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.

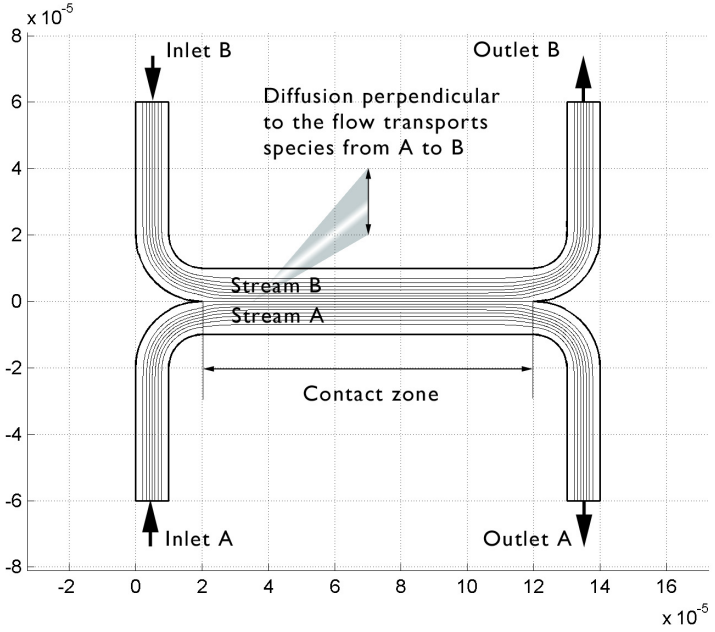

Figure 1: Diagram of the H-microcell (dimensions in metres).

Model Definition

The geometry of the microcell (Figure 2) 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.

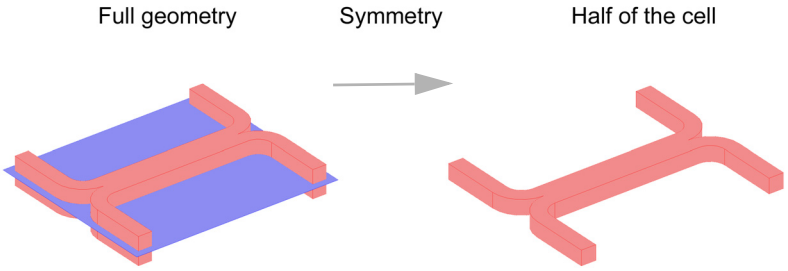

Figure 2: Model geometry. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry.

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, a value typical for microchannels. Thus 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 Navier-Stokes equations at steady state:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I}+\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] \tag{2}$$

$$\nabla\cdot(\rho\mathbf{u}) = 0$$

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

$$-\nabla \cdot (-D\nabla c + c\mathbf{u}) = 0 . \quad (3)$$

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 3 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 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:

  $$\mu = \mu_0(1 + \alpha c^2) . \quad (4)$$

  Here α is a constant of dimension (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.

Next, consider the boundary conditions, starting with the Navier-Stokes equations. For the relevant boundary conditions, refer to Figure 3.

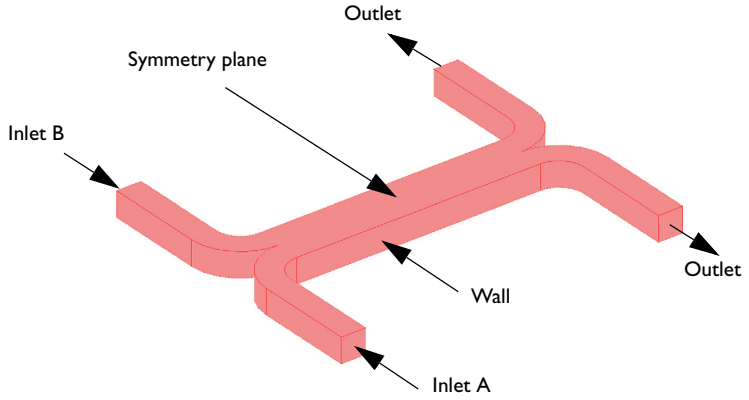

Figure 3: Model domain boundaries.

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

$$\begin{aligned} p &= p_0 \\ \mathbf{n} \cdot \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) &= 0 \end{aligned} \tag{5}$$

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, using the *Symmetry* boundary condition sets the velocity component in the normal direction of the surface to zero:

$$\begin{aligned} \mathbf{n} \cdot \mathbf{u} &= 0 \\ \mathbf{t} \cdot \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} &= 0 \end{aligned} \tag{6}$$

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

$$(u, v, w) = (0, 0, 0) \qquad \text{at the walls} \tag{7}$$

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:

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$$\begin{aligned} c &= c_0 \quad \text{at inlet A} \\ c &= 0 \quad \text{at inlet B} \end{aligned} \tag{8}$$

Model the symmetry plane and cell walls with the *No Flux* condition:

$$(-D\nabla c + c\mathbf{u}) \cdot \mathbf{n} = 0 \quad \text{at the symmetry plane and walls} \tag{9}$$

This equation states that the flux of species perpendicular to the boundary equals zero. 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:

$$(-D\nabla c) \cdot \mathbf{n} = 0 \quad \text{at the outlets} \tag{10}$$

This condition eliminates concentration gradients in the flow direction.

Results

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

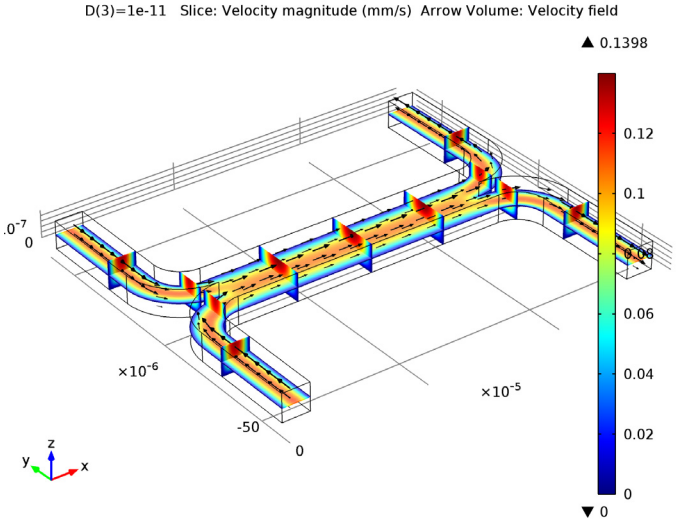

Figure 4: Flow velocity field.

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

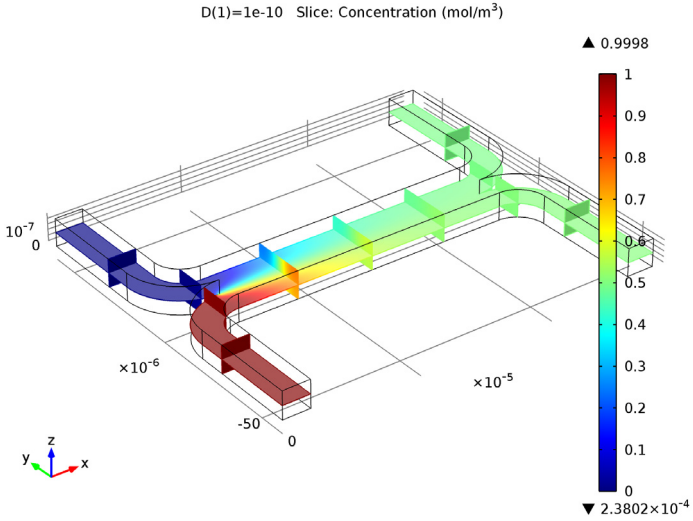

Figure 5: Concentration distribution for a species with diffusivity 10^{-10} m^2/s.

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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.

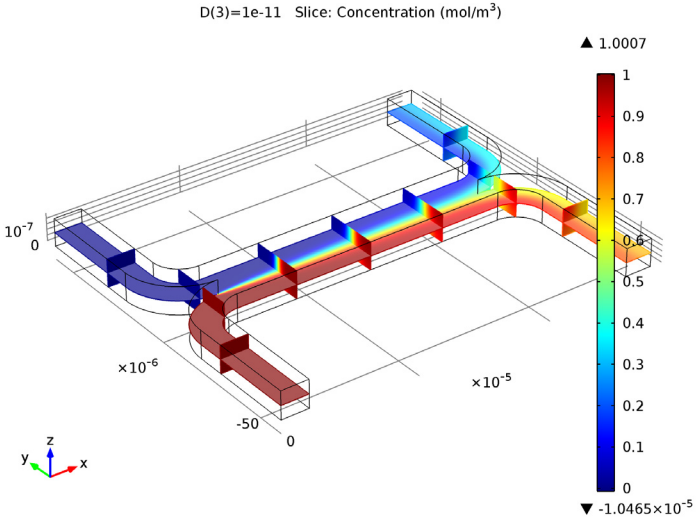

Figure 6: Concentration distribution for a species with diffusivity $1 \cdot 10^{-11} m^2/s$.

The concentration distribution in Figure 6 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 7 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 8 with Figure 6.

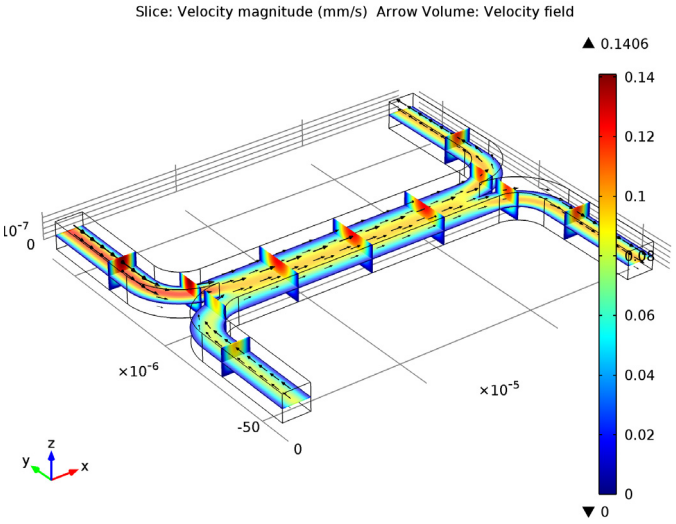

Figure 7: Velocity field. The viscosity varies with the concentration according to Equation 4 *with* $\alpha = 0.5$ $(m^3/mol)^2$. *The figure shows that the velocity field is affected by variations in concentration. Compare it to the velocity field in* Figure 4.

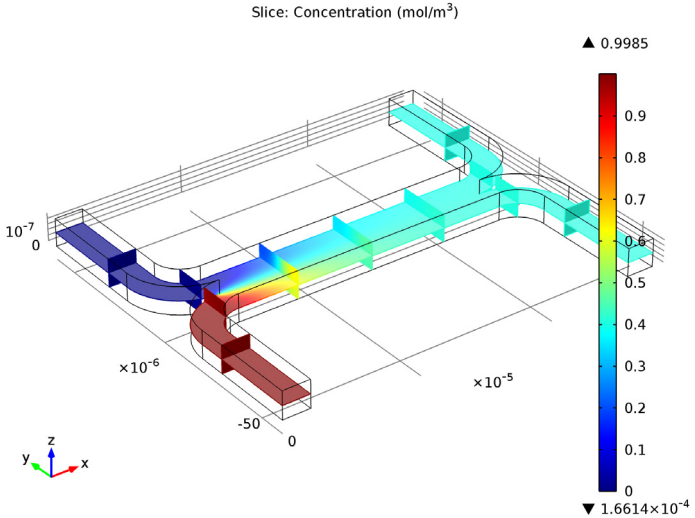

Figure 8: Concentration distribution for the species with diffusivity $1{\cdot}10^{-10} m^2/s$ *for the case where the fluid viscosity varies with concentration. Comparison with the plot in* Figure 5 *shows that fewer molecules of the species are transported to outlet B.*

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Model Library path: `Chemical_Reaction_Engineering_Module/Mass_Transport/microchannel_h_cell`

Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click **Next**.

3 In the **Add physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

4 Click **Add Selected**.

5 In the **Add physics** tree, select **Chemical Species Transport>Transport of Diluted Species (chds)**.

6 Click **Add Selected**.

7 Click **Next**.

8 Find the **Studies** subsection. In the tree, select **Preset Studies for Selected Physics>Stationary**.

9 Click **Finish**.

GEOMETRY 1

Start by building one face of the microchannel H-cell using a Work Plane as follows:

Work Plane 1

In the **Model Builder** window, right-click **Geometry 1** and choose **Work Plane**.

Rectangle 1

1 In the **Model Builder** window, under **Model 1>Geometry 1>Work Plane 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 `14`.

4 In the **Height** edit field, type `6`.

5 Click the **Build Selected** button.

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

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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 12.

4 In the **Height** edit field, type 5.

5 Locate the **Position** section. In the **xw** edit field, type 1.

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

7 Click the **Build Selected** button.

Difference 1

1 Right-click **Plane Geometry** and choose **Boolean Operations>Difference**.

2 Select the object **r1** only.

3 In the **Difference** settings window, locate the **Difference** section.

4 Under **Objects to subtract**, click **Activate Selection**.

5 Select the object **r2** only.

6 Click the **Build Selected** button.

Fillet 1

1 Right-click **Plane Geometry** and choose **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 1.

5 Click the **Build Selected** button.

Fillet 2

1 Right-click **Plane Geometry** and choose **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 2.

5 Click the **Build Selected** button.

Mirror 1

1 Right-click **Plane Geometry** and choose **Transforms>Mirror**.

2 Select the object **fil2** only.

3 In the **Mirror** settings window, locate the **Input** section.

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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 Right-click **Plane Geometry** and choose **Boolean Operations>Union**.

2 Select the objects **fil2** and **mir1** 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.

Now, extrude the work plane to get the 3D geometry:

Extrude 1

1 In the **Model Builder** window, under **Model 1>Geometry 1** right-click **Work Plane 1** and choose **Extrude**.

2 Right-click **Extrude 1** and choose **Build Selected**.

Scale 1

1 Right-click **Geometry 1** and choose **Transforms>Scale**.

2 Select the object **ext1** only.

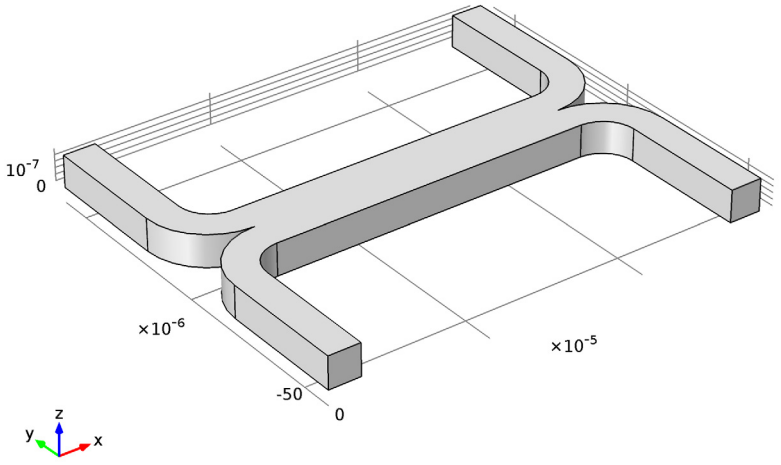
3 In the **Scale** settings window, locate the **Scale Factor** section.

4 In the **Factor** edit field, type `1e-5`.

5 Click the **Build Selected** button.

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

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



GLOBAL DEFINITIONS

Parameters

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

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

MATERIALS

Material Browser

1 In the **Model Builder** window, under **Model 1** right-click **Materials** and choose **Open Material Browser**.

2 In the **Material Browser** window, locate the **Materials** section.

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

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4 Right-click and choose **Add Material to Model** from the menu.

For microfluidic flows, second order elements are more accurate and computationally efficient than the linear elements. Increase the element order for both the fluid flow and the mass transport.

LAMINAR FLOW

1 In the **Model Builder** window's toolbar, click the **Show** button and select **Discretization** in the menu.

2 In the **Model Builder** window, under **Model 1** click **Laminar Flow**.

3 In the **Laminar Flow** settings window, click to expand the **Discretization** section.

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

TRANSPORT OF DILUTED SPECIES

1 In the **Model Builder** window, under **Model 1** click **Transport of Diluted Species**.

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

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

LAMINAR FLOW

Inlet 1

1 In the **Model Builder** window, under **Model 1** right-click **Laminar Flow** and choose **Inlet**.

2 Select Boundaries 2 and 8 only.

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

4 From the **Boundary condition** list, choose **Pressure, no viscous stress**.

5 Locate the **Pressure, No Viscous Stress** section. In the p_0 edit field, type `p0`.

Outlet 1

1 In the **Model Builder** window, right-click **Laminar Flow** and choose **Outlet**.

2 Select Boundaries 20 and 22 only.

Symmetry 1

1 Right-click **Laminar Flow** and choose **Symmetry**.

2 Select Boundary 4 only.

TRANSPORT OF DILUTED SPECIES

Convection and Diffusion 1

1 In the **Model Builder** window, expand the **Model 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 $\mathbf{u}$ list, choose **Velocity field (spf/fp1)**.

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

Concentration 1

1 In the **Model Builder** window, right-click **Transport of Diluted Species** 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 `c0`.

Concentration 2

1 Right-click **Transport of Diluted Species** 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.

Outflow 1

1 Right-click **Transport of Diluted Species** and choose **Outflow**.

2 Select Boundaries 20 and 22 only.

MESH 1

1 In the **Model Builder** window, under **Model 1** click **Mesh 1**.

2 In the **Mesh** settings window, locate the **Mesh Settings** section.

3 From the **Sequence type** list, choose **Physics-controlled mesh**.

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

Size 1

1 Right-click **Model 1>Mesh 1** and choose **Edit Physics-Induced Sequence**.

2 In the **Model Builder** window, under **Model 1>Mesh 1** click **Size 1**.

3 In the **Size** settings window, locate the **Element Size** section.

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

5 Click the **Build Selected** button.

Size 2

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

2 In the **Size** settings window, 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 edit field, type `1.5E-6`.

Free Tetrahedral 1

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

2 Click the **Build All** button.

STUDY 1

Use two stationary solver steps, the first one solving for the fluid flow only.

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
Transport of Diluted Species (chds)	×

Add a second stationary steps that solves the mass transport using the previously computed flow field.

Step 2: Stationary 2

1 In the **Model Builder** window, right-click **Study 1** and choose **Study Steps>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
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 **Continuation** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Continuation parameter	Parameter value list
D	`1e-10 5e-11 1e-11`

7 Right-click **Study 1** and choose **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.

8 Right-click **Study 1** and choose **Compute**.

RESULTS

Velocity (spf)

To generate Figure 4 follow these steps:

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

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

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

4 Click the **Plot** button.

5 Right-click **Results>Velocity (spf)>Slice 1** and choose **Duplicate**.

6 In the **Slice** settings window, click to expand the **Title** section.

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

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

9 In the **Planes** edit field, type 2.

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

11 Click the **Plot** button.

12 Right-click **Results>Velocity (spf)>Slice 2** and choose **Duplicate**.

13 In the **Slice** settings window, locate the **Plane Data** section.

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

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

16 Click the **Plot** button.

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

18 In the **Arrow Volume** settings window, locate the **Arrow Positioning** section.

19 Find the **x grid points** subsection. In the **Points** edit field, type 14.

20 Find the **y grid points** subsection. In the **Points** edit field, type 21.

21 Find the **z grid points** subsection. In the **Points** edit field, type 3.

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

23 Click the **Plot** button.

Proceed to plot the concentration distribution (Figure 5) .

Concentration (chds)

1 In the **Model Builder** window, under **Results** click **Concentration (chds)**.

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

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

4 In the **Model Builder** window, under **Results>Concentration (chds)** right-click **Slice 1** and choose **Duplicate**.

5 In the **Slice** settings window, click to expand the **Title** section.

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

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

8 In the **Planes** edit field, type 2.

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

10 Click the **Plot** button.

11 Right-click **Results>Concentration (chds)>Slice 2** and choose **Duplicate**.

12 In the **Slice** settings window, locate the **Plane Data** section.

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

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

15 Click the **Plot** button.

Generate Figure 6 using the parameter value 10^{-11}.

16 In the **Model Builder** window, click **Concentration (chds)**.

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

18 From the **Parameter value (D)** list, choose **1e-11**.

19 Click the **Plot** button.

Add a correction term in the viscosity.

LAMINAR FLOW

Fluid Properties 1

1 In the **Model Builder** window, under **Model 1>Laminar Flow** click **Fluid Properties 1**.

2 In the **Fluid Properties** settings window, locate the **Fluid Properties** section.

3 From the μ list, choose **User defined**. In the associated edit 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.

ROOT

In the **Model Builder** window, right-click the root node and choose **Add Study**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Find the **Studies** subsection. In the tree, select **Preset Studies for Selected Physics>Stationary**.

3 Click **Finish**.

STUDY 2

Step 1: Stationary

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 Click the **Compute** button.

RESULTS

Velocity (spf) 1

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

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

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3 From the **Data set** list, choose **Solution 3**.

4 Click the **Plot** button.

Concentration (chds) 2

1 In the **Model Builder** window, under **Results** right-click **Concentration (chds)** 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 Click the **Plot** button.

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