

# Introduction to Microfluidics Module





## Introduction to the Microfluidics Module

© 1998-2013 COMSOL

Protected by U.S. Patents 7,519,518; 7,596,474; and 7,623,991. Patents pending.

This Documentation and the Programs described herein are furnished under the COMSOL Software License Agreement (www.comsol.com/sla) and may be used or copied only under the terms of the license agreement.

COMSOL, COMSOL Multiphysics, Capture the Concept, COMSOL Desktop, and LiveLink are either registered trademarks or trademarks of COMSOL AB. All other trademarks are the property of their respective owners, and COMSOL AB and its subsidiaries and products are not affiliated with, endorsed by, sponsored by, or supported by those trademark owners. For a list of such trademark owners, see <a href="https://www.comsol.com/tm">www.comsol.com/tm</a>.

Version: May 2013 COMSOL 4.3b

# Contact Information

Visit the Contact Us page at <a href="www.comsol.com/contact">www.comsol.com/contact</a> to submit general inquiries, contact Technical Support, or search for an address and phone number. You can also visit the Worldwide Sales Offices page at <a href="www.comsol.com/contact/offices">www.comsol.com/contact/offices</a> for address and contact information.

If you need to contact Support, an online request form is located at the COMSOL Access page at www.comsol.com/support/case.

Other useful links include:

- Support Center: www.comsol.com/support
- Download COMSOL: www.comsol.com/support/download
- Product Updates: www.comsol.com/support/updates
- COMSOL Community: www.comsol.com/community
- Events: www.comsol.com/events
- COMSOL Video Center: www.comsol.com/video
- Support Knowledge Base: www.comsol.com/support/knowledgebase

Part No. CM021902

# Contents

The Microfluidics Module
Microfluidic Devices: Physics and Applications
The Microfluidics Module Physics Guide
Physics List by Space Dimension and Preset Study Type 13
The Model Library15
Tutorial Example: A Controlled Diffusion Micromixer

### The Microfluidics Module

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.

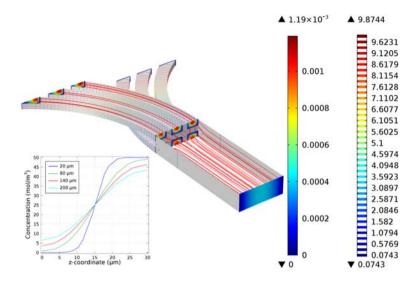
To model a microfluidic device the geometry is first defined in the software. Then appropriate materials are selected and a suitable Microfluidics interface is added. Initial conditions and boundary conditions are set up within the interface. Next, the mesh is defined—in many cases COMSOL's default mesh, 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

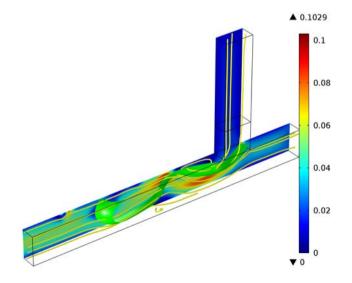
Microfluidic flows occur on length scales that are orders of magnitude smaller than macroscopic flows. Manipulation of fluids at the microscale has a number of advantages—typically microfluidic systems are smaller, operate faster, and require less fluid than their macroscopic equivalents. Energy inputs 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<sup>2</sup>, 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.

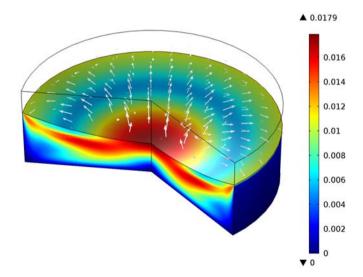


When multiple phases are present, surface tension effects become important relative to gravity and inertia at small length scales. The Laplace pressure (the pressure jump across a two phase boundary), capillary force, and Marangoni forces all scale as 1/L. The figure below shows the break up of oil droplets 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

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.

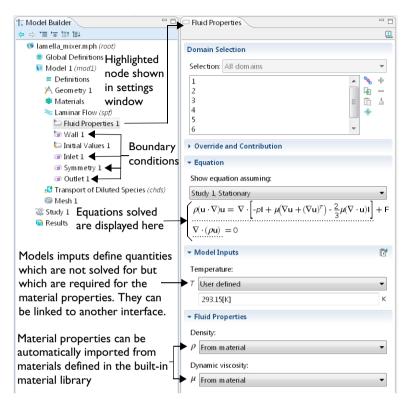


Figure 1: The Model Builder (to the left), and the Fluid Properties I settings window for the selected feature node (to the right). The Equation section in the settings window shows the model equations. The terms added to the equation system by the feature are underlined with a dotted line.

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.

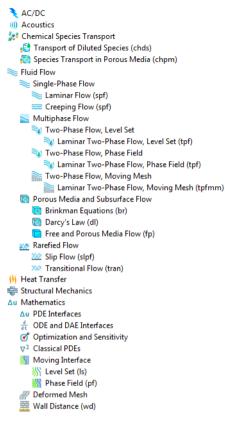


Figure 2: The Microfluidics Module physics interfaces as displayed in the Model Wizard. Note that this is for 3D models.

#### 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 (XXX) 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.

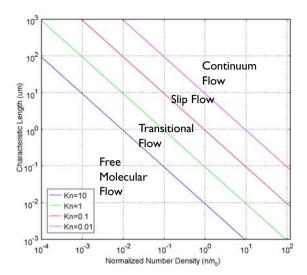


Figure 3: Plot showing the main fluid flow regimes for rarefied gas flows. Different regimes are separated by lines of constant Knudsen number. The number density of the gas is normalized to the number density of an ideal gas at a pressure of 1 atmosphere and a temperature of  $0^{\circ}$  C (n0).

# Physics List by Space Dimension and Preset Study Type

The table below list 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		
Chemical Species Transport						
Transport of Diluted Species*	:	chds	all dimensions	stationary; time dependent		
Species Transport in Porous Media	<b>3</b>	chpm	all dimensions	stationary; time dependent		
€ Fluid Flow						
Single-Phase Flow						
Laminar Flow*		spf	3D, 2D, 2D axisymmetric	stationary; time dependent		
Creeping Flow	=	spf	3D, 2D, 2D axisymmetric	stationary; time dependent		
Multiphase Flow						
Two-Phase Flow, Level Set						
Laminar Two-Phase Flow, Level Set	₹	tpf	3D, 2D, 2D axisymmetric	transient with initialization		
Two-Phase Flow, Phase Field						
Laminar Two-Phase Flow, Phase Field	₹	tpf	3D, 2D, 2D axisymmetric	transient with initialization		
Two-Phase Flow, Moving Mesh						
Laminar Two-Phase Flow, Moving Mesh		tpfmm	3D, 2D, 2D axisymmetric	time dependent		
Porous Media and Subsurface Flow						
Brinkman Equations	1	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		
Rarefied Flow						
Slip Flow	<u>2008</u>	slpf	3D, 2D, 2D axisymmetric	stationary; time dependent		
<b>## Heat Transfer</b>						
Heat Transfer in Porous Media	(88)	ht	all dimensions	stationary; time dependent		
Δu Mathematics						
Moving Interface						
Level Set	<b>3</b> 88	ls	all dimensions	transient with initialization		
Phase Field	<b>\$</b> \$\$	pf	all dimensions	time dependent; transient with initialization		
* This is an enhanced interface, wadded functionality for this modul	/hich is i		vith the base COI	initi		

# The Model Library

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 III 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 ( \big| ) 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 oicon. 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.



# Controlled Diffusion Micromixer I

<sup>1.</sup> 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.

#### Introduction

This model treats an H-shaped microfluidic device for controlled mixing through diffusion. The device puts two different laminar streams in contact for a controlled period of time. The contact surface is well defined, and by controlling the flow rate it is possible to control the amount of species transported from one stream to the other through diffusion. The device concept is illustrated in Figure 1.

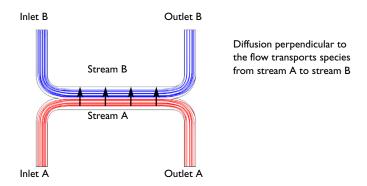


Figure 1: Diagram of the device.

# Model Definition

The geometry of the device is shown in Figure 2. The device geometry is split in two because of symmetry. The design aims to maintain a laminar flow field when the two streams, A and B, are united and thus prevent uncontrolled convective mixing. The transport of species between streams A and B should take place only by diffusion in order that species with low diffusion coefficients stay in their respective streams.

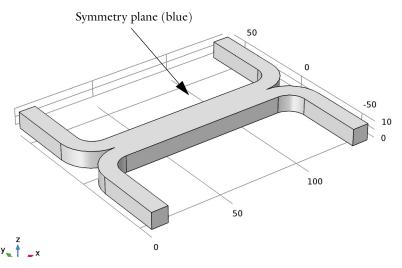


Figure 2: Model geometry. To avoid any type of convective mixing, the design must smoothly let both streams come in contact with each other. Due to symmetry, it is sufficient to model half the geometry, so the actual channel is twice as high in the z-direction.

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

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

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

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

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

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

In this model, the parametric solver is used to solve Equation 1 for three different species, each with different values of D:  $1\times10^{-11}$  m<sup>2</sup>/s,  $5\times10^{-11}$  m<sup>2</sup>/s, and  $1\times10^{-10}$  m<sup>2</sup>/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.

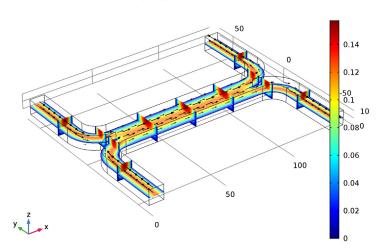
Two versions of the model are solved:

- In the first version, it is assumed that a change in solute concentration does not influence the fluid's density and viscosity. This implies that it is possible to first solve the Navier-Stokes equations and then solve the mass balance equation.
- In the second version, the viscosity depends quadratically on the concentration:

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

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

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



D(3)=1E-11 Slice: Velocity magnitude (mm/s) Arrow Volume: Velocity field

Figure 3: Flow velocity field.



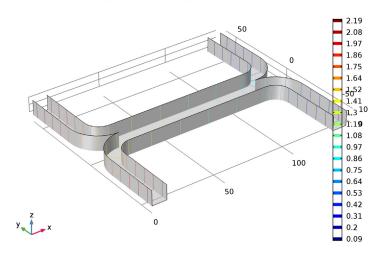


Figure 4: Pressure distribution on the channel walls.



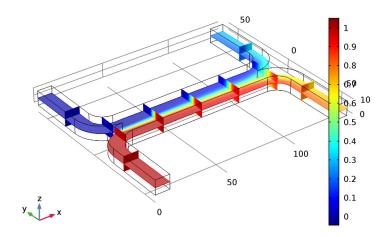


Figure 5: Concentration distribution for a species with diffusivity  $1\cdot 10^{-11}~\text{m}^2/\text{s}$ .

#### D(2)=5E-11 Slice: Concentration (mol/m³)

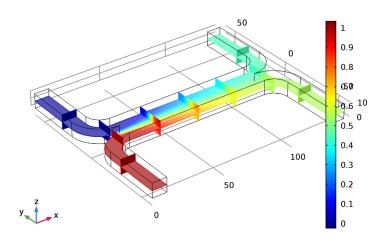


Figure 6: Concentration distribution for a species with diffusivity  $5\cdot 10^{-11}~\text{m}^2/\text{s}$ .



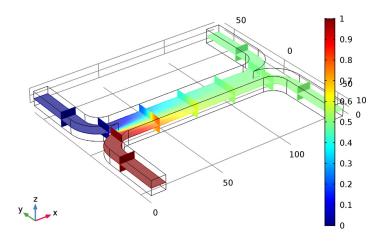


Figure 7: Concentration distribution for a species with diffusivity  $1 \cdot 10^{-10} \text{ m}^2/\text{s}$ .

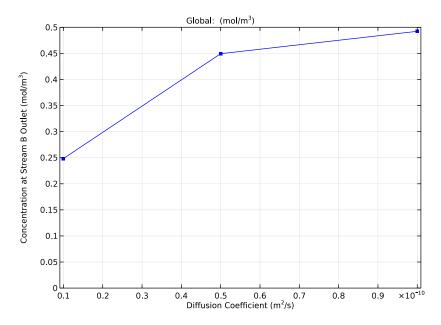


Figure 8: Average concentration at the outlet of stream B as a function of the diffusion coefficient.

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

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

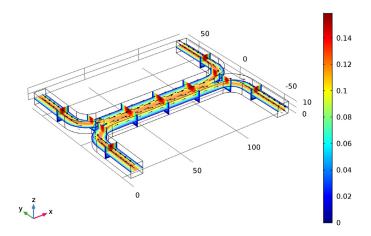


Figure 9: Velocity field. The viscosity varies with the concentration according to  $\mu = \mu_0 (1 + \alpha c)$  with  $\alpha = 0.5$  (m/mol)<sup>2</sup>. It is difficult to see the differences between this figure and that in Figure 3, but careful inspection reveals a slight change in the velocity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



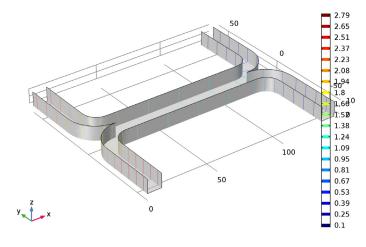


Figure 10: Pressure distribution. The viscosity varies with the concentration according to  $\mu = \mu_0 (1 + \alpha c^2)$  with  $\alpha = 0.5$  (m<sup>3</sup>/mol)<sup>2</sup>. This figure should be compared to Figure 4. There are significant differences between the two cases.



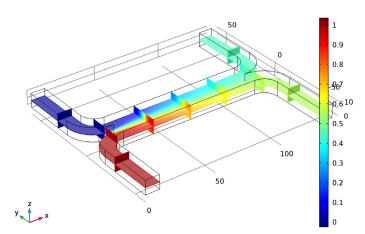


Figure 11: Concentration distribution for the species with diffusivity  $5\cdot 10^{-11}$  m<sup>2</sup>/s for the case where the fluid viscosity varies with concentration. This plot is very similar to the corresponding plot for an uncoupled flow, shown in Figure 6.

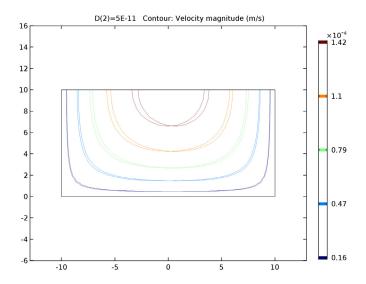


Figure 12: Comparison of the velocity field for the uncoupled and coupled flow simulations showing the difference between the two cases. The coupled flow, in which the fluid viscosity is a function of concentration, is asymmetric.

**Application Library path:** Microfluidics Module/Micromixers/ controlled\_diffusion\_micromixer

# 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>Creeping 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 Preset Studies for Selected Physics Interfaces>Stationary.
- 8 Click Done.

#### **GEOMETRY I**

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

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.
- 3 From the Length unit list, choose µm.

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

Work Plane I (wpl)

- I On the Geometry toolbar, click Work Plane.
- 2 In the Settings window for Work Plane, click Show Work Plane.

#### Rectangle I (rI)

- I On the Work Plane toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type 140.
- **4** In the **Height** text field, type **60**.
- 5 Right-click Rectangle I (rI) and choose Build Selected.

#### Rectangle 2 (r2)

- I On the Work Plane toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type 120.
- 4 In the **Height** text field, type 50.
- **5** Locate the **Position** section. In the **xw** text field, type 10.
- **6** In the **yw** text field, type 10.
- 7 Right-click Rectangle 2 (r2) and choose Build Selected.

#### Difference I (dif1)

- I On the Work Plane toolbar, click Booleans and Partitions and choose Difference.
- **2** Select the object **r1** only.
- 3 In the Settings window for Difference, locate the Difference section.
- **4** Find the **Objects to subtract** subsection. Select the **Active** toggle button.
- **5** Select the object **r2** only.
- 6 Right-click Difference I (dif1) and choose Build Selected.

#### Fillet I (fill)

- I On the Work Plane toolbar, click Fillet.
- 2 On the object difl, select Points 3 and 5 only.
- 3 In the Settings window for Fillet, locate the Radius section.
- 4 In the Radius text field, type 10.
- 5 Right-click Fillet I (fill) and choose Build Selected.

#### Fillet 2 (fil2)

- I On the Work Plane toolbar, click Fillet.
- 2 On the object fill, select Points 1 and 9 only.
- 3 In the Settings window for Fillet, locate the Radius section.

- 4 In the Radius text field, type 20.
- 5 Right-click Fillet 2 (fil2) and choose Build Selected.

Mirror I (mirl)

- I On the Work Plane toolbar, click Transforms and choose Mirror.
- **2** Select the object **fil2** only.
- 3 In the Settings window for Mirror, 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 text field, type 0.
- 6 In the yw text field, type 1.
- 7 Right-click Mirror I (mirl) and choose Build Selected.

Union I (uni I)

- I On the Work Plane toolbar, click Booleans and Partitions and choose Union.
- 2 Click in the **Graphics** window and then press Ctrl+A to select both objects.
- 3 In the Settings window for Union, locate the Union section.
- 4 Clear the Keep interior boundaries check box.
- 5 Right-click Union I (unil) and choose Build Selected.

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

Work Plane I (wpl)

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

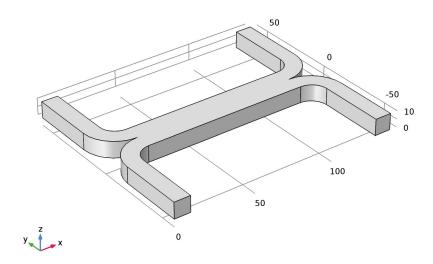
Extrude I (ext I)

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

Distances (µm)
10

4 Right-click Extrude I (extl) and choose Build Selected.

#### 5 Click the Zoom Extents button on the Graphics toolbar.



Create parameters to define the model.

#### **GLOBAL DEFINITIONS**

#### **Parameters**

- I On the Home toolbar, click Parameters.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
D	5e-11[m^2/s]	5E-II m²/s	Diffusion constant
fr	15[pl/s]	1.5E-14 m <sup>3</sup> /s	Inlet flow rate
c0	1[mol/m^3]	I mol/m³	Inlet concentration
alpha	0.5[(m^3/mol)^2]	0.5 m^6/mol <sup>2</sup>	Viscosity c^2-term prefactor

Create an average operator to compute the mean output concentration.

#### DEFINITIONS

Average I (aveop1)

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

Add material properties to the model.

#### MATERIALS

In the Model Builder window, under Component I (compl) right-click Materials and choose Blank Material.

Material I (mat I)

- I In the Settings window for Material, locate the Material Contents section.
- 2 In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Density	rho	1000	kg/m³	Basic
Dynamic viscosity	mu	1e-3	Pa·s	Basic

#### CREEPING FLOW (SPF)

Add a Laminar flow inlet boundary condition.

Inlet I

- I On the Physics toolbar, click Boundaries and choose Inlet.
- 2 Select Boundary 2 only.
- 3 In the Settings window for Inlet, locate the Boundary Condition section.
- 4 From the list, choose Laminar inflow.
- 5 Locate the Laminar Inflow section. Click the Flow rate button.
- **6** In the  $V_0$  text field, type fr/2.

Set the flow rate to one half of the parameter value, since only half of the geometry is modeled.

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

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

#### Inlet 2

- I Right-click Inlet I and choose Duplicate.
- 2 In the Settings window for Inlet, locate the Boundary Selection section.
- 3 Click Clear Selection.
- 4 Select Boundary 8 only.

Add an outlet with a **Pressure** boundary condition.

#### Outlet I

- I On the Physics toolbar, click Boundaries and choose Outlet.
- **2** Select Boundaries 20 and 22 only.

The default pressure of 0 Pa is appropriate in this case.

Add a **Symmetry** boundary condition in the symmetry plane.

#### Symmetry I

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

Now set up the mass transport physics.

#### TRANSPORT OF DILUTED SPECIES (TDS)

#### Transport Properties I

Use the computed velocity field for the species convection.

- I In the Model Builder window, expand the Component I (compl)>Transport of Diluted Species (tds) node, then click Transport Properties I.
- 2 In the Settings window for Transport Properties, locate the Model Inputs section.
- 3 From the **u** list, choose **Velocity field (spf)**.

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

- **4** Locate the **Diffusion** section. In the  $D_c$  text field, type D.
  - Specify the concentration at the two inlets.
- 5 In the Model Builder window, click Transport of Diluted Species (tds).

#### Concentration 1

- I On 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 On 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.

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

Use the **Outflow** condition to allow species to leave the domain by convection.

### Outflow I

- I On the Physics toolbar, click Boundaries and choose Outflow.
- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- 3 Click Paste Selection.
- 4 In the Paste Selection dialog box, type 20 22 in the Selection text field.
- 5 Click OK.

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

### MESH I

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

### Free Quad I

Select Boundary 4 only.

#### Size

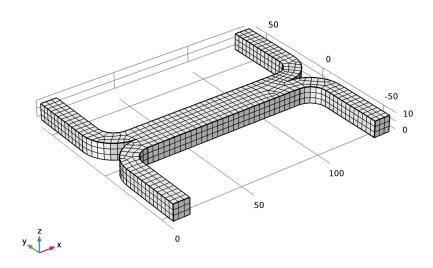
- I In the Model Builder window, under Component I (compl)>Mesh I click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 From the Calibrate for list, choose Fluid dynamics.
- 4 From the Predefined list, choose Coarse.

Next, sweep the mesh through the domain.

# Swept I

I In the Model Builder window, right-click Mesh I and choose Swept.

# 2 In the Settings window for Swept, click Build All.



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

#### STUDY I

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

- I In the Settings window for Study, locate the Study Settings section.
- 2 Clear the Generate default plots check box. For **Step 1**, solve only the creeping flow problem.

## Step 1: Stationary

- I In the Model Builder window, under Study I click Step I: Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- 3 In the table, clear the Solve for check box for the Transport of Diluted Species interface. Add a second study step.

## Stationary 2

On the Study toolbar, click Study Steps and choose Stationary>Stationary.

### Step 2: Stationary 2

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.

- I In the Settings window for Stationary, locate the Physics and Variables Selection section.
- 2 In the table, clear the **Solve for** check box for the **Creeping Flow** interface.
- 3 Click to expand the Values of dependent variables section. Locate the Values of Dependent Variables section. Find the Values of variables not solved for subsection. From the Settings list, choose User controlled.
- 4 From the Method list, choose Solution.
- 5 From the Study list, choose Study I, Stationary. Solve the diffusion problem for three values of the diffusion coefficient.
- 6 Click to expand the **Study extensions** section. Locate the **Study Extensions** section. Select the Auxiliary sweep check box.
- 7 Click Add.
- **8** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
D	1e-10 5e-11 1e-11	

**9** On the **Study** toolbar, click **Compute**.

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

#### RESULTS

Surface 1

- I On the Results toolbar, click More Data Sets and choose Surface.
- **2** Select Boundaries 1, 3, 5–7, 9–19, 21, 23, and 24 only. First plot the velocity of the flow within the channel.

3D Plot Group 1

I On the Results toolbar, click 3D Plot Group.

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

Slice 1

- I In the Model Builder window, right-click 3D Plot Group I and choose Slice.
- 2 In the Settings window for Slice, locate the Expression section.
- 3 From the Unit list, choose mm/s.

3D Plot Group 1

Add additional slices in different directions.

Slice 2

- I In the Model Builder window, under Results right-click 3D Plot Group I and choose Slice.
- 2 In the **Settings** window for Slice, locate the **Expression** section.
- 3 From the Unit list, choose mm/s.
- 4 Locate the Plane Data section. From the Plane list, choose xy-planes.
- 5 In the Planes text field, type 1.

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

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

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

7 Click to expand the **Title** section. From the **Title type** list, choose **None**. Add slices in a third plane.

Slice 3

- I Right-click Results>3D Plot Group I>Slice 2 and choose Duplicate.
- 2 In the Settings window for Slice, locate the Plane Data section.
- 3 From the Plane list, choose zx-planes.
- 4 In the Planes text field, type 2.

Use the **Arrow Volume** plot to visualize the flow direction.

3D Plot Group 1

In the Model Builder window, under Results right-click 3D Plot Group I and choose Arrow Volume.

Arrow Volume 1

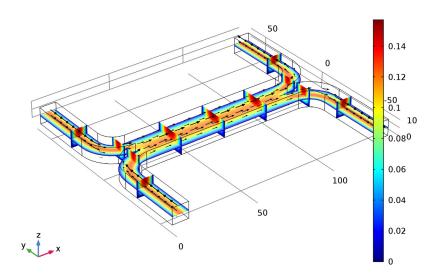
- I In the **Settings** window for Arrow Volume, locate the **Arrow Positioning** section.
- 2 Find the x grid points subsection. In the Points text field, type 14.
- 3 Find the y grid points subsection. In the Points text field, type 21.

- 4 Find the z grid points subsection. In the Points text field, type 3.
- 5 Locate the Coloring and Style section. From the Color list, choose Black. Rename the plot.

# 3D Plot Group 1

- I Right-click **3D Plot Group I** and choose **Rename**.
- 2 In the Rename 3D Plot Group dialog box, type Velocity (uncoupled flow) in the New label text field.
- 3 Click OK.
- 4 On the Velocity (uncoupled flow) toolbar, click Plot.

D(3)=1E-11 Slice: Velocity magnitude (mm/s) Arrow Volume: Velocity field



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

## 3D Plot Group 2

- I On the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Data set list, choose Surface 1. First add a uniformly colored surface, to highlight the channel walls.

## Surface I

I Right-click 3D Plot Group 2 and choose Surface.

- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the Expression text field, type 1.
- 4 Locate the Coloring and Style section. From the Coloring list, choose Uniform.
- 5 From the Color list, choose Gray.

Next use contours to visualize the pressure.

## 3D Plot Group 2

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

### Contour I

I In the Settings window for Contour, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Creeping Flow> Velocity and pressure>p - Pressure.

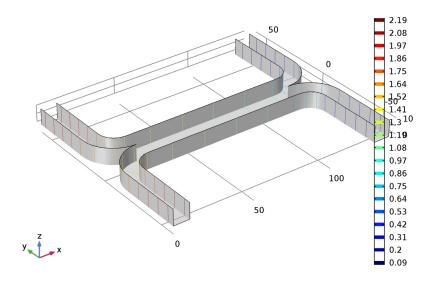
Finally rename the plot.

## 3D Plot Group 2

- I Right-click 3D Plot Group 2 and choose Rename.
- 2 In the Rename 3D Plot Group dialog box, type Pressure (uncoupled flow) in the New label text field.
- 3 Click OK.

# 4 On the Pressure (uncoupled flow) toolbar, click Plot.

D(3)=1E-11 Surface: 1 (1) Contour: Pressure (Pa)



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)

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

Velocity (uncoupled flow) I

Re-name the plot.

- I In the Model Builder window, under Results right-click Velocity (uncoupled flow) I and choose Rename.
- 2 In the Rename 3D Plot Group dialog box, type Concentration (uncoupled flow) in the New label text field.
- 3 Click OK.

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

Slice 1

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

2 In the Settings window for Slice, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Transport of Diluted Species>c - Concentration.

Slice 2

- I In the Model Builder window, under Results>Concentration (uncoupled flow) click Slice 2.
- 2 In the Settings window for Slice, click Replace Expression in the upper-right corner of the **Expression** section. From the menu, choose **c** - **Concentration**.

Slice 3

- I In the Model Builder window, under Results>Concentration (uncoupled flow) click Slice 3.
- 2 In the Settings window for Slice, click Replace Expression in the upper-right corner of the **Expression** section. From the menu, choose **c** - **Concentration**.

Disable the **Arrow Volume** plot.

Arrow Volume 1

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

Concentration (uncoupled flow)

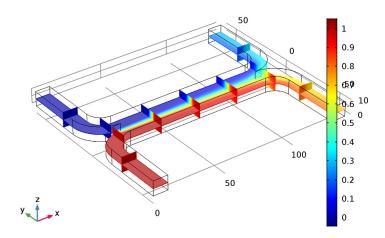
- I In the Model Builder window, under Results click Concentration (uncoupled flow).
- 2 On the Concentration (uncoupled flow) toolbar, click Plot.

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

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

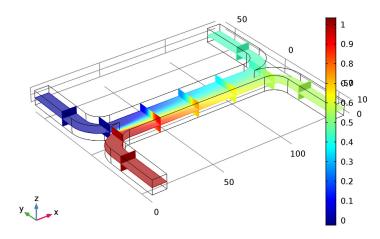
## 3 Click Plot.

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



- 4 In the Settings window for 3D Plot Group, locate the Data section.
- 5 From the Parameter value (D) list, choose 5E-11.
- 6 On the Concentration (uncoupled flow) toolbar, click Plot.

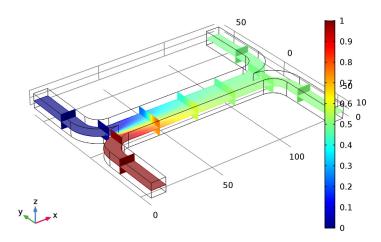
D(2)=5E-11 Slice: Concentration (mol/m<sup>3</sup>)



7 From the Parameter value (D) list, choose IE-10.

# 8 On the Concentration (uncoupled flow) toolbar, click Plot.

D(1)=1E-10 Slice: Concentration (mol/m<sup>3</sup>)



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

## ID Plot Group 4

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

### Global I

I On the ID Plot Group 4 toolbar, click Global.

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

- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
aveop1(c)	mol/m^3	

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

- 4 Click to expand the **Legends** section. Clear the **Show legends** check box. Add a marker in the computed datapoints.
- 5 Click to expand the Coloring and style section. Locate the Coloring and Style section. Find the Line markers subsection. From the Marker list, choose Point.

6 From the Positioning list, choose In data points.

Change the axis titles. Note that html tags and a range of mathematical symbols and Greek letters can be entered in the axis and plot titles.

## ID Plot Group 4

- I In the Model Builder window, under Results click ID Plot Group 4.
- 2 In the Settings window for 1D Plot Group, locate the Plot Settings section.
- 3 Select the x-axis label check box.
- 4 In the associated text field, type Diffusion Coefficient (m<sup>2</sup>/s).
- 5 Select the y-axis label check box.
- 6 In the associated text field, type Concentration at Stream B Outlet (mol/m<sup> 3</sup>).

Change the axis limits for the plot.

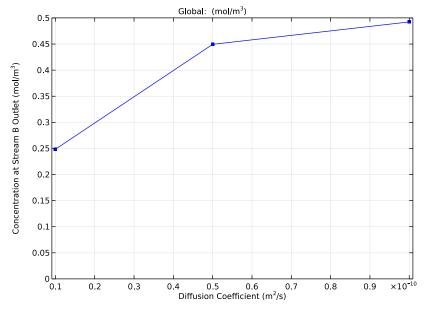
- 7 Click to expand the Axis section. Select the Manual axis limits check box.
- **8** In the **y minimum** text field, type 0.
- **9** In the **y maximum** text field, type **0.5**. Finally re-name the plot.
- 10 Right-click Results>1D Plot Group 4 and choose Rename.
- II In the Rename ID Plot Group dialog box, type Output Concentration (uncoupled flow) in the New label text field.

I2 Click OK.

# 13 On the Output Concentration (uncoupled flow) toolbar, click Plot.

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

In some cases, particularly if the solution consists of large macromolecules, the dissolved species has a large influence on the liquid's viscosity. In such situations, the Navier-Stokes and the convection-diffusion equations become coupled, and so they must be solved simultaneously.



Now set up the fully coupled problem. To make the viscosity a function of the species concentration simply type an expression into the Dynamic viscosity field of the Fluid **Properties** node.

### CREEPING FLOW (SPF)

On the Physics toolbar, click Transport of Diluted Species (tds) and choose Creeping Flow (spf).

Fluid Properties 1

I In the Model Builder window, under Component I (compl)>Creeping 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 1e-3[Pa\*s]\*(1+ alpha\*c^2).

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

#### ADD STUDY

- I On 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 Preset Studies>Stationary.
- 4 Click Add Study in the window toolbar.

### STUDY 2

Turn off the default plot groups again.

- I In the Model Builder window, click Study 2.
- 2 In the Settings window for Study, locate the Study Settings section.
- 3 Clear the Generate default plots check box.
- 4 On the Home toolbar, click Compute.

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

### RESULTS

Surface I

In the Model Builder window, under Results>Data Sets right-click Surface I and choose Duplicate.

Surface 2

- I In the **Settings** window for Surface, locate the **Data** section.
- 2 From the Data set list, choose Study 2/Solution 3 (sol3).

Re-create the velocity, pressure and concentration plots for the fully coupled problem.

Velocity (uncoupled flow)

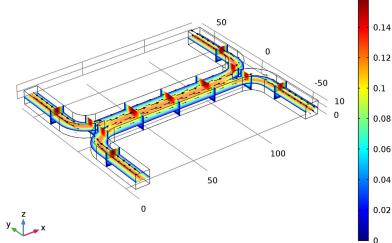
In the Model Builder window, under Results right-click Velocity (uncoupled flow) and choose Duplicate.

Velocity (uncoupled flow) I

- I In the **Settings** window for 3D Plot Group, locate the **Data** section.
- 2 From the Data set list, choose Study 2/Solution 3 (sol3).
- 3 Right-click Results>Velocity (uncoupled flow) I and choose Rename.
- 4 In the Rename 3D Plot Group dialog box, type Velocity (coupled flow) in the New label text field.
- 5 Click OK.
- 6 On the Velocity (coupled flow) toolbar, click Plot.

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

Slice: Velocity magnitude (mm/s) Arrow Volume: Velocity field



Pressure (uncoupled flow)

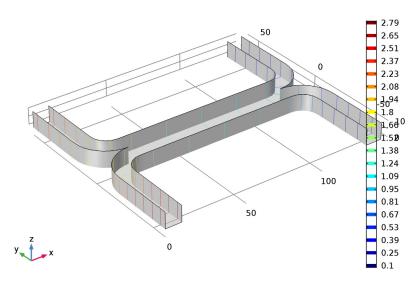
In the Model Builder window, under Results right-click Pressure (uncoupled flow) and choose Duplicate.

Pressure (uncoupled flow) I

- I In the Settings window for 3D Plot Group, locate the Data section.
- 2 From the Data set list, choose Surface 2.

- 3 Right-click Results>Pressure (uncoupled flow) I and choose Rename.
- 4 In the Rename 3D Plot Group dialog box, type Pressure (coupled flow) in the New label text field.
- 5 Click OK.
- 6 On the Pressure (coupled flow) toolbar, click Plot.

The pressure distribution in the channel has changed significantly as a result of the increased viscosity of the fluid that contains the added species. Thus the two inlets must be maintained at different pressures. This may be possible for a single stage, but it would significantly complicate the design of a multiple stage device.



Surface: 1 (1) Contour: Pressure (Pa)

Concentration (uncoupled flow)

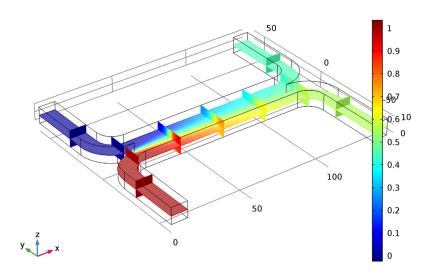
In the Model Builder window, under Results right-click Concentration (uncoupled flow) and choose **Duplicate**.

Concentration (uncoupled flow) I

- I In the Settings window for 3D Plot Group, locate the Data section.
- 2 From the Data set list, choose Study 2/Solution 3 (sol3).
- 3 Right-click Results>Concentration (uncoupled flow) I and choose Rename.
- 4 In the Rename 3D Plot Group dialog box, type Concentration (coupled flow) in the New label text field.

- 5 Click OK.
- 6 On the Concentration (coupled flow) toolbar, click Plot.

Slice: Concentration (mol/m3)



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.

## Cut Plane I

- I On the Results toolbar, click Cut Plane.
- 2 In the Settings window for Cut Plane, locate the Plane Data section.
- 3 In the x-coordinate text field, type 70.

### Cut Plane 2

- I Right-click Cut Plane I and choose Duplicate.
- 2 In the Settings window for Cut Plane, locate the Data section.
- 3 From the Data set list, choose Study 2/Solution 3 (sol3).

## Cut Plane I

Then add a **Contour** plot of the velocity magnitude.

## 2D Plot Group 8

- I On the Results toolbar, click 2D Plot Group.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Data set list, choose Cut Plane 1.
- 4 From the Parameter value (D) list, choose 5E-11.

#### Contour I

- I Right-click 2D Plot Group 8 and choose Contour.
- 2 In the Settings window for Contour, locate the Levels section.
- 3 In the Total levels text field, type 5.

Create a duplicate **Contour** plot, using the same colors and scales, but showing the coupled data.

#### Contour 2

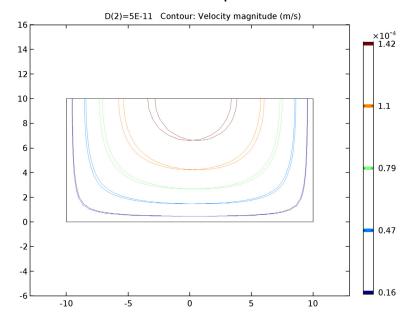
- I Right-click Results>2D Plot Group 8>Contour I and choose Duplicate.
- 2 In the Settings window for Contour, locate the Data section.
- 3 From the Data set list, choose Cut Plane 2.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 5 Click to expand the Inherit style section. Locate the Inherit Style section. From the Plot list, choose Contour 1.

### 2D Plot Group 8

Rename the plot.

- I In the Model Builder window, under Results right-click 2D Plot Group 8 and choose Rename.
- 2 In the Rename 2D Plot Group dialog box, type Velocity Comparison in the New label text field.
- 3 Click OK.
- 4 On the Velocity Comparison toolbar, click Plot.

5 Click the Zoom Extents button on the Graphics toolbar.



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.

### Global Evaluation 1

- I On the Results toolbar, click Global Evaluation.
- 2 In the Settings window for Global Evaluation, locate the Expressions section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
aveop1(c)	mol/m^3	

### 4 Click Evaluate.

### Global Evaluation 2

- I Right-click Global Evaluation I and choose Duplicate.
- 2 In the Settings window for Global Evaluation, locate the Data section.
- 3 From the Data set list, choose Study 2/Solution 3 (sol3).
- 4 Click New Table.

## TABLE

# I Go to the Table window.

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