Created in COMSOL Multiphysics 5.6

Microchannel H-Cell

Introduction

This example models an H-microcell for separation through diffusion. In Figure 1, it is shown how 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. 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.

The model utilizes the Laminar Flow and Transport of Diluted Species interfaces to fully capture the separation within the cell.

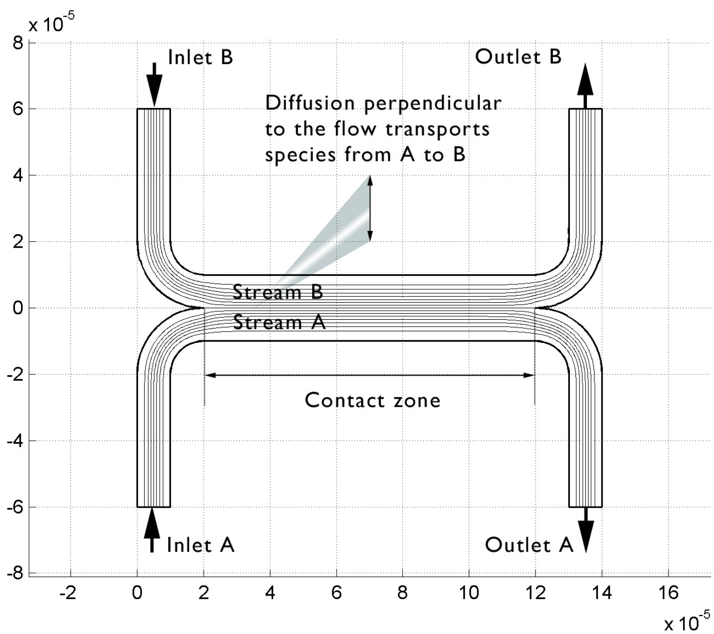


Figure 1: Diagram of the H-microcell (dimensions in meters).

Model Definition

The geometry of the microcell is shown in Figure 2. Due to symmetry, the model geometry can be simplified to half of it.

The design is aimed to eliminate upsets in the flow field when the two streams, A and B, are united. Thus, the cell enables mixing of A and B solely through diffusion. A system allowing convection would mix all species equally and lead to loss of control over the separation abilities.

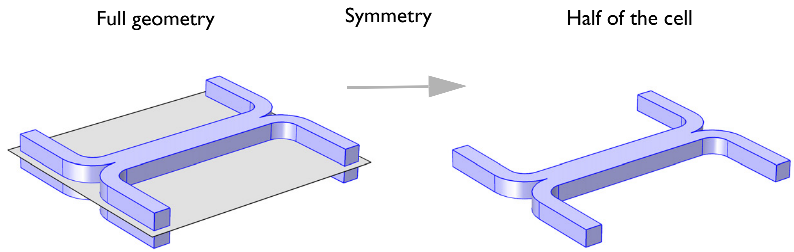


Figure 2: Model geometry as given by Albert Witarsa's and Professor Finlayson. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry.

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:

$$\mathrm{Re} = \frac{d\rho u}{\mu} = \frac{1\cdot 10^{-5}\cdot 1\cdot 10^{3}\cdot 1\cdot 10^{-4}}{1\cdot 10^{-3}} \tag{1}$$

Equation 1 gives a Reynolds number of 0.001 for a water solution and the channel dimensions given in Figure 1. This value is typical for microchannels. Additionally, this indicates that it is easy to get a numerical solution of the full momentum balance and continuity equations with a reasonable number of elements. The Laminar Flow interface can set up and solve the incompressible Navier-Stokes equations at steady state:

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

Here ρ denotes density (SI unit: $\mathrm{kg/m^3}$), $\mathbf{u}$ is the velocity (SI unit: m/s), μ denotes viscosity (SI unit: Pa·s), and p equals pressure (SI unit: 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. Use the Transport of Diluted Species interface to set up and solve the appropriate stationary mass-balance equation:

$$-\nabla\cdot(-D\nabla c+c\mathbf{u}) = 0 \qquad (2)$$

In this equation, D denotes the diffusion coefficient (SI unit: m^2/s) and c represents the concentration (SI unit: mol/m^3). In this model, you use the parametric solver to solve Equation 2 for three different values of D — $1\cdot10^{-11}$ m^2/s, $5\cdot10^{-11}$ m^2/s, and $1\cdot10^{-10}$ 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 concentration does not influence the fluid's density and viscosity. This implies that it is possible to first solve for the fluid flow and then for the mass transport.
- In the second version, you include a correction term in the viscosity that depends quadratically on the concentration in Equation 1:

$$\mu = \mu_0(1+\alpha c^2) \qquad (3)$$

  Here α is a constant of dimension (SI unit: m^6/mol^2). An influence of concentration on viscosity of this kind is usually observed in solutions of larger molecules. In this case the flow and mass transport equations have to be solved simultaneously.

Last, consider the boundary conditions. All boundaries are visualized in Figure 3.

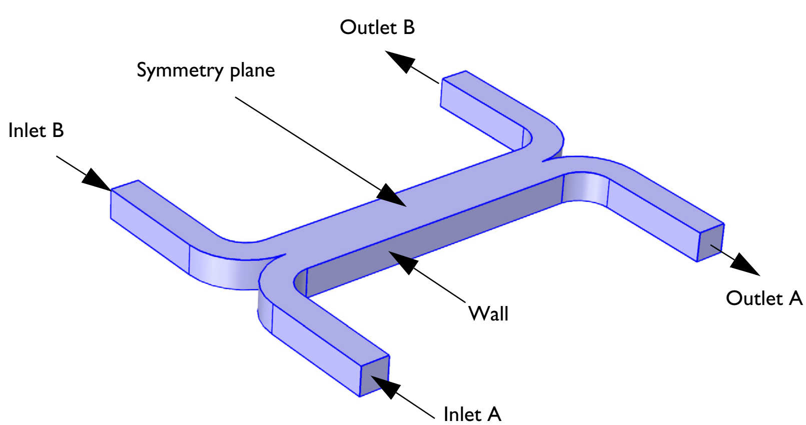


Figure 3: Model domain boundaries.

For the Laminar Flow interface:

- At the inlets and outlets, Pressure conditions apply along with vanishing viscous stress. 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 walls, No slip conditions state that the velocity is zero.
- At the symmetry plane, using the Symmetry boundary condition sets the velocity component in the normal direction of the surface to zero.

For the Transport of Diluted Species:

- At the inlets, use the Concentration boundary condition to set concentration. At inlets A and B the concentration are 1 mol/m^3 and 0 mol/m^3, respectively.
- At the outlets, apply the convective flux condition through the Outflow boundary condition, stating that the diffusive transport perpendicular to the boundary normal is negligible. This condition will thus eliminate concentration gradients in the flow direction.
- Model the symmetry plane and cell walls with the No Flux condition. This equation states that the flux of species perpendicular to the boundary equals zero.

Results and Discussion

Figure 4 shows the velocity field for the whole microcell. The flow is symmetric and is not influenced by the concentration field.

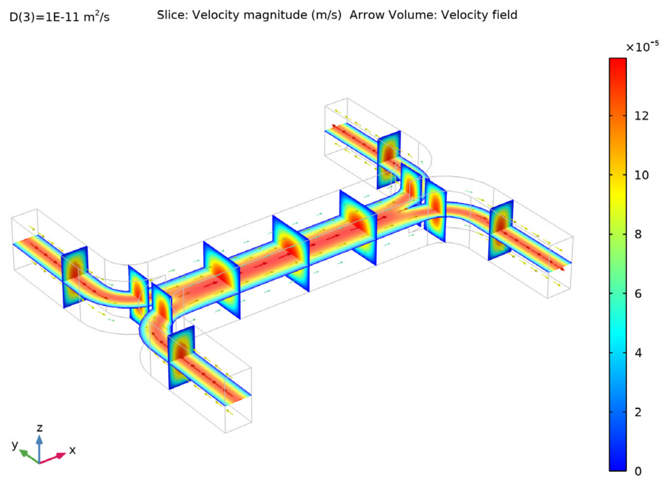


Figure 4: Flow velocity field.

Figure 5 shows the concentration distribution for the species with the highest simulated diffusivity.

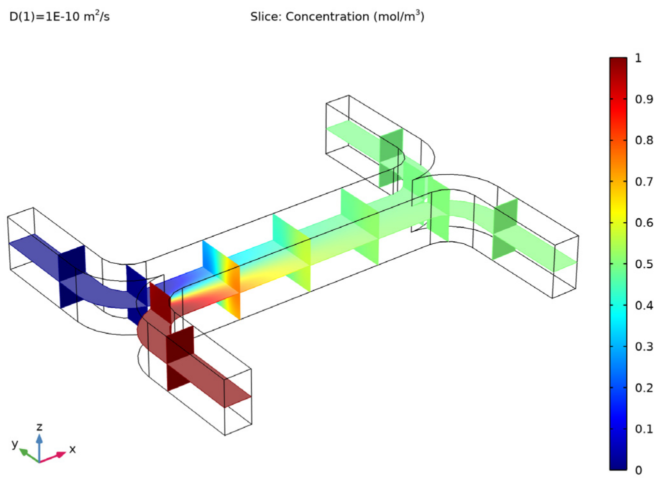


Figure 5: Concentration distribution for a species with diffusivity 10^{-10} m^2/s.

Because of the relatively large diffusion coefficient, the degree of mixing is almost perfect. The species with a diffusion coefficient ten times smaller shows a different result. The concentration distribution in Figure 6 shows that the diffusion coefficient for the species too low for achieving significant mixing of the streams.

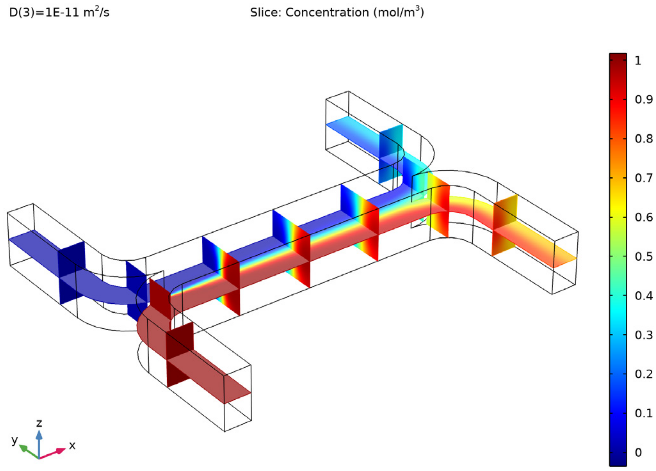


Figure 6: Concentration distribution for a species with diffusivity $1 \cdot 10^{-11} m^2/s$.

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 model needs to be fully coupled and solve both interfaces simultaneously. Figure 7 shows the results of such a simulation. Here, the changes in viscosity have caused an asymmetry in the velocity. As a consequence of the modified flow field, the transport of molecules to outlet B is also different from the constant flow field case (Figure 8 versus Figure 5).

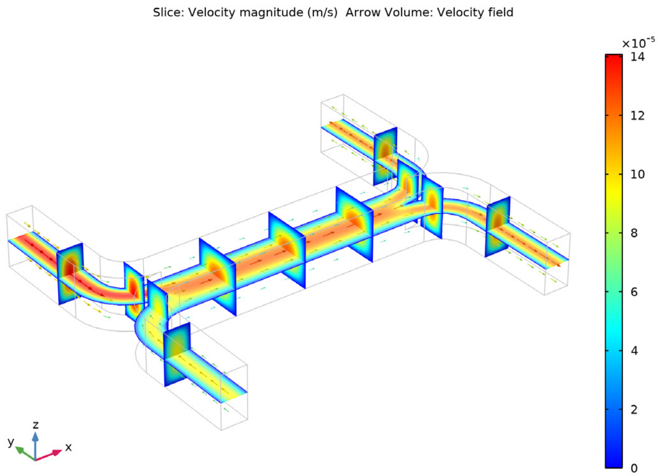


Figure 7: Velocity field. The viscosity varies with the concentration according to Equation 3 *with* $\alpha = 0.5\ (m^3/mol)^2$*. The figure shows that the velocity field is affected by variations in concentration..*

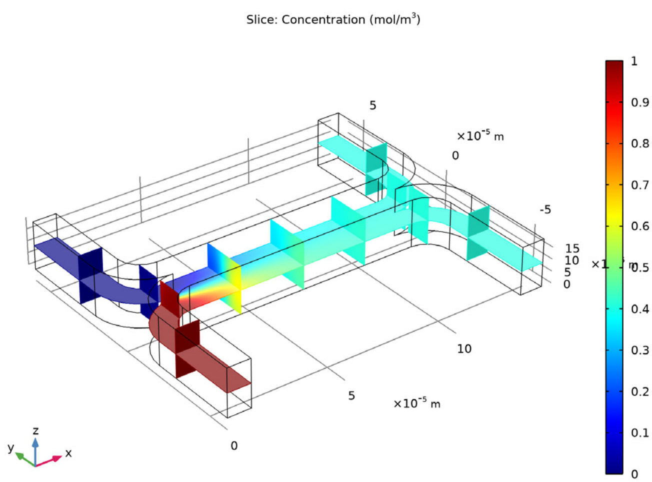


Figure 8: Concentration distribution for the species with diffusivity $1\cdot 10^{-10} m^2/s$ *for the case where the fluid viscosity varies with concentration. Comparison with the plot in* Figure 5 *shows that fewer molecules of the species are transported to outlet B.*

Application Library path: `Chemical_Reaction_Engineering_Module/Mixing_and_Separation/microchannel_h_cell`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

5 Click **Add**.

6 Click **Study**.

7 In the **Select Study** tree, select **General Studies>Stationary**.

8 Click **Done**.

GEOMETRY 1

Create the geometry. To simplify this step, insert a prepared geometry sequence.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

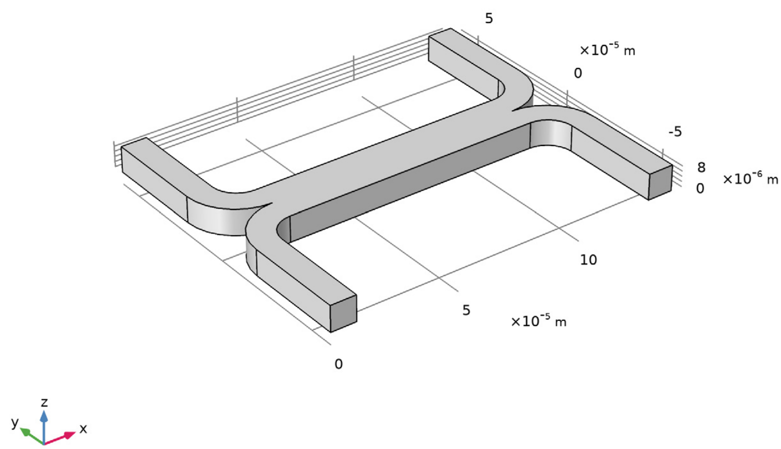
2 In the **Geometry** toolbar, click **Insert Sequence**.

3 Browse to the model's Application Libraries folder and double-click the file `microchannel_h_cell.mph`.

Work Plane 1 (wp1)

1 Click the **Zoom Extents** button in the **Graphics** toolbar.

This completes the geometry modeling stage. The geometry should now look like that in the figure below.



ROOT

Import the model parameters from a text file.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `microchannel_h_cell_parameters.txt`.

The material properties of water are available within the **Material Library**.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Built-in>Water, liquid**.

4 Click **Add to Component** in the window toolbar.

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

For microfluidic flows, second order elements are more accurate and computationally efficient than the linear elements. Increase the element order for both interfaces in the model.

LAMINAR FLOW (SPF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, click to expand the **Discretization** section.

3 From the **Discretization of fluids** list, choose **P2+P1**.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species (tds)**.

2 In the **Settings** window for **Transport of Diluted Species**, click to expand the **Discretization** section.

3 From the **Concentration** list, choose **Quadratic**.

LAMINAR FLOW (SPF)

In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 Select Boundaries 2 and 8 only.

3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

4 From the list, choose **Pressure**.

5 Locate the **Pressure Conditions** section. In the p_0 text field, type `p0`.

Outlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.

2 Select Boundaries 20 and 22 only.

3 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

4 Select the **Normal flow** check box.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.
2 Select Boundary 4 only.

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species (tds)** click **Transport Properties 1**.
2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.
3 In the D_c text field, type `D`.

Concentration 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.
2 Select Boundary 2 only.
3 In the **Settings** window for **Concentration**, locate the **Concentration** section.
4 Select the **Species c** check box.
5 In the $c_{0,c}$ text field, type `c0`.

Concentration 2

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

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.
2 Select Boundaries 20 and 22 only.

MULTIPHYSICS

Reacting Flow, Diluted Species 1 (rfd1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Coarse**.

Size

Right-click **Component 1 (comp1)>Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size 1

1 In the **Settings** window for **Size**, locate the **Element Size** section.

2 From the **Predefined** list, choose **Coarser**.

3 Click **Build Selected**.

Size 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Points 19, 20, 25, and 26 only.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

7 In the associated text field, type `4.5E-6`.

Free Tetrahedral 1

1 In the **Model Builder** window, right-click **Free Tetrahedral 1** and choose **Build Selected**.

2 In the **Settings** window for **Free Tetrahedral**, click **Build All**.

Use two **Stationary** solver steps. In the first only the **Laminar Flow** interface is solved.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Transport of Diluted Species (tds)**.

Add a second stationary step that solves the **Transport of Diluted Species** interface using the previously computed flow field.

Stationary 2

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Laminar Flow (spf)**.

Within this study step, enable the parametric continuation solver to solve the mass transport problem for several diffusion coefficients.

4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
D (Diffusion constant)	`1e-10 5e-11 1e-11`	`m^2/s`

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

By default, the solution from the first step will be applied to the (fluid) variables not solved for in the second step.

2 In the **Settings** window for **Solution**, click **Compute**.

Create a **Mirror 3D Data Set** that enables plotting of the whole geometry, i.e. both sides of the symmetry plane.

RESULTS

Mirror 3D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 3D**.

2 In the **Settings** window for **Mirror 3D**, locate the **Plane Data** section.

3 From the **Plane** list, choose **xy-planes**.

4 In the **z-coordinate** text field, type `1e-5`.

Velocity (spf)

To generate Figure 4 follow these steps:

Slice

1 In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Slice**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

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

4 In the **Velocity (spf)** toolbar, click **Plot**.

Slice 2

1 Right-click **Slice** and choose **Duplicate**.

2 In the **Settings** window for **Slice**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plane Data** section. From the **Plane** list, choose **zx-planes**.

5 In the **Planes** text field, type `2`.

6 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice**.

7 In the **Velocity (spf)** toolbar, click **Plot**.

Slice 3

1 Right-click **Slice 2** and choose **Duplicate**.

2 In the **Settings** window for **Slice**, locate the **Plane Data** section.

3 From the **Plane** list, choose **xy-planes**.

4 In the **Planes** text field, type `1`.

5 From the **Entry method** list, choose **Coordinates**.

6 In the **z-coordinates** text field, type `1e-5`.

7 In the **Velocity (spf)** toolbar, click **Plot**.

Arrow Volume 1

1 In the **Model Builder** window, right-click **Velocity (spf)** and choose **Arrow Volume**.

2 In the **Settings** window for **Arrow Volume**, locate the **Arrow Positioning** section.

3 Find the **x grid points** subsection. In the **Points** text field, type `14`.

4 Find the **y grid points** subsection. In the **Points** text field, type `21`.

5 Find the **z grid points** subsection. In the **Points** text field, type `3`.

6 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

7 In the **Velocity (spf)** toolbar, click **Plot**.

Velocity (spf)

1 In the **Model Builder** window, click **Velocity (spf)**.

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

3 From the **Dataset** list, choose **Mirror 3D 1**.

4 Locate the **Plot Settings** section. From the **Color** list, choose **Gray**.

5 Click the **Show Grid** button in the **Graphics** toolbar.

Slice

1 In the **Model Builder** window, click **Slice**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 From the **Unit** list, choose **m/s**.

4 Click to expand the **Quality** section. From the **Resolution** list, choose **Fine**.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **RainbowLight**.

Slice 2

1 In the **Model Builder** window, click **Slice 2**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 From the **Unit** list, choose **m/s**.

Slice 3

1 In the **Model Builder** window, click **Slice 3**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 From the **Unit** list, choose **m/s**.

Color Expression 1

1 In the **Model Builder** window, right-click **Arrow Volume 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **RainbowLight**.

Arrow Volume 1

1 In the **Model Builder** window, click **Arrow Volume 1**.

2 In the **Settings** window for **Arrow Volume**, locate the **Coloring and Style** section.

3 Select the **Scale factor** check box.

4 In the associated text field, type `0.04`.

5 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice**.

6 In the **Velocity (spf)** toolbar, click **Plot**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

8 In the **Velocity (spf)** toolbar, click **Plot**.

Proceed to plot the concentration distribution Figure 5.

Concentration, Slice

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

2 In the **Settings** window for **3D Plot Group**, type `Concentration, Slice` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Mirror 3D 1**.

4 From the **Parameter value (D (m^2/s))** list, choose **1E-10**.

Slice 1

1 Right-click **Concentration, Slice** and choose **Slice**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Diluted Species>Species c>c - Concentration - mol/m³**.

Slice 2

1 Right-click **Slice 1** and choose **Duplicate**.

2 In the **Settings** window for **Slice**, locate the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plane Data** section. From the **Plane** list, choose **zx-planes**.

5 In the **Planes** text field, type `2`.

6 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

7 In the **Concentration, Slice** toolbar, click **Plot**.

Slice 3

1 Right-click **Slice 2** and choose **Duplicate**.

2 In the **Settings** window for **Slice**, locate the **Plane Data** section.

3 From the **Plane** list, choose **xy-planes**.

4 In the **Planes** text field, type `1`.

5 From the **Entry method** list, choose **Coordinates**.

6 In the **z-coordinates** text field, type `1e-5`.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

8 In the **Concentration, Slice** toolbar, click **Plot**.

Concentration, Slice

Generate Figure 6 using the diffusion coefficient value $1E^{-11}\ m^2/s$.

1 In the **Model Builder** window, click **Concentration, Slice**.

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

3 From the **Parameter value (D (m^2/s))** list, choose **1E-11**.

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

5 In the **Concentration, Slice** toolbar, click **Plot**.

Add a correction term in the viscosity.

LAMINAR FLOW (SPF)

Fluid Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Fluid Properties 1**.

2 In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.

3 From the μ list, choose **User defined**. In the associated text field, type `mu*(1+alpha*c^2)`.

When viscosity is concentration dependent you must solve all equations simultaneously. Add a second study for the fully coupled problem.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

1 In the **Model Builder** window, click **Study 2**.

2 In the **Settings** window for **Study**, locate the **Study Settings** section.

3 Clear the **Generate default plots** check box.

4 In the **Home** toolbar, click **Compute**.

Create Figure 7 and Figure 8 by following these steps.

RESULTS

Mirror 3D 2

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 3D**.

2 In the **Settings** window for **Mirror 3D**, locate the **Plane Data** section.

3 From the **Plane** list, choose **xy-planes**.

4 In the **z-coordinate** text field, type `1e-5`.

5 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 3 (sol3)**.

Velocity (spf) 1

1 In the **Model Builder** window, right-click **Velocity (spf)** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Mirror 3D 2**.

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

5 In the **Velocity (spf) 1** toolbar, click **Plot**.

6 Click the **Show Grid** button in the **Graphics** toolbar.

Concentration, Slice 1

1 In the **Model Builder** window, right-click **Concentration, Slice** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Mirror 3D 2**.

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

5 In the **Concentration, Slice 1** toolbar, click **Plot**.

6 Click the **Show Grid** button in the **Graphics** toolbar.