

Microchannel H-Cell

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.

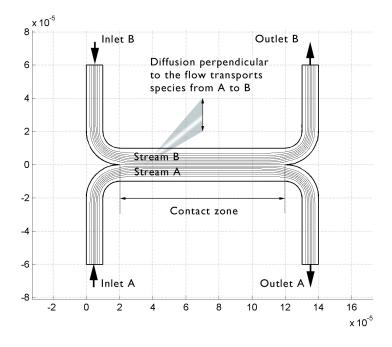


Figure 1: Diagram of the H-microcell (dimensions in meters).

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.

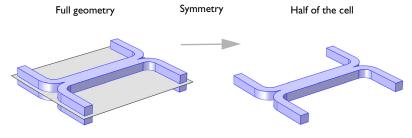


Figure 2: Model geometry as given by Albert Witarsa's and Professor Finlayson. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry.

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:

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

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

Here ρ denotes density (SI unit: kg/m³), **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:

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

In this equation, D denotes the diffusion coefficient (SI unit: m^2/s) and c represents the concentration (SI unit: mol/m³). In this model, you use the parametric solver to solve Equation 2 for three different values of $D - 1.10^{-11}$ m²/s, 5.10^{-11} m²/s, and 1.10^{-10} m²/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:

$$\mu = \mu_0 (1 + \alpha c^2) \tag{3}$$

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.

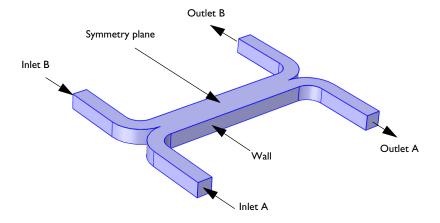


Figure 3: Model domain boundaries.

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/m³ and 0 mol/m³, 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.

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

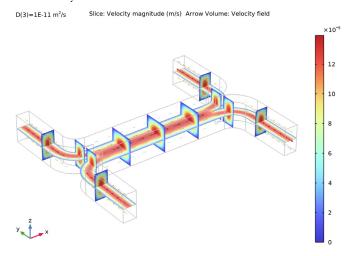


Figure 4: Flow velocity field.

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

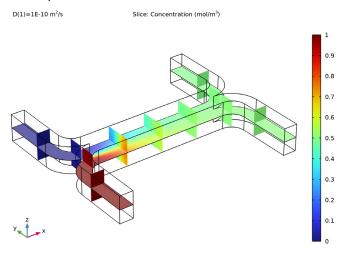


Figure 5: Concentration distribution for a species with diffusivity $10^{-10} \ m^2/s$.

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.

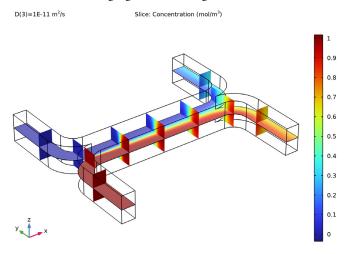


Figure 6: Concentration distribution for a species with diffusivity $1 \cdot 10^{-11} \text{m}^2/\text{s}$.

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).



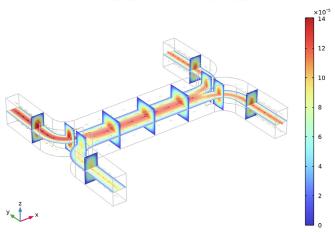
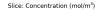


Figure 7: Velocity field. The viscosity varies with the concentration according to Equation 3 with $\alpha = 0.5 \ (m^3/mol)^2$. The figure shows that the velocity field is affected by variations in concentration.



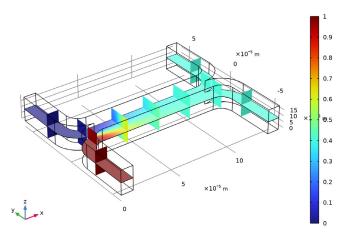


Figure 8: Concentration distribution for the species with diffusivity $1\cdot 10^{-10} m^2/s$ for the case where the fluid viscosity varies with concentration. Comparison with the plot in Figure 5 shows that fewer molecules of the species are transported to outlet B.

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

- I 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 M Done.

GEOMETRY I

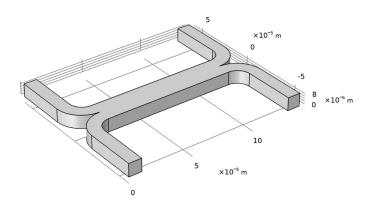
Create the geometry. To simplify this step, insert a prepared geometry sequence.

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 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 I (wpl)

I 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

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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

I 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 Radd 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)

- I In the Model Builder window, under Component I (compl) 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.

Inlet 1

- I 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 I

- I 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 I

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

TRANSPORT OF DILUTED SPECIES (TDS)

- I In the Model Builder window, under Component I (compl) 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.

Transport Properties 1

- I In the Model Builder window, under Component I (compl)> Transport of Diluted Species (tds) click Transport Properties 1.
- 2 In the Settings window for Transport Properties, locate the Diffusion section.
- **3** In the $D_{\rm c}$ text field, type D.

Concentration I

- I 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

- I 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 I

- I 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 I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 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 I (compl)>Mesh I and choose Edit Physics-Induced Sequence.

Size 1

I In the Settings window for Size, locate the Element Size section.

- 2 From the Predefined list, choose Coarser.
- 3 Click **Build Selected**.

Size 2

- I In the Model Builder window, right-click Mesh I 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.
- 7 Select the Maximum element size check box. In the associated text field, type 4.5E-6.

Free Tetrahedral I

- I In the Model Builder window, right-click Free Tetrahedral I 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.

VISCOSITY NOT DEPENDING ON CONCENTRATION

- I In the Model Builder window, click Study I.
- 2 In the Settings window for Study, type Viscosity Not Depending on Concentration in the Label text field.

Laminar Flow

- I In the Model Builder window, under Viscosity Not Depending on Concentration click Step 1: Stationary.
- 2 In the Settings window for Stationary, type Laminar Flow in the Label text field.
- 3 Locate the Physics and Variables Selection section. 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.

Transport of Diluted Species

- I In the Study toolbar, click Study Steps and choose Stationary>Stationary.
- 2 In the Settings window for Stationary, type Transport of Diluted Species in the Label text field.

3 Locate the Physics and Variables Selection section. 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 I (soll)

I 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 dataset that enables plotting of the whole geometry, that is, both sides of the symmetry plane.

RESULTS

Mirror 3D I

- I 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

- I 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

I 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

- I 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

- I 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)

- I 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

- I 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. Click Change Color Table.
- 6 In the Color Table dialog box, select Rainbow>RainbowLight in the tree.
- 7 Click OK.

Slice 2

- I 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

- I 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

- I In the Model Builder window, right-click Arrow Volume I and choose Color Expression.
- 2 In the Settings window for Color Expression, locate the Coloring and Style section.
- 3 Click Change Color Table.
- 4 In the Color Table dialog box, select Rainbow>RainbowLight in the tree.
- 5 Click OK.

Arrow Volume 1

- I In the Model Builder window, click Arrow Volume I.
- 2 In the Settings window for Arrow Volume, locate the Coloring and Style section.
- **3** Select the **Scale factor** check box. In the associated text field, type 0.04.
- 4 Click to expand the Inherit Style section. From the Plot list, choose Slice.
- 5 In the Velocity (spf) toolbar, click Plot.
- 6 Click the Zoom Extents button in the Graphics toolbar.
- 7 In the Velocity (spf) toolbar, click Plot.

Proceed to plot the concentration distribution Figure 5.

Concentration, Slice (1E-10)

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

- 2 In the Settings window for 3D Plot Group, type Concentration, Slice (1E-10) 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 IE-10.

Slice 1

- I Right-click Concentration, Slice (IE-10) 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 I (compl)>** Transport of Diluted Species>Species c>c - Concentration - mol/m3.

Slice 2

- I Right-click Slice I 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.

Slice 3

- I 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.
- Generate Figure 6 using the diffusion coefficient value $1E^{-11}$ m²/s by duplicating Concentration, Slice (IE-I0).

Concentration, Slice (IE-II)

I In the Model Builder window, right-click Concentration, Slice (IE-10) and choose Duplicate.

- 2 In the Settings window for 3D Plot Group, type Concentration, Slice (1E-11) in the Label text field.
- 3 Locate the Data section. From the Parameter value (D (m^2/s)) list, choose IE-II.

Add a correction term in the viscosity.

LAMINAR FLOW (SPF)

Fluid Properties 1

- I In the Model Builder window, under Component I (compl)>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

- I 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.

VISCOSITY DEPENDING ON CONCENTRATION

- I In the Model Builder window, click Study 2.
- 2 In the Settings window for Study, type Viscosity Depending on Concentration in the Label text field.
- 3 Locate the Study Settings section. 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

I 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 Viscosity Depending on Concentration/Solution 3 (sol3).

Velocity (Concentration Dependent)

- I In the Model Builder window, right-click Velocity (spf) and choose Duplicate.
- 2 In the Settings window for 3D Plot Group, type Velocity (Concentration Dependent) in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Mirror 3D 2.
- **4** Click the **Zoom Extents** button in the **Graphics** toolbar.
- 5 In the Velocity (Concentration Dependent) toolbar, click **Plot**.
- 6 Click the Show Grid button in the Graphics toolbar.

Concentration, Slice (IE-10, Concentration Dependent) I

- I In the Model Builder window, right-click Concentration, Slice (IE-10) and choose Duplicate.
- 2 In the Settings window for 3D Plot Group, type Concentration, Slice (1E-10, Concentration Dependent) 1 in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Mirror 3D 2.
- 4 In the Concentration, Slice (IE-10, Concentration Dependent) I toolbar, click 🕥 Plot.
- 5 Click the Show Grid button in the Graphics toolbar.