics toolbar.



Create parameters to define the model.

## GLOBAL DEFINITIONS

### Parameters

- On the **Home** toolbar, click **Parameters**.
- In the **Parameters** settings window, locate the **Parameters** section.
- In the table, enter the following settings:

Name	Expression	Value	Description
D	$5e-11$ [m <sup>2</sup> /s]	5.000E-11 m <sup>2</sup> /s	Diffusion constant
fr	15 [pl/s]	1.500E-14 m <sup>3</sup> /s	Inlet flow rate
c0	1 [mol/m <sup>3</sup> ]	1.000 mol/m <sup>3</sup>	Inlet concentration
alpha	$0.5$ [(m <sup>3</sup> /mol) <sup>2</sup> ]	0.5000 m <sup>6</sup> /mol <sup>2</sup>	Viscosity c <sup>2</sup> -term prefactor

Create an average operator to compute the mean output concentration.

## DEFINITIONS

### Average 1

- On the **Definitions** toolbar, click **Component Couplings** and choose **Average**.
- In the **Average** settings window, locate the **Source Selection** section.
- From the **Geometric entity level** list, choose **Boundary**.
- Select Boundary 22 only.

Note that there are several methods to select a geometric entity. To select, for example, a boundary, place the cursor over the boundary in the graphics window. If

the required boundary is not highlighted in red then rotate the scroll wheel until it is highlighted, then left-click to select it (the up and down arrow keys can also be used instead of the scroll wheel). Alternatively, use the **Selection list** to display a list of the available boundary numbers (available from the Home>More Windows menu if you are using windows, or from the Windows menu on other platforms).

Boundaries are added to the selection by first left clicking on the boundary and then right-clicking and selecting Add to selection. To add several boundaries, hold the Ctrl key down when left clicking.

For more information about selecting geometric entities in the **Graphics** window, see the COMSOL Multiphysics User's Guide.

Add material properties to the model.

## MATERIALS

### *Material 1*

- 1 In the **Model Builder** window, under **Component 1** right-click **Materials** and choose **New Material**.
- 2 In the **Material** settings window, locate the **Material Contents** section.
- 3 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Density	rho	1000	kg/m <sup>3</sup>	Basic
Dynamic viscosity	mu	1e-3	Pa·s	Basic

## CREEPING FLOW

Because you are dealing with a liquid flow, you can set the flow type to incompressible.

- 1 In the **Model Builder** window, under **Component 1** click **Creeping Flow**.
- 2 In the **Creeping Flow** settings window, locate the **Physical Model** section.
- 3 From the **Compressibility** list, choose **Incompressible flow**.

Note that several default nodes have been added automatically to the model tree. The 'D' in the upper left corner of the node icon indicates that a node has been added by default.

Add a laminar flow inlet boundary condition.

### *Inlet 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Inlet**.
- 2 Select Boundary 2 only.

- 3 In the **Inlet** settings window, locate the **Boundary Condition** section.
- 4 From the **Boundary condition** list, choose **Laminar inflow**.
- 5 Locate the **Laminar Inflow** section. Click the **Flow rate** button.
- 6 In the  $V_0$  edit field, type  $fr/2$ .  
Set the flow rate to one half of the parameter value, since only half of the geometry is modeled.
- 7 In the  $L_{\text{entr}}$  edit field, type  $100[\text{um}]$ .  
The entrance length should be set to a value large enough for a laminar flow to develop.

#### *Inlet 2*

- 1 Right-click **Component 1 >Creeping Flow >Inlet 1** and choose **Duplicate**.
- 2 In the **Inlet** settings window, locate the **Boundary Selection** section.
- 3 Click **Clear Selection**.
- 4 Select Boundary 8 only.  
Add an outlet with a pressure boundary condition.

#### *Outlet 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Outlet**.
- 2 Select Boundaries 20 and 22 only.  
The default pressure of 0 Pa is appropriate in this case.  
Add a symmetry boundary condition in the symmetry plane.

#### *Symmetry 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.
- 2 Select Boundary 4 only.  
Now set up the mass transport physics.

### **TRANSPORT OF DILUTED SPECIES**

#### *Convection and Diffusion 1*

Use the computed velocity field for the species convection.

- 1 In the **Model Builder** window, expand the **Component 1 >Transport of Diluted Species** node, then click **Convection and Diffusion 1**.
- 2 In the **Convection and Diffusion** settings window, locate the **Model Inputs** section.

- 3 From the **u** list, choose **Velocity field (spf/fp I)**.

The diffusion coefficient is set to use the parameter previously defined.

- 4 Locate the **Diffusion** section. In the  $D_c$  edit field, type D.

Specify the concentration at the two inlets.

#### *Concentration 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Concentration**.
- 2 Select Boundary 2 only.
- 3 In the **Concentration** settings window, locate the **Concentration** section.
- 4 Select the **Species c** check box.
- 5 In the  $c_{0,c}$  edit field, type  $c_0$ .

#### *Concentration 2*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Concentration**.
- 2 Select Boundary 8 only.
- 3 In the **Concentration** settings window, locate the **Concentration** section.
- 4 Select the **Species c** check box.

In this case the concentration should take the default value of 0.

Use the outflow condition to allow species to leave the domain by convection.

#### *Outflow 1*

- 1 On the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
- 2 In the **Outflow** settings window, locate the **Boundary Selection** section.
- 3 Click **Paste Selection**.
- 4 Go to the **Paste Selection** dialog box.
- 5 In the **Selection** edit field, type 20 22.
- 6 Click the **OK** button.

Set up the mesh. Microfluidic devices are frequently extruded 2D geometries. It is therefore frequently convenient to extrude a 2D mesh. First mesh the top face of the device with a 2D quad mesh.

## **MESH 1**

#### *Free Quad 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **More Operations>Free Quad**.

- 2 Select Boundary 4 only.

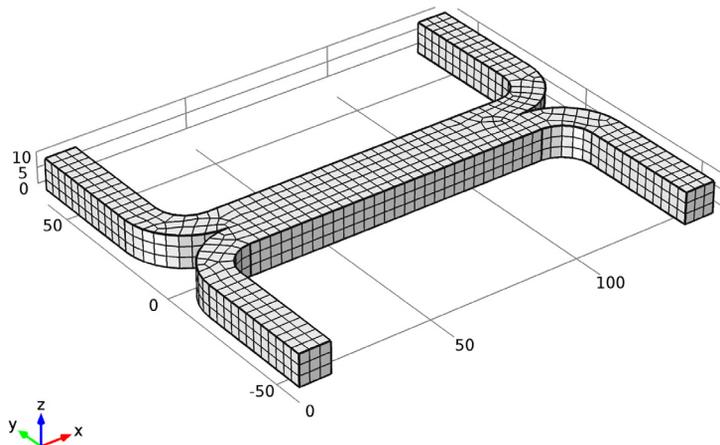
*Size*

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.
- 2 In the **Size** settings window, locate the **Element Size** section.
- 3 From the **Calibrate for** list, choose **Fluid dynamics**.
- 4 From the **Predefined** list, choose **Coarse**.

Next, sweep the mesh through the domain.

*Swept 1*

- 1 In the **Model Builder** window, right-click **Mesh 1** and choose **Swept**.
- 2 Right-click **Swept 1** and choose **Build All**.



Now set up a study to solve the problem. Initially it is assumed that the fluid flow and diffusion problems are uncoupled. In this case it makes sense to solve the fluid flow problem first and then to use the velocity field as an input for the diffusion problem. This will save time and memory, particularly since the diffusion problem is solved for three parameters.

**STUDY 1**

Since the study will automatically generate a large number of default plots, default plots are disabled.

- 1 In the **Model Builder** window, click **Study 1**.
  - 2 In the **Study** settings window, locate the **Study Settings** section.
  - 3 Clear the **Generate default plots** check box.
- For step 1, solve only the creeping flow problem.

*Step 1: Stationary*

- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.
- 2 In the **Stationary** settings window, locate the **Physics and Variables Selection** section.
- 3 In the table, enter the following settings:

Physics	Solve for	Discretization
Transport of Diluted Species	×	Physics settings

Add a second study step.

*Step 2: Stationary 2*

- 1 On the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.  
Disable the solution of the creeping flow problem for this step, but import the previously computed solution into the relevant dependent variables so that they can be used to compute the convective species transport.
- 2 In the **Stationary** settings window, locate the **Physics and Variables Selection** section.
- 3 In the table, enter the following settings:

Physics	Solve for	Discretization
Creeping Flow	×	Physics settings

- 4 Click to expand the **Values of dependent variables** section. Locate the **Values of Dependent Variables** section. Select the **Values of variables not solved for** check box.
- 5 From the **Method** list, choose **Solution**.
- 6 From the **Study** list, choose **Study 1, Stationary**.  
Solve the diffusion problem for three values of the diffusion coefficient.
- 7 Click to expand the **Study extensions** section. Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.
- 8 Click **Add**.

9 In the table, enter the following settings:

Auxiliary parameter	Parameter value list
D (Diffusion constant)	1e-10 5e-11 1e-11

10 On the **Home** toolbar, click **Compute**.

Create a surface data set to view the pressure on the channel walls.

## RESULTS

### Data Sets

1 On the **Results** toolbar, click **More Data Sets** and choose **Surface**.

2 Select Boundaries 1, 3, 5–7, 9–19, 21, 23, and 24 only.

First plot the velocity of the flow within the channel.

### 3D Plot Group 1

1 On the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

Use a slice plot to view the data on one or more slices through the geometry.

2 In the **Model Builder** window, under **Results** right-click **3D Plot Group 1** and choose **Slice**.

3 In the **Slice** settings window, locate the **Expression** section.

4 From the **Unit** list, choose **mm/s**.

Add additional slices in different directions.

5 In the **Model Builder** window, right-click **3D Plot Group 1** and choose **Slice**.

6 In the **Slice** settings window, locate the **Expression** section.

7 From the **Unit** list, choose **mm/s**.

8 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

9 In the **Planes** edit field, type 1.

The extra slices should use the same scale and colors for the velocity plot as the existing slice.

10 Click to expand the **Inherit style** section. Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

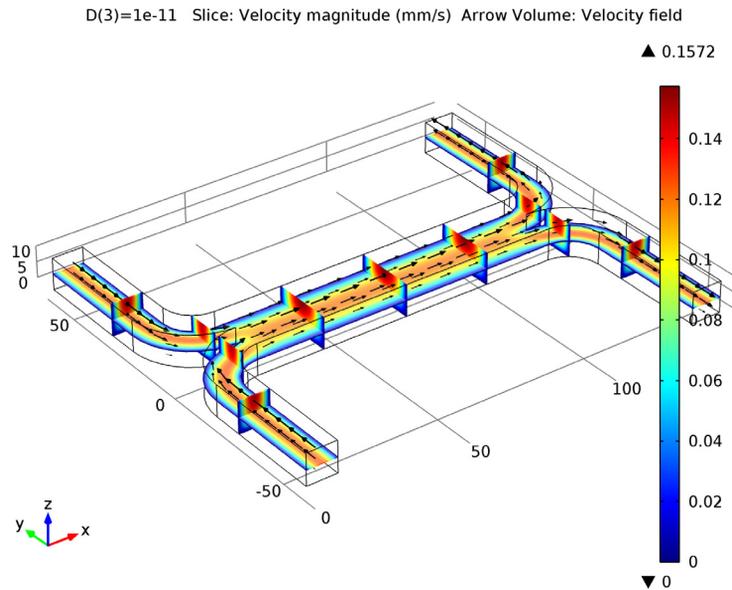
To avoid duplicate titles, turn off the title for additional slices.

11 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Add slices in a third plane.

- 12** Right-click **Results>3D Plot Group 1>Slice 2** and choose **Duplicate**.
- 13** In the **Slice** settings window, locate the **Plane Data** section.
- 14** From the **Plane** list, choose **zx-planes**.
- 15** In the **Planes** edit field, type 2.  
Use the arrow volume plot to visualize the flow direction.
- 16** In the **Model Builder** window, right-click **3D Plot Group 1** and choose **Arrow Volume**.
- 17** In the **Arrow Volume** settings window, locate the **Arrow Positioning** section.
- 18** In the **x Grid Points** edit field, type 14.
- 19** In the **y Grid Points** edit field, type 21.
- 20** In the **z Grid Points** edit field, type 3.
- 21** Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.  
Rename the plot.
- 22** Right-click **3D Plot Group 1** and choose **Rename**.
- 23** Go to the **Rename 3D Plot Group** dialog box and type **Velocity (uncoupled flow)** in the **New name** edit field.
- 24** Click **OK**.

5 On the **3D Plot Group** toolbar, click **Plot**.



Next add a pressure plot, using the data set created previously.

### 3D Plot Group 2

1 On the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **3D Plot Group** settings window, locate the **Data** section.

3 From the **Data set** list, choose **Surface 1**.

First add a uniformly colored surface, to highlight the channel walls.

4 Right-click **Results>3D Plot Group 2** and choose **Surface**.

5 In the **Surface** settings window, locate the **Expression** section.

6 In the **Expression** edit field, type 1.

7 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

8 From the **Color** list, choose **Gray**.

Next use contours to visualize the pressure.

9 In the **Model Builder** window, right-click **3D Plot Group 2** and choose **Contour**.

10 In the **Contour** settings window, locate the **Expression** section.

**11** Select **Creeping Flow>Pressure (p)** in the **Replace expression** menu, which is accessed in the upper-right corner of the section.

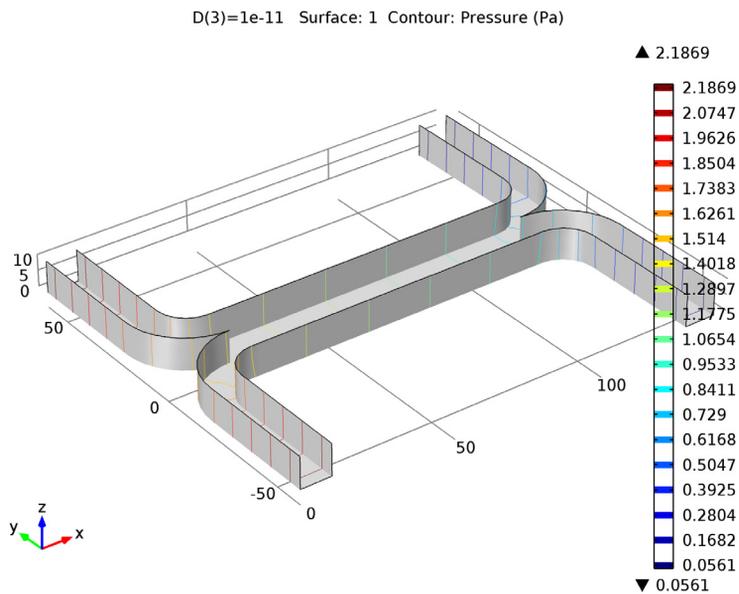
Finally rename the plot.

**12** Right-click **3D Plot Group 2** and choose **Rename**.

**13** Go to the **Rename 3D Plot Group** dialog box and type **Pressure (uncoupled flow)** in the **New name** edit field.

**14** Click **OK**.

**15** On the **3D Plot Group** toolbar, click **Plot**.



Next create a slice plot to visualize the concentration in the device. Use the existing velocity slice plot as a basis for this plot.

*Velocity (uncoupled flow) 1*

**1** In the **Model Builder** window, under **Results** right-click **Velocity (uncoupled flow)** and choose **Duplicate**.

Re-name the plot.

**2** In the **Model Builder** window, under **Results** right-click **Velocity (uncoupled flow) 1** and choose **Rename**.

**3** Go to the **Rename 3D Plot Group** dialog box and type **Concentration (uncoupled flow)** in the **New name** edit field.

**4** Click **OK**.

For each of the slice sub-nodes, change the plotted quantity to concentration.

*Concentration (uncoupled flow)*

**1** In the **Model Builder** window, expand the **Results>Concentration (uncoupled flow)** node, then click **Slice 1**.

**2** In the **Slice** settings window, locate the **Expression** section.

**3** Select **Transport of Diluted Species>Species c>Concentration (c)** in the **Replace expression** menu, which is accessed in the upper-right corner of the section.

**4** In the **Model Builder** window, under **Results>Concentration (uncoupled flow)** click **Slice 2**.

**5** In the **Slice** settings window, locate the **Expression** section.

**6** Select **Transport of Diluted Species>Species c>Concentration (c)** in the **Replace expression** menu.

**7** In the **Model Builder** window, under **Results>Concentration (uncoupled flow)** click **Slice 3**.

**8** In the **Slice** settings window, locate the **Expression** section.

**9** Select **Transport of Diluted Species>Species c>Concentration (c)** in the **Replace expression** menu.

Disable the arrow volume plot.

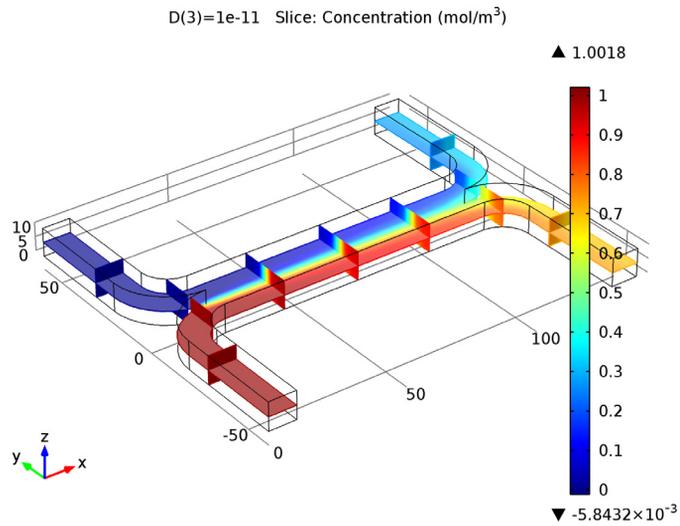
**10** In the **Model Builder** window, under **Results>Concentration (uncoupled flow)** right-click **Arrow Volume 1** and choose **Disable**.

**11** On the **3D Plot Group** toolbar, click **Plot**.

Look at the plot for each of the three diffusion coefficient levels.

The plots on the next page show the results for each of the diffusion coefficients solved for. For the heaviest species, which has the smallest diffusivity, there is limited mixing between streams A and B. For the lightest species, which has the largest diffusion coefficient, the mixing is almost perfect.

**12** On the **3D Plot Group** toolbar, click **Plot**.

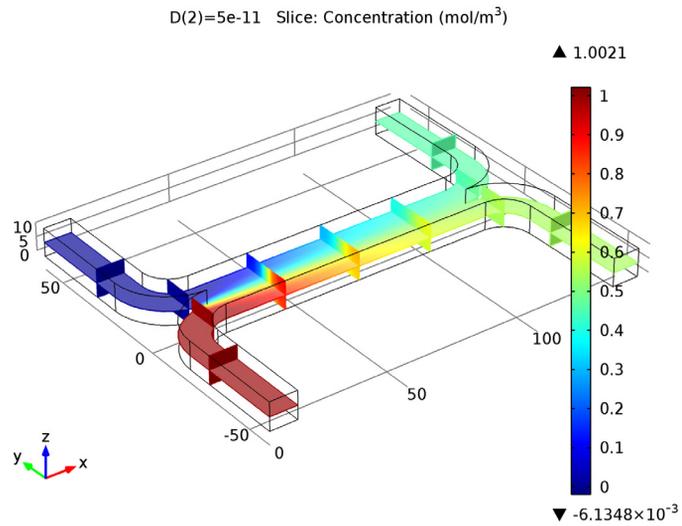


**13** In the **Model Builder** window, click **Concentration (uncoupled flow)**.

**14** In the **3D Plot Group** settings window, locate the **Data** section.

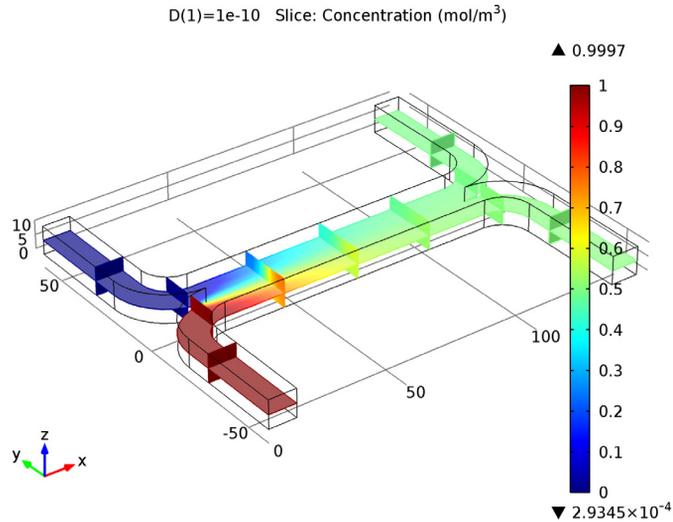
**15** From the **Parameter value (D)** list, choose **5e-11**.

16 On the **3D Plot Group** toolbar, click **Plot**.



17 From the **Parameter value (D)** list, choose **1e-10**.

**18** On the **3D Plot Group** toolbar, click **Plot**.



Add a global plot to show how the concentration at the output differs with diffusion coefficient.

#### *ID Plot Group 4*

**1** On the **Home** toolbar, click **Add Plot Group** and choose **ID Plot Group**.

**2** On the **ID Plot Group** toolbar, click **Global**.

Use the previously defined average operator to compute the average concentration at the device output.

**3** In the **Global** settings window, locate the **y-Axis Data** section.

**4** In the table, enter the following settings:

Expression	Unit	Description
aveop1(c)	mol/m <sup>3</sup>	

No legend is necessary for this plot, as only one quantity is plotted.

**5** Click to expand the **Legends** section. Clear the **Show legends** check box.

Add a marker in the computed datapoints.

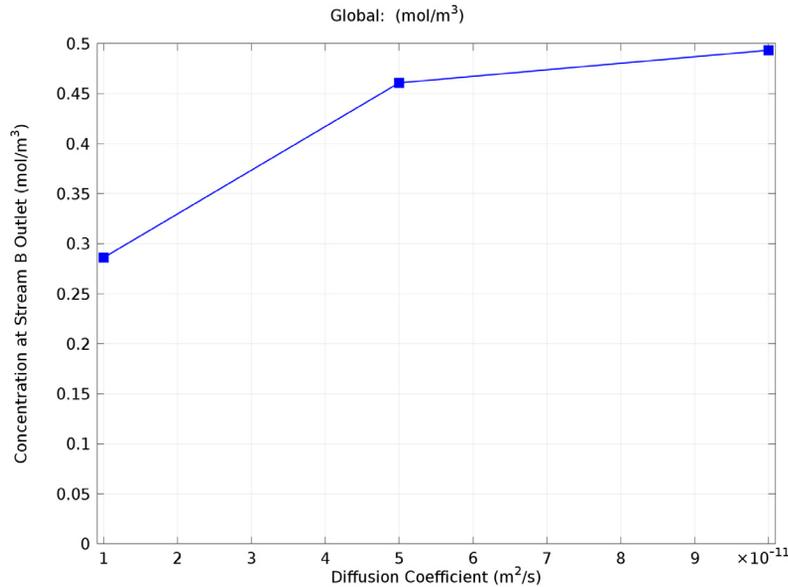
**6** Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Point**.

- 7 From the **Positioning** list, choose **In data points**.  
Change the axes titles. Note that html tags and a range of mathematical symbols and greek letters can be entered in the axes and plot titles.
- 8 In the **Model Builder** window, click **ID Plot Group 4**.
- 9 In the **ID Plot Group** settings window, locate the **Plot Settings** section.
- 10 Select the **x-axis label** check box.
- 11 In the associated edit field, type Diffusion Coefficient ( $m^{2}/s$ ).
- 12 Select the **y-axis label** check box.
- 13 In the associated edit field, type Concentration at Stream B Outlet ( $mol/m^{3}$ ).  
Change the axis limits for the plot.
- 14 Click to expand the **Axis** section. Select the **Manual axis limits** check box.
- 15 In the **y minimum** edit field, type 0.
- 16 In the **y maximum** edit field, type 0.5.  
Finally re-name the plot.
- 17 Right-click **ID Plot Group 4** and choose **Rename**.
- 18 Go to the **Rename ID Plot Group** dialog box and type Output Concentration (uncoupled flow) in the **New name** edit field.
- 19 Click **OK**.
- 20 On the **ID Plot Group** toolbar, click **Plot**.

This plot shows that the concentration of the species at the output is strongly dependent on the diffusion coefficient of the molecule. Thus the device could be used to separate species with different diffusion coefficients, particularly if multiple stages of the device were arranged in series.

In some cases, particularly if the solution consists of large macromolecules, the dissolved species has a large influence on the liquid's viscosity. In such situations, the

Navier-Stokes and the convection-diffusion equations become coupled, and so they must be solved simultaneously.



Now set up the fully coupled problem. To make the viscosity a function of the species concentration simply type an expression into the viscosity setting of the fluid properties node.

## CREEPING FLOW

### *Fluid Properties I*

- 1** In the **Model Builder** window, under **Component I >Creeping Flow** click **Fluid Properties I**.
- 2** In the **Fluid Properties** settings window, locate the **Fluid Properties** section.
- 3** From the  $\mu$  list, choose **User defined**. In the associated edit field, type  $1e-3[\text{Pa}\cdot\text{s}]\cdot(1+\alpha\cdot c^2)$ .

Add a study to solve the fully coupled problem. In this instance only a single diffusion coefficient will be solved for, so no parametric sweep will be required. The model will default to the parameter entered on the parameters node for the diffusion constant:  $5e-11 \text{ m}^2/\text{s}$

## ROOT

On the **Home** toolbar, click **Add Study**.

## ADD STUDY

- 1 Go to the **Add Study** window.
- 2 Find the **Studies** subsection. In the tree, select **Preset Studies>Stationary**.
- 3 In the **Add study** window, click **Add Study**.

## STUDY 2

Turn off the default plot groups again.

- 1 In the **Model Builder** window, click **Study 2**.
- 2 In the **Study** settings window, locate the **Study Settings** section.
- 3 Clear the **Generate default plots** check box.
- 4 On the **Home** toolbar, click **Compute**.  
Add another surface data set that points to the new solution.

## RESULTS

### *Data Sets*

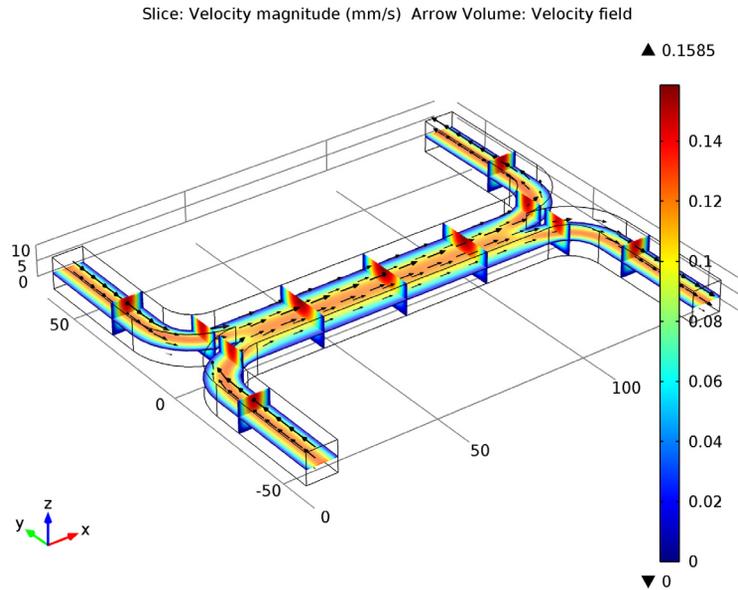
- 1 In the **Model Builder** window, under **Results>Data Sets** right-click **Surface 1** and choose **Duplicate**.
- 2 In the **Surface** settings window, locate the **Data** section.
- 3 From the **Data set** list, choose **Solution 3**.  
Re-create the velocity, pressure and concentration plots for the fully coupled problem.

### *Velocity (coupled flow)*

- 1 In the **Model Builder** window, under **Results** right-click **Velocity (uncoupled flow)** and choose **Duplicate**.
- 2 In the **3D Plot Group** settings window, locate the **Data** section.
- 3 From the **Data set** list, choose **Solution 3**.
- 4 Right-click **Results>Velocity (uncoupled flow) 1** and choose **Rename**.
- 5 Go to the **Rename 3D Plot Group** dialog box and type **Velocity (coupled flow)** in the **New name** edit field.
- 6 Click **OK**.

**7** On the **3D Plot Group** toolbar, click **Plot**.

There are significant differences in the flow pattern, although these are hard to see when comparing this plot with the similar one generated previously. The flow through a slice of the channel will be investigated in more detail later to better highlight these differences.

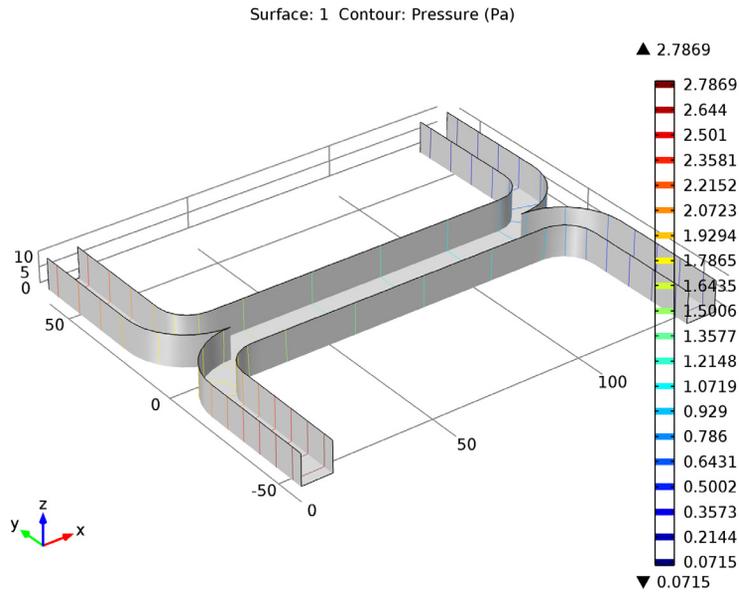


*Pressure (uncoupled flow) 1*

- 1** In the **Model Builder** window, under **Results** right-click **Pressure (uncoupled flow)** and choose **Duplicate**.
- 2** In the **3D Plot Group** settings window, locate the **Data** section.
- 3** From the **Data set** list, choose **Surface 2**.
- 4** Right-click **Results>Pressure (uncoupled flow) 1** and choose **Rename**.
- 5** Go to the **Rename 3D Plot Group** dialog box and type **Pressure (coupled flow)** in the **New name** edit field.
- 6** Click **OK**.
- 7** On the **3D Plot Group** toolbar, click **Plot**.

The pressure distribution in the channel has changed significantly as a result of the increased viscosity of the fluid that contains the added species. Thus the two inlets

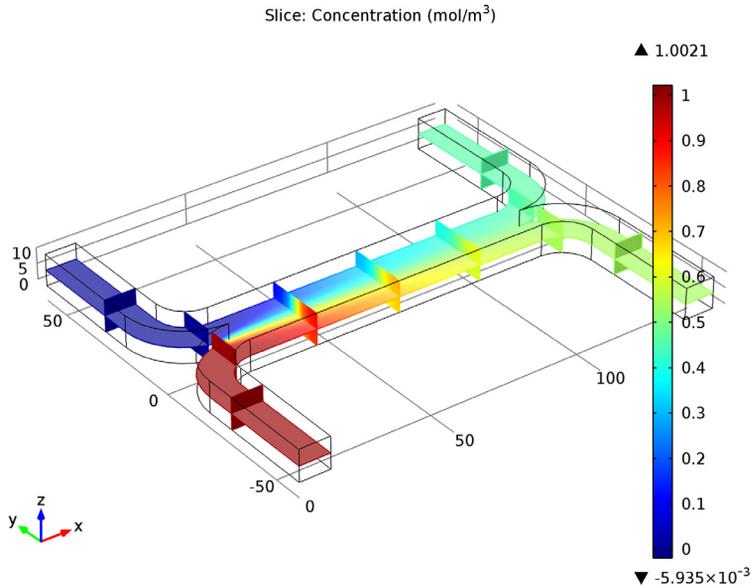
must be maintained at different pressures. This may be possible for a single stage, but it would significantly complicate the design of a multiple stage device.



#### Concentration (uncoupled flow) I

- 1 In the **Model Builder** window, under **Results** right-click **Concentration (uncoupled flow)** and choose **Duplicate**.
- 2 In the **3D Plot Group** settings window, locate the **Data** section.
- 3 From the **Data set** list, choose **Solution 3**.
- 4 Right-click **Results>Concentration (uncoupled flow) I** and choose **Rename**.
- 5 Go to the **Rename 3D Plot Group** dialog box and type **Concentration (coupled flow)** in the **New name** edit field.
- 6 Click **OK**.

- 7 On the **3D Plot Group** toolbar, click **Plot**.



The concentration distribution is affected only slightly by the coupling between the flow and the concentration.

Next add a cut plane data set in the center of the channel, for both the uncoupled and fully coupled solutions. These will be used to visualize the change in the flow profile induced by the coupling.

#### Data Sets

- 1 On the **Results** toolbar, click **Cut Plane**.
- 2 In the **Cut Plane** settings window, locate the **Plane Data** section.
- 3 In the **x-coordinate** edit field, type 70.
- 4 Right-click **Results>Data Sets>Cut Plane 1** and choose **Duplicate**.
- 5 In the **Cut Plane** settings window, locate the **Data** section.
- 6 From the **Data set** list, choose **Solution 3**.

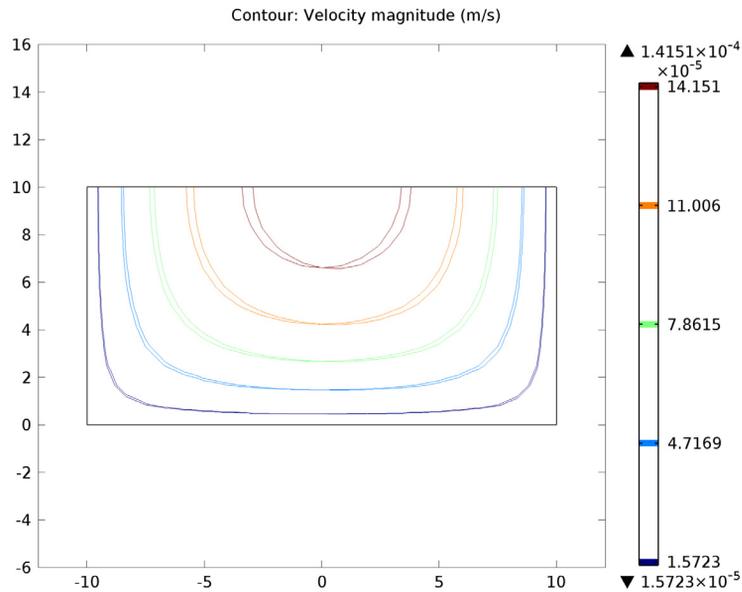
Then add a 2D contour plot of the velocity magnitude.

#### 2D Plot Group 8

- 1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

- 2** In the **2D Plot Group** settings window, locate the **Data** section.
- 3** From the **Data set** list, choose **Cut Plane 1**.
- 4** From the **Parameter value (D)** list, choose **5e-11**.
- 5** Right-click **Results>2D Plot Group 8** and choose **Contour**.
- 6** In the **Contour** settings window, locate the **Levels** section.
- 7** In the **Total levels** edit field, type 5.  
Create a duplicate contour plot, using the same colors and scales, but showing the coupled data.
- 8** Right-click **Results>2D Plot Group 8>Contour 1** and choose **Duplicate**.
- 9** In the **Contour** settings window, locate the **Data** section.
- 10** From the **Data set** list, choose **Cut Plane 2**.
- 11** Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 12** Click to expand the **Inherit style** section. Locate the **Inherit Style** section. From the **Plot** list, choose **Contour 1**.  
Rename the plot.
- 13** In the **Model Builder** window, right-click **2D Plot Group 8** and choose **Rename**.
- 14** Go to the **Rename 2D Plot Group** dialog box and type **Velocity Comparison** in the **New name** edit field.
- 15** Click **OK**.

**16** On the **2D Plot Group** toolbar, click **Plot**.



Now it is possible to compare the velocity distributions more carefully. It is clear that the coupling has introduced an asymmetry into the flow pattern, as a result of the higher viscosity in the fluid containing the dissolved species.

Finally compare the output concentration between the two solutions.

#### Derived Values

- 1** On the **Results** toolbar, click **Global Evaluation**.
- 2** In the **Global Evaluation** settings window, locate the **Expression** section.
- 3** In the **Expression** edit field, type `aveop1(c)`.
- 4** Click the **Evaluate** button.

#### TABLE

Right-click **Results>Derived Values>Global Evaluation 1** and choose **Duplicate**.

#### RESULTS

##### Derived Values

- 1** In the **Global Evaluation** settings window, locate the **Data** section.

- 2 From the **Data set** list, choose **Solution 3**.
- 3 Right-click **Results>Derived Values>Global Evaluation 2** and choose **Evaluate>New Table**.

Only a small difference occurs in the output concentration as a result of the coupling between the problems. However the coupling would make adding multiple stages of the device together much more difficult, as different pressures are required at the two inlets to obtain the same flow velocity in the two streams.

