

# Introduction to Microfluidics Module



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# The Microfluidics Module

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The Microfluidics Module is used by engineers and scientists to understand, predict, and design microfluidic systems. The use of simulation tools in the design cycle is becoming more widespread as they can improve understanding, reduce prototyping costs, and speed up development. The Microfluidics Module allows users to quickly and accurately model single-phase flows, multiphase flows, flow through porous media, electrokinetic flows, and slightly rarefied gas flows.

The Microfluidics Module can solve stationary and time-dependent flows in two-dimensional and three-dimensional spaces. Formulations suitable for different types of flow are set up as predefined user interfaces, referred to as Microfluidics interfaces. The fluid-flow interfaces use physical quantities, such as pressure and flow rate, and physical properties, such as viscosity and density, to define a fluid-flow problem. Different interfaces are available to cover a range of microfluidic flows. Examples include: laminar flow, creeping flow, two-phase flow (phase field, level set, and moving mesh), porous media flow (Darcy's Law, the Brinkman equations, or Free and Porous Media Flow—which combines the Brinkman equations with laminar flow) and slip flow. The transport of multiple species can also be treated with the Transport of Diluted Species interface. These physics interfaces can easily be coupled with, for example, COMSOL's Electrostatics or Electric Currents user interfaces to solve multiphysics problems such as electrokinetic flows.

For each of the Microfluidics interfaces, the underlying physical principles are expressed in the form of partial differential equations, together with corresponding initial and boundary conditions. COMSOL's design emphasizes the physics by providing users with the equations solved by each feature and offering the user full access to the underlying equation system. There is also tremendous flexibility to add user-defined equations and expressions to the system. For example, to model the transport of a species that significantly affects the viscosity of the fluid, simply type in concentration-dependent viscosity—no scripting or coding is required (this is demonstrated in the tutorial example on page 16). When COMSOL compiles the equations the complex couplings generated by these user-defined expressions are automatically included in the equation system. The equations are then solved using the finite element method and a range of industrial-strength solvers. Once a solution is obtained a vast range of postprocessing tools are available to interrogate the data, and predefined plots are automatically generated to show the device response. COMSOL offers the flexibility to evaluate a wide range of physical quantities including predefined quantities such as the pressure, velocity, shear rate, or the vorticity (available through easy-to-use menus), as well as arbitrary user-defined expressions.

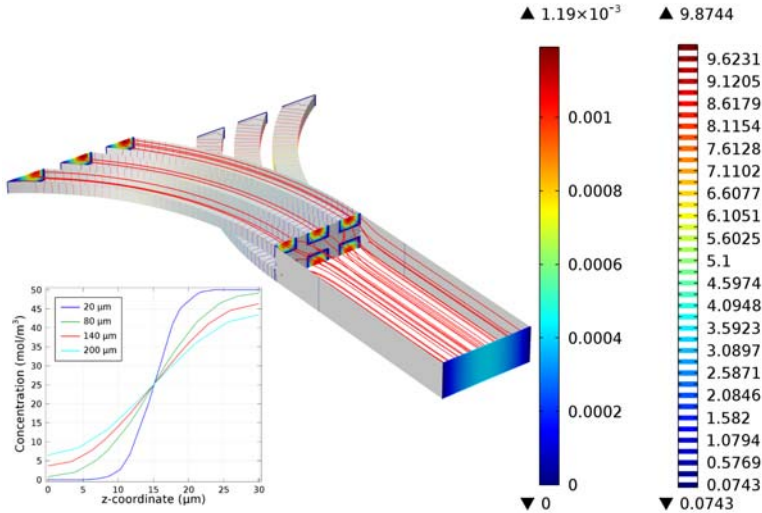
To model a microfluidic device the geometry is first defined in the software. Then appropriate materials are selected and a suitable Microfluidics interface is added. Initial conditions and boundary conditions are set up within the interface. Next, the mesh is defined—in many cases COMSOL’s default mesh, which is produced from physics-dependent defaults, will be appropriate for the problem. A solver is selected, again with defaults appropriate for the relevant physics, and the problem is solved. Finally the results are visualized. All these steps are accessed from the COMSOL Desktop.

## Microfluidic Devices: Physics and Applications

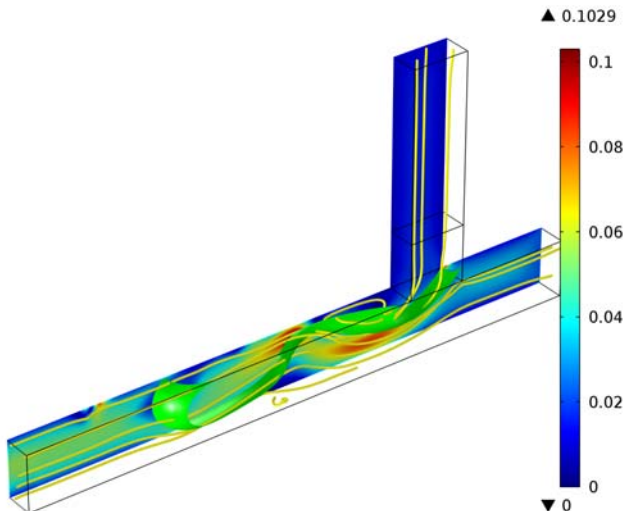
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Microfluidic flows occur on length scales that are orders of magnitude smaller than macroscopic flows. Manipulation of fluids at the microscale has a number of advantages—typically microfluidic systems are smaller, operate faster, and require less fluid than their macroscopic equivalents. Energy inputs and outputs are also easier to control (for example, heat generated in a chemical reaction) because the surface-to-area volume ratio of the system is much greater than that of a macroscopic system.

In general, as the length scale ( $L$ ) of the fluid flow is reduced, properties that scale with the surface area of the system become comparatively more important than those that scale with the volume of the flow. This is apparent in the fluid flow itself as the viscous forces, which are generated by shear over the isovelocity surfaces (scaling as  $L^2$ ), dominate over the inertial forces (which scale volumetrically as  $L^3$ ). The Reynolds number ( $Re$ ), which characterizes the ratio of these two forces, is typically low, so the flow is usually laminar ( $Re < 1000$ ). In many cases the creeping (Stokes) flow regime applies ( $Re < 1$ ). Laminar and creeping flows make mixing particularly difficult, so mass transport is often diffusion limited. The diffusion time scales as  $L^2$ , but even in microfluidic systems diffusion is often a slow process. This has implications for chemical transport within microfluidic systems. The figure below shows flow in a device designed to enhance the mixing of two fluids in a lamella flow. Pressure contours are shown on the walls of the mixer, and the velocity magnitude is shown at the inlets and outlets of the mixer as well as at the point where the two sets of channels (carrying different fluids) converge. Streamlines (in red) are also plotted. The inset shows the concentration of a diffusing species present in only one of the fluids. It is plotted along vertical lines located progressively further down the center of the mixer.



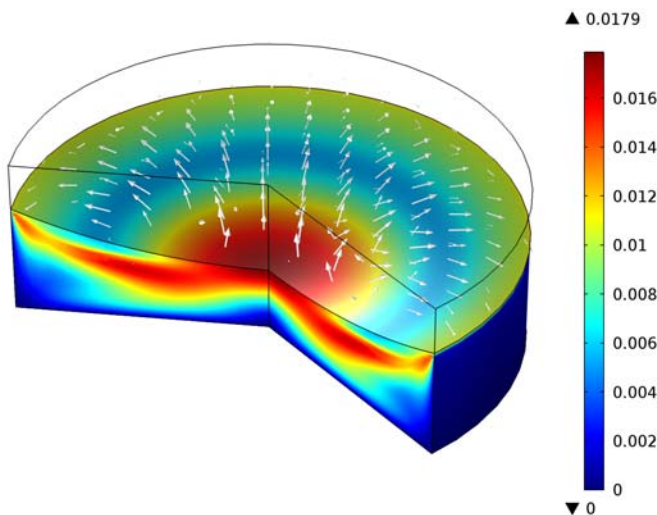
When multiple phases are present, surface tension effects become important relative to gravity and inertia at small length scales. The Laplace pressure (the pressure jump across a two phase boundary), capillary force, and Marangoni forces all scale as  $1/L$ . The figure below shows the break up of oil droplets to produce an emulsion as the oil flows into a channel carrying a second fluid. Velocity streamlines are shown and the fluid velocity is plotted on the symmetry plane. The two-phase boundary is shown in green.





Flow through porous media can also occur on microscale geometries. Because the permeability of a porous media scales as  $L^2$  (where  $L$  is the average pore radius) the flow is often friction dominated when the pore size is in the micron range and Darcy's law can be used. For intermediate flows this module also provides a user interface to model flows where Brinkman equation is appropriate.

At the microscale a range of electrohydrodynamic effects can be exploited to influence the fluid flow. The electric field strength for a given applied voltage scales as  $1/L$ , making it easier to apply relatively large fields to the fluid with moderate voltages. In electroosmosis the uncompensated ions in the charged electric double layer (EDL) present on the fluid surfaces are moved by an electric field, causing a net fluid flow. Electrophoretic and dielectrophoretic forces on charged or polarized particles in the fluid can be used to induce particle motion, as can diamagnetic forces in the case of magnetophoresis. The manipulation of contact angles by the electrowetting phenomena is also easy in microscale devices, a phenomenon that has been exploited as a basis for various new display technologies. The figure below shows an adjustable focus liquid lens, whose radius of curvature can be adjusted using the electrowetting effect. The colors show the fluid velocity magnitude in a lower, oil filled part of the lens and the arrow plot shows the velocity in the liquid above the oil lens.



As the length scale of the flow becomes comparable to intermolecular length scale more complex kinetic effects become important. For gases the ratio of the molecular mean free path to the flow geometry size is given by the Knudsen number ( $Kn$ ). Clearly,  $Kn$  scales as  $1/L$ . For  $Kn < 0.01$  fluid flow is usually well

described by the Navier-Stokes equations with no-slip boundary conditions. In the slip flow regime ( $0.01 < Kn < 0.1$ ) appropriate slip boundary conditions can be used with the Navier-Stokes equations to describe the flow away from the boundary. The Microfluidics Module includes an interface to deal with these slightly rarefied gas flows: the Slip Flow interface. For more highly rarefied flows the Molecular Flow Module should be used.

# The Microfluidics Module Physics Guide

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The Microfluidics physics interfaces are used to set up a simulation problem. Each physics interface expresses the relevant physical phenomena in the form of sets of partial or ordinary differential equations, together with appropriate boundary and initial conditions. Each feature added to the interface represents a term or condition in the underlying equation set. These features are usually associated with a geometric entity within the model, such as a domain, boundary, edge (for 3D models), or point. Figure 1 uses the Lamella Mixer model (found in the Microfluidics Module Model Library) to show the Model Builder and the settings window for the selected Fluid Properties 1 feature node. This node adds the Navier-Stokes equations to the simulation within the domains selected. Under the Fluid Properties section lists indicate that the fluid density and viscosity are inherited from the material properties assigned to the domain. The material properties can be set up as functions of dependent variables in the model, for example, temperature and pressure. The wall, inlet, symmetry, and outlet boundary conditions are also highlighted in the model tree. The Wall boundary condition is applied by default to all surfaces in the model and adds a no-slip constraint to the flow. The inlet and outlet features include a range of options to allow fluid to enter or leave the simulation domain.

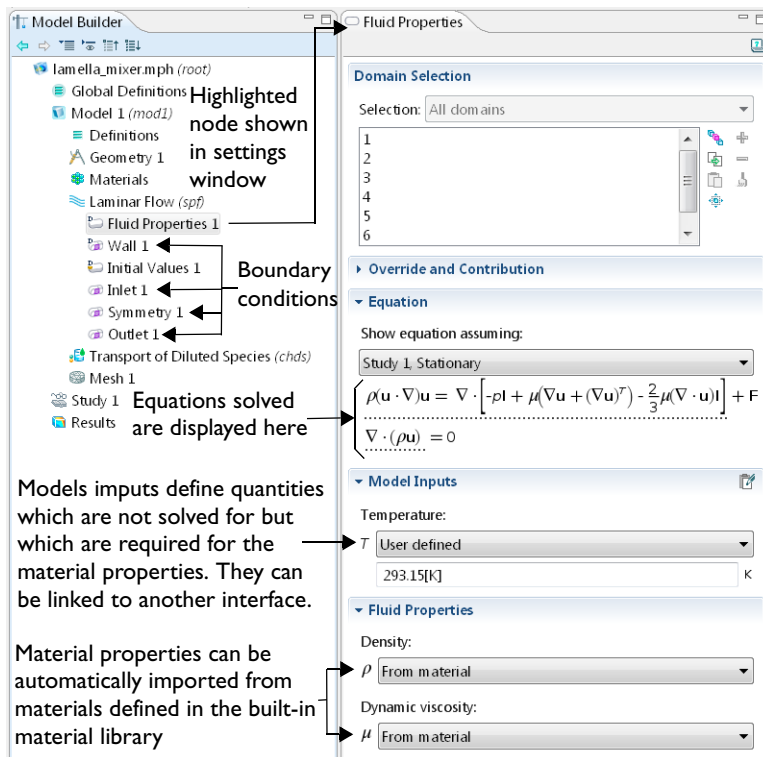


Figure 1: The Model Builder (to the left), and the Fluid Properties I settings window for the selected feature node (to the right). The Equation section in the settings window shows the model equations. The terms added to the equation system by the feature are underlined with a dotted line.


The Microfluidics Module includes a number of interfaces for modeling different types of microfluidic device. When a new model is started, these interfaces are selected from the Model Wizard. Figure 2 shows the Model Wizard with the physics interfaces included with the Microfluidics Module highlighted. Also see “Physics List by Space Dimension and Preset Study Type” on page 13. Below, a brief overview of each of the Microfluidics Module physics interfaces is given.


- AC/DC
- Acoustics
- Chemical Species Transport
  - Transport of Diluted Species (chds)
  - Species Transport in Porous Media (chpm)
- Fluid Flow
  - Single-Phase Flow
    - Laminar Flow (spf)
    - Creeping Flow (spf)
  - Multiphase Flow
    - Two-Phase Flow, Level Set
      - Laminar Two-Phase Flow, Level Set (tpf)
    - Two-Phase Flow, Phase Field
      - Laminar Two-Phase Flow, Phase Field (tpf)
    - Two-Phase Flow, Moving Mesh
      - Laminar Two-Phase Flow, Moving Mesh (tpfmm)
  - Porous Media and Subsurface Flow
    - Brinkman Equations (br)
    - Darcy's Law (dl)
    - Free and Porous Media Flow (fp)
  - Rarefied Flow
    - Slip Flow (slpf)
    - Transitional Flow (tran)
- Heat Transfer
- Structural Mechanics
- Mathematics
  - PDE Interfaces
    - ODE and DAE Interfaces
  - Optimization and Sensitivity
  - Classical PDEs
    - Moving Interface
      - Level Set (ls)
      - Phase Field (pf)
    - Deformed Mesh
    - Wall Distance (wd)

Figure 2: The Microfluidics Module physics interfaces as displayed in the Model Wizard. Note that this is for 3D models.




## SINGLE-PHASE FLOW

Microfluidic flows usually occur at low Reynolds numbers. The Reynolds number ( $Re$ ) is a measure of the ratio of the fluid viscous to the inertial forces acting on the fluid and is given by:  $Re = \rho UL / \mu$ , where  $\rho$  is the fluid density,  $U$  is a characteristic velocity,  $L$  is a characteristic length scale, and  $\mu$  is the dynamic viscosity.


The Laminar Flow interface () applies when the Reynolds number is less than approximately 1000. The interface solves the Navier-Stokes equations, for incompressible and weakly compressible flows (weakly compressible implies that the Mach number ( $Ma$ ), given by  $Ma = U/c$ , where  $c$  is the velocity of sound in the fluid, is less than 0.3). This fluid-flow interface also allows for simulation of non-Newtonian fluid flow.


The Creeping Flow interface () approximates the Navier-Stokes equations for the case when the Reynolds number is significantly less than 1. This is often referred to as Stokes flow and is appropriate for use when viscous flow is dominant. It is usually applicable for microfluidic devices.


## MULTIPHASE FLOW

The Two-Phase Flow, Level Set interface () , the Two-Phase Flow, Phase Field interface () , and the Two Phase Flow, Moving Mesh interface () are used to model two fluids separated by a fluid interface. The moving interface is tracked in detail using either the level set method, the phase field method, or by a moving mesh, respectively. The level set and phase field methods use a fixed mesh and solve additional equations to track the interface location. The moving mesh method solves the Navier Stokes equations on a moving mesh with boundary conditions to represent the interface. In this case equations must be solved for the mesh deformation. These interfaces support both compressible (Mach number,  $Ma < 0.3$ ) and incompressible laminar flows, where one or both fluids can be non-Newtonian.

## POROUS MEDIA AND SUBSURFACE FLOW


The Brinkman Equations interface () models flow through a porous medium where shear stresses cannot be neglected. The physics interface supports both the Stokes-Brinkman formulation, suitable for very low flow velocities, and Forchheimer drag, which is used to account for effects at higher velocities. The fluid can be either incompressible or compressible, provided that the Mach number is less than 0.3.

The Darcy's Law interface () models relatively slow flows through porous media. Shear stresses perpendicular to the flow are neglected.




The Free and Porous Media Flow interface () models both porous media (using the Brinkman Equations) and laminar flow, automatically providing the coupling between them.

These interfaces are appropriate for microfluidic porous media flow. Example applications include paper microfluidics and transport in biological tissue.

## TRANSPORT OF DILUTED SPECIES

The Transport of Diluted Species interface () simulates chemical species transport through diffusion, convection (when coupled to fluid flow), and migration in electric fields for mixtures where one component, a solvent, is present in excess (90 mol% or greater). It is typically employed to model the performance of mixers. For modeling chemical reactions in microfluidic devices the chemical reaction engineering module is recommended.

## RAREFIED GAS FLOWS

Rarefied gas flow occurs when the mean free path,  $\lambda$ , of the molecules becomes comparable with the length scale of the flow,  $L$ . The Knudsen number,  $Kn = \lambda/L$ , characterizes the importance of rarefaction effects on the flow. As the gas becomes rarefied (corresponding to increasing Knudsen number), the Knudsen layer, which is present within one mean free path of the wall, begins to have a significant effect on the flow. For Knudsen numbers below 0.01 rarefaction can be neglected, and the Navier Stokes equations can be solved with non-slip boundary conditions (the Laminar Flow () or Creeping Flow () interfaces can be used in this instance). For slightly rarefied gases ( $0.01 < Kn < 0.1$ ), the Knudsen layer can be modeled by appropriate boundary conditions at the walls together with the continuum Navier-Stokes equations in the domain. In this instance the Slip Flow interface () is appropriate. To model higher Knudsen numbers the Molecular Flow Module is required. The figure below shows how high Knudsen numbers can be obtained either by reducing the size of the geometry, or by reducing the pressure or number density of the gas.

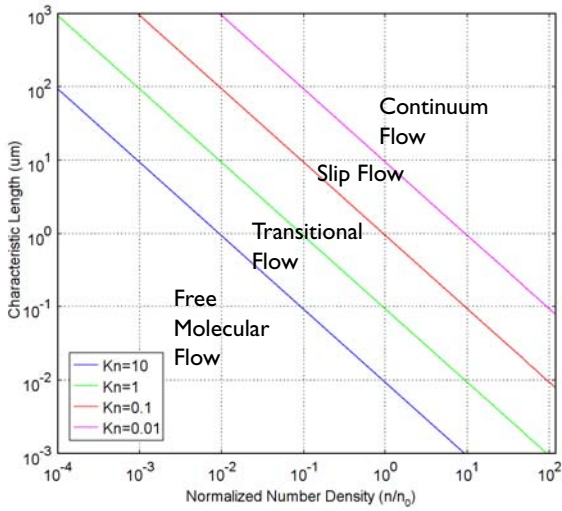




















Figure 3: Plot showing the main fluid flow regimes for rarefied gas flows. Different regimes are separated by lines of constant Knudsen number. The number density of the gas is normalized to the number density of an ideal gas at a pressure of 1 atmosphere and a temperature of 0° C ( $n_0$ ).



## Physics List by Space Dimension and Preset Study Type

The table below lists the physics interfaces available specifically with this module in addition to the COMSOL Multiphysics basic license.

Physics	Icon	Tag	Space Dimension	Available Preset Study Type
<b>Chemical Species Transport</b>				
Transport of Diluted Species*		chds	all dimensions	stationary; time dependent
Species Transport in Porous Media		chpm	all dimensions	stationary; time dependent
<b>Fluid Flow</b>				
<i>Single-Phase Flow</i>				
Laminar Flow*		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Creeping Flow		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
<b>Multiphase Flow</b>				
<i>Two-Phase Flow, Level Set</i>				
Laminar Two-Phase Flow, Level Set		tpf	3D, 2D, 2D axisymmetric	transient with initialization
<i>Two-Phase Flow, Phase Field</i>				
Laminar Two-Phase Flow, Phase Field		tpf	3D, 2D, 2D axisymmetric	transient with initialization
<i>Two-Phase Flow, Moving Mesh</i>				
Laminar Two-Phase Flow, Moving Mesh		tpfmm	3D, 2D, 2D axisymmetric	time dependent
<b>Porous Media and Subsurface Flow</b>				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent


Physics	Icon	Tag	Space Dimension	Available Preset Study Type
Free and Porous Media Flow		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
 <b>Rarefied Flow</b>				
Slip Flow		slpf	3D, 2D, 2D axisymmetric	stationary; time dependent
 <b>Heat Transfer</b>				
Heat Transfer in Porous Media		ht	all dimensions	stationary; time dependent
 <b>Mathematics</b>				
 <b>Moving Interface</b>				
Level Set		ls	all dimensions	transient with initialization
Phase Field		pf	all dimensions	time dependent; transient with initialization


\* This is an enhanced interface, which is included with the base COMSOL package but has added functionality for this module.

# The Model Library



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The Microfluidics Module Model Library illustrates the Microfluidics interfaces and the available features using tutorial examples. These examples include analyses of existing Microfluidic devices, tutorial models and benchmark models.

To open any Microfluidics Module model, select View>Model Library  from the main menu in COMSOL Multiphysics. In the Model Library window that opens, expand the Microfluidics Module folder and browse or search the contents of the folders. Click Open Model and PDF to open both the model in COMSOL Multiphysics and a PDF to read background theory including the step-by-step instructions on how to build it.

The Model Library is updated on a regular basis by COMSOL in order to add new models and to improve existing models. Choose View>Model Library Update  to update the model library.

The MPH-files in the COMSOL model libraries can have two formats—Full MPH-files or Compact MPH-files.

- Full MPH-files, including all meshes and solutions. In the Model Library these models appear with the  icon. If the MPH-file's size exceeds 25MB, a tip with the text “Large file” and the file size appears when you position the cursor at the model's node in the Model Library tree.
- Compact MPH-files with all settings for the model but without built meshes and solution data to save space on the DVD (a few MPH-files have no solutions for other reasons). You can open these models to study the settings and to mesh and re-solve the models. It is also possible to download the full versions—with meshes and solutions—of most of these models through Model Library Update. In the Model Library these models appear with the  icon. If you position the cursor at a compact model in the Model Library window, a No solutions stored message appears. If a full MPH-file is available for download, the corresponding node's context menu includes a Model Library Update item.

A model from the Model Library is used as a tutorial in this guide. See “Tutorial Example: A Controlled Diffusion Micromixer” on page 16.

# Tutorial Example: A Controlled Diffusion Micromixer<sup>1</sup>

This example 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 4. 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 transport of species between streams A and B should take place only by diffusion in order that species with low diffusion coefficients stay in their respective streams.

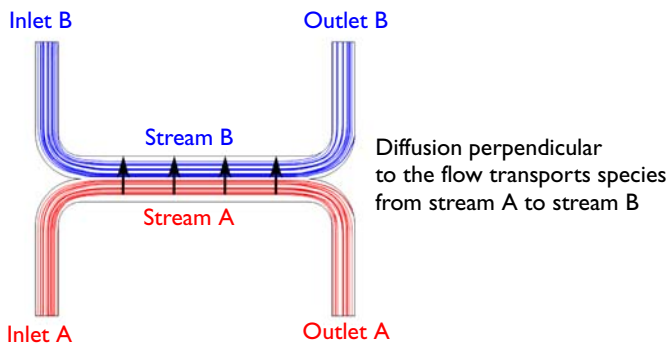


Figure 4: Device concept.

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:

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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.

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

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:

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

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

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

In this example, 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 is required when solving Fick's equation. COMSOL automatically includes the stabilization by default, so no explicit settings are required.

The example is solved in two stages:

- 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.

The geometry of the device is shown in Figure 5. 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 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.

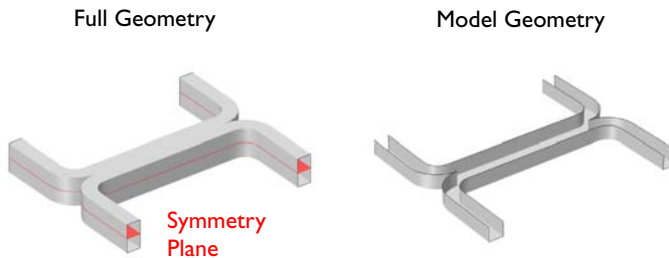










Figure 5: Left: Device geometry showing symmetry plane. Right: Model geometry. Only half of the device needs to be simulated, as the flow is symmetric about the midplane.

## Model Wizard


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- 1 Double-click the COMSOL Multiphysics icon on the desktop.
- 2 In the Model Wizard, the default Space Dimension selected is 3D. Click Next .
- 3 On the Add Physics page, under Fluid Flow>Single-Phase Flow, double-click Creeping Flow (spf)  to add it to the Selected physics list. You can also click the Add Selected button  or right-click and choose  Add Selected.
- 4 Under Chemical Species Transport, double-click Transport of Diluted Species (chds) .
- 5 Click Next .
- 6 On the Studies window under Preset Studies, click Stationary .
- 7 Click Finish .

## Geometry 1

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For many microfluidic devices it is convenient to specify the geometry dimensions using micrometers. Since the device is symmetric, it is only necessary to model half of it.

- 1 In the Model Builder, under Model 1 click Geometry 1 .
- 2 In the Geometry settings window, locate the Units section.
- 3 From the Length unit list, choose  $\mu\text{m}$ .



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

- 4 Right-click Model 1>Geometry 1  and choose Work Plane .




### *Rectangle 1*

- 1 In the Model Builder, 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 field, enter 140.
- 4 In the Height field, enter 60.
- 5 Click the Build Selected button .



### *Rectangle 2*

- 1 In the Model Builder, 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 field, enter 120.
- 4 In the Height field, enter 50.
- 5 Locate the Position section. In the xw field, enter 10.
- 6 In the yw field, enter 10.
- 7 Click the Build Selected button .



### *Difference 1*

- 1 In the Model Builder, under Model 1>Geometry 1>Work Plane 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 In the Model Builder, under Model 1>Geometry 1>Work Plane 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 field, enter 10.
- 5 Click the Build Selected button .

### *Fillet 2*




- 1 In the Model Builder, under Model 1>Geometry 1>Work Plane 1 right-click Plane Geometry  and choose Fillet.
- 2 On the object fill, select Points 1 and 9 only.
- 3 In the Fillet settings window, locate the Radius section.
- 4 In the Radius field, enter 20.
- 5 Click the Build Selected button .

### *Mirror 1*

- 1 In the Model Builder, under Model 1>Geometry 1>Work Plane 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.
- 4 Select the Keep input objects check box.
- 5 Locate the Normal Vector to Line of Reflection section. In the xw field, enter 0.
- 6 In the yw field, enter 1.
- 7 Click the Build Selected button .





### Union 1

- 1 In the Model Builder, under Model 1>Geometry 1>Work Plane 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 .

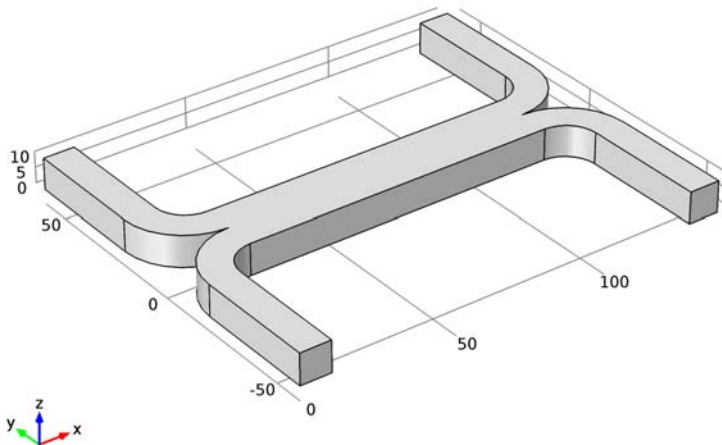
### Extrude 1

Extrude the 2D geometry to create a 3 dimensional geometry.

- 1 In the Model Builder, under Model 1>Geometry 1 right-click Work Plane 1  and choose Extrude .
- 2 In the Extrude settings window, locate the Distances from Plane section.
- 3 In the table, enter the following settings:

DISTANCES ( $\mu\text{m}$ )
10

- 4 Click the Build Selected button .





## Global Definitions

---

### Parameters

Create parameters to define the model.

- 1 In the Model Builder, right-click Global Definitions  and choose Parameters .
- 2 In the Parameters settings window, locate the Parameters section.
- 3 In the table, enter the following settings:


NAME	EXPRESSION	DESCRIPTION
D	$5e-11$ [m <sup>2</sup> /s]	Diffusion constant
fr	15 [pl/s]	Inlet flow rate
c0	1 [mol/m <sup>3</sup> ]	Inlet concentration
alpha	$0.5$ [(m <sup>3</sup> /mol) <sup>2</sup> ]	Viscosity c <sup>2</sup> -term prefactor


## Definitions

---

### Average I

Create an average operator to compute the mean output concentration.

- 1 In the Model Builder, under Model 1 right-click Definitions  and choose Model Couplings>Average.
- 2 In the Average settings window, locate the Source Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 22 only.



Note that there are several methods to select a geometric entity. To select, for example, a boundary, left click in the geometry until the required boundary is highlighted, then right click. Alternatively, in the View menu, choose Selection list  to display a list of the available boundary numbers. Once again boundaries are added to the selection by first left clicking and then right clicking the item in the list. For more information about selecting geometric entities in the Graphics window, see the *COMSOL Multiphysics Reference Manual*.

## Materials

---

Add material properties to the model.

### Material 1


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


PROPERTY	NAME	VALUE
Density	rho	1000
Dynamic viscosity	mu	1e-3

## Creeping Flow

---



Since we are dealing with a liquid flow we can set the flow type to incompressible.

- 1 In the Model Builder, under Model 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 indicates these default nodes.

### Inlet 1




Add a laminar flow inlet boundary condition.

- 1 In the Model Builder, right-click Creeping Flow  and choose the boundary condition 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  $V_0$  field, enter  $fr/2$ . The flow rate is set to one half of the parameter value, since only half of the geometry is modeled.

7 In the  $L_{\text{entr}}$  field, enter 100[um].


The entrance length should be set to a value large enough for a laminar flow to develop.

### *Inlet 2*

- 1 Right-click Model 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.



### *Outlet 1*

Add an outlet with a pressure boundary condition.

- 1 In the Model Builder, right-click Creeping Flow  and choose the boundary condition Outlet.
- 2 Select Boundaries 20 and 22 only. The default pressure of 0 Pa is appropriate in this case.

### *Symmetry 1*

Add a symmetry boundary condition in the symmetry plane.

- 1 In the Model Builder, right-click Creeping Flow  and choose the boundary condition Symmetry .
- 2 Select Boundary 4 only.

## **Transport of Diluted Species**

---

Now set up the mass transport physics.

### *Convection and Diffusion 1*

Use the computed velocity field for the species convection.

- 1 In the Model Builder, 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 **u** list, choose Velocity field (spf/fp1).

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


4 Locate the Diffusion section. In the  $D_c$  field, enter D.

### *Concentration 1*

Specify the concentration at the two inlets.


- 1 In the Model Builder, right-click Transport of Diluted Species and choose the boundary condition 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  $c_{0,c}$  field, enter c0.

### *Concentration 2*

- 1 In the Model Builder, right-click Transport of Diluted Species and choose the boundary condition 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.

### *Outflow 1*

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


- 1 In the Model Builder, right-click Transport of Diluted Species and choose the boundary condition Outflow .
- 2 In the Outflow settings window, locate the Boundary Selection section.
- 3 Select Boundaries 20 and 22.

## Mesh 1


---

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

### *Free Quad 1*

- 1 In the Model Builder, under Model 1 right-click Mesh 1  and choose More Operations>Free Quad.
- 2 Select Boundary 4 only.

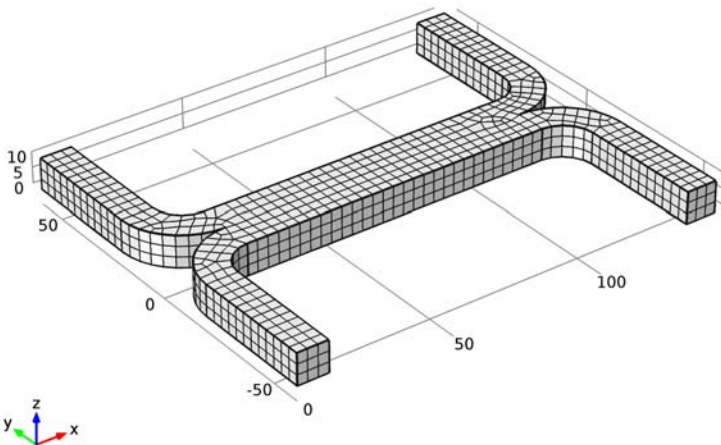
### *Size*

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






## Study 1

---

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.



- 1 In the Model Builder, click Study 1 .
- 2 In the Study settings window, locate the Study Settings section.
- 3 Clear the Generate default plots check box. Since the study will automatically generate a large number of default plots, default plots are disabled.
- 4 For step 1, solve only the creeping flow problem.

### Step 1: Stationary



- 1 In the Model Builder, under Study 1 click Step 1: Stationary .
- 2 In the Stationary settings window, under Physics and Variables Selection, click the Transport of Diluted Species row in the Physics column. In the table, click the Solve for column and click to change the check mark  to an  to remove the physics interface from Study 1.

Add a second study step.

### Step 2: Stationary 2

- 1 In the Model Builder, right-click Study 1  and choose Study Steps>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, under Physics and Variables Selection, click the Creeping Flow row in the Physics column. In the table, click the Solve for column and click to change the check mark  to an  to remove the physics interface from Study 1.
- 3 Click to expand the Values of Dependent Variables section. Select the Values of variables not solved for check box.
- 4 From the Method list, choose Solution.
- 5 From the Study list, choose Study 1: Stationary.

Solve the diffusion problem for three values of the diffusion coefficient.

- 6 In the Stationary settings window, click to expand the Study Extensions section.
- 7 Select the Continuation check box.

8 Click Add .

9 In the table, enter the following settings:

CONTINUATION PARAMETER	PARAMETER VALUE LIST
D (Diffusion constant)	1e-10 5e-11 1e-11


10 In the Model Builder, right click Study 1  and select Compute .

## Results

---





### Data Sets



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

- 1 In the Model Builder, under Results right-click Data Sets  and choose Surface.
- 2 In the Surface settings window, locate the Selection section.
- 3 From the Selection list, choose Manual.
- 4 Select Boundaries 1, 3, 5–7, 9–19, 21, 23, and 24 only.

### 3D Plot Group 1

First plot the velocity of the flow within the channel.

- 1 In the Model Builder, right-click Results  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, 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, 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 field, enter 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. 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 field, enter 2.

Use the arrow volume plot to visualize the flow direction.

**16** In the Model Builder, right-click 3D Plot Group 1  and choose Arrow Volume.

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

**18** Find the x grid points subsection. In the Points field, enter 14.

**19** Find the y grid points subsection. In the Points field, enter 21.

**20** Find the z grid points subsection. In the Points field, enter 3.



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

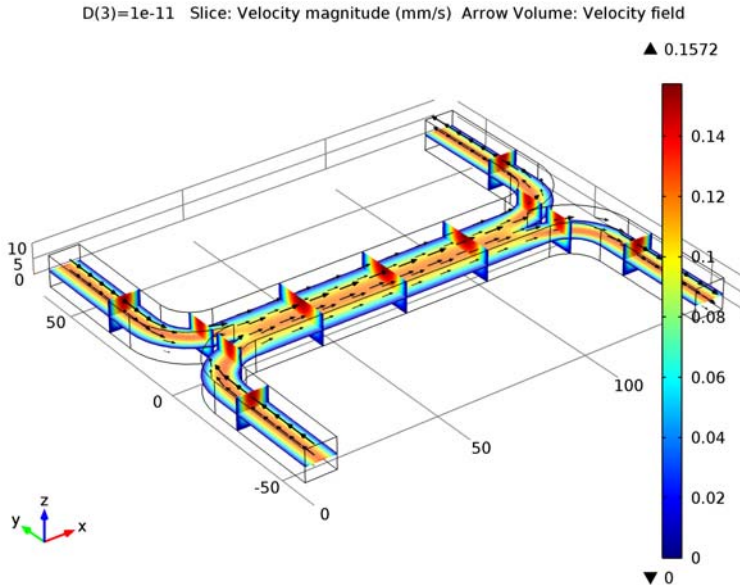
Rename the plot.

**22** In the Model Builder, right-click 3D Plot Group 1  and choose Rename .

**23** Go to the Rename 3D Plot Group dialog box and enter `Velocity (uncoupled flow)` in the New name field.



**24** Click OK.

**25** Right-click 3D Plot Group 1  and choose Plot .



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

### 3D Plot Group 2

1 Right-click Results  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 field, enter 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.

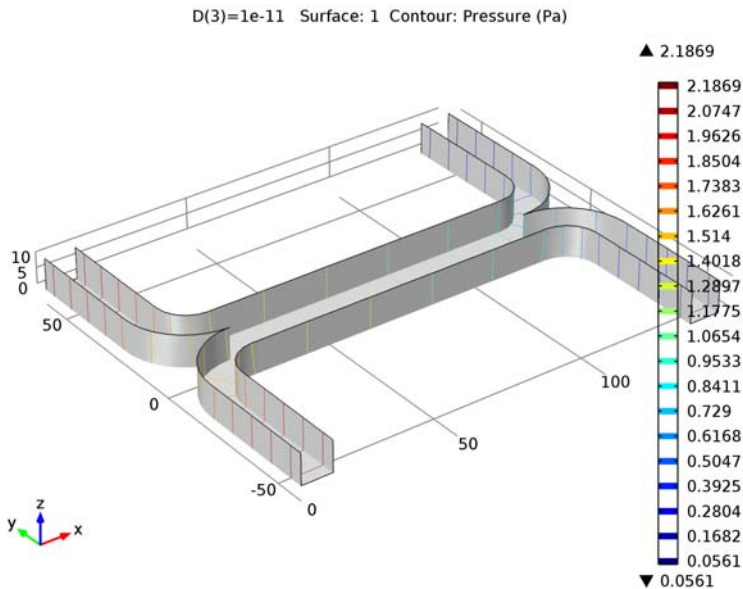
9 In the Model Builder, right-click 3D Plot Group 2  and choose Contour.

10 In the Contour settings window, click Replace Expression  in the upper-right corner of the Expression section. From the menu, choose Creeping Flow>Pressure (p).

Finally rename the plot.


11 In the Model Builder, right-click 3D Plot Group 2  and choose Rename .

- 12 Go to the Rename 3D Plot Group dialog box and enter Pressure (uncoupled flow) in the New name field.
- 13 Click OK.
- 14 Right-click 3D Plot Group 2  and choose 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, under Results right-click Velocity (uncoupled flow) and choose Duplicate .

Re-name the plot.






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

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


- 4 Click OK.

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

### Concentration (uncoupled flow)

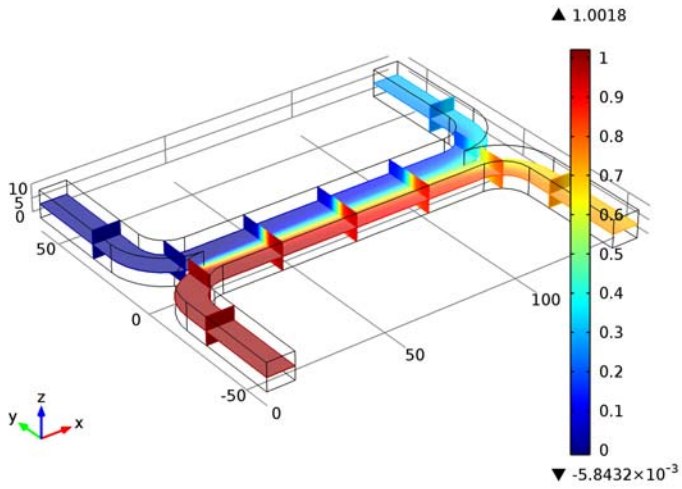
- 1 In the Model Builder, expand the Results>Concentration (uncoupled flow) node, then click Slice 1 .
- 2 In the Slice settings window, click Replace Expression  in the upper-right corner of the Expression section. From the menu, choose Transport of Diluted Species>Species c>Concentration (c).
- 3 In the Model Builder, under Results>Concentration (uncoupled flow) click Slice 2 .
- 4 In the Slice settings window, click Replace Expression  in the upper-right corner of the Expression section. From the menu, choose Concentration (c).
- 5 Repeat steps 3 and 4 for Slice 3 .

Disable the arrow volume plot.

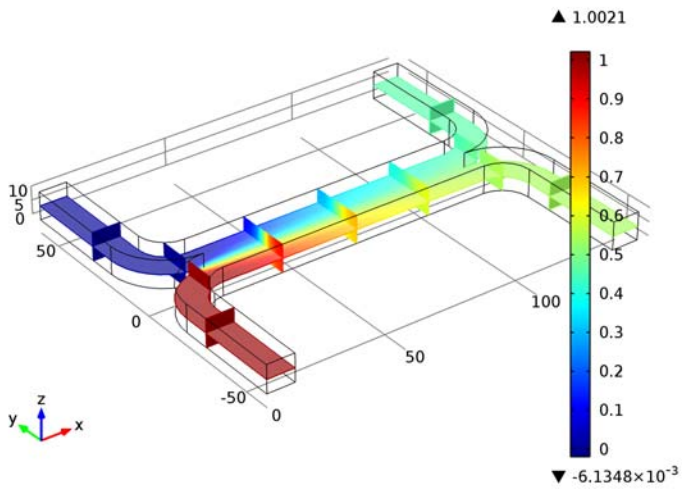
- 6 In the Model Builder, under Results>Concentration (uncoupled flow) right-click Arrow Volume 1 and choose Disable.
- 7 Right-click Concentration (uncoupled flow) and choose Plot.  
Look at the plot for each of the three diffusion coefficient levels.
- 8 In the Model Builder, click Concentration (uncoupled flow).
- 9 In the 3D Plot Group settings window, locate the Data section.
- 10 From the Parameter value (D) list, choose each of the values: 1e-11, 5e-11 and 1e-10, clicking the Plot button  after each selection.

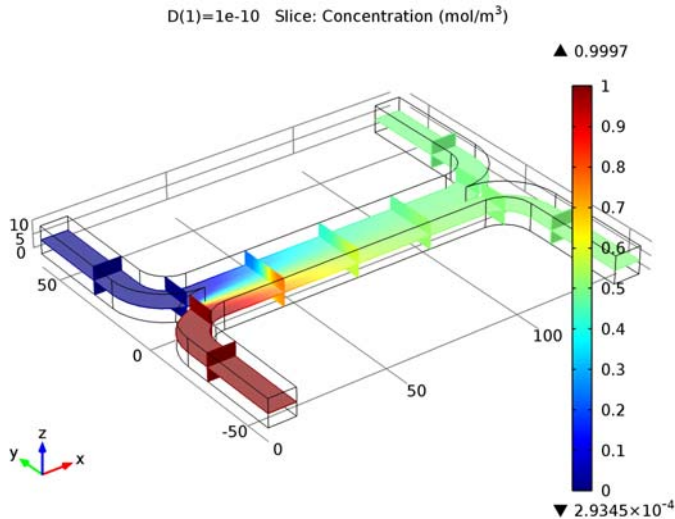
The plots on the next page show the results for each of the diffusion coefficients solved for. For the heaviest species, which has the smallest diffusivity, there is limited mixing between streams A and B. For the lightest species, which has the largest diffusion coefficient, the mixing is almost perfect.

D(3)=1e-11 Slice: Concentration (mol/m<sup>3</sup>)



D(2)=5e-11 Slice: Concentration (mol/m<sup>3</sup>)





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

#### 1D Plot Group 4

1 In the Model Builder, right-click Results and choose 1D Plot Group .

2 Right-click 1D Plot Group 4 and choose 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>	

5 Click to expand the Legends section. Clear the Show legends check box (no legend is necessary for this plot, as only one quantity is plotted).


Add a marker in the computed data points.

6 Click to expand 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. See *Using Special*





*Formats and Symbols in Titles* in the *Results Evaluation and Visualization Chapter* of the *COMSOL Multiphysics user guide* for further information.

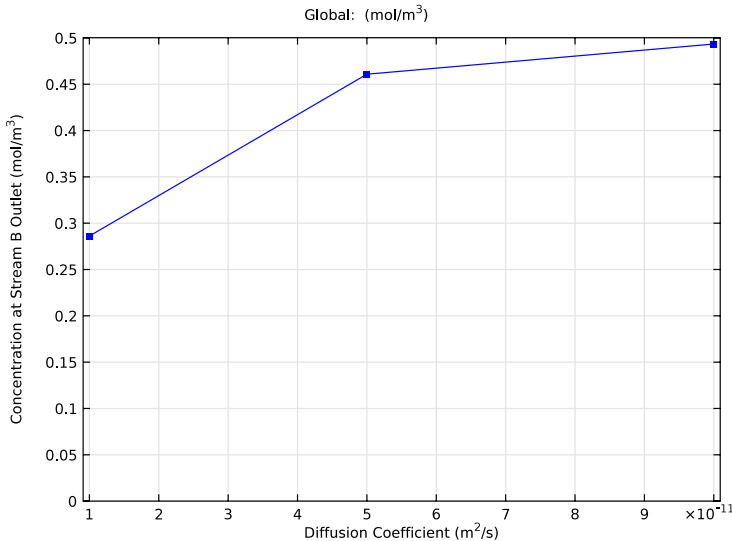
- 8 In the Model Builder, click 1D Plot Group 4 .
- 9 In the 1D Plot Group settings window, locate the Plot Settings section.
- 10 Select the x-axis label check box.
- 11 In the associated field, enter Diffusion Coefficient ( $\text{m}^2/\text{s}$ ).
- 12 Select the y-axis label check box.
- 13 In the associated field, enter Concentration at Stream B Outlet ( $\text{mol}/\text{m}^3$ ).

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 field, enter 0.
- 16 In the y maximum field, enter 0.5.

Finally re-name the plot.

- 17 Right-click 1D Plot Group 4  and choose Rename .
- 18 Go to the Rename 1D Plot Group dialog box and enter Output Concentration (uncoupled flow) in the New name field.
- 19 Click OK.
- 20 Right-click 1D Plot Group 4  and choose 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.

## Creeping Flow

---

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





### *Fluid Properties 1*

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

## Study 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:  $5\times 10^{-11} \text{ m}^2/\text{s}$ .

- 1 In the Model Builder, right-click the root node  and choose Add Study .
- 2 Go to the Model Wizard window.
- 3 Find the Studies subsection. In the tree, select Preset Studies for Selected Physics>Stationary .
- 4 Click Finish .

Turn off the default plot groups again.




- 5 In the Model Builder, click Study 2 .
- 6 In the Study settings window, locate the Study Settings section.
- 7 Clear the Generate default plots check box.
- 8 Click the Compute button .

## Results

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Add another surface data set that points to the new solution.

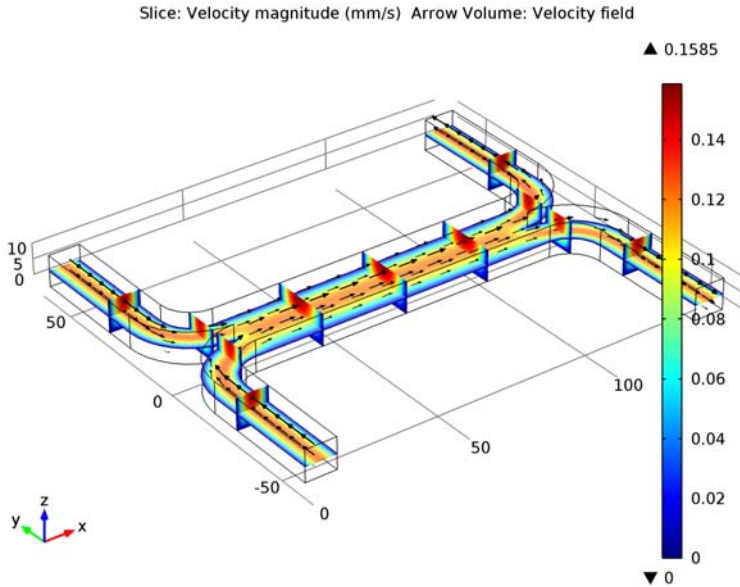
### *Data Sets*

- 1 In the Model Builder, 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 (uncoupled flow) 1*

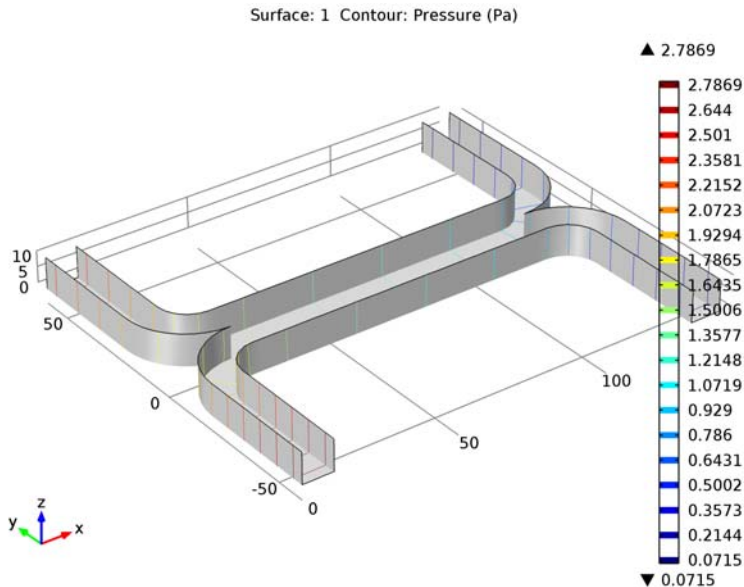
- 1 In the Model Builder, under Results right-click Velocity (uncoupled flow) and choose Duplicate .
- 2 In the 3D Plot Group settings window, locate the Data section.
- 3 From the Data set list, choose Solution 3.
- 4 Right-click Results>Velocity (uncoupled flow) 1 and choose Rename .
- 5 Go to the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

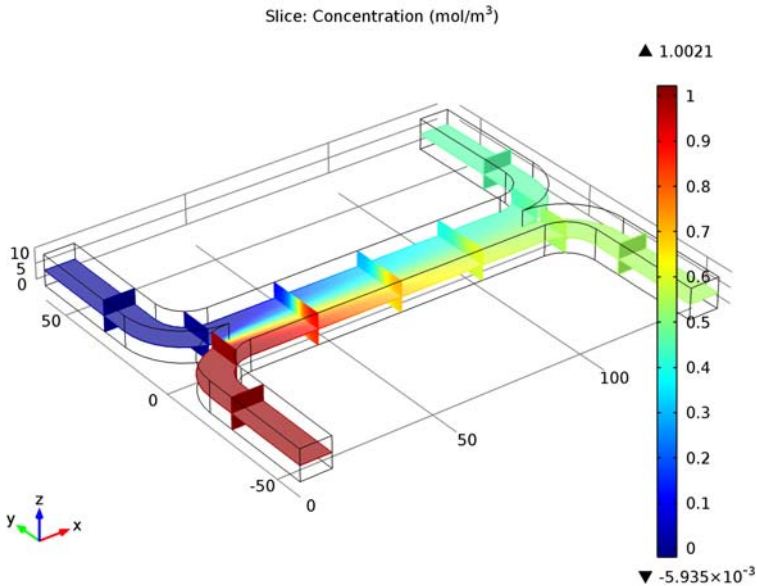
- 1 In the Model Builder, under Results right-click Pressure (uncoupled flow) and choose Duplicate .
- 2 In the 3D Plot Group settings window, locate the Data section.
- 3 From the Data set list, choose Surface 2.
- 4 Right-click Results>Pressure (uncoupled flow) 1 and choose Rename .
- 5 Go to the Rename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



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) 1*





- 1 In the Model Builder, 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) 1 and choose Rename .
- 5 Go to the Rename 3D Plot Group dialog box and enter Concentration (coupled flow) in the New name field.
- 6 Click OK.
- 7 Click the Plot button .



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 In the Model Builder, under Results right-click Data Sets  and choose Cut Plane .
- 2 In the Cut Plane settings window, locate the Plane Data section.
- 3 In the x-coordinates field, enter 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 In the Model Builder, right-click Results and choose 2D Plot Group .
- 2 In the 2D Plot Group settings window, locate the Data section.

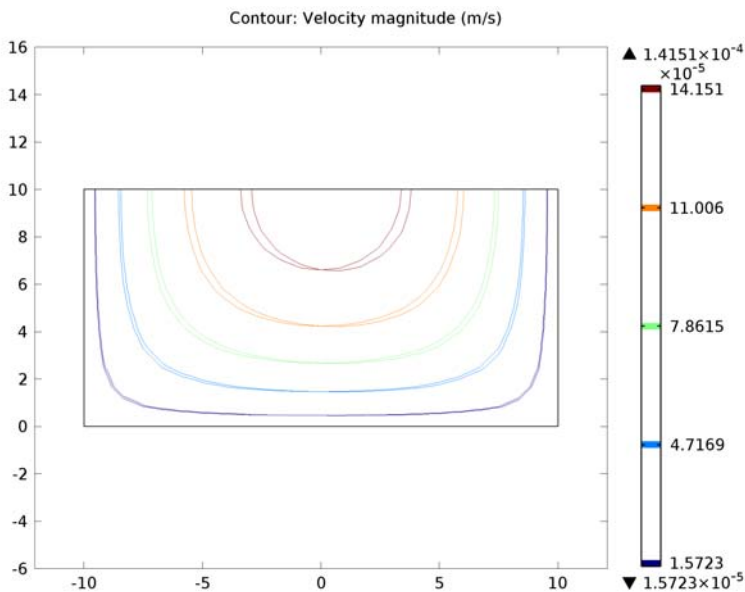
- 3 From the Data set list, choose Cut Plane 1.
- 4 From the Parameter value (D) list, choose 5e-11.
- 5 Right-click Results>2D Plot Group 8 and choose Contour.
- 6 In the Contour settings window, locate the Levels section.
- 7 In the Total levels field, enter 5.

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 Locate the Title section. From the Title type list, choose None.
- 12 Locate the Inherit Style section. From the Plot list, choose Contour 1.

Rename the plot.



- 13 In the Model Builder, right-click 2D Plot Group 8  and choose Rename .
- 14 Go to the Rename 2D Plot Group dialog box and enter Velocity Comparison in the New name field.
- 15 Click OK.
- 16 Right-click 2D Plot Group 8  and choose 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 In the Model Builder, under Results right-click Derived Values 8.85  
e-12 and choose Global Evaluation 8.85  
e-12.
- 2 In the Global Evaluation settings window, locate the Expression section.
- 3 In the Expression field, enter  $\text{aveop1}(c)$ .
- 4 Click the Evaluate button . When the diffusion coefficient is  $5 \times 10^{-11} \text{ m}^2/\text{s}$  the mean concentration at the outlet is  $0.463 \text{ mol}/\text{m}^3$ .
- 5 Right-click Results>Derived Values>Global Evaluation 1 8.85  
e-12 and choose Duplicate .
- 6 In the Global Evaluation settings window, locate the Data section.
- 7 From the Data set list, choose Solution 3.
- 8 Right-click Results>Derived Values>Global Evaluation 2 8.85  
e-12 and choose Evaluate>New Table. For the fully coupled problem, the mean outlet concentration is  $0.463 \text{ mol}/\text{m}^3$  for  $D=5 \times 10^{-11} \text{ m}^2/\text{s}$ .

No significant 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.