



INTRODUCTION TO
Microfluidics Module

Introduction to the Microfluidics Module

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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 physics interfaces, referred to as Microfluidics physics 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 physics 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 interfaces to solve multiphysics problems such as electrokinetic flows.

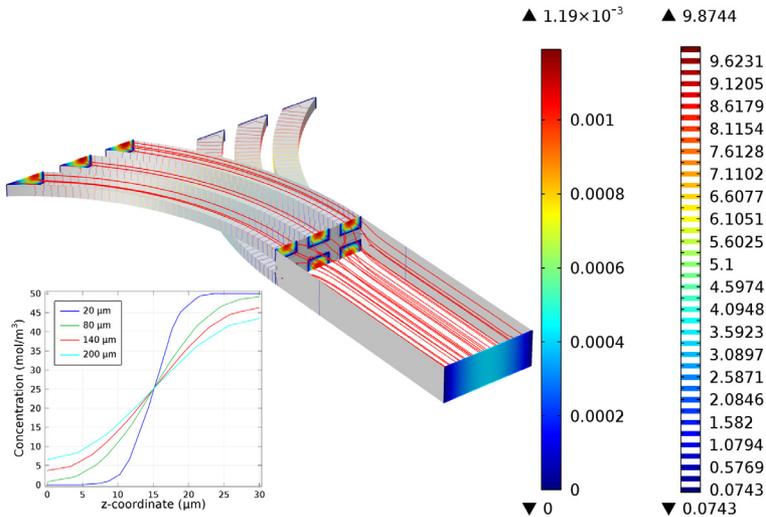
For each of the Microfluidics physics interfaces, the underlying physical principles are expressed in the form of partial differential equations, together with corresponding initial and boundary conditions. COMSOL's design emphasizes the physics by providing users with the equations solved by each feature 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 a concentration-dependent viscosity—no scripting or coding is required (this is demonstrated in the [Tutorial Example: A Controlled Diffusion Micromixer](#)). 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 physics interface is added. Initial conditions and boundary conditions are set up within the physics 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 interface, and the problem is solved. Finally the results are visualized. All these steps are accessed from the COMSOL Desktop.

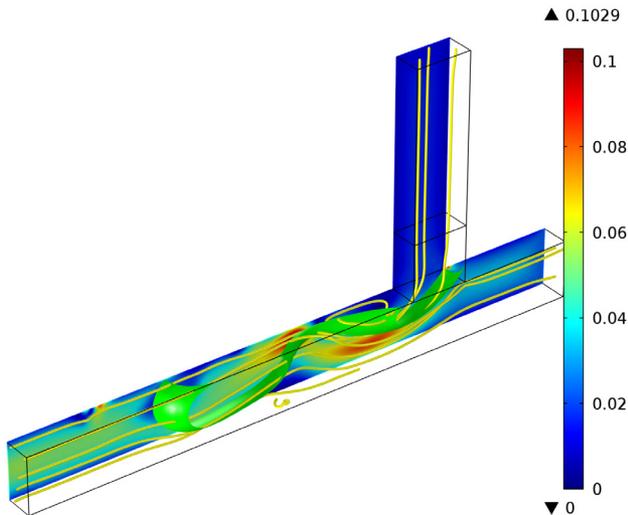
Microfluidic Devices: Physics and Applications

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^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.

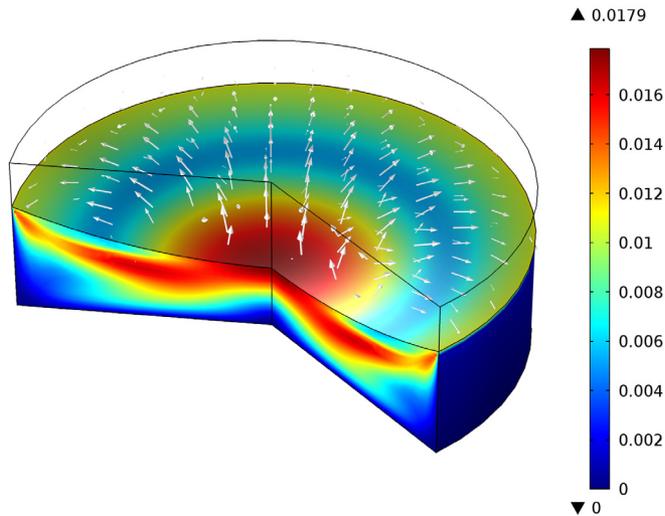


When multiple phases are present, surface tension effects become important relative to gravity and inertia at small length scales. The Laplace pressure (the pressure jump across a two phase boundary), capillary force, and Marangoni forces all scale as $1/L$. The figure below shows the break up of oil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

At the microscale, a range of electrohydrodynamic effects can be used 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 used 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 ($0.01 < \text{Kn} < 0.1$), appropriate slip boundary conditions can be used with the Navier-Stokes equations to describe the flow away from the boundary. The Microfluidics Module includes a physics 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 Interface 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 physics 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 components), or point. [Figure 1](#) uses the Lamella Mixer model (found in the Microfluidics Module application 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 the settings 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.

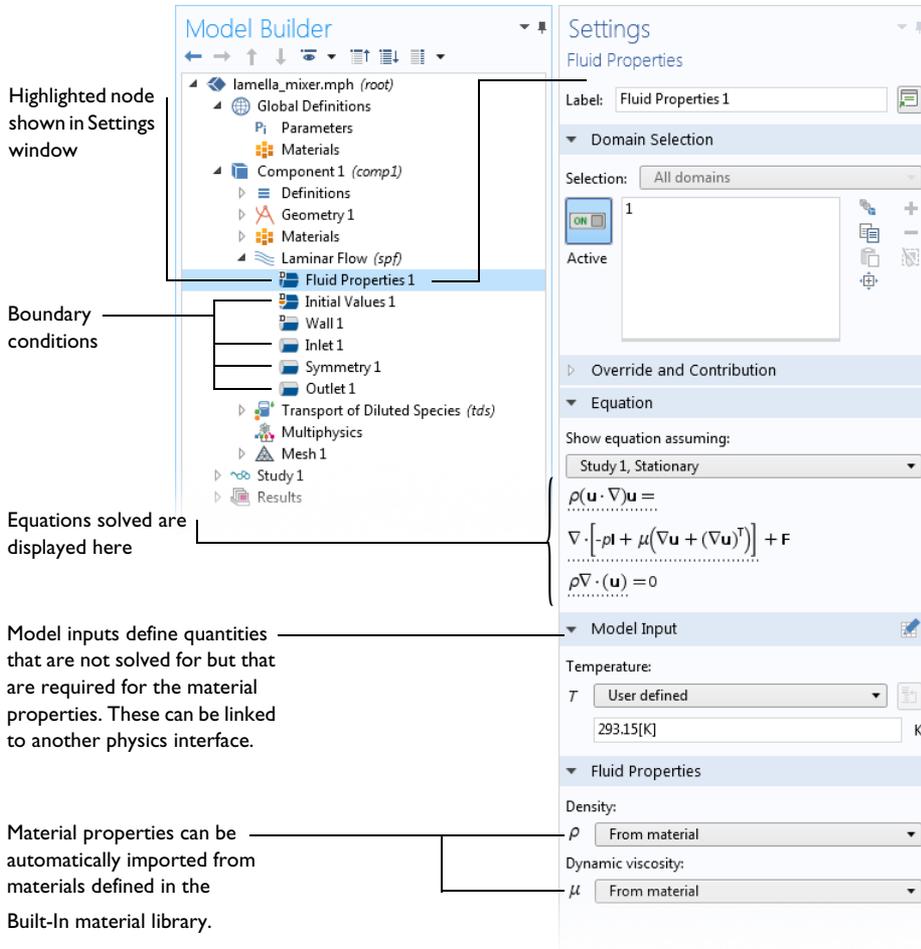


Figure 1: The Model Builder (to the left), and the Settings window for Fluid Properties I for the selected feature node (to the right). The Equation section in the Settings window shows the model equations. The terms added to the equation system by the feature are underlined with a dotted line.

The Microfluidics Module includes a number of physics interfaces for modeling different types of microfluidic devices. When a new model is started, these physics interfaces are selected from the Model Wizard. Figure 2 shows the Model Wizard with the physics interfaces included with the Microfluidics Module. Also see [Physics Interface Guide by Space Dimension and Study Type](#). Below, a brief overview of each of the Microfluidics Module physics interfaces is given.

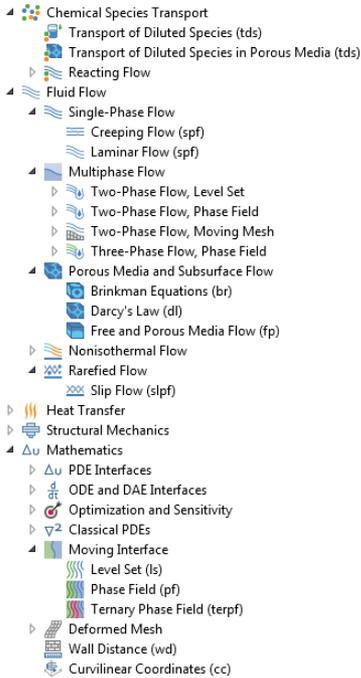


Figure 2: The Microfluidics Module physics interfaces as displayed in the Model Wizard. Note that this is for 3D components.

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 ρ is the fluid density, U is a characteristic velocity, L is a characteristic length scale, and μ is the dynamic viscosity.

The Laminar Flow interface (\approx) applies when the Reynolds number is less than approximately 1000. The physics 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 the simulation of non-Newtonian flows.

The Creeping Flow interface (\approx) 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. Since a surface in the geometry is used to represent the interface between the two fluids in the Moving Mesh interface, the interface itself cannot break up into multiple disconnected surfaces. This means that the Moving Mesh interface cannot be applied to problems such as droplet formation in inkjet devices (in these applications the level set or phase field interfaces are appropriate). All three physics interfaces support both compressible (Mach number, $Ma < 0.3$) and incompressible laminar flows, where one or both fluids can be non-Newtonian.

The Laminar Three-Phase Flow, Phase Field interface () models laminar flow of three incompressible phases which may be either Newtonian or non-Newtonian. The moving fluid-fluid interfaces between the three phases are tracked in detail using the phase-field method.

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 physics 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, λ , of the molecules becomes comparable with the length scale of the flow, L . The Knudsen number, $\text{Kn} = \lambda/L$, 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 ($0.01 < \text{Kn} < 0.1$), 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.

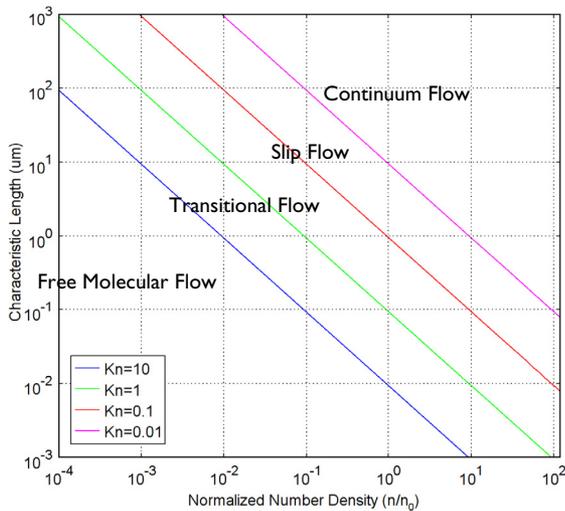


Figure 3: Plot showing the main fluid flow regimes for rarefied gas flows. Different regimes are separated by lines of constant Knudsen number. The number density of the gas is normalized to the number density of an ideal gas at a pressure of 1 atmosphere and a temperature of 0° C (n_0).

Physics Interface Guide by Space Dimension and Study Type

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

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Chemical Species Transport				
Transport of Diluted Species ¹		tds	all dimensions	stationary; time dependent
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent
Reacting Flow				
Laminar Flow, Diluted Species ¹		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 Fluid Flow				
 Single-Phase Flow				
Creeping Flow		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow ¹		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
 Multiphase Flow				
 Two-Phase Flow, Level Set				
Laminar Two-Phase Flow, Level Set		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
 Two-Phase Flow, Phase Field				
Laminar Two-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization
 Three-Phase Flow, Phase Field				
Laminar, Three-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent
 Two-Phase Flow, Moving Mesh				
Laminar Two-Phase Flow, Moving Mesh		—	3D, 2D, 2D axisymmetric	time dependent
 Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Free and Porous Media Flow		fp	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 Rarefied Flow				
Slip Flow		slpf	3D, 2D, 2D axisymmetric	stationary; time dependent
 Mathematics				
 Moving Interface				
Level Set		ls	all dimensions	time dependent with phase initialization
Phase Field		pf	all dimensions	time dependent; time dependent with phase initialization
Ternary Phase Field		terpf	3D, 2D, 2D axisymmetric	time dependent
¹ This physics interface is included with the core COMSOL package but has added functionality for this module.				

Tutorial Example: A Controlled Diffusion Micromixer¹

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.

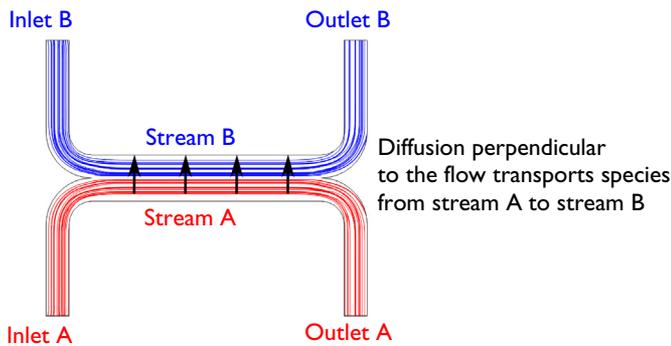


Figure 4: Device concept.

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 ρ is the fluid density (1000 kg/m³), U is a characteristic velocity of the flow (0.1 mm/s), μ 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:

1. This example was originally formulated by Albert Witsarsa 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 (m^2/s) and c is its concentration (mol/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 with two versions:

- 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 α is a constant of dimension $\text{m}^6/(\text{mol})^2$ and μ_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.

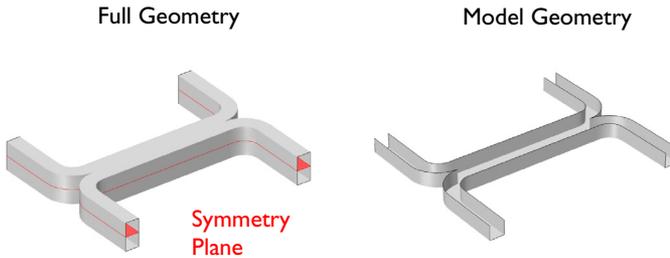


Figure 5: Left: Device geometry showing symmetry plane. Right: Model geometry. Only half of the device needs to be simulated, as the flow is symmetric about the midplane.

Model Wizard

Note: These instructions are for the user interface on Windows but apply, with minor differences, also to Linux and Mac.

- 1 To start the software, double-click the COMSOL icon on the desktop. When the software opens, you can choose to use the Model Wizard to create a new COMSOL model or Blank Model to create one manually. For this tutorial, click the Model Wizard button.

If COMSOL is already open, you can start the Model Wizard by selecting New  from the File menu and then click Model Wizard .

The Model Wizard guides you through the first steps of setting up a model. The next window lets you select the dimension of the modeling space.

- 2 In the Select Space Dimension window click the 3D button .
- 3 In the Select Physics tree under Fluid Flow>Single-Phase Flow click Creeping Flow (spf) .
- 4 Click Add.
- 5 In the Select Physics tree under Chemical Species Transport click Transport of Diluted Species (tds) .
- 6 Click Add and then the Study button .
- 7 In the tree under General Studies click Stationary .
- 8 Click Done .

Geometry 1

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 Component 1 click Geometry 1 .
- 2 In the Settings window for Geometry locate the Units section. From the Length unit list, choose μm .

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

- 3 On the Geometry toolbar click Work Plane .

Rectangle 1

- 1 In the Model Builder, under Geometry 1>Work Plane 1, right-click Plane Geometry  and choose Rectangle.
- 2 In the Settings window for Rectangle locate the Size section.
 - In the Width text field, enter 140.
 - In the Height text field, enter 60.
- 3 Click the Build Selected button .

Rectangle 2

- 1 Right-click Plane Geometry  and choose Rectangle.
- 2 In the Settings window for Rectangle locate the Size section.
 - In the Width text field, enter 120.
 - In the Height text field, enter 50.
- 3 Locate the Position section.
 - In the xw text field, enter 10.
 - In the yw text field, enter 10.
- 4 Click the Build Selected button .

Difference 1

- 1 Right-click Plane Geometry  and choose Booleans and Partitions>Difference.
- 2 Select the object r1 only.
- 3 In the Settings window for Difference locate the Difference section. Under Objects to subtract, toggle the Active button.
- 4 Select the object r2 only.

- 5 Click the Build Selected button  .

Fillet 1

- 1 Right-click Plane Geometry  and choose Fillet.
- 2 On the object dif1, select Points 3 and 5 only.
- 3 In the Settings window for Fillet locate the Radius section. In the Radius text field, enter 10.
- 4 Click the Build Selected button  .

Fillet 2

- 1 Right-click Plane Geometry  and choose Fillet.
- 2 On the object fill, select Points 1 and 9 only.
- 3 In the Settings window for Fillet locate the Radius section. In the Radius text field, enter 20.
- 4 Click the Build Selected button  .

Mirror 1

- 1 Right-click Plane Geometry  and choose Transforms>Mirror.
- 2 Select the object fil2 only.
- 3 In the Settings window for Mirror locate the Input section. Select the Keep input objects check box.
- 4 Locate the Normal Vector to Line of Reflection section.
 - In the xw text field, enter 0.
 - In the yw text field, enter 1.
- 5 Click the Build Selected button  .

Union 1

- 1 Right-click Plane Geometry  and choose Booleans and Partitions>Union .
- 2 Select the objects fil2 and mir1 only.
- 3 Click the Build Selected button  .

Extrude 1

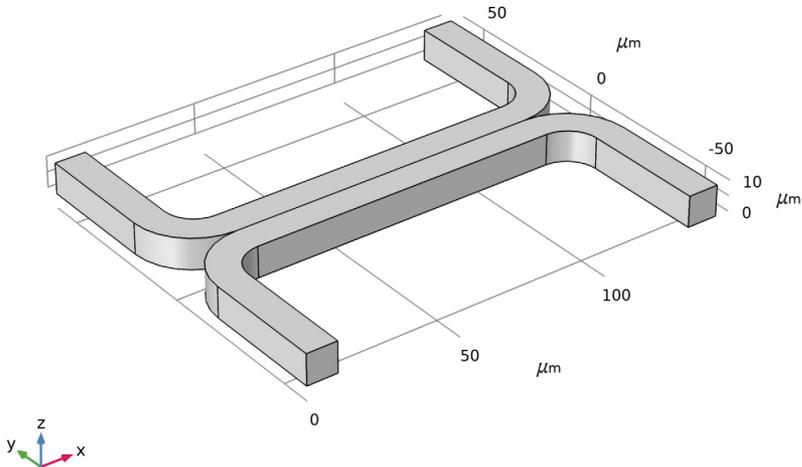
Extrude the 2D geometry to create a 3D geometry.

- 1 Right-click Work Plane 1  and choose 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 Click the Build Selected button  .



Global Definitions

Parameters

1 On the Home toolbar click Parameters P_i and select Parameters 1 P_i .

Note: On Linux and Mac, the Home toolbar refers to the specific set of controls near the top of the Desktop.

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

3 In the table, enter the following settings:

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

Materials

Add material properties to the model.

Material 1

- 1 On the Materials toolbar click Blank Material .
- 2 In the Settings window for Material 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

Note: There are several methods to select a geometric entity. To select, for example, a boundary, place the cursor over the boundary in the graphics window. If the required boundary is not highlighted in red then rotate the scroll wheel until it is highlighted, then left-click to select it (the up and down arrow keys can also be used instead of the scroll wheel). Alternatively, use the Selection list to display a list of the available boundary numbers (available from the Home> Windows menu if you are using windows, or from the Windows menu on other platforms). Boundaries are added to the selection by first clicking on the boundary and then right-clicking and selecting Add to selection. To add several boundaries, hold the Ctrl key down when clicking. For more information about selecting geometric entities in the Graphics window, see the *COMSOL Multiphysics Reference Manual*.

- 1 In the Model Builder under Component 1 click Creeping Flow .

Note: Several default nodes are added automatically to the model tree. The  'D' in the upper left corner of the node indicates these are default nodes.

Inlet 1

Add a fully developed flow inlet boundary condition.

- 1 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. From the Boundary condition list, choose Fully developed flow.

4 Locate the Fully developed flow section. Click the Flow rate button.

- In the V_0 text field, enter $fr/2$.

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

Inlet 2

- 1 Under Creeping Flow, right-click Inlet 1  and choose Duplicate .
- 2 In the Settings window for Inlet locate the Boundary Selection section. Click Clear Selection .
- 3 Select Boundary 10 only.

Outlet 1

Add an outlet with a pressure boundary condition.

- 1 On the Physics toolbar click Boundaries  and choose Outlet.
- 2 Select Boundaries 23 and 25 only.
The default pressure of 0 Pa is appropriate in this case.

Symmetry 1

Add a symmetry boundary condition in the symmetry plane.

- 1 On the Physics toolbar click Boundaries  and choose Symmetry.
- 2 Select Boundaries 4 and 9 only.

Transport of Diluted Species

Now set up the mass transport physics features.

Transport Properties 1

Use the computed velocity field for the species convection.

- 1 In the Model Builder, expand the Component 1>Transport of Diluted Species node, then click Transport Properties 1.
- 2 In the Settings window for Transport Properties locate the Model Inputs section. From the **u** list, choose Velocity field (spf).
The diffusion coefficient is set to use the parameter previously defined.
- 3 Locate the Diffusion section. In the D_c text field, enter **D**.

Concentration 1

Specify the concentration at the two inlets.

- 1 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. Select the Species c check box.
- 4 In the $c_{0,c}$ text field, enter c_0 .

Concentration 2

- 1 On the Physics toolbar click Boundaries  and choose Concentration.
- 2 Select Boundary 10 only.
- 3 In the Settings window for Concentration locate the Concentration section. 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 On the Physics toolbar click Boundaries  and choose Outflow.
- 2 Click Paste Selection .
- 3 Go to the Paste Selection dialog box. In the Selection text field, type 23.
- 4 Click OK.

Outflow 2

- 1 On the Physics toolbar click Boundaries  and choose Outflow.
- 2 Click Paste Selection .
- 3 Go to the Paste Selection dialog box. In the Selection text field, type 25.
- 4 Click OK.

Mesh 1

Set up the mesh. By default, COMSOL will create a mesh for the physics currently in the model. Often this is good enough, but in this case, we want to make some small edits to the default mesh sequence. By default, the fine mesh is not applied to interior boundaries. Typically this is wanted, since interior boundaries are transparent to the fluid flow. However, in this case, the mixing of the two streams occurs close to this interior boundary, so we can add boundary 16 to the Size 1 and also the Boundary Layer Properties 1 mesh feature.

Size

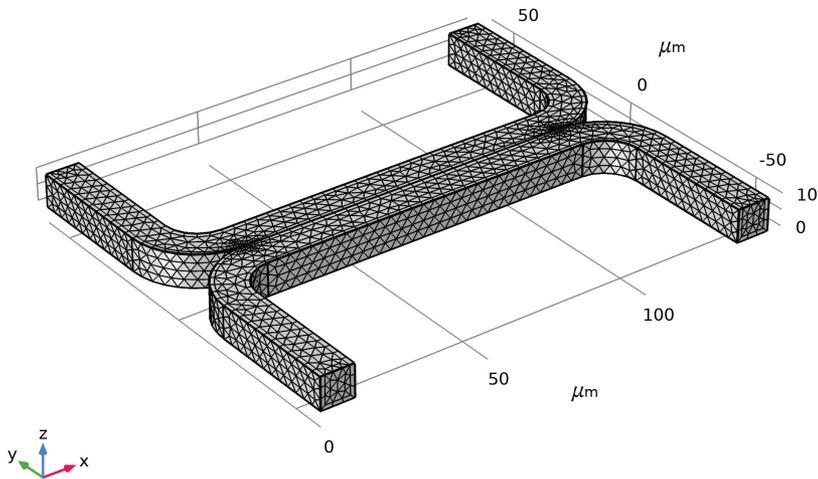
- 1 In the Model Builder window, under Component 1 right-click Mesh 1  and choose Edit Physics-Induced Sequence.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 From the Predefined list, choose Extra coarse.

Size 1

- 1 In the Model Builder window, under Component 1 (comp1)>Mesh 1 click Size 1.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 From the Predefined list, choose Coarse.
- 4 Locate the Geometric Entity Selection section. Click Paste Selection .
- 5 In the Paste Selection dialog box, type 16 in the Selection text field.
- 6 Click OK.

Boundary Layer Properties 1

- 1 In the Model Builder window, expand the Component 1 (comp1)>Mesh 1>Boundary Layers 1  node, then click Boundary Layer Properties 1 .
- 2 In the Settings window for Boundary Layer Properties, locate the Boundary Selection section.
- 3 Click Paste Selection .
- 4 In the Paste Selection dialog box, type 16 in the Selection text field.
- 5 Click OK.
- 6 Right-click Component 1 (comp1)>Mesh 1>Boundary Layers 1>Boundary Layer Properties 1 and choose 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 Settings window for Study locate the Study Settings section. Clear the Generate default plots check box.

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

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 Settings window for Stationary under Physics and Variables Selection, click the Transport of Diluted Species row in the Physics interface column.
- 3 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 On the Study toolbar click Study Steps  and choose Stationary>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 these can be used to compute the convective species transport.
- 2 In the Settings window for Stationary under Physics and Variables Selection, click the Creeping Flow row in the Physics interface column.
- 3 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.
- 4 Click to expand the Values of Dependent Variables section.
 - In the Values of variables not solved for area, from the Settings list, choose User controlled.
 - From the Method list, choose Solution.
 - From the Study list, choose Study 1, Stationary.Solve the diffusion problem for three values of the diffusion coefficient.
- 5 In the Settings window for Stationary click to expand the Study Extensions section. Select the Auxiliary Sweep check box.
- 6 Click Add .
- 7 In the table, enter the following settings:

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

- 8 On the Home toolbar click Compute. .

Results

Data Sets

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

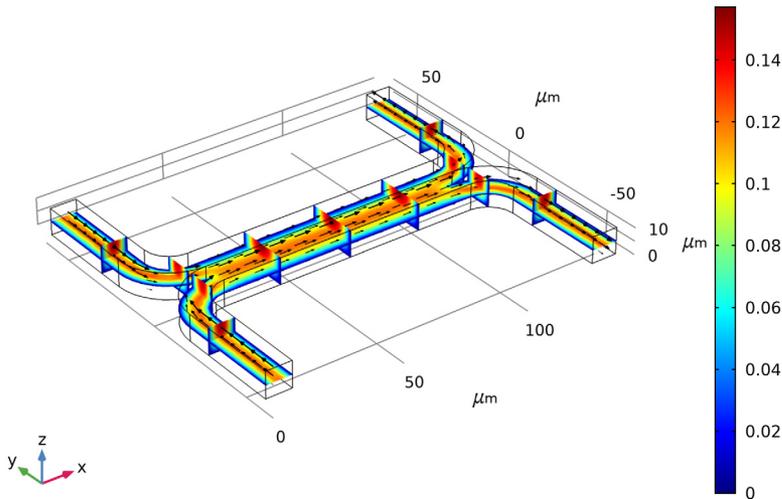
- 1 On the Results toolbar click More Data Sets  and choose Surface .
- 2 In the Settings window for Surface locate the Selection section. Click Paste Selection .
- 3 In the Paste Selection dialog, In the Selection text field, type 1 3 5 6 7 11 12 13 14 15 17 18 19 20 21 22 24 26 27.
- 4 Click OK.

3D Plot Group 1

First plot the velocity of the flow within the channel.

- 1 On the Home toolbar click Add Plot Group  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 right-click 3D Plot Group 1  and choose Slice .
- 3 In the Settings window for Slice locate the Expression section. From the Unit list, choose mm/s.
Add additional slices in different directions.
- 4 Right-click 3D Plot Group 1  and choose Slice .
- 5 In the Settings window for Slice locate the Expression section. From the Unit list, choose mm/s.
- 6 Locate the Plane Data section.
 - From the Plane list, choose xy-planes.
 - In the Planes text field, enter 1.The extra slices should use the same scale and colors for the velocity plot as the existing slice.
- 7 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.
- 8 Click to expand the Title section. From the Title type list, choose None.
Add slices in a third plane.
- 9 Under 3D Plot Group 1 right-click Slice 2  and choose Duplicate .
- 10 In the Settings window for Slice locate the Plane Data section.
 - From the Plane list, choose zx-planes.
 - In the Planes text field, enter 2.Use the arrow volume plot to visualize the flow direction.
- 11 Right-click 3D Plot Group 1  and choose Arrow Volume.
- 12 In the Settings window for Arrow Volume locate the Arrow Positioning section.
 - Find the x grid points subsection. In the Points text field, enter 14.
 - Find the y grid points subsection. In the Points text field, enter 21.
 - Find the z grid points subsection. In the Points text field, enter 3.
- 13 Locate the Coloring and Style section. From the Color list, choose Black.
- 14 Click 3D Plot Group 1. In the Label text field enter Velocity (uncoupled flow).
- 15 On the 3D plot group toolbar, click Plot .

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



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

3D Plot Group 2

1 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. From the Data set list, choose Surface 1.

Add a uniformly colored surface to highlight the channel walls.

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

4 In the Settings window for Surface locate the Expression section. In the Expression text field, enter 1.

5 Locate the Coloring and Style section.

- From the Coloring list, choose Uniform.
- From the Color list, choose Gray.

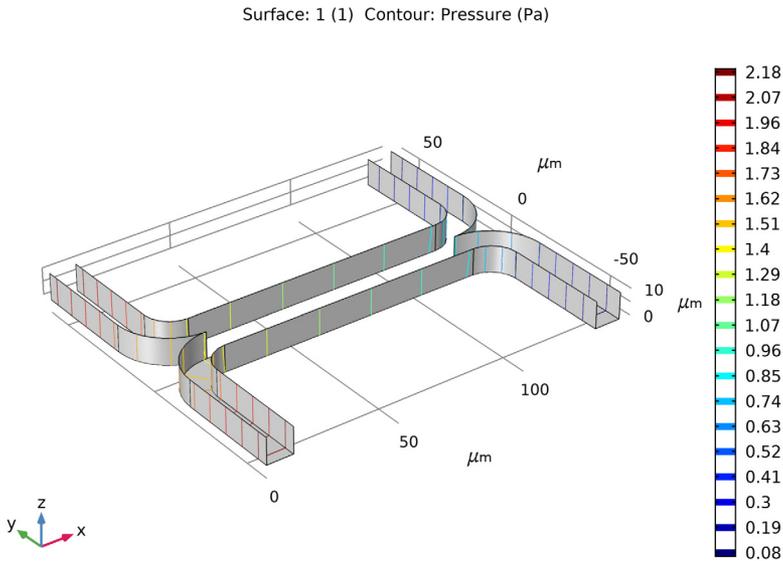
Next use contours to visualize the pressure.

6 Right-click 3D Plot Group 2  and choose Contour .

7 In the Settings window for Contour click Replace Expression  in the upper-right corner of the Expression section. From the menu, choose Creeping Flow > p – Pressure.

8 Click 3D Plot Group 2. In the Label text field enter Pressure (uncoupled flow).

9 Click 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 .
- 2 In the Label text field enter Concentration (uncoupled flow).
- 3 Click Plot .

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

Concentration (uncoupled flow)

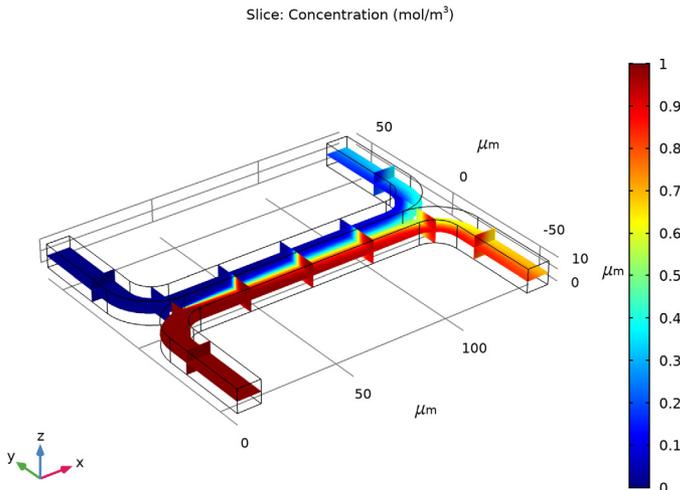
- 1 Expand the Results>Concentration (uncoupled flow) node, then click Slice 1 .
- 2 In the Settings window for Slice click Replace Expression  in the upper-right corner of the Expression section. From the menu, choose Transport of Diluted Species > c – Concentration.
- 3 Click Slice 2 .
- 4 In the Settings window for Slice click Replace Expression  in the upper-right corner of the Expression section. From the menu, choose c – Concentration.

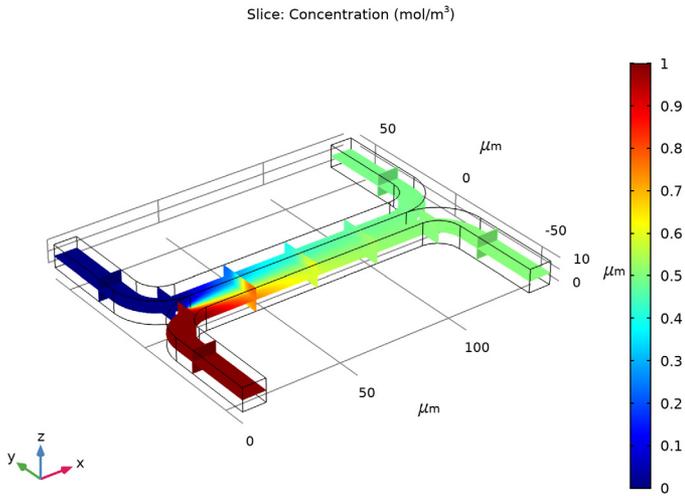
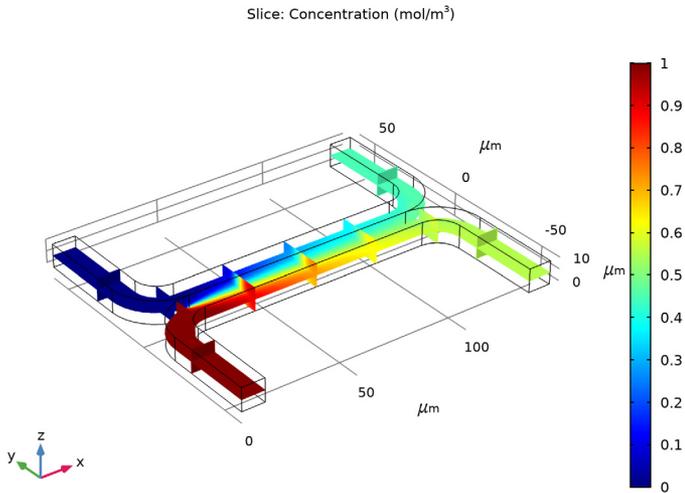
- 5 Repeat steps 3 and 4 for Slice 3 .

Disable the arrow volume plot.
- 6 Right-click Arrow Volume 1  and choose Disable .
- 7 On the 3D plot group toolbar click Plot .

Look at the plot for each of the three diffusion coefficient levels.
- 8 Click Concentration (uncoupled flow) .
- 9 In the Settings window for 3D Plot Group locate the Data section. From the Parameter value (D) list, choose each of the values: $1\text{e-}11$, $5\text{e-}11$ and $1\text{e-}10$, 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.





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

1D Plot Group 4

On the Home toolbar click Add Plot Group  and choose 1D Plot Group .

- 2 On the 1D plot group toolbar click Global .

Use the previously defined average operator to compute the average concentration at the device output.
- 3 In the Settings window for Global, click Replace Expression in the upper-right corner of the y-axis data section. From the menu, choose Component 1>Transport of Diluted Species>tds.out2.c0_avg_c - Concentration.
- 4 Locate the x-Axis Data section. Under Parameter, select Expression and in the Expression edit field, enter D.
- 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.
 - From the Positioning list, choose In data points.

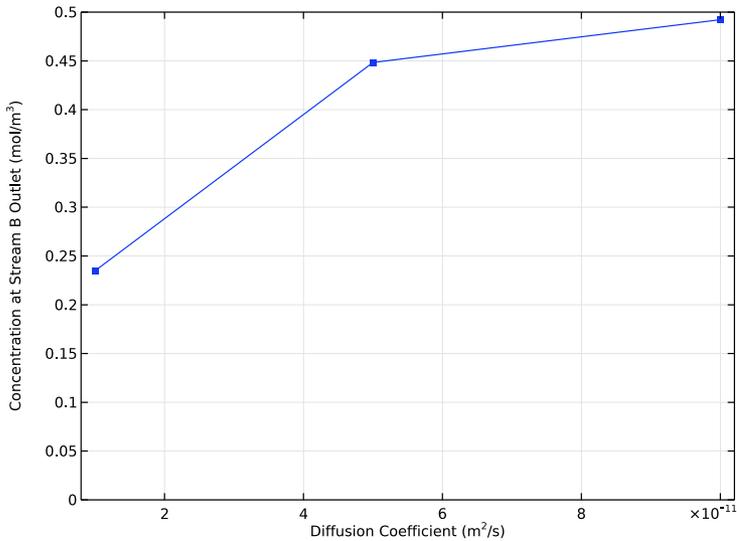
Change the axes titles.

Note: 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 Reference Manual* for more information.

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

Change the axis limits for the plot.
- 9 Click to expand the Axis section. Select the Manual axis limits check box.
 - In the y minimum text field, enter 0.
 - In the y maximum text field, enter 0.5.
- 10 Click 1D Plot Group 4  and in the Label text field enter Output Concentration (uncoupled flow).

|| 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.

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 Creeping Flow, 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, enter $1e-3[\text{Pa}\cdot\text{s}](1+\alpha\cdot c^2)$.

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 On the Home toolbar click Add Study .
- 2 Find the Studies subsection. In the tree under General Studies, click Stationary .
- 3 In the Add study window click Add Study.
Turn off the default plot groups again.
- 4 In the Model Builder click Study 2 .
- 5 In the Settings window for Study locate the Study Settings section. Clear the Generate default plots check box.
- 6 On the Home toolbar click Compute .

Results

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

Data Sets

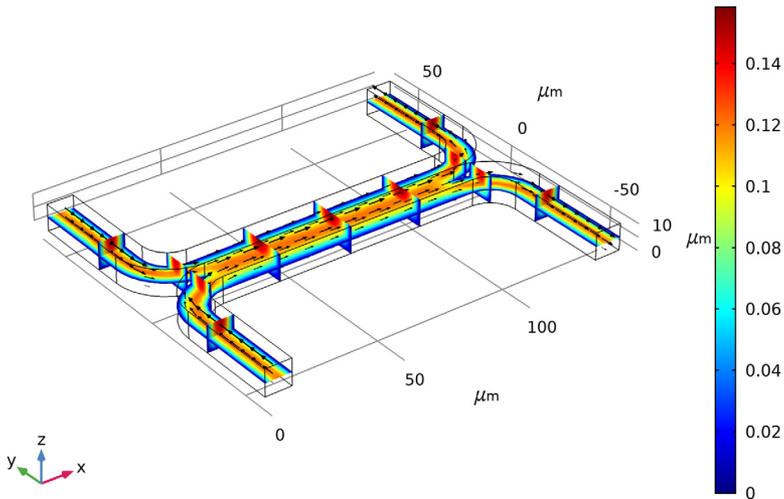
- 1 In the Model Builder under Results>Data Sets, right-click Surface 1  and choose Duplicate .
- 2 In the Settings window for Surface locate the Data section. From the Data set list, choose Study 2/Solution 3.

Recreate 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 Settings window for 3D Plot Group locate the Data section. From the Data set list, choose Study 2/Solution 3.
- 3 In the Label text field enter Velocity (coupled flow).
- 4 On the 3D plot group toolbar click Plot .

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

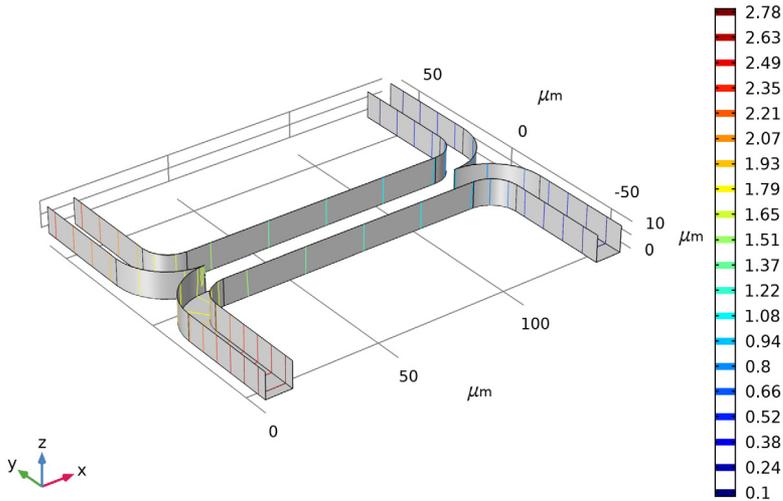


There are significant differences in the flow pattern, although these are hard to see when comparing this plot with the similar one generated previously. The flow through a slice of the channel will be investigated in more detail later to better highlight these differences.

Pressure (uncoupled flow) I

- 1 In the Model Builder under Results, right-click Pressure (uncoupled flow)  and choose Duplicate .
- 2 In the Settings window for 3D Plot Group locate the Data section. From the Data set list, choose Surface 2.
- 3 In the Label text field enter Pressure (coupled flow).
- 4 On the 3D plot group toolbar click Plot .

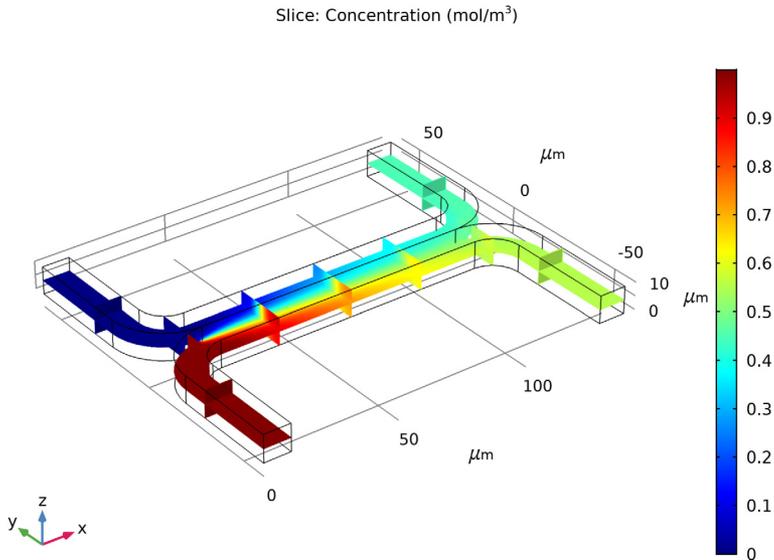
Surface: 1 (1) Contour: Pressure (Pa)



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 Settings window for 3D Plot Group locate the Data section. From the Data set list, choose Study 2/Solution 3.
- 3 In the Label text field enter Concentration (coupled flow).
- 4 On the 3D plot group toolbar click Plot .



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

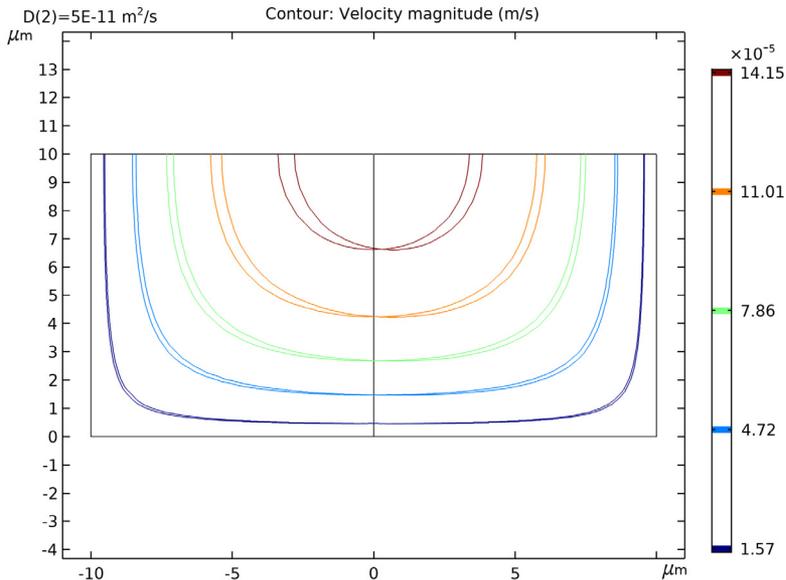
- 1 On the Results toolbar click Cut Plane .
- 2 In the Settings window for Cut Plane locate the Plane Data section. In the x-coordinates text field, enter 70.
- 3 Under Data Sets, right-click Cut Plane 1  and choose Duplicate .
- 4 In the Settings window for Cut Plane locate the Data section. From the Data set list, choose Study 2/Solution 3.

Add a 2D contour plot of the velocity magnitude.

2D Plot Group 8

- 1 On the Results toolbar click 2D Plot Group .

- 2 In the Settings window for 2D Plot Group locate the Data section.
 - From the Data set list choose Cut Plane 1.
 - From the Parameter value (D) list choose 5e-11.
- 3 Right-click 2D Plot Group 8  and choose Contour .
- 4 In the Settings window for Contour locate the Levels section. In the Total levels text field, enter 5.
Create a duplicate contour plot, using the same colors and scales, but showing the coupled data.
- 5 Under 2D Plot Group 8, right click Contour 1  and choose Duplicate .
- 6 In the Settings window for Contour locate the Data section. From the Data set list, choose Cut Plane 2.
- 7 Click to expand the Title section. From the Title type list, choose None.
- 8 Click to expand the Inherit Style section. From the Plot list, choose Contour 1.
- 9 Click 2D Plot Group 8 .
- 10 In the Label text field enter Velocity Comparison.
- 11 On the 2D Plot Group toolbar click 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 On the Results toolbar, in the Derived Values area, choose Global Evaluation .
- 2 In the Settings window for Global Evaluation, click Replace Expression in the upper-right corner of the Expressions section. From the menu, choose Component 1>Transport of Diluted Species>tds.out2.c0_avg_c - Concentration.
- 3 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 0.448 mol/m^2 .
- 4 Under Derived Values, right-click Global Evaluation 1  and choose Duplicate .
- 5 In the Settings window for Global Evaluation locate the Data section. From the Data set list, choose Study 2/Solution 3.
- 6 Right-click Global Evaluation 2  and choose Evaluate>New Table.
For the fully coupled problem, the mean outlet concentration is 0.4497 mol/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.

